SUPPORTING INFORMATION

Dynamics and the Regiochemistry of Nitration of Toluene

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Experimental Procedures

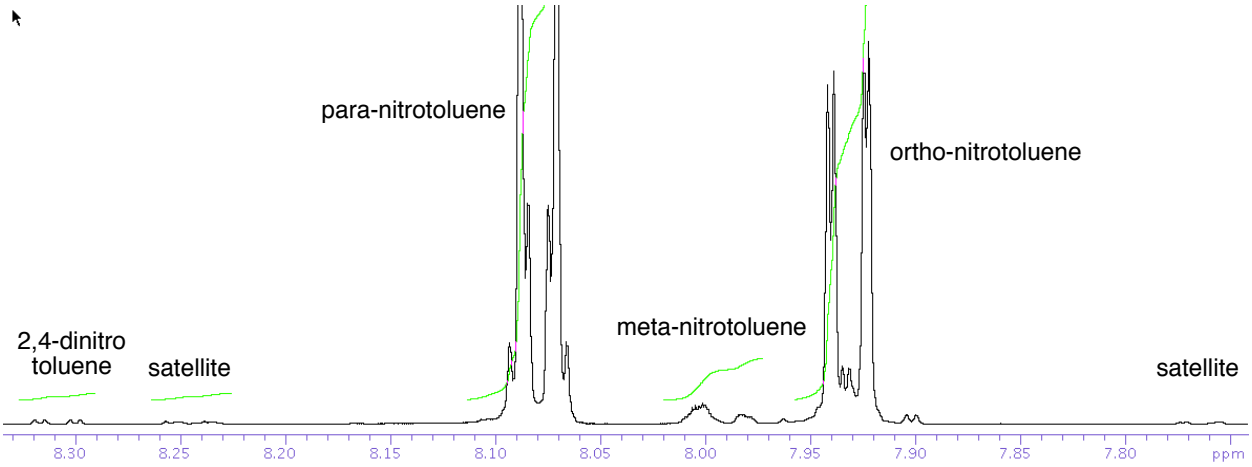
Reaction Procedures for Nitration of Toluene:

Nitration of Toluene using Nitronium Tetrafluoroborate in CH_2Cl_2. Example Procedure: To a rapidly stirred mixture of 0.72 g (5.4 mmol) of nitronium tetrafluoroborate in 217 mL of CH_2Cl_2 was added in one portion a mixture of 4.6 mL (3.99 g, 43.3 mmol) of toluene and 217 mL of CH_2Cl_2. The reaction mixture was stirred for 2 h at 25 ºC, and the reaction was quenched by addition of 50 mL of water. The aqueous phase was extracted with three 50-mL portions of CH_2Cl_2. The combined organic layers were rinsed with 50 mL of brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The residue was then analyzed directly by ^{1}H NMR. The characteristic peaks for the

products were: *o*-nitrotoluene: ^{1}H NMR ($CDCl_3$): δ 2.58 (s, 3H), 7.32 (m, 2H), 7.48 (t, J=8 Hz, 1H), 7.94 (d, J=8 Hz, 1H); *m*-nitrotoluene: ^{1}H NMR ($CDCl_3$): δ 2.42 (s, 3H), 7.38 (t, J=7.8 Hz, 1H), 7.47 (d, J=7.8 Hz, 1H), 7.95 (s, 1H), 7.97 (s, 1H); *p*-nitrotoluene: ^{1}H NMR ($CDCl_3$): δ 2.44 (s, 3H), 7.29 (d, J=8.2 Hz, 2H), 8.08 (d, J=8.2 Hz, 2H).

Approximately 0.6% of material tentatively identified as 2,4-dinitrotoluene was observed under these conditions. This assignment was made based on characteristic peaks at δ 8.78 (d, J=2.3 Hz), 8.31 (d of d, J=8.5 and 2.3 Hz), and 7.54 (d, 8.5 Hz).

Figure S1. Expansion of the downfield aromatic region of the ^{1}H NMR of the product mixture from the nitration of toluene with nitronium tetrafluoroborate.



Nitration of Toluene using Nitronium Tetrafluoroborate without Solvent: To 10.0 mL (8.67 g, 94.4 mmol) of toluene was added, in one portion, 0.63 g (4.7 mmol) of nitronium tetrafluoroborate. The resulting mixture was stirred for 1 h at 25 °C. The reaction was quenched by addition of 15 mL of water. The organics were washed with 15 mL of brine and dried over anhydrous Na_2SO_4, then analyzed directly by ^{1}H NMR.

Product Ratio Determination

The product ratios were determined from the crude mixture by ^{1}H NMR. The signals used for the product ratio determination were those for the aromatic protons *ortho* to the nitro group in each compound, allowing for the number of hydrogens in the signals integrated. The percentage of each isomer, the average, standard deviation and 95% confidence interval are shown in Table S1.

Table S1: Product ratios, average, standard deviation and 95% confidence interval for the nitration of toluene

	Para (%)	**Ortho (%)**	**Meta (%)**
	41.05	57.03	1.93
	41.94	56.02	2.04
	41.25	56.93	1.82
	40.64	57.08	2.28
	40.84	57.10	2.06
	40.73	57.13	2.14
Average	41.07	56.88	2.05
Stdve.	0.48	0.43	0.16
95% conf.	0.50	0.45	0.17

Product Ratio vs Concentration for Nitration of Toluene: To evaluate the possible role of more complicated mechanistic possibilities on the nitration regiochemistry, the selectivity was examined at a range of concentrations, including neat toluene, 2 M, 1 M, 0.1 M, and 0.01 M, by procedures matching or analogous to those described above. The results are shown in Table S2.

Table S2: Product ratios vs concentrations for nitration of toluene

Concentration	Para (%)	Ortho (%)	Meta (%)
No solvent	41.1	56.3	2.6
2 M	40.7	56.6	2.7
1 M	39.5	57.9	2.7
0.1 M	41.1	56.9	2.0
0.01 M	41.1	56.6	2.2

Computational Procedures and Supporting Computational Results

General

Calculations of structures, energies, and frequencies employed default procedures in Gaussian09[1,2,3] unless otherwise noted. Complete structures and energetics are provided in sections below. All absolute energies are in Hartrees. All relative energies are presented in kcal/mol.

While most calculated structures were obtained using the default grid, in some cases it was necessary to employ an ultrafine grid to obtain satisfactory structure convergence or frequencies. Structures obtained with an ultrafine grid have the label "uft". For all such structures, single-point energies with the default grid were obtained to ensure that the change in grid had no significant effect on the potential energy.

The program suite PROGDYN used for dynamics is a series of component programs written as either Unix shell scripts or awk programs. Gaussian09 was used to calculate the forces at each point in trajectories. A full description of PROGDYN including listings of the subprograms can be found in a later section. The latest version of this program can be obtained by emailing Daniel Singleton at singleton@chem.tamu.edu. The original version of this program was published in the Supporting Information of a previous paper.[4]

The program PROGMC is a new program consisting of a series of component programs written as either Unix shell scripts or awk programs. Gaussian09 was used to calculate the raw energies for each test geometry, and PROGMC adjusts these energies by biasing potentials and a potential used to maintain a spherical solvent cluster. A full description of PROGMC including listings of the subprograms can be found in a later section.

IRCs were not conducted for all structures; rather, they were only conducted for structures where an examination of the transition vector left the outcome of the IRC in reasonable doubt. In some cases, particularly when IRC calculations failed, trajectory calculations were carried out to determine the products from a transition structure, and it was presumed that the IRC would lead to the major product from the trajectories. There are cases where this assumption would be incorrect, but in those cases we would argue that trajectories provide a *better* measure of the product from a transition structure than an IRC.

Additional Comments on the ONIOM Model and the Conditions for Simulations.

As discussed in the main text, the simulations in explicit solvent employed a two-layer ONIOM calculation, using M06-2X/6-311G* for the toluene / NO_2^+ and PM3 for the BF_4^- and CH_2Cl_2. There were a number of considerations in this choice and there are some advantages and disadvantages to the calculational method chosen.

For the reaction of NO_2^+ with toluene, the energetics of the NO_2^+ interaction with toluene were considered paramount. The main text discusses our choice of M06-2X/6-311G* for this interaction, and a later section describes in detail the validation studies with respect to this interaction. It is important to note that the method performs very well versus CCSD(T) calculations on the critical part of the energy surface, as well as on the relative energies of the isomeric s-complexes. It should also be noted that increasing the size of the basis set did not improve performace on the validation studies.

For the NO_2^+ interaction with the BF_4^- counterion, the most pressing priority was avoid the unreal decomposition of the NO_2BF_4. Any method maintains the long-range electrostatic attraction of the ions, and a later section details the unsurprisingly excellect performace of the ONIOM calculations at long range. While DFT methods underestimate the barrier for this reaction, the PM3 portion of the ONIOM overestimates the stability of the NO_2BF_4, and it underestimates the gas-phase attraction of the ions at close range – see page S123. The former is not a problem, while the latter will tend to make the counterion act like a larger counterion. In toluene solvent, NO_2BF_4, NO_2PF_6, NO_2ClO_4, $NO_2Cl/TiCl_4$, $NO_2Cl/SnCl_4$, NO_2Cl/BF_3, and NO_2Cl/PF_5 all provide product ratios that are within experimental error of each other. For this reason, it was viewed that the tightness of counterion to the NO_2^+ is not a major factor in the reaction's selectivity, so the error in the ONIOM surface was considered acceptable.

For the solvent, our concerns were that the solvent have a reasonable the dipole moment and that it be polarizable. The PM3 calculations underestimate the dipole moment (1.36 D versus 1.6 D) so our computational solvent is less polar than pure CH_2Cl_2. However, our experimental solvent contains toluene, making it less polar, and we used a range of concentrations up to 2 M with little change in the product ratio.

All semi-empirical methods underestimate the polarizability of molecule, and the PM3 calculations do so with CH_2Cl_2. The α_{xx}, α_{xy}, α_{yy}, α_{xz}, α_{yz}, α_{zz} tensors for CH_2Cl_2 for PM3 are 39.3, 0, 20, 0, 0, and 7.7, respectively. For comparison, the tensors calculated M062X/6-311+G(2df,2pd) are 51, 0, 34.8, 0, 0, and 30.2. Along the most polarizable axis, the PM3 polarizability is about 77% of the actual polarizability.

A significant issue then with using PM3 CH_2Cl_2 as solvent is that it is a gas at 25 °C. For this reason, the spheres and cubes of solvent described below are compressed at approximately 400 bar to maintain a density of 1.3. The solvent's heat of vaporization is only about 2.4 kcal/mol, compared to the experimental value of 6.8 kcal/mol. In this regard the solvent is not very realistic but this was not expected to be a critical factor in the simulation.

Initialization of Trajectories and Additional Details on Trajectories

Trajectories were initialized in differing ways depending on the details of the calculation. All trajectories started from transition structures (simple potential energy saddle points) or canonical variational transition structures (CVTSs) were quasiclassical. This includes trajectories started from **4a**‡, **4b**‡, **4c**‡, **5a**‡, **5b**‡, **5c**‡, **6a**‡, **6b**‡, **6c**‡, and related transition structures.

For quasiclassical trajectories, each normal mode in the transition structure of interest was given its zero-point energy plus a Boltzmann distribution of quantized vibrational energies. The desired energy in each of the normal modes of the transition structure was mapped from a random number generator to a Boltzmann distribution set at 25 °C. The phase of each of the normal modes was mapped from a Gaussian distribution of random numbers. This distribution is not correct for a classical oscillator but would be approximately correct for a quantum oscillator in its ground state (only ignoring mode displacements outside of the classical limit), and has the advantage that a larger portion of the trajectories start with an energy approximating the initially desired energy. The sign on the velocity of the normal modes was randomized. After an energy/force calculation on the initial geometry, the total initial energy was calculated and the trajectory was thrown out if the energy did not agree satisfactorily (within 1 kcal/mol) with the desired energy. (This is a variation of the conventional practice of scaling energies.[5]) The mode corresponding to the transition vector was treated classically. A sample PROGDYN parameter file (progdyn.conf) is given in a later section.

The trajectories in explicit solvent and related supporting studies were fully classical, and their initation is described in subsequent sections.

PMF Trajectory Initialization, PMF in a Solvent Cube, and Extended Data

The process for generating starting structures for trajectories in a sphere of 101 CH_2Cl_2 molecules was circuitous. Initial structures were generated by surrounding molecules of toluene and NO_2^+ with 102 CH_2Cl_2 molecules, using a cube of CH_2Cl_2 geometries generated with an Excel spreadsheet. The distance between the aromatic ring carbons and the ipso and para carbons of toluene was constrained at ≈4 Å using the *fixedatom* resource in PROGDYN, and six random trajectories were initiated at 1000 Kelvin using a PM3 surface. The solvent molecules were forced into a cube with 22.4 Å sides using the *boxon* facility in PROGDYN, and the six trajectories were equilibrated at 1000 Kelvin for 5 ps, then cooled slowly to 25 °C using the thermostat facility in PROGDYN with thermostatmult set at 0.999 (removing 0.1% of the energy per fs), and equilibration at 298 K was continued for 5 ps.

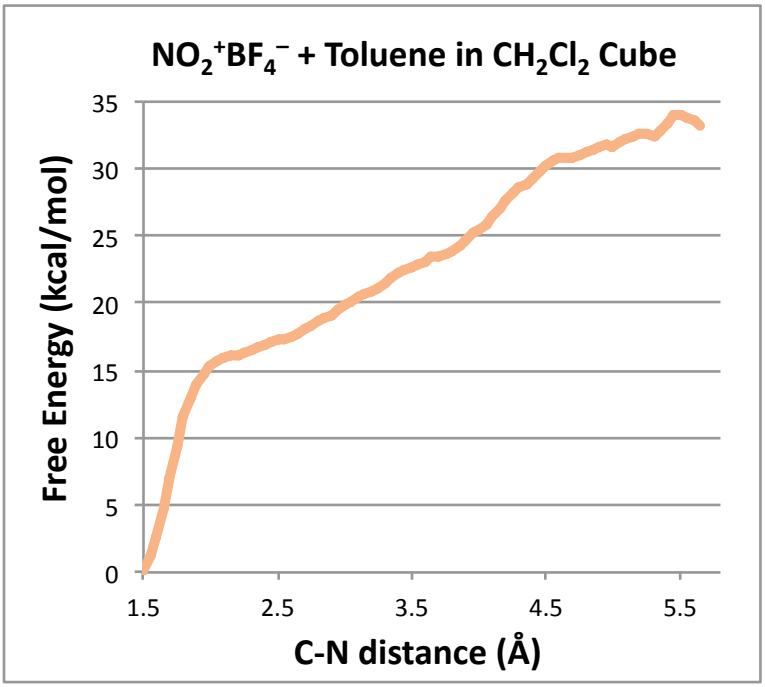
The set of six trajectories was then duplicated to give two sets. The first set of six trajectories will be used in a later section. For the second set of six, a CH_2Cl_2 molecule was converted into a BF_4^- molecule. The latter were equilibrated for 5 additional ps in PM3 calculations, using at this stage a harmonic potential to maintain a 3 Å separation between the NO_2^+ and the BF_4^- ions. The two sets of six trajectories were then equilibrated at 25 °C with only the nitrogen atom – arene carbon constraint for 5 ps in ONIOM calculations using M06-2X/6-311G* for the toluene / NO_2^+ and PM3 for the BF_4^- (when present) and CH_2Cl_2.

The six sets of trajectories including $NO_2^+BF_4^-$ were then duplicated five times (for a total of 36 sets of trajectories) and dispersed using a series of interlocking-sphere biasing potentials (see the section below for details) using the *applyforce* facility in PROGDYN. All other constraints were turned off. The biasing potential sphere radii and number of assigned trajectories for these potentials were 2.1 Å (5), 2.2 Å (3), 2.5 Å (3), 2.8 Å (3), 3.1 Å (3), 3.4 Å (3), 3.7 Å (3), 4.0 Å (3), 4.3 Å (2), 4.6 Å (2), 4.9 Å (2), 5.2 Å (2), and 5.5 Å (2). These trajectories were equilibrated for 5 ps, then nitrogen-carbon distance data was collected and analyzed using the weighted-histogram analysis method (see reference in main text and sample files in a later section).

A total of 240 ps of MD was obtained, and the results are shown in Figure S2. The PMF

exhibits the same absence of a barrier seen later. It was judged however that the use of a cubic box of solvent was non-optimum, in part because the rigid box facility in PROGDYN is relatively subject to edge effects and in part because of the non-isotopic distribution of solvent molecules.

Figure S2. Potential of mean force curve for approach of $NO_2^+BF_4^-$ to toluene in a 22.4 Å cube of 101 CH_2Cl_2 molecules.

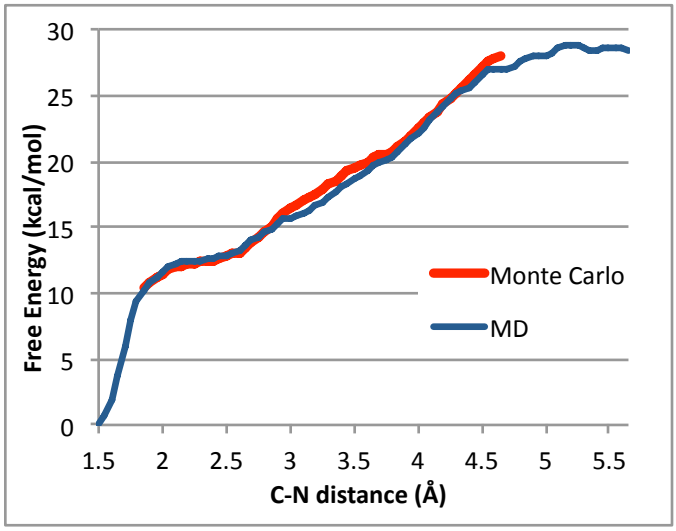


Each of the cubic structures was then molded into a sphere with a soft 25.8 Å diameter using the *sphereon* facility in PROGDYN, and equilibrated for 5 ps after achieve a spherical shape. Once in a sphere, the N atom of the NO_2^+ was constrained to the center of the sphere by a weak harmonic potential (with k = 0.119 kcal/mol/Å^2) to the middle of the sphere, using the *zeroatom* facility in PROGDYN. The sphere was maintained with a density of 1.3 by a harmonic restoring potential (with k = 11.86 kcal/mol/Å^2) on atoms outside of 12.9 Å from the center of the sphere. That is, a force is applied to atoms that are outside of 12.9 Å from the center of the sphere, along a vector toward the center of the sphere. The magnitude of the force was set to (distance to center -12.9 Å) x 11.86 kcal/mol/Å^2. These parameters are set with the "*sphereon* 1", "*spheresize* 12.9", and "*sphereforce* 0.01" keywords in PROGDYN. A later section gives the complete PROGDYN parameter file (progdyn.conf) for these trajectories.

Duplication of trajectories and dispersal with differing biasing potentials ultimately generated a total of 66 separate trajectories from which MD data was collected. In all cases care was taken to maximize the independence of separate trajectories. In some cased the trajectories were cut short and were not restartable. This arose from a bug in PROGDYN; if a PROGDYN run cannot write to disk (as occurs when a disk quota maximum is reached), the files necessary for restarting runs can be lost. As a result, the length of the separate trajectories varies from 4 ps to 52 ps. The biasing potential sphere radii and number of assigned trajectories for these potentials were 1.9 Å (7), 2.0 Å (7), 2.1 Å (6), 2.2 Å (11), 2.35 Å (6), 2.5 Å (3), 2.8 Å (4), 3.1 Å (3), 3.4 Å (4), 3.7 Å (3), 4.0 Å (3), 4.3 Å (2), 4.6 Å (2), 4.9 Å (2), 5.2 Å (2), and 5.5 Å (2).

Figure S3 below shows an extended version of Figure 1 from the main text, including all data. The roughness of the PMF surface at long C-N distances is most likely due to limited data in this range.

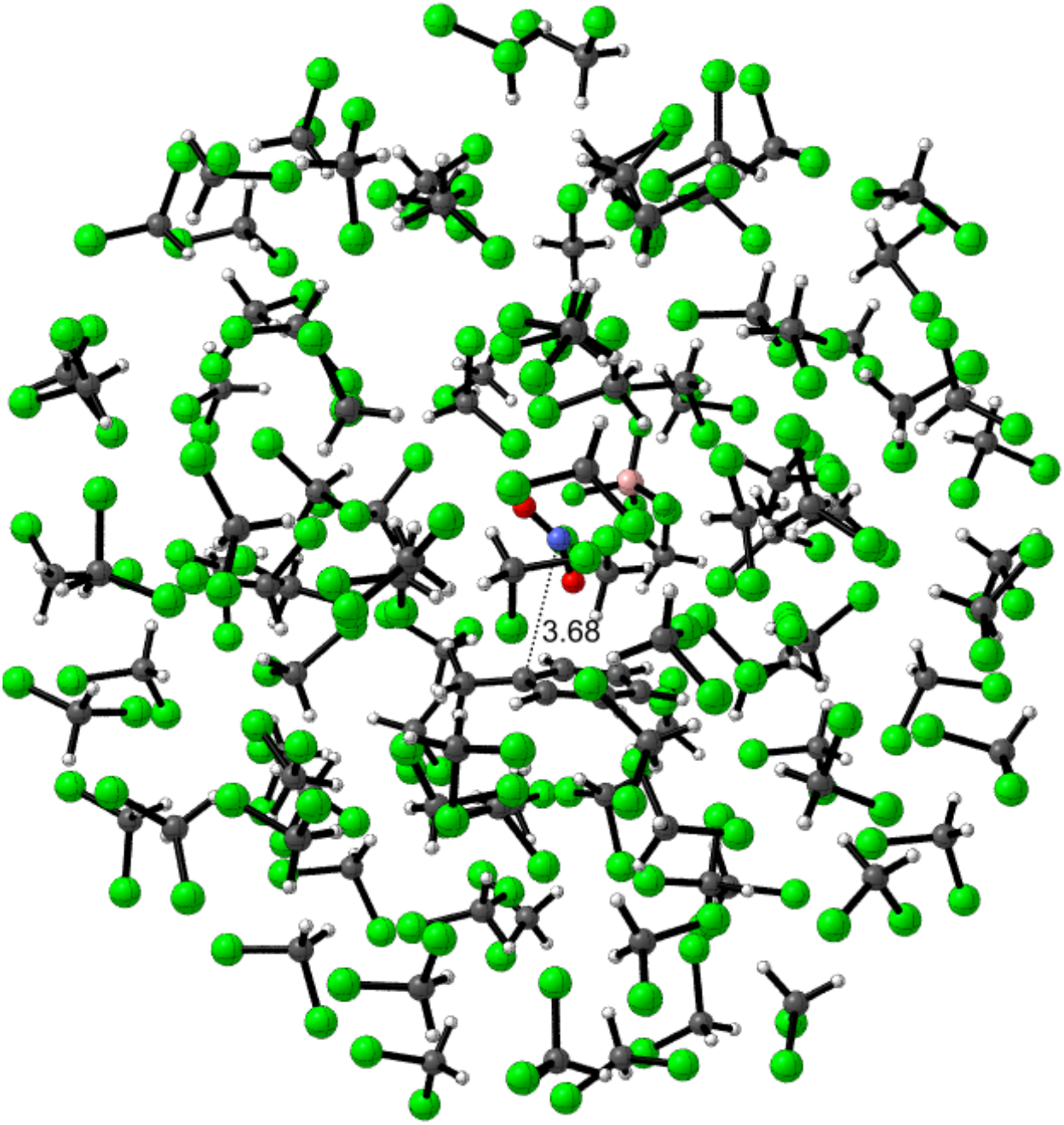
Figure S3. Extended version of Figure 1 from main text showing all available MD data.



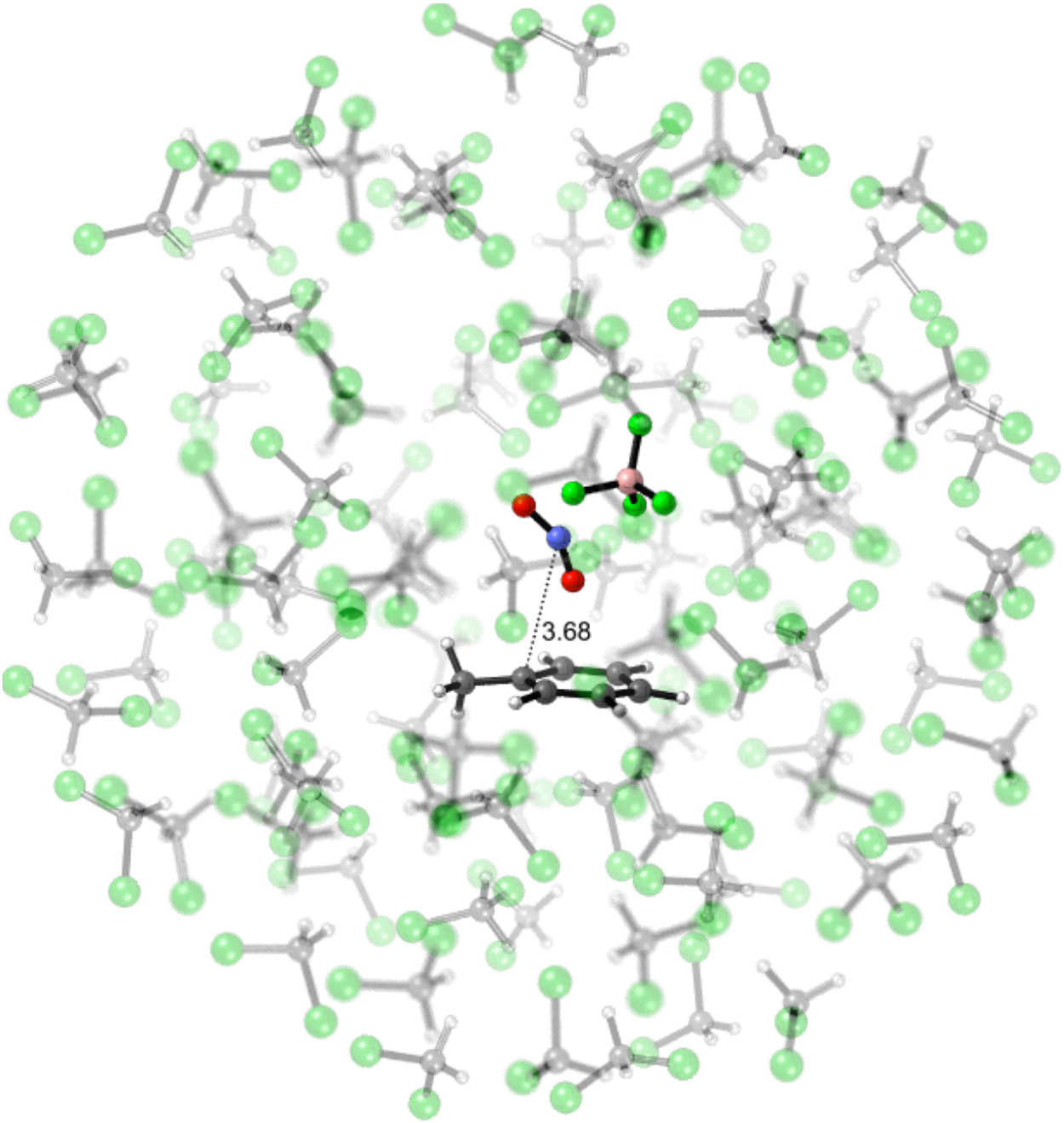
Product-Forming Trajectories for the Full Model

To generate product-forming trajectories, PMF trajectories above in which the interlocking-sphere biasing potential was zero at 3.4-4.0 Å were used as "feeder" trajectories to provide starting points. At 250 fs intervals the helper program *prodynsam* (listed in a later section) was used to create a *geoPlusVel* file for use in PROGDYN. The *progdynsam* program leads to trajectories with all atoms moving at their current velocity. Each resulting unconstrained trajectory was integrated forward and backward in time until one of the regioisomers of **2** (defined by a C-N distance of <1.6 Å) was formed.

A typical starting point for product-forming trajectories is shown below in two formats. In the first, there are no special effects for the picture. The solvent molecules are seen clearly but the reactants are somewhat obscured.



In the second view below, the solvent molecules are "transparent" and a focal point is set in the area of the reactants.



Product-Forming Trajectories using $NO_2^+BF_4^-$ in Implicit Solvent.

A series of six trajectories containing only toluene and $NO_2^+BF_4^-$ were created by taking six of the PMF trajectories in implicit solvent from above and deleting all of the solvent molecules, then continuing the trajectories with a PCM implicit solvent model for CH_2Cl_2 and the same interlocking-sphere biasing potential as in the source trajectories. The biasing potential sphere radii and number of assigned sequences for these potentials were 3.4 Å (1), 3.7 Å (2), 4.0 Å (2), and 4.3 Å (1). These "feeder" trajectories were then equilibrated and thermostated at 25 °C for 2 ps. The energy surface was ONIOM / PCM(CH_2Cl_2), using M06-2X/6-311G* for the

toluene and NO_2^+ and PM3 for the BF_4^-.

After equilibration, at 250 fs intervals the helper program *prodynsam* (listed in a later section) was used to create a *geoPlusVel* file for use in PROGDYN. The *progdynsam* program leads to trajectories with all atoms moving at their current velocity. Each resulting unconstrained trajectory was integrated forward and backward in time until one of the regioisomers of **2** (defined by a C-N distance of <1.6 Å) was formed, or the NO_2^+ dissociated as judged by a C-N distance > 5.0 Å.

A total of 151 results were obtained:

32 – dissociated

48 – formed the para product

19 – formed the meta product

38 – formed the ortho product

14 – formed the ipso product

Product-Forming Trajectories using NO_2^+ in Implicit Solvent.

A series of six trajectories containing only toluene and NO_2^+ were created by taking six of the PMF trajectories in implicit solvent from above and deleting all of the solvent molecules and the BF_4^-, then continuing the trajectories with a PCM implicit solvent model for CH_2Cl_2 and interlocking-sphere biasing potentials with radii 3.7 Å. These "feeder" trajectories were then equilibrated and thermostated at 25 °C for 2 ps. The energy surface was M06-2X/6-311G*/PCM(CH_2Cl_2).

After equilibration, at 250 fs intervals the helper program *prodynsam* (listed in a later section) was used to create a *geoPlusVel* file for use in PROGDYN. The *progdynsam* program leads to trajectories with all atoms moving at their current velocity. Each resulting unconstrained trajectory was integrated forward and backward in time until one of the regioisomers of **2** (defined by a C-N distance of <1.6 Å) was formed, or the NO_2^+ dissociated as judged by a C-N distance > 5.0 Å.

A total of 149 results were obtained:

0 – dissociated

41 – formed the para product

34 – formed the meta product

37 – formed the ortho product

37 – formed the ipso product

Product-Forming Trajectories using NO_2^+ in Explicit CH_2Cl_2.

A previous section described the creation of a set of six trajectories including toluene and NO_2^+ but no counterion in 102 explicit CH_2Cl_2 molecules. After the previously described equilibration, these trajectories were continued with constrained C-N distances of ≈4.0 on the ONIOM energy surface. At 250 fs intervals the helper program *prodynsam* (listed in a later section) was used to create a *geoPlusVel* file for use in PROGDYN. The *progdynsam* program leads to trajectories with all atoms moving at their current velocity. Each resulting unconstrained trajectory was integrated forward and backward in time until one of the regioisomers of **2** (defined by a C-N distance of <1.6 Å) was formed, or the NO_2^+ dissociated as judged by a C-N distance > 5.0 Å.

A total of 209 results were obtained:

0 – dissociated

67 – formed the para product

37 – formed the meta product

97 – formed the ortho product

8 – formed the ipso product

It should be noted that these trajectories were conducted in a cube of solvent, not a sphere. Exploratory studies did not find any significant difference between product-forming trajectories in a cube versus a sphere.

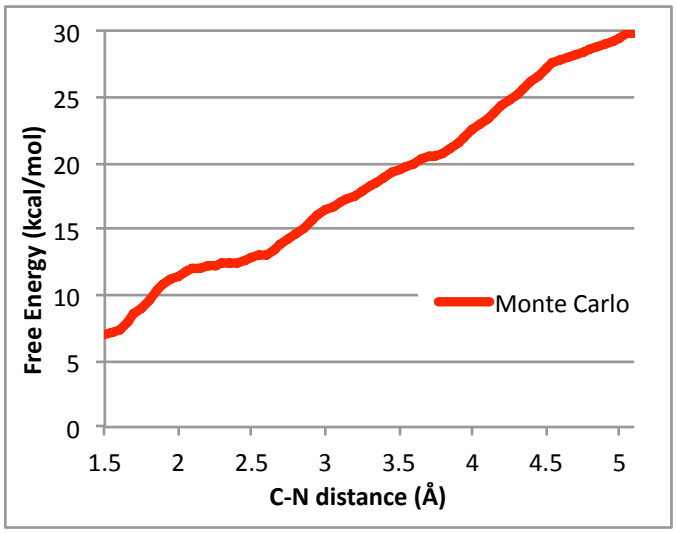
Monte Carlo Starting Points, Equilibration, and Extended Data

The starting geometries for a series of 48 Monte Carlo geometry sequences were taken from MD structures in the later half of their data collection. The biasing potential sphere radii and number of assigned sequences for these potentials were 1.8 Å (6), 2.0 Å (6), 2.1 Å (5), 2.2 Å (6), 2.35 Å (6), 2.5 Å (2), 2.8 Å (2), 3.1 Å (3), 3.4 Å (2), 3.7 Å (2), 4.0 Å (2), 4.3 Å (2), 4.6 Å (2), and 4.9 Å (2). The resulting geometries were equilibrated for 1000 steps when the biasing potential was unchanged versus the MD source of the geometry, and for 5000 steps when the biasing potential was changed versus the MD source.

As internal checks of the Monte Carlo data, we monitored whether the overall average C-N distance varied systematically as the sequences proceeded, and we monitored whether independent sequences provided equivalent data. Some of the data obtained failed these internal checks, and these data were not included in Figure 1 of the main text. This requires some explanation.

In a Monte Carlo program, a central problem is how to explore coordinate space in a fully representative way in as few of steps as possible while keeping a reasonable percentage of the steps acceptable. PROGMC approaches this problem by dividing the system into molecules, performing translations and rotations on the molecules as a whole, stepping the bond lengths in each molecule by necessarily relatively small steps, and stepping angles and dihedral angles by larger steps using an algorithm that steps along two vectors that are orthogonal to the bond stretch and each other. The program was judged nicely efficient at dealing with the NO_2^+, BF_4^-, and 101 CH_2Cl_2 molecules. It had trouble however dealing with the large distortions of the toluene ring that are associated with NO_2^+ attack. This trouble was associated with a common problem with ring structures and internal coordinates; small changes in internal coordinates in rings can have large effects on the "last" bond in a ring, that is, the one that is not directly determined by an internal coordinate. This is a well-known solvable problem but is not solved yet in the current code. The code instead decreased the motion of atoms in the toluene ring, but this slows large geometry changes in the ring. Because of the problem with slow equilibration in the area of the surface associated with NO_2^+ attack, we did not include that portion of the data in Figure 1. Figure S4 displays the complete data. The Monte Carlo results still show the same qualitative pattern as the MD data, but, lacking a full exploration of the space associated with **2**, the energy dip in this area (with a C-N distance less than 1.85 Å) is far less pronounced.

Figure S4. Extended version of the Monte Carlo data from Figure 1 of the main text showing all available data.

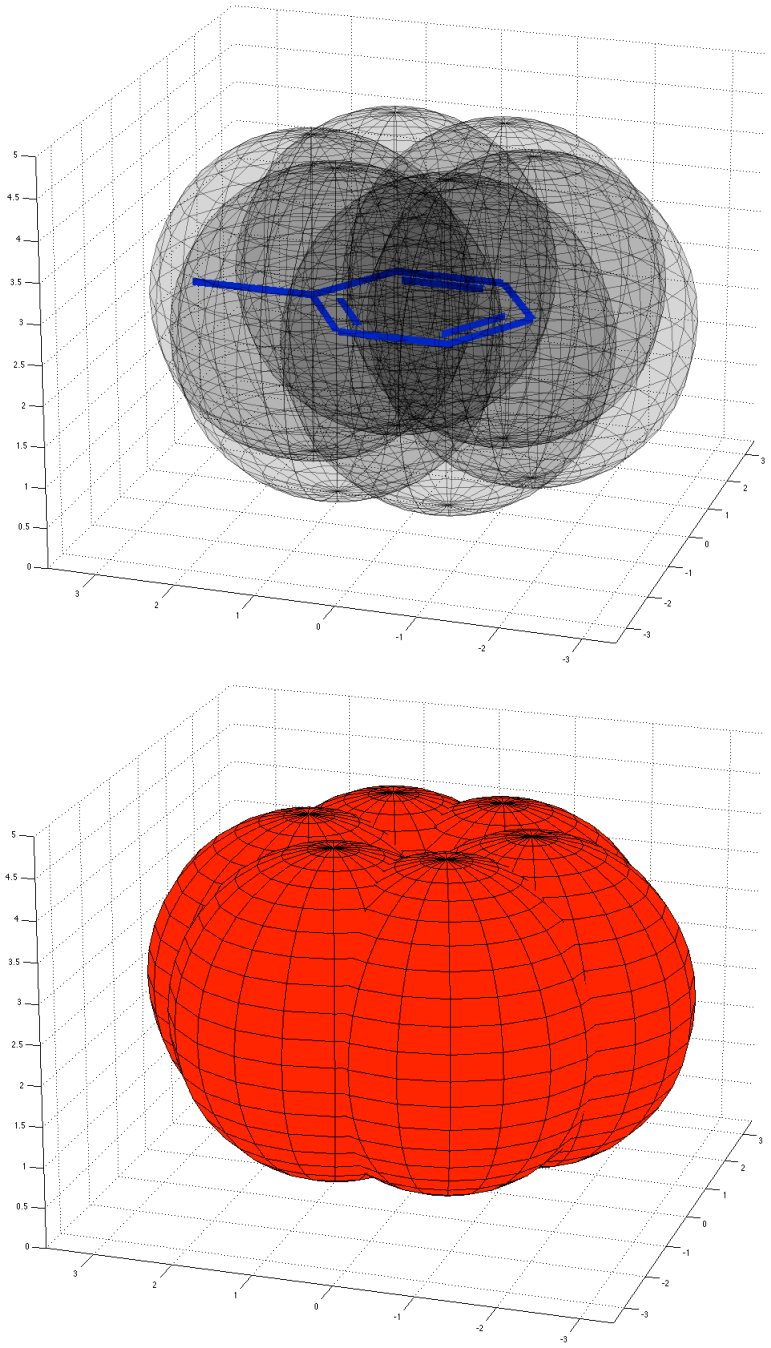


The Interlocking Sphere Biasing Potential

The use of simple biasing potentials based on the distance of the nitrogen atom from a chosen carbon atom, such as the *para* carbon, fails. The failure occurs because the NO_2^+ remains free to attack the other aromatic carbons, and it invariably does so except when the biasing potential sets very short C-N distances. This problem was avoided using the more complicated biasing potential to be described here. The next section discusses in more detail the meaning of the PMF curve for this complex biasing potential.

The MD and Monte Carlo calculations employed biasing potentials that were based on interlocking spheres centered on the arene ring carbons. The surface of the spheres represents the zero of the potential, and the applied potential was 0.5 * 118.6 kcal/mol/Å^2 * r^2 where r is the distance of the nitrogen atom from the closest surface point of the spheres. For Monte Carlo calculations, this potential was simply added to the energy of the system. For MD calculations, the nitrogen atom and the carbon atom at the center of the closest sphere were subjected to a restoring force along their internuclear axis.

The first picture below illustrates the interlocking spheres when at a radius of 2.5 Å from the carbon nuclei, using transparency to show the positions of the carbon nuclei. It should be noted that the spheres move with the motion of the carbon atoms, and that no sphere was place around the methyl-group carbon. The second picture shows the solid zero-potential surface.



Additional Discussion of the Meaning of the Figure 1 PMF Curves

The interlocking-sphere biasing potential that was employed lets the NO_2^+ roam from carbon to carbon in the MD and Monte Carlo simulations. However, the energetics of the system can restrict the roaming, depending on the distance of the NO_2^+ from the ring. Some discussion

of these effects on roaming and how they affect the meaning of the PMF curves will be given here.

Table S3 below shows the radius of the spheres in the biasing potential (which we will simplistically call the "C-N distance"), the total MD time for each radius, the number of "switches" for each radius where a "switch" is a change of closest carbon from one carbon to another (a simple measure of the roaming of the NO_2^+), the average time between switches, and the percentage of the time that the MD trajectories were nearest the para, meta, ortho, or ipso carbons.

We first consider the roaming of the NO_2^+ at relatively long C-N distances. In a medium range between C-N distances of 2.8 Å and 4.3 Å, switches are common. At the longest C-N distances (4.6 Å or greater), switches become less common. This is likely to be simply a geometry effect – the spheres have become bigger and their surface near the plane of the aromatic becomes accessible, so the NO_2^+ must roam a greater average distance to switch from carbon to carbon. At C-N distances between 3.4 and 4.0 Å, the distribution of para / meta / ortho / ipso carbons as closest to the NO_2^+ appears roughly statistical (allowing for a factor of 2 as appropriate), as mentioned in the main text. The distribution also appears to be statistical at longer distances, though there is more fluctuation in the numbers, perhaps due to the lower total time of the MD simulations.

Table S3. Roaming Information in MD trajectories with a biasing potential.

potential sphere radius	total time (fs)	"switches"	time (fs) / switch	% para	%meta	%ortho	%ipso
2 Å	125539	18	6974	45	15	35	5
2.1 Å	129184	39	3312	91	2	7	0
2.2 Å	140594	271	519	57	9	18	16
2.35 Å	108354	682	159	35	9	27	29
2.5 Å	107698	1025	105	26	10	20	44
2.8 Å	119991	2102	57	4	7	32	57
3.1 Å	47370	767	62	37	35	23	5
3.4 Å	47016	1286	37	17	25	35	23
3.7 Å	46588	1296	36	20	25	35	20
4 Å	46943	1989	24	24	32	30	14
4.3 Å	28072	1029	27	20	29	33	18
4.6 Å	26652	546	49	18	29	20	32
4.9 Å	20823	316	66	15	33	32	20
5.2 Å	19389	165	118	11	43	31	16
5.5 Å	15219	79	193	17	36	39	8

At C-N distances of 2.8 and 2.5 Å, the NO_2^+ appears to prefer to be near the ipso carbon. In this distance range we see a similar preference for the NO_2^+ to be near the ipso carbon in PCM calculations. As mentioned in the main text, the most stable transition structure for attack of NO_2^+ on toluene in PCM calculations was one for attack at the ipso carbon. At 2.35 and 2.2 Å, a preference for the NO_2^+ to be near the para carbon emerges.

At distances shorter than 2.2 Å, there is a significant complication in the data. That is,

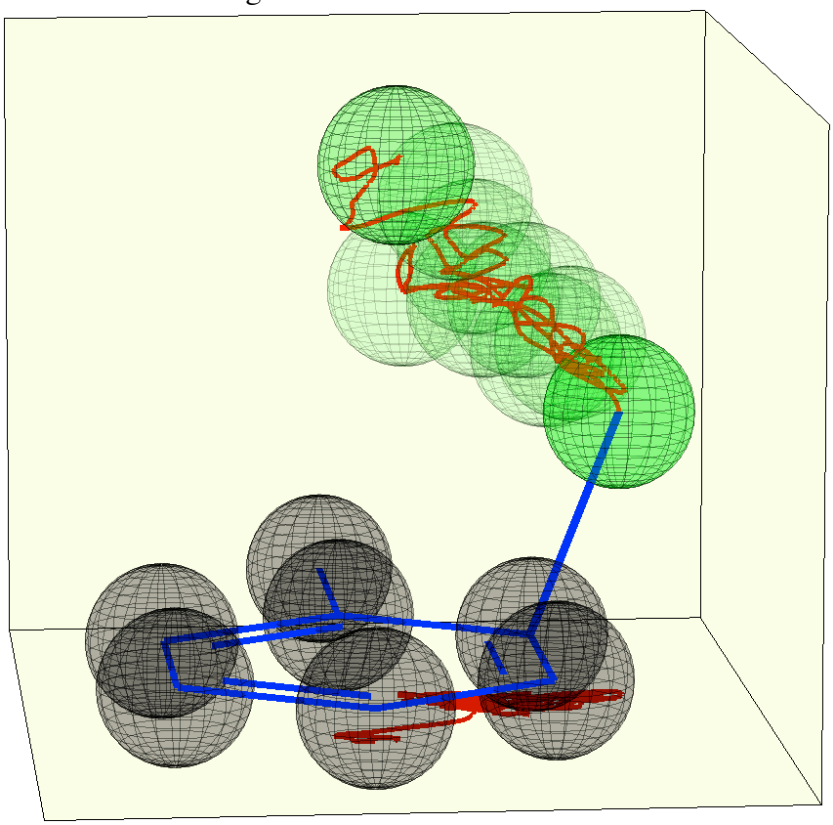
switches are sufficiently uncommon that we can no longer expect the ratio of the closest carbons to reflect a thermodynamic preference. Random statistical effects impact all of the para / meta / ortho / ipso ratios in the table, but at the shortest distances the ratios depend on the starting points. The 2 Å data contains a significant amount of time in which the meta and ipso carbons were closest simply because the starting points afforded significant amounts of these points. The 2 Å data should be recognized as a range that includes C-N distances down to 1.5 Å. At the shortest distances it is far more stable for the NO_2^+ to be near the para carbon. When trajectories switch from meta or ipso to ortho or para and stay there for > 500 fs, they never switch back. For this reason, the meta and ipso 2 Å data are questionable, since they do not appear to be the result of a full equilibration. A reanalysis leaving out this data had no significant effect on the MD PMF curve.

This brings up an important caveat on our conclusions. That is, because we have no fully-defensible data for MD with the NO_2^+ nearest the meta or ipso carbons, we do not know whether there is a barrier for the formation of the meta or ipso isomers of **2**. We can only say that there is no free-energy barrier along the C-N distance coordinate for attack at the *para* and *ortho* carbons.

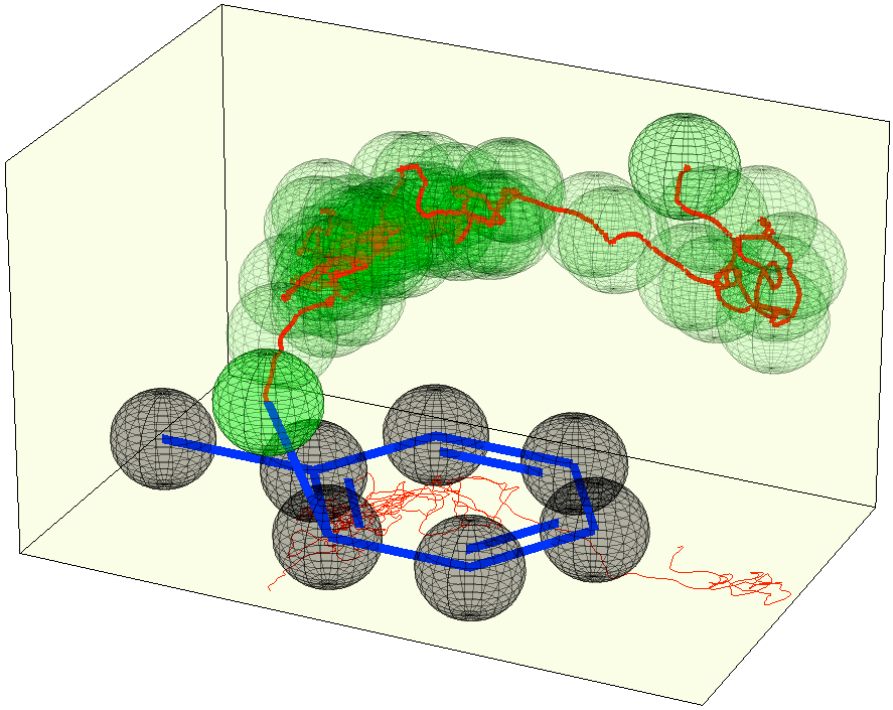
Additional Plots of Trajectories, Comments

Full Model (Explicit Solvent, $NO_2^+ BF_4^-$)

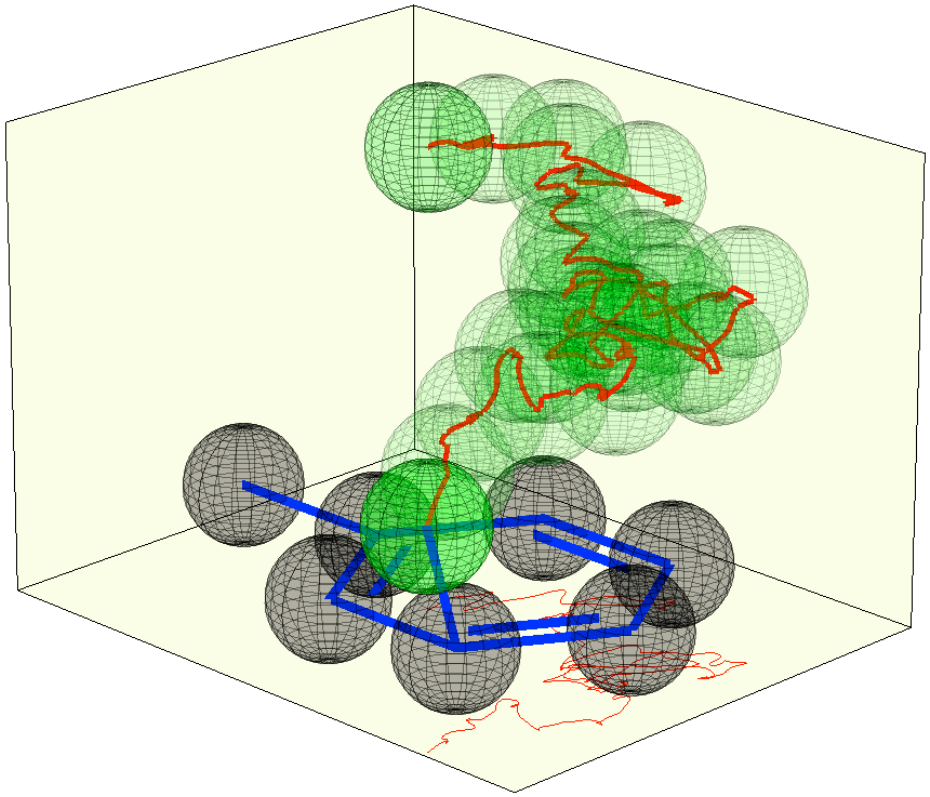
This short trajectory illustrates how the nitronium can approach a carbon to within 2 Å then pull back without reacting.



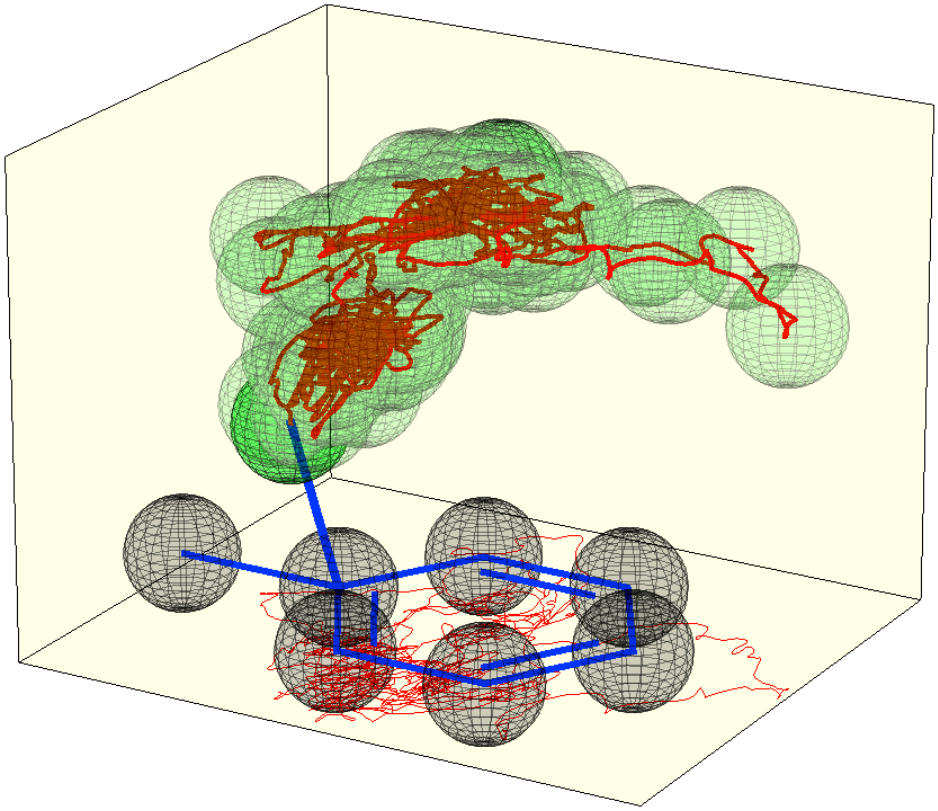
The nitrogen roams in its relative position versus the carbons quickly when the nitrogen is far from the ring carbons, but the roaming slows as the nitrogen approached the ring.



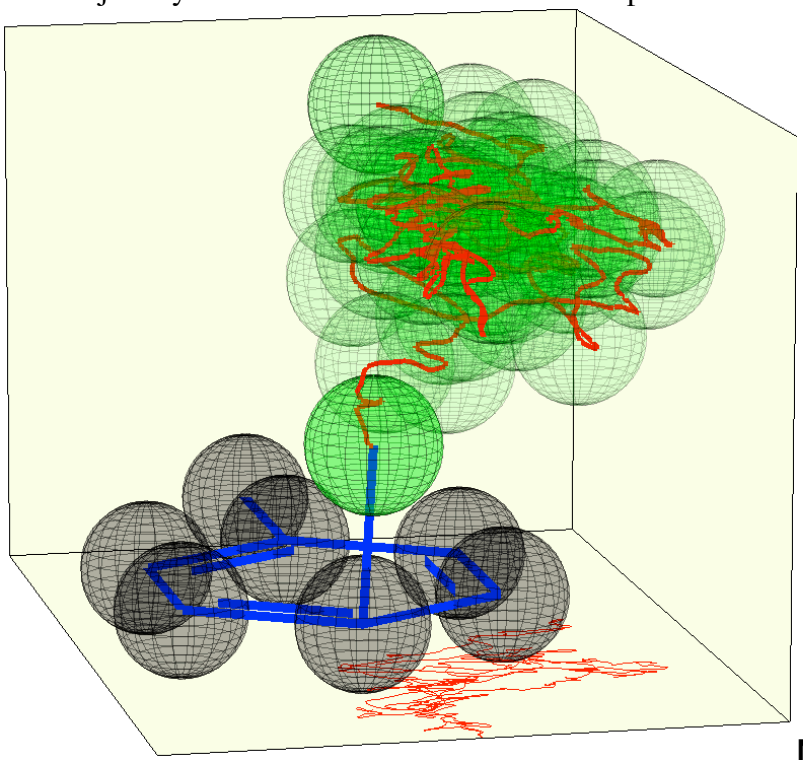
This trajectory switches from approach to the para carbon to meta attack at the very end.



This latter part of this trajectory has the NO_2^+ in between the ortho and ipso carbons, before finally seeing attack at the ipso position.

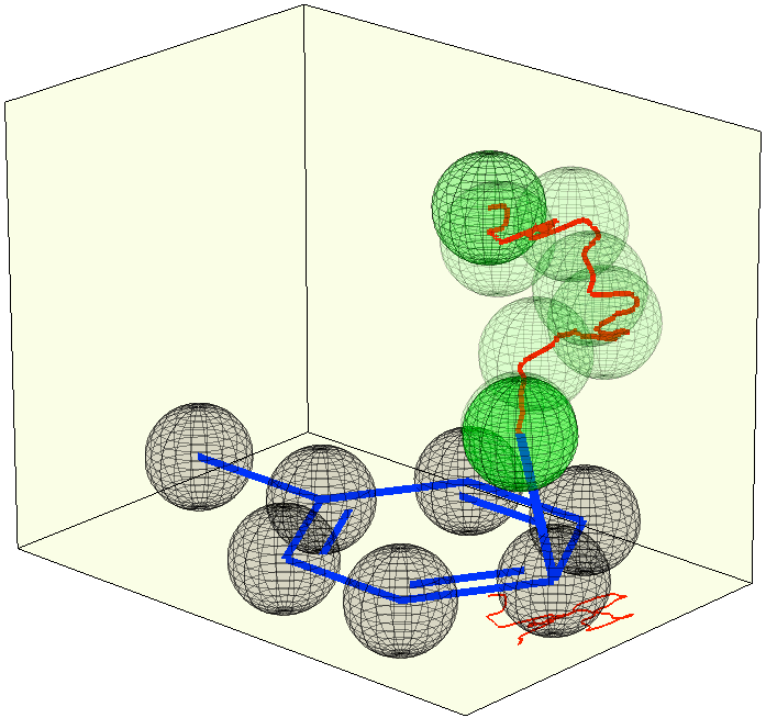


This trajectory makes a late switch from meta to para attack.

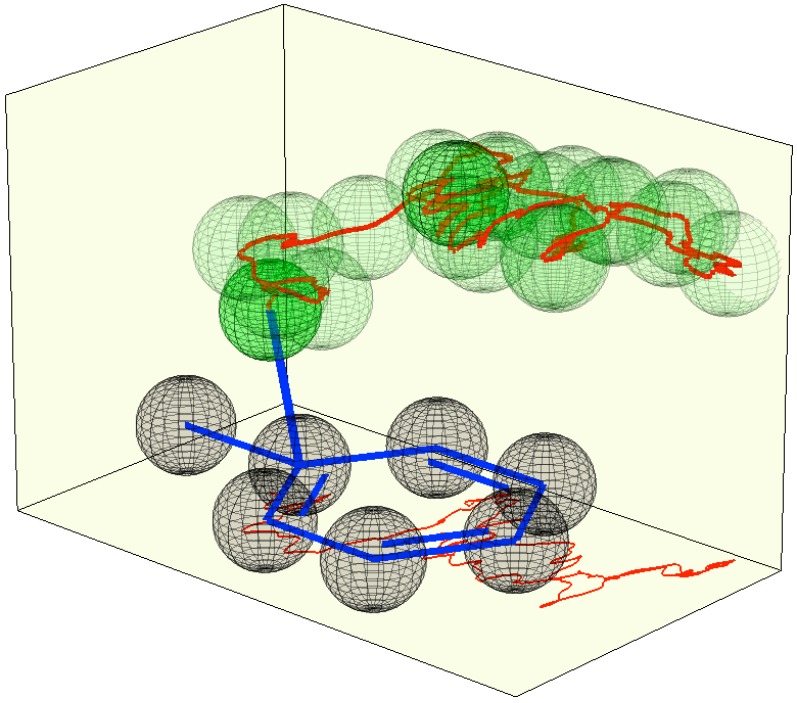


$NO_2^+ BF_4^-$ in a PCM Model

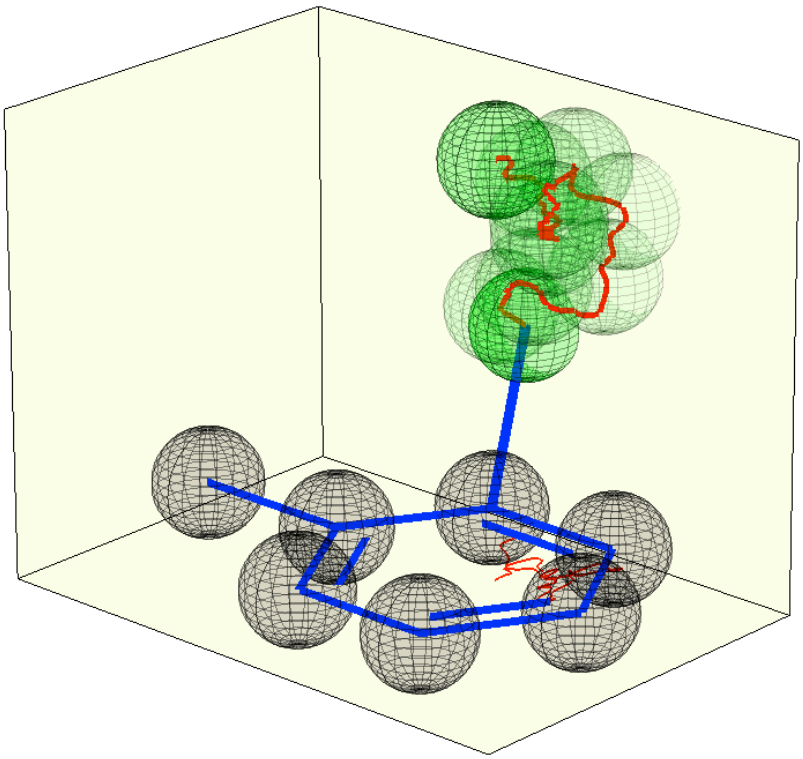
The median time of 1150 fs includes many short trajectories like this one, affording the para σ-complex in 426 fs.



Here is one of the longer trajectories in explicity solvent, taking 1787 fs to afford the ipso product. The nitronium spends most of the time at >3 Å from the arene carbons, then rapidly forms product after approaching closer.

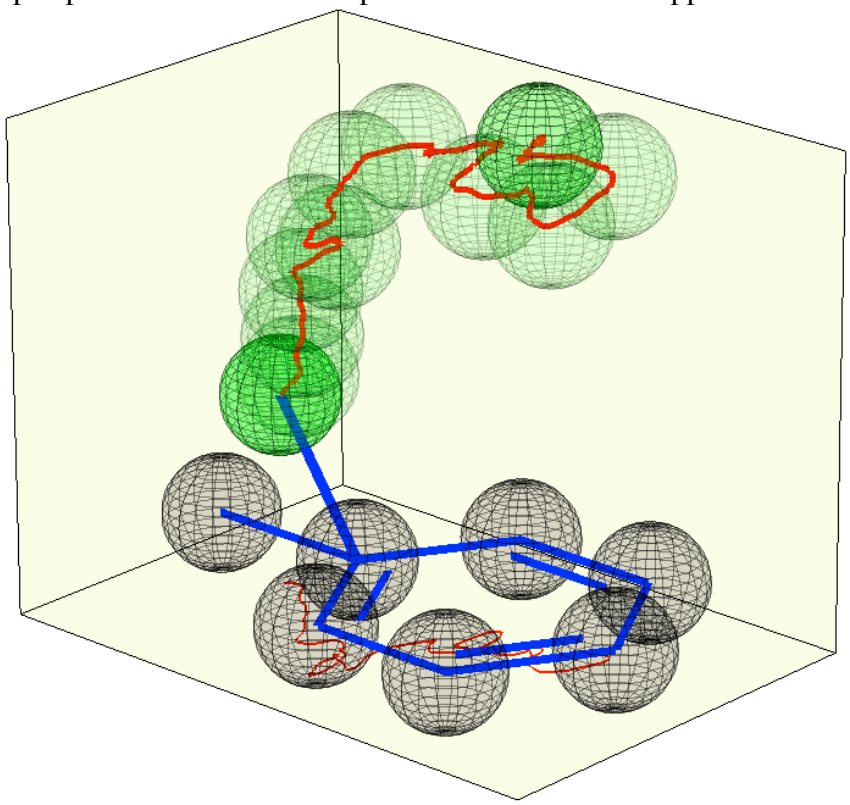


Ortho product formation in 631 fs. Notice how little the trace meanders before product formation.

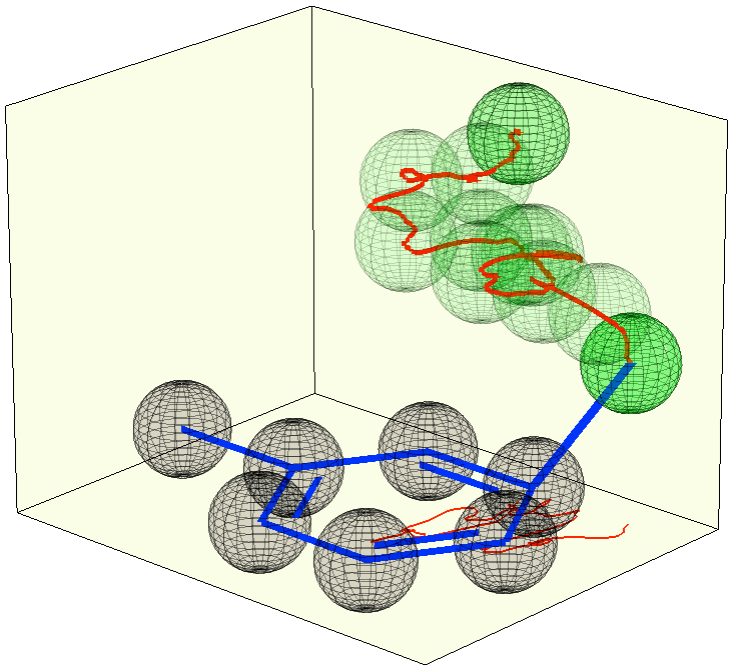


NO_2^+ with no counterion in Explicit Solvent

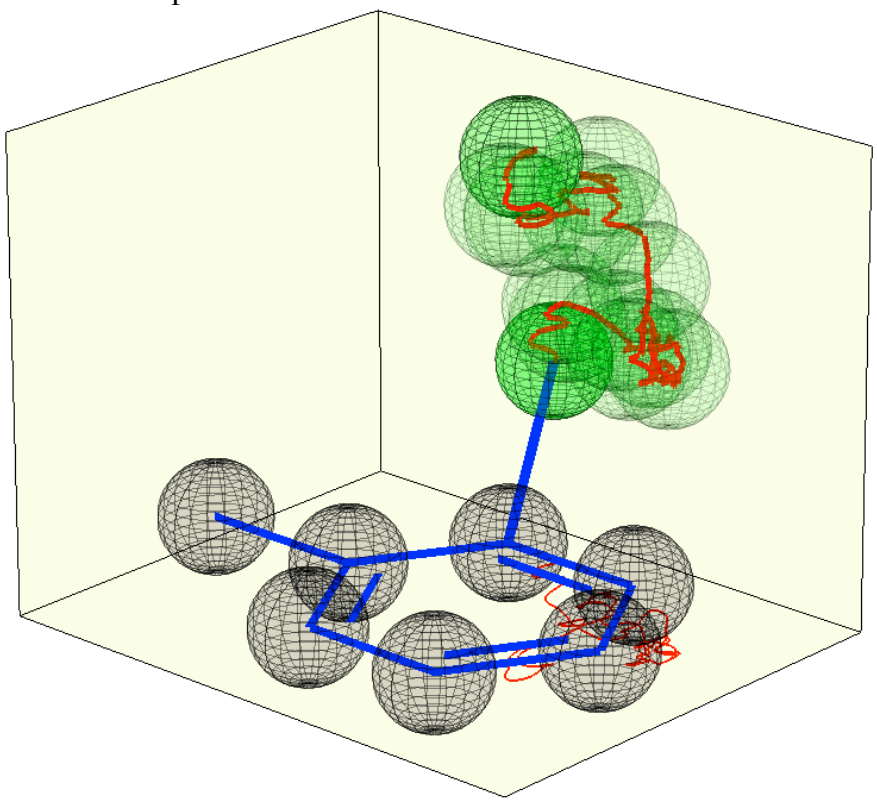
Ipso product formation is rapid after the nitronium approaches the carbon.



Meta product formation.



This trajectory shows an exception to the usual rapid descent to product. The nitronium at first approaches the meta carbon to within 1.9 Å, then moves over to the ortho carbon at the end. Such reversal can occur in explicit solvent but they are far less common than when the counterion is present.



Results and Selectivity Predictions for Trajectories based on Conventional Transition Stuctures

Trajectories for Toluene / NO_2^+ M06-2X/6-311G*/PCM (CH_2Cl_2)

For the five TSs located for the reaction of toluene with NO_2^+ in M06-2X/6-311G*/PCM(CH_2Cl_2) calculations, the table below shows the nominal (Gaussian 09 output, harmonic approximation) thermal free energy, the Boltzmann factor for each structure, the weighting of each structure, the raw trajectory results, trajectory percentages, and weighted percentages that add up to the predicted selectivity. The TSs are labeled by unique code numbers, e.g. 190031) that correspond to the codes that later label their specific geometry later in this document.

The Boltzmann factors have allowed for a factor of 2 for chiral structures relative to the achiral lowest-energy structure.

	G (Hartrees)	Erel (kcal/mol)	Boltzmann Factor	Boltzmann weighting
TS 190031	-476.190031	0.0	1.00	0.040
TS 187860	-476.18786	1.4	0.20	0.008
TS 188821	-476.188821	0.8	0.56	0.022
TS 189331	-476.189331	0.4	0.95	0.038

TS 189465	-476.189465	0.4	1.10	0.044

	trajectory results raw			
	ipso	ortho	meta	para
TS 190031	25	6		
TS 187860		37	11	1
TS 188821		58	19	
TS 189331			7	55
TS 189465			9	72

	trajectory percentages			
	ipso	ortho	meta	para
TS 190031	0.81	0.19	0.00	0.00
TS 187860	0.00	0.76	0.22	0.02
TS 188821	0.00	0.75	0.25	0.00
TS 189331	0.00	0.00	0.11	0.89
TS 189465	0.00	0.00	0.11	0.89

	weighted percentages			
	ipso	ortho	meta	para
TS 190031	0.21	0.05	0.00	0.00
TS 187860	0.00	0.04	0.01	0.00
TS 188821	0.00	0.11	0.04	0.00
TS 189331	0.00	0.00	0.03	0.22
TS 189465	0.00	0.00	0.03	0.26

	ipso	ortho	meta	para
Selectivity	0.21	0.20	0.11	0.48

Trajectories for Toluene / $NO_2^+BF_4^-$ M06-2X/6-311G*/PCM (CH_2Cl_2)

The table below shows the nominal (Gaussian 09 output, harmonic approximation) thermal free energy for the complete set of TSs obtained for the reaction of toluene with $NO_2^+BF_4^-$ in M06-2X/6-311G*/PCM(CH_2Cl_2) calculations. For those structures where trajectories were run, the table then shows the Boltzmann factor for each structure, the weighting of each structure, the raw trajectory results, trajectory percentages, and weighted percentages that add up to the predicted selectivity. The TSs are labeled by unique code numbers, e.g. 3.440_824095) that correspond to the codes that later label their specific geometry later in this document.

	G (Hartrees)	Erel (kcal/mol)	Boltzman Factor	Boltzmann weighting
TS 3.440_824095	-900.824095	0.00	1.00	0.33
TS 3.4399_824088	-900.824088	0.00	0.99	0.33

TS 3.440_824085	-900.824085	0.01	0.99	0.33
TS 3.426_824053	-900.824053	0.03	0.96	0.32
TS 3.393_822143	-900.822143	1.22	0.13	0.04
TS 3.3794_822005	-900.822005	1.31	0.11	0.04
TS 3.332_821966	-900.821966	1.34	0.10	0.03
TS 2.434_821714	-900.821714	1.49	0.08	0.03
TS 2.429_821508	-900.821508	1.62	0.06	0.02
TS 2.4410_821447	-900.821447	1.66		
TS 2.419_821322	-900.821322	1.74		
TS 2.4198_821288	-900.821288	1.76		
TS 2.435_821006	-900.821006	1.94		
TS 2.424_820983	-900.820983	1.95		
TS 2.398_820850	-900.820850	2.04		
TS 2.3272_820767	-900.820767	2.09		
TS 2.387_820745	-900.820745	2.10		
TS 3.444_820739	-900.820739	2.11		
TS 3.1392_820578	-900.820578	2.21		
TS 3.1409_820572	-900.820572	2.21		
TS 3.055_820543	-900.820543	2.23		
TS 2.4184_820386	-900.820386	2.33		
TS 2.306_820365	-900.820365	2.34		
TS 2.2457_820277	-900.820277	2.40		
TS 2.386_820166	-900.820166	2.47		
TS 3.298_819960	-900.819960	2.59		
TS 3.271_819957	-900.819957	2.60		
TS 2.6887_819594	-900.819594	2.82		
TS 2.586_819521	-900.819521	2.87		
TS 2.8006_818867	-900.818867	3.28		
TS 2.801_818858	-900.818858	3.29		
TS 2.8758_818627	-900.818627	3.43		
TS 2.778_818581	-900.818581	3.46		
TS 2.840_818475	-900.818475	3.53		
TS 3.1393_818379	-900.818379	3.59		
TS 3.052_818171	-900.818171	3.72		
TS 2.8774_817851	-900.817851	3.92		
TS 2.776_817301	-900.817301	4.26		

	trajectory results raw			
	ipso	ortho	meta	para
TS 3.440_824095	18			
TS 3.4399_824088	14			
TS 3.440_824085	17	1		

TS 3.426_824053	18	23		
TS 3.393_822143	1	31		
TS 3.3794_822005	3	36		
TS 3.332_821966	21	2	0	0
TS 2.434_821714			3	43
TS 2.429_821508				59

	trajectory percentages			
	ipso	ortho	meta	para
TS 3.440_824095	1.00	0.00	0.00	0.00
TS 3.4399_824088	1.00	0.00	0.00	0.00
TS 3.440_824085	0.94	0.06	0.00	0.00
TS 3.426_824053	0.44	0.56	0.00	0.00
TS 3.393_822143	0.03	0.97	0.00	0.00
TS 3.3794_822005	0.08	0.92	0.00	0.00
TS 3.332_821966	0.91	0.09	0.00	0.00
TS 2.434_821714	0.00	0.00	0.07	0.93
TS 2.429_821508	0.00	0.00	0.00	1.00

	weighted percentages			
TS 3.440_824095	ipso	ortho	meta	para
TS 3.4399_824088	0.23	0.00	0.000	0.00
TS 3.440_824085	0.22	0.00	0.000	0.00
TS 3.426_824053	0.21	0.01	0.000	0.00
TS 3.393_822143	0.09	0.12	0.000	0.00
TS 3.3794_822005	0.00	0.03	0.000	0.00
TS 3.332_821966	0.00	0.02	0.000	0.00
TS 2.434_821714	0.02	0.00	0.000	0.00
TS 2.429_821508	0.00	0.00	0.001	0.02
TS 3.440_824095	0.00	0.00	0.000	0.01
	total			
	ipso	ortho	meta	para
Selectivity	0.78	0.19	0.0012	0.032

Trajectories for Toluene / $NO_2^+BF_4^-$ ONIOM(M06-2X/6-311G*:PM3)/PCM (CH_2Cl_2)

The table below shows the nominal (Gaussian 09 output, harmonic approximation) thermal free energy for the complete set of TSs and CVTSs obtained for the reaction of toluene with $NO_2^+BF_4^-$ in ONIOM(M06-2X/6-311G*:PM3)/PCM (CH_2Cl_2) calculations. For those structures where trajectories were run, the table then shows the raw trajectory results.

As discussed in the main text, the located transition structures were biased for TSs associated with barriers, with attack *para* or *meta* (e.g., **6a**‡ and **6a**‡) over those that face no

barrier. This posed a problem for the prediction of the product ratios from the calculations, because it was impractical to perform an exhaustive search for all of the CVTSs associated with attack ortho or ipso. We assume that approximately the same ensemble of counterion positions that was observed for para and meta attack also exists for ortho or ipso attack, even though the latter cannot be fully accounted for. To approximately allow for all of the possibilities, we choose a series of four structures in which the counterion occupies approximately the same relative position, and we estimated the selectivity based on this limited series. The table below then only shows Boltzmann factors and weightings for those four structures. The weighted percentages were added up to predict the selectivity. It may be argued that this is only a very crude way to estimate the selectivity. A better method to predict the selectivity based on random starting points (described in a previous section) gives roughly the same results.

If the selectivity were predicted based on all low-energy structures for which trajectories were obtained, the prediction would be 4% *ipso*, 6% *ortho*, 17% *meta*, and 69% *para*. This has no effect on any argument in the main text, but it does serve to illustrate the problem with relying too much on located TSs without consideration of what was not located.

The TSs are labeled by unique code numbers, e.g. 3.440_824095 that correspond to the codes that later label their specific geometry later in this document.

	G (Hartrees)	Erel (kcal/mol)	Boltzman Factor	Boltzmann weighting
TS 2.609_94138	-476.94139	0.00		
TS 2.998_94130	-476.9413	0.06	0.91	0.38
TS 2.706_94118	-476.941183	0.13	0.80	0.33
TS 2.612_94115	-476.941158	0.14		
TS 2.605_94114	-476.941143	0.15		
TS 2.702_94087	-476.940877	0.3		
TS 2.742_94075	-476.940751	0.4		
TS 2.613_94072	-476.940723	0.4		
TS 2.711_94072	-476.94072	0.4		
TS 2.613_94064	-476.940644	0.5		
TS 2.611_94056	-476.94056	0.5		
CVTS 940511	-476.940511	0.6	0.39	0.16
TS 2.704_94050	-476.940501	0.6		
TS 2.610_94049	-476.940492	0.6		
TS 2.693_94047	-476.940476	0.6		
TS 2.622_94034	-476.940348	0.7		
CVTS 940237	-476.940237	0.7	0.30	0.12
TS 2.596_94018	-476.940182	0.8		
TS 3.138_94010	-476.940108	0.8		
TS 2.678_94009	-476.940097	0.8		
TS 2.598_94007	-476.940072	0.8		
TS 2.687_93987	-476.93987	1.0		
TS 2.776_93985	-476.939853	1.0		

TS 2.615_93980	-476.939809	1.0
TS 3.093_93959	-476.939593	1.1
TS 2.607_93956	-476.939561	1.1
TS 2.610_93954	-476.93954	1.2
TS 3.125_93949	-476.939494	1.2
TS 3.130_93946	-476.939465	1.2
TS 2.684_93941	-476.939419	1.2
TS 3.119_93935	-476.939352	1.3
TS 3.092_93920	-476.9392	1.4
TS 2.967_93897	-476.938974	1.5
TS 3.146_93865	-476.938658	1.7
TS 2.609_93861	-476.938616	1.7
TS 3.118_93853	-476.938536	1.8
TS 2.635_93808	-476.938082	2.1
TS 3.139_93772	-476.937723	2.3
TS 3.077_93756	-476.937563	2.4
TS 2.629_93703	-476.937037	2.7
TS 3.182_93693	-476.936936	2.8
TS 3.107_93658	-476.936587	3.0
TS 3.341_93655	-476.936553	3.0
TS 3.099_93449	-476.934492	4.3

	trajectory results raw			
	ipso	ortho	meta	para
TS 2.609_94138			9	66
TS 2.998_94130		62	88	0
TS 2.706_94118			10	67
TS 2.612_94115			5	47
TS 2.605_94114				42
TS 2.702_94087			8	53
TS 2.742_94075			25	30
TS 2.613_94072		1	10	78
TS 2.711_94072			10	71
TS 2.613_94064			11	76
TS 2.611_94056			8	59
VTS940511	37	14		
VTS940237	4	60		

	trajectory percentages			
	ipso	ortho	meta	para
TS 2.609_94138	0.00	0.00	0.12	0.88
TS 2.998_94130	0.00	0.41	0.59	0.00

TS 2.706_94118	0.00	0.00	0.13	0.87
TS 2.612_94115	0.00	0.00	0.10	0.90
TS 2.605_94114	0.00	0.00	0.00	1.00
TS 2.702_94087	0.00	0.00	0.13	0.87
TS 2.742_94075	0.00	0.00	0.45	0.55
TS 2.613_94072	0.00	0.01	0.11	0.88
TS 2.711_94072	0.00	0.00	0.12	0.88
TS 2.613_94064	0.00	0.00	0.13	0.87
TS 2.611_94056	0.00	0.00	0.12	0.88
VTS940511	0.73	0.27	0.00	0.00
VTS940237	0.06	0.94	0.00	0.00

	weighted percentages			
	ipso	ortho	meta	para
TS 2.998_94130	0.00	0.16	0.222	0.00
TS 2.706_94118	0.00	0.00	0.043	0.29
VTS940511	0.12	0.05	0.000	0.00
VTS940237	0.01	0.12	0.000	0.00

	total			
	ipso	ortho	meta	para
Selectivity	0.12	0.20	0.27	0.29

Trajectories for Toluene / NO_2^+ / H_2SO_4 M06-2X/6-311G*/PCM (ε=109)

The table below shows the nominal (Gaussian 09 output, harmonic approximation) thermal free energy for the complete set of TSs obtained for the reaction of toluene with NO_2^+ / H_2SO_4 in M06-2X/6-311G* calculations with a PCM model based on that used in Koleva, G.; Galabov, B.; Hadjieva, B.; Schaefer, H. F.; Schleyer, P. v. R. *Angew. Chem. Int. Ed.* **2015**, *54*, 14123-14127 (ε=109, epsinf=2.016,rsolv=2.5). For those structures where trajectories were run, the table then shows the Boltzmann factor for each structure, the weighting of each structure, the raw trajectory results, trajectory percentages, and weighted percentages that add up to the predicted selectivity. The TSs are labeled by unique code numbers, e.g. 3.45_370364 that correspond to the codes that later label their specific geometry later in this document.

	G (Hartrees)	Erel (kcal/mol)	Boltzman Factor	Boltzmann weighting
TS 3.45_370364	-1176.370364	0.000	1.000	0.133
TS 3.42_370300	-1176.370300	0.040	0.934	0.125
TS 3.41_370239	-1176.370239	0.078	0.876	0.117
TS 3.44_370143	-1176.370143	0.139	0.791	0.105
TS 3.46_370093	-1176.370093	0.170	0.750	0.100
TS 3.43_369922	-1176.369922	0.277	0.626	0.083
TS 3.46_369483	-1176.369483	0.553	0.393	0.052

TS 3.46_369466	-1176.369466	0.564	0.386	0.051
TS 3.41_369431	-1176.369431	0.585	0.372	0.050
TS 2.46_368778	-1176.368778	0.995	0.186	0.025
TS 2.46_368547	-1176.368547	1.140	0.146	0.019
TS 3.45_368434	-1176.368434	1.211	0.129	0.017
TS 2.45_368346	-1176.368346	1.266	0.118	0.016
TS 2.44_368221	-1176.368221	1.345	0.103	0.014
TS 3.42_368199	-1176.368199	1.359	0.101	0.013
TS 2.43_368154	-1176.368154	1.387	0.096	0.013
TS 2.50_368101	-1176.368101	1.420	0.091	0.012
TS 2.45_367948	-1176.367948	1.516	0.077	0.010
TS 3.47_367776	-1176.367776	1.624	0.064	0.009
TS 2.45_367760	-1176.367760	1.634	0.063	0.008
TS 2.47_367357	-1176.367357	1.887	0.041	0.006
TS 2.47_367350	-1176.367350	1.891	0.041	0.005
TS 3.27_367301	-1176.367301	1.922	0.039	0.005
TS 3.08_366987	-1176.366987	2.119	0.028	0.004
TS 3.32_366879	-1176.366879	2.187	0.025	0.003
TS 3.34_366676	-1176.366676	2.314	0.020	0.003
TS 2.48_366653	-1176.366653	2.329		
TS 3.33_365619	-1176.365619	2.978		

trajectory results raw

	ipso	ortho	meta	para
TS 3.45_370364	13	21		
TS 3.42_370300	6	32		
TS 3.41_370239	3	35		
TS 3.44_370143	5	34		
TS 3.46_370093	8	23		
TS 3.43_369922	5	29		
TS 3.46_369483	23	3		
TS 3.46_369466	19	2		
TS 3.41_369431	2	36		
TS 2.46_368778			2	44
TS 2.46_368547			8	32
TS 3.45_368434	8	33		
TS 2.45_368346			1	47
TS 2.44_368221			2	62
TS 3.42_368199	5	22		
TS 2.43_368154				55
TS 2.50_368101			2	53
TS 2.45_367948			8	39
TS 3.47_367776	51	2		

TS 2.45_367760			5	47
TS 2.47_367357			4	38
TS 2.47_367350				34
TS 3.27_367301		48		
TS 3.08_366987		21	5	
TS 3.32_366879		48		
TS 3.34_366676		77		

	trajectory percentages			
	ipso	ortho	meta	para
TS 3.45_370364	0.382	0.618	0.000	0.000
TS 3.42_370300	0.158	0.842	0.000	0.000
TS 3.41_370239	0.079	0.921	0.000	0.000
TS 3.44_370143	0.128	0.872	0.000	0.000
TS 3.46_370093	0.258	0.742	0.000	0.000
TS 3.43_369922	0.147	0.853	0.000	0.000
TS 3.46_369483	0.885	0.115	0.000	0.000
TS 3.46_369466	0.905	0.095	0.000	0.000
TS 3.41_369431	0.053	0.947	0.000	0.000
TS 2.46_368778	0.000	0.000	0.043	0.957
TS 2.46_368547	0.000	0.000	0.200	0.800
TS 3.45_368434	0.195	0.805	0.000	0.000
TS 2.45_368346	0.000	0.000	0.021	0.979
TS 2.44_368221	0.000	0.000	0.031	0.969
TS 3.42_368199	0.185	0.815	0.000	0.000
TS 2.43_368154	0.000	0.000	0.000	1.000
TS 2.50_368101	0.000	0.000	0.036	0.964
TS 2.45_367948	0.000	0.000	0.170	0.830
TS 3.47_367776	0.962	0.038	0.000	0.000
TS 2.45_367760	0.000	0.000	0.096	0.904
TS 2.47_367357	0.000	0.000	0.095	0.905
TS 2.47_367350	0.000	0.000	0.000	1.000
TS 3.27_367301	0.000	1.000	0.000	0.000
TS 3.08_366987	0.000	0.808	0.192	0.000
TS 3.32_366879	0.000	1.000	0.000	0.000
TS 3.34_366676	0.000	1.000	0.000	0.000

	weighted percentages			
	ipso	ortho	meta	para
TS 3.45_370364	0.051	0.082	0.000	0.000
TS 3.42_370300	0.020	0.105	0.000	0.000
TS 3.41_370239	0.009	0.108	0.000	0.000

TS 3.44_370143	0.014	0.092	0.000	0.000
TS 3.46_370093	0.026	0.074	0.000	0.000
TS 3.43_369922	0.012	0.071	0.000	0.000
TS 3.46_369483	0.046	0.006	0.000	0.000
TS 3.46_369466	0.047	0.005	0.000	0.000
TS 3.41_369431	0.003	0.047	0.000	0.000
TS 2.46_368778	0.000	0.000	0.001	0.024
TS 2.46_368547	0.000	0.000	0.004	0.016
TS 3.45_368434	0.003	0.014	0.000	0.000
TS 2.45_368346	0.000	0.000	0.000	0.015
TS 2.44_368221	0.000	0.000	0.000	0.013
TS 3.42_368199	0.002	0.011	0.000	0.000
TS 2.43_368154	0.000	0.000	0.000	0.013
TS 2.50_368101	0.000	0.000	0.000	0.012
TS 2.45_367948	0.000	0.000	0.002	0.009
TS 3.47_367776	0.008	0.000	0.000	0.000
TS 2.45_367760	0.000	0.000	0.001	0.008
TS 2.47_367357	0.000	0.000	0.001	0.005
TS 2.47_367350	0.000	0.000	0.000	0.005
TS 3.27_367301	0.000	0.005	0.000	0.000
TS 3.08_366987	0.000	0.003	0.001	0.000
TS 3.32_366879	0.000	0.003	0.000	0.000
TS 3.34_366676	0.000	0.003	0.000	0.000

total			
ipso	ortho	meta	para
0.241	0.630	0.0100	0.119

Programs for Calculations

Program Suite PROGDYN

A full listing of the subprograms of PROGDYN is given below. To allow the reader to understand or make use of PROGDYN, we describe here first the overall structure of the program. We also list and describe in this section a number of helper programs that were used to analyze the data from the trajectory calculations.

The master control program for dynamics, in the form of a Unix Shell Script, is called *progdynstarterHP*. For a user to start to use *progdynstarterHP*, some early lines in it that assign the scratch space and the location of the program files and input files would have to be modified for the local environment. These lines are between lines 45 and 55 and should be apparent. The location of the scratch space is usually passed to *progdynstarterHP* as a parameter.

progdynstarterHP takes as input files:

freqinHP - This is the standard output from a Gaussian 98, 03, or 09 frequency calculation using freq=hpmodes. For isotopically labeled compounds, use freq=(hpmodes,readisotopes).

progdyn.conf – This is a file giving a variety of configuration options, called on by many of the subprograms. progdyn.conf examples are listed below and contains explanations of the program options.

isomernumber - A number in file isomernumber provides a start for numbering runs. The default is 1.

detour – A signal file that, by existing, signals the program to do a side calculations

nogo – A signal file that, by existing, signals the program to stop between points

bypassproggen - A signal file that, by existing, signals the program to use a supplied input file *geoPlusVel* instead of generating one for itself. This pathway for initialization is important here because it is used when the program progdynsam, described later, is used to generate the geoPlusVel file.

methodfile – A file that contains lines to be added to the end of each g09.com input file, such as lines that call for an NMR calculation

ZMAT – An input file for the CFOUR (http://www.cfour.de) suite of programs. When ZMAT is supplied, *progdynstarterHP* will automatically run call CFOUR (which must be set up independently by the user) by making use of the script *progcfour*.

cannontraj – A file containing a vector for each atom, used to fire an initial geometry in a particular direction.

progdynstarterHP calls the following programs:

proggenHP - An awk program that starts a trajectory, giving each mode its zero point energy (if a quasiclassical calculation) plus random additional excitations depending on the temperature.

prog1stpoint – Awk program that creates the first Gaussian input file for each run

prog2ndpoint – Awk program that creates the second Gaussian input file for each run. prog2ndpoint also checks the energy of the first point to see if it fits with the desired energy, and aborts the run if it does not by creating appropriate output in file Echeck

progdynb – Creates subsequent Gaussian input files until run is completed, written in awk

proganal – A program to analyze the latest point and see if a run is done. This program must be redone for each new system. Elaborate changes are sometimes programmed into proganal, such as the automatic changing of configuration variables. proganal creates the output to dynfollowfile and NMRlist or NMRlistdis

randgen – A program that generates random numbers between 0 and 1. These are generated all at once and stored in a file for use by proggenHP.

progcfour – A control script to run CFOUR calculations (not needed for most kinds of runs).

progdynstarterHP has the following output files:

isomernumber – A running tab of the trajectory number

runpointnumber – a running tab of the point in the trajectory

Echeck – output form where prog2ndpoint checks the energy of the trajectory to see if it fits with the desired energy

geoRecord – A record of all of the geoPlusVel files.

geoPlusVel – Created by proggen, this gives the starting positions, velocities, isotopic masses, excitations of the normal modes, and initial displacements of the normal modes for current run.

g09.com – Created by prog1stpoint, prog2ndpoint, and progdynb, this is the latest input file for Gaussian09 for current run and latest point.

olddynrun, *olddynrun2, olddynrun3* – files containing the last three outputs from Gaussian, for creation of the next point

traj, traj1, traj2, traj3, etc. – files containing the geometries and energies for each trajectory, numbered by the isomernumber, in a format suitable for reading by Molden.
dynfollowfile – A short record of the runs and their results. The data desired for *dynfollowfile* must be programed into the script *proganal* as needed for each system studied.
NMRlist or *NMRlistdis* – output of NMR predictions at each point in a trajectory, when desired
skipstart - A signal file that, by existing, tells progdynstarterHP that we are in the middle of a run. For trajectories that are propagated forward and backward in time, skipstart keeps track of whether one is in the forward or reverse part.
diagnostics – optional output that follows which subprograms are running and configuration variables, decided by variable in progdyn.conf
vellist – optional output that lists the velocities of each atom, decided by variable in progdyn.conf, or lists the total kinetic energy in the system and the classical temperature, often also keeps track of the density
A number of files starting with *'temp'* are created then later erased.

The following helper programs were used for the current study.
progdynsam – an awk program that generates a geoPlusVel file based on input from a *traj* file. Typically, the traj file is a trajectory performed with constraints, and the new geoPlusVel will be started without constraints. *progdynsam* must be modified for the desired temperature, and it takes as input the variable pt to decide which points in the traj file are used to define the geoPlusVel. For previously constrained atoms, *progdynsam* gives the atoms a Boltzmann-random velocity and direction of motion appropriate for the desired temperature. The program is invoked with awk –v pt=## –f progdynsam traj where ## is the trajectory point used to start a new geoPlusVel, and traj is the output file from above containing the list of trajectory points.
progwhere – an awk program used to analyze the output data in *dynfollowfile*. It is involked with awk –f progtrajlength dynfollowfile where dynfollowfile is a list of one or more of the dynfollowfile output files described above.
whamnit – a shell script that extracts data from the dynfollowfile files, sets up and runs wham to calculate the PMF, and keeps track of some general aspects of trajectories
progseries – an AWK script used by whamnit to extract data from the dynfollowfile files
wham – a program from Grossfield, Alan, "WHAM: the weighted histogram analysis method", version 2.0.9, http://membrane.urmc.rochester.edu/content/wham that performs the wham analysis
prog3dpath – a program that takes the output from dynfollowfile and generates the data for a 3d path relative to the aveage position of the arene carbons, used for generating the the pictures in Figure 2 of the paper.
nitrationPara1.m – This is an example of the Matlab version 2014 b code that was used to generate along with the data from prog3dpath to generate the Figures in Figure 2.

Program progdynstarterHP

```
#!/bin/bash
#progdynstarterHP, made to use high-precision modes from Gaussian output with freq=hpmodes
#updated to create a random number file temp811 that is used by proggenHP
#version September 16, 2005, made for workstations
#version August 2007 to allow periodic copying of g09.log to dyn putting it under control of progdynb
#version Feb 2008 moves variables like the scratch directory and location of randgen to the beginning
#version March 2008 added proganal reporting to points 1 and 2
#version Jan 2009 fixed bug generator of having proganal run twice in checking for complete runs
#version May 2009 Echeck catches bad energies after only one point, other lines written simpler, triple while loop, revised comments
#version Aug 2010 isomernumber adds words to ease parsing, increased elements up to bromine, runpointnumber checked for more appropriate restarts
#version Aug 2011 runpointnumber starts better, restart better if died during first few points, awk bug fix
#version Aug 2012 freqinHP reads with only 3 freqs, goingwell and other temp files moved to $scratchdir
#version Aug 2013 adds ability to automatically run a CFOUR program if the file ZMAT exists
#
#version Nov 2013 adds ability to bypass generation of geoPlusVel using the signal file bypassproggen
#version Nov 2015 makes using guess=read easier, improves ability to restart after disk write failures, partially allows for MM runs in Gaussian
#LIMITATIONS - standard version only handles elements up to bromine, must change program to do higher atomic numbers
#   only handles up to 4000th excited state for modes - this could start to affect the initialization of classical modes or transition vectors at
#    extremely high temperatures
#   The routine that checks whether the actual energy approximately equals the desired energy checks for lines containing "SCF
```

```
Done" or "EUMP2 =" or " Energy="
#   This should handle ordinary calculations HF, DFT, ONIOM, and MP2 calculatons but the routine in prog2ndpoint would have to be changed for other calcs.
#
#                                   OUTLINE
# A. initilize to perform Gaussian jobs, set the scratch, program, and other directores, remove errant control files
#    start outermost loop L1L1L1L1L1L1L1L1
#    start loop 2 L2L2L2L2L2L2L2L2L2
# B. branch on whether there is a file named "skipstart"
#    if there is, skip B1, B2, B3 entirely
#    if no file named "skipstart" then generate a new isomer.  Instructions: Get rid of skipstart to start new isomer.
#    the B loop generates geoPlusVel, adds it to geoRecord, generates and runs first and second points, and sets up for continuous loop
#  B1. generates geoPlusVel, isomernumber, runpointnumber=1, then makes g09.com for point 1
#  B2. checks for success of B1 or exits, then sets geoRecord then runs g09.com.  Checks for its success or exits.
#  B3. runpointnumber=2, kills run if XXXX in dynfollowfile due to bad energy probably, makes g09.com for point 2, runs it
#      checks for its success or exits
#      runpointnumber=3, uses progdynb to make g09.com for point 3
#      sets skipstart=forward
#  B4. Only runs if skipstart=ireverserestart, performs reverserestart, ends with runpointnumber=3
#      sets skipstart=reverse
# C. loop over propagation steps
#
#
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
#
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
#
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
#origdir, randdir, scratchdir, g09root, logfile all may need varied from system to system and assigned here or by program calling this one
export LC_ALL=C
echo $1
scratchdir=$1
export g09root=/software/lms/g09_D01
. $g09root/g09/bsd/g09.profile
origdir=`pwd`
cd $origdir
logfile=docslog
randdir=~/bin
proggramdir=~/binall500
freqfile=~/binall500/freqinHP
echo
echo ORIGDIR at the beginning of run:
echo $origdir
ls $origdir
echo
echo SCRATCHDIR at the beginning of run:
echo $scratchdir
ls $scratchdir
echo
echo PROGGRAMDIR at the beginning of run::
echo $proggramdir
ls $proggramdir

rm -f nogo    # assume that if someone is starting a job, they want it to go.
```

```
rm -f diagnostics goingwell tempdone # diagnostics contains extra info from previous runs, other two files are from older
versions of progdyn
if (test -s g09.com) then
  sed -i '/guess=tcheck/d' g09.com      # no chk file on first point
fi

#### Triple 'while' loop - will have to break multiple times to get out, but advantage is ability to control starting over
#L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1
L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1L1
while (true)
do
# As long as there is a file "goingwell" the program will not exit entirely by itself
rm -f $scratchdir/goingwell
#L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2
L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2L2
while (true)
do
#  BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB
  if (test -f skipstart) then
    echo "skipping start and continuing from previous runs"
  else
#  B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1B1 generate geoPlusVel and first input file
    if [ `cat runpointnumber` = "1" ]; then
      echo "X did not complete first point so new isomer started" >> dynfollowfile
    fi
    if [ `cat runpointnumber` = "2" ]; then
      echo "X did not complete second point so new isomer started" >> dynfollowfile
    fi
    if [ `cat runpointnumber` = "3" ]; then
      echo "X did not complete third point so new isomer started" >> dynfollowfile
    fi
    cd $origdir
    if (test -f bypassproggen) then
      echo "taking starting conditions from pre-generated geoPlusVel"
    else
      $randdir/randgen > temp811
# the next 8 lines would have to be changed to use low-precision modes
      awk '/        1         2/,/Harmonic frequencies/ {print}' $freqfile > temp401
      awk '/Frequencies --/ {print $3;print $4;print $5;print $6;print $7}' temp401 > tempfreqs
      awk '/Reduced masses/ {print $4;print $5;print $6;print $7;print $8}' temp401 > tempredmass
      awk '/Force constants/ {print $4;print $5;print $6;print $7;print $8}' temp401 > tempfrc
      awk '/0/ && ((length($1) < 2) && ($1 < 4)) {print}' temp401 > tempmodes
      awk '/has atomic number/ {print}' $freqfile > tempmasses
      awk '/Standard orientation:/,/tional const/ {if (($3==0) || (substr($3,1,2)==10)) print}' $freqfile > tempstangeos
      awk '/Input orientation:/,/Stoichiometry/ {if (($3==0) || (substr($3,1,2)==10)) print}' $freqfile > tempinputgeos
      awk -f $proggramdir/proggenHP $freqfile > geoPlusVel
    fi
    if (test -f isomernumber) then
      cp isomernumber temp533
      awk 'BEGIN {getline;i=$1+1;print i,"----trajectory isomer number----"}' temp533 > isomernumber
      rm temp533
    else
      echo "1 ----trajectory isomer number----" > isomernumber
    fi
    echo 1 > runpointnumber
    rm g09.com
    awk -f $proggramdir/prog1stpoint isomernumber > g09.com
#  B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2B2  if first part successfule then
clean up and run the first input file, otherwise die
    if (test -s g09.com) then
      rm tempfreqs tempredmass tempfrc tempmodes tempstangeos tempmasses temp401 temp811 tempinputgeos
      cat isomernumber >> geoRecord
```

```
        cat geoPlusVel >> geoRecord
        rm -f $scratchdir/goingwell
        cd $scratchdir
        cp $origdir/g09.com $scratchdir/g09.com
        $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
        cd $origdir
        grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
        if (test -s $scratchdir/goingwell) then
          cp $scratchdir/g09.log olddynrun2
        else
          cp $scratchdir/g09.log $origdir/g09.log
          break
        fi
      else
        break
      fi
#  B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3B3 if B2 worked then you are here.
create 2nd point, run it, and set up for propagation loop
      rm g09.com
      echo 2 > runpointnumber
      awk -f $proggramdir/prog2ndpoint $scratchdir/g09.log > g09.com
# before we decide to run this, check the energy
      awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
      rm -f $scratchdir/tempdone
      tail -1 dynfollowfile | awk '/XXXX/ {print}' > $scratchdir/tempdone
      if (test  -s $scratchdir/tempdone) then
        rm -f dyn
        rm -f traj
        echo 0 > runpointnumber
        break
      fi
      if (test -s g09.com) then
        rm -f $scratchdir/goingwell
        cd $scratchdir
        cp $origdir/g09.com $scratchdir/g09.com
        $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
        cd $origdir
        grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
        if (test -s $scratchdir/goingwell) then
          cp $scratchdir/g09.log olddynrun
          awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
          awk '/Input orientation/,/Distance matrix/ {print};/Matrix orientation/,/Stoichiometry/ {print}' olddynrun | awk '{if
(($2>.5) && ($2<100)) print}' > old
          awk '/Input orientation/,/Distance matrix/ {print};/Matrix orientation/,/Stoichiometry/ {print}' olddynrun2 | awk '{if
(($2>.5) && ($2<100)) print}' > older
          echo 3 > runpointnumber
          if (test -f bypassproggen) then
            cat bypassproggen > runpointnumber
            echo 3 > bypassproggen
          fi
          awk -f $proggramdir/progdynb olddynrun > g09.com
          rm -f old older
        else
          cp $scratchdir/g09.log $origdir/g09.log
          break
        fi
      else
        break
      fi
# we've just completed a start, so lets skipstart until instructed otherwise
      echo "forward" > skipstart
    fi
```

```
#
B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4
B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4B4
# Reverse trajectories starter routine
  if [ `cat skipstart` = "reverserestart" ]; then
    cd $origdir
    rm g09.com
    echo 1 > runpointnumber
    awk -f $proggramdir/prog1stpoint isomernumber > g09.com
    if (test -s g09.com) then
      rm -f $scratchdir/goingwell
      cd $scratchdir
      cp $origdir/g09.com $scratchdir/g09.com
      $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
      cd $origdir
      grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
      if (test -s $scratchdir/goingwell) then
        cp $scratchdir/g09.log olddynrun2
      else
        cp $scratchdir/g09.log $origdir/g09.log
        break
      fi
    else
      break
    fi
    rm g09.com
    echo 2 > runpointnumber
    awk -f $proggramdir/prog2ndpoint $scratchdir/g09.log > g09.com
    awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
    rm -f $scratchdir/tempdone
    if (test -s g09.com) then
      rm -f $scratchdir/goingwell
      cd $scratchdir
      cp $origdir/g09.com $scratchdir/g09.com
      $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
      cd $origdir
      grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
      if (test -s $scratchdir/goingwell) then
        cp $scratchdir/g09.log olddynrun
        cat $scratchdir/g09.log >> dyn
        awk -f $proggramdir/proganal $scratchdir/g09.log >> dynfollowfile
        awk '/Input orientation/,/Distance matrix/ {print};/Matrix orientation/,/Stoichiometry/ {print}' olddynrun | awk '{if
(($2>.5) && ($2<100)) print}' > old
        awk '/Input orientation/,/Distance matrix/ {print};/Matrix orientation/,/Stoichiometry/ {print}' olddynrun2 | awk '{if
(($2>.5) && ($2<100)) print}' > older
        echo 3 > runpointnumber
        if (test -f bypassproggen) then
          cat bypassproggen > runpointnumber
        fi
        awk -f $proggramdir/progdynb olddynrun > g09.com
        rm -f old older
      else
        cp $scratchdir/g09.log $origdir/g09.log
        break
      fi
    else
      break
    fi
# we've just completed a reversestart, so lets skipstart until instructed otherwise
    echo "reverse" > skipstart
  fi
```

```
#  END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___END_of_B___

#  CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC  propagation loop
  while (true)
  do
    rm -f $scratchdir/goingwell
    cd $scratchdir
    cp $origdir/g09.com $scratchdir/g09.com
    $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
    cd $origdir
    grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
    if (test -s $scratchdir/goingwell) then
      awk -f $proggramdir/proganal $scratchdir/g09.log >> $origdir/dynfollowfile
      mv olddynrun2 olddynrun3
      mv olddynrun olddynrun2
      awk '/Input orientation/,/Distance matrix/ {print};/Matrix orientation/,/Stoichiometry/ {print}' $scratchdir/g09.log | awk '{if
(($2>.5) && ($2<100)) print}' > old
      cp $scratchdir/g09.log olddynrun
      awk '/Input orientation/,/Distance matrix/ {print};/Matrix orientation/,/Stoichiometry/ {print}' olddynrun2 | awk '{if
(($2>.5) && ($2<100)) print}' > older
      #increment runpointnumber
      cp runpointnumber $scratchdir/temp533
      awk 'BEGIN {getline;i=$1+1;print i}' $scratchdir/temp533 > runpointnumber
      rm $scratchdir/temp533
      awk -f $proggramdir/progdynb $scratchdir/g09.log > g09.com
      rm -f old older
    else
      cp $scratchdir/g09.log $origdir/g09.log
      break
    fi
# kludge to do a side calculation of NMR using progcfour.  If ZMAT is there then it gets ran and renamed.
# creation of ZMAT is under the control of progdynb, which is controlled by keyword NMRcc in progdyn.conf
# decisions to be made: erase ZMAT at beginning?  what to do if cfour calc dies?
    if (test  -f ZMAT) then
      cp ZMAT $scratchdir
      cd $scratchdir
      $scratchdir/progcfour $origdir $scratchdir
      cd $origdir
      mv ZMAT temp.ZMAT
      echo "generic one two three" `cat runpointnumber` "runisomer" `cat isomernumber` >> NMRlistcc
      awk '/Nuclear Magnetic Resonance/,/HF-SCF/ {if ($2=="C") print $1,$2,"Isotropic =",$3; if ($2=="H") print
$1,$2,"Isotropic =",$3}' x.log >> NMRlistcc
    fi

# here is a cool link that lets you interupt the dynamics with a short job, then
# it automatically goes back to the dynamics  just make the file 'detour' and it
# will delete detour, run run.com, then go back to dynamics
    if (test  -f detour) then
      rm detour
      date >> $logfile
      cat run.com >> $logfile
      cp run.log temp.log
      cd $scratchdir
      $g09root/g09/g09 $origdir/run.com > $origdir/run.log
      cd $origdir
    fi

#stop it all nicely by creating a nogo file
    if (test  -f nogo) then
      break
    fi
```

```
#figure out if this isomer is done - change in april 2013 is to move proganal call up from here
     rm -f $scratchdir/tempdone
     tail -2 dynfollowfile | awk '/XXXX/ {print}' > $scratchdir/tempdone
     if (test  -s $scratchdir/tempdone) then
       if [ `awk '/reversetraj/ {if ($1=="reversetraj") print $2}' progdyn.conf` = "true" ]; then
         if [ `cat skipstart` = "reverse" ]; then
           rm -f skipstart
           rm -f geoPlusVel
           rm -f olddynrun
           rm -f olddynrun2
           rm -f olddynrun3
           a=`awk '{print $1}' isomernumber`
           mv traj traj$a
         fi
         if [ `cat skipstart` = "forward" ]; then
           echo reverserestart > skipstart
         fi
       else
         rm -f skipstart
         rm -f geoPlusVel
         rm -f olddynrun
         rm -f olddynrun2
         rm -f olddynrun3
         a=`awk '{print $1}' isomernumber`
         mv traj traj$a
       fi
       break
     fi
   done
#
END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_L
oop____

# We've got to break a second time to get out of this loop
# if we really want to quit.  Otherwise, it will start over
# at the top
   if (test  -f nogo) then
     break
   fi
   if (test  -s $scratchdir/goingwell) then
     echo "starting a new point or a new direction"
   else
     break
   fi
done

   if (test  -f nogo) then
     break
   fi
   if (test  -s $scratchdir/goingwell) then
     echo "starting a new point or a new direction2"
   else
     break
   fi
done
exit 0
```

Program proggenHP

```
BEGIN {
# 2014 - avoids bug with a box on, so that starts without modes use input geometry, not standard orientation
# aug 2013 summary of changes
```

```
#includes molecular rotation, ability to do multiple NMR calculations, ONIOM with link atoms,
#nonstandard routes, handling of linear molecules using geometry linear, fixed but with atoms over 99 but
#bug varies with version of Gaussian, randomization based on PROCINFO (solved many problems), added initialDiss 3 for
random
#phase of normal modes
# Aut 2010 changes classicalSpacing to 2 and upped possible excited states to 4000
# Jan 2009 - a number of little changes to improve reporting, precision, etc, specification of displacement on particular modes
# Jan 2009 cannonball trajectories.  adds desired energy to initial velocities based on file cannontraj, so one can shoot toward a ts
# updated Nov 2008 to incorporate running DRPs
# updated Nov 2008 to allow for start without an initial freq calc using classical = 2
# updated Aug 2008 added to atom list to handle a large number of atoms without changes needed
# updated June 2008 to incorportate new method for choosing displacements with initialdis 2
# updated Jan 17 2008 - bug fix for > 99 atoms, 300 excitations of low modes possible
# version August 2007 - incorporates classical trajectory calculation option
#also allows listing of number of imaginary frequencies
# version Sept 16, 2005 - incorportates searchdir but not yet rotation
# now reads random numbers from temp811, starting at a random place
# The input files are generated before this and are tempfreqs, tempredmass,
# tempfrc, tempmodes, and tempstangeos.
# It will count the number of atoms.

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
charge=0; multiplicity=1; method="HF/3-21G"; memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999
conver1=4.184E26 #dividing by this converts amu angs^2 /s^2 to kcal/mol
geometry="nonlinear";rotationmode=0

#initialization and constants
for (i=1;i<=10000;i++) {disMode[i]=-1}
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0; classicalSpacing=2
zpeGauss=0; zpeGaussK=0; zpePlusE=0; potentialE=0

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="initialdis") initialDis=$2
  if ($1=="timestep") timestep=$2
  if ($1=="scaling") scaling=$2
  if ($1=="temperature") temp=$2
  if ($1=="searchdir") searchdir=$2
  if ($1=="classical") classical=$2
  if ($1=="numimag") numimag=$2
  if ($1=="geometry") geometry=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="boxon") boxon=$2
  if ($1=="boxsize") boxsize=$2
```

```
  if ($1=="DRP") DRP=$2; if (DRP==1) classical=2 #this lets one start a DRP from a point that is not a freq calc
  if ($1=="maxAtomMove") maxAtomMove=$2
  if ($1=="cannonball") cannonball=$2
  if ($1=="displacements") disMode[$2]=$3
  if ($1=="controlphase") controlPhase[$2]=$3
  if ($1=="rotationmode") rotationmode=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag>=1) print "***************** starting proggen *****************" >> "diagnostics"
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag>=1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag>=1) print "processors,checkpoint,title,initialdis,timestep,scaling,temperature" >> "diagnostics"
if (diag>=1) print processors,checkpoint,title1,title2,title3,title4,initialDis,timestep,scaling,temp >> "diagnostics"
if (diag>=1) print "classical,numimag,highlevel,boxon,boxsize,DRP,maxAtomMove,cannonball" >> "diagnostics"
if (diag>=1) print classical,numimag,highlevel,boxon,boxsize,DRP,maxAtomMove,cannonball >> "diagnostics"

# put geometries into array, also figure out number of atoms
# note that this picks out the last geometry in a file, assuming
# that if there is an optimization followed by a freq, nothing else follows
# kludgy - repeats last line twice - must be a better way
do {
  getline < "tempstangeos"
  if (oldline==$0) $0=""
  oldline=$0
  atom = $1
  if (atom>numAtoms) numAtoms=atom
  atNum[atom]=$2
  geoArr[atom,1]=$4; geoArr[atom,2]=$5; geoArr[atom,3]=$6
  geoArrOrig[atom,1]=$4; geoArrOrig[atom,2]=$5; geoArrOrig[atom,3]=$6
  velArr[atom,1]=0; velArr[atom,2]=0; velArr[atom,3]=0
  }
while (length($0) > 0)

#output the number of atoms, used in many routines
print numAtoms

# put in atomic symbols and atomic weights - assigns a default mass but then reads it from tempmasses when possible
for (i=1;i<=numAtoms;i++) {
  getline < "tempmasses"
  if (atNum[i]==1) {atSym[i]="H";atWeight[i]=1.00783}
  if (atNum[i]==2) {atSym[i]="He";atWeight[i]=4.0026}
  if (atNum[i]==3) {atSym[i]="Li";atWeight[i]=6.941}
  if (atNum[i]==4) {atSym[i]="Be";atWeight[i]=9.012}
  if (atNum[i]==5) {atSym[i]="B";atWeight[i]=10.811}
  if (atNum[i]==6) {atSym[i]="C";atWeight[i]=12.}
  if (atNum[i]==7) {atSym[i]="N";atWeight[i]=14.007}
  if (atNum[i]==8) {atSym[i]="O";atWeight[i]=15.9994}
  if (atNum[i]==9) {atSym[i]="F";atWeight[i]=18.9984}
  if (atNum[i]==10) {atSym[i]="Ne";atWeight[i]=20.1797}
  if (atNum[i]==11) {atSym[i]="Na";atWeight[i]=22.989}
  if (atNum[i]==12) {atSym[i]="Mg";atWeight[i]=24.305}
  if (atNum[i]==13) {atSym[i]="Al";atWeight[i]=26.98154}
  if (atNum[i]==14) {atSym[i]="Si";atWeight[i]=28.0855}
  if (atNum[i]==15) {atSym[i]="P";atWeight[i]=30.9738}
  if (atNum[i]==16) {atSym[i]="S";atWeight[i]=32.066}
```

```
  if (atNum[i]==17) {atSym[i]="Cl";atWeight[i]=35.4527}
  if (atNum[i]==18) {atSym[i]="Ar";atWeight[i]=39.948}
  if (atNum[i]==19) {atSym[i]="K";atWeight[i]=39.0983}
  if (atNum[i]==20) {atSym[i]="Ca";atWeight[i]=40.078}
  if (atNum[i]==21) {atSym[i]="Sc";atWeight[i]=44.96}
  if (atNum[i]==22) {atSym[i]="Ti";atWeight[i]=47.867}
  if (atNum[i]==23) {atSym[i]="V";atWeight[i]=50.94}
  if (atNum[i]==24) {atSym[i]="Cr";atWeight[i]=51.9961}
  if (atNum[i]==25) {atSym[i]="Mn";atWeight[i]=54.938}
  if (atNum[i]==26) {atSym[i]="Fe";atWeight[i]=55.845}
  if (atNum[i]==27) {atSym[i]="Co";atWeight[i]=58.933}
  if (atNum[i]==28) {atSym[i]="Ni";atWeight[i]=58.693}
  if (atNum[i]==29) {atSym[i]="Cu";atWeight[i]=63.546}
  if (atNum[i]==30) {atSym[i]="Zn";atWeight[i]=65.38}
  if (atNum[i]==31) {atSym[i]="Ga";atWeight[i]=69.723}
  if (atNum[i]==32) {atSym[i]="Ge";atWeight[i]=72.64}
  if (atNum[i]==33) {atSym[i]="As";atWeight[i]=74.9216}
  if (atNum[i]==34) {atSym[i]="Se";atWeight[i]=78.96}
  if (atNum[i]==35) {atSym[i]="Br";atWeight[i]=79.904}
  if (atNum[i]==46) {atSym[i]="Pd";atWeight[i]=106.42}
  if (atNum[i]==53) {atSym[i]="I";atWeight[i]=126.90447}
# gets actual weight from freqinHP when possible so a prior calc with readisotopes gets you isotopic substitution
  if ((i<100) && ($9>0)) atWeight[i]=$9
#  if ((i>99) && ($8>0)) atWeight[i]=$8

  if ((diag>1) && (i==1)) print "atNum[i],atSym[i],atWeight[i],geoArr[i,1],geoArr[i,2],geoArr[i,3]" >> "diagnostics"
  if (diag>1) print atNum[i],atSym[i],atWeight[i],geoArr[i,1],geoArr[i,2],geoArr[i,3] >> "diagnostics"
  }

# read in frequencies, scale them, read in Reduced masses, read in force
#constants, replace negative frequencies by 2 wavenumbers
numFreq=3*numAtoms-6
if (geometry=="linear") numFreq=3*numAtoms-5
for (i=1;i<=numFreq;i++) {
  $0=""
  getline < "tempfreqs"
  freq[i]=$0*scaling
  if (freq[i]<0) freq[i]=2
  }
for (i=1;i<=numFreq;i++) {
  $0=""
  getline < "tempredmass"
  redMass[i]=$0
  if (redMass[i]=="") redMass[i]=1.
  }
for (i=1;i<=numFreq;i++) {
  $0=""
  getline < "tempfrc"
  frc[i]=$0
  if (frc[i]=="") frc[i]=0.0001
  if (frc[i]==0) frc[i]=0.0001
  if ((diag>1) && (i==1)) print "freq[i],redMass[i],frc[i]" >> "diagnostics"
  if (diag>1) print freq[i],redMass[i],frc[i] >> "diagnostics"
  }

# read in the modes - note that trajectories always need a freq calc with freq=hpmodes unless classical=2
if (classical!=2) {
  for (i=1;i<=numFreq;i+=5) {
    for (j=1;j<=(3*numAtoms);j++) {
      getline < "tempmodes"
      mode[i,$2,$1]=$4; mode[i+1,$2,$1]=$5; mode[i+2,$2,$1]=$6; mode[i+3,$2,$1]=$7; mode[i+4,$2,$1]=$8
      }
```

```
    }
  }
if (diag>2) {for (i=1;i<=numFreq;i++) {print mode[i,1,1],mode[i,1,2],mode[i,1,3] >> "modesread"}}

# if doing a cannonball trajectory, read in the vector
if (cannonball>0) {
  for (i=1;i<=numAtoms;i++) {
    getline < "cannontraj"
    cannonArr[i,1]=$1; cannonArr[i,2]=$2; cannonArr[i,3]=$3
    }
  }

# collect a series of random numbers from file temp811, generated from an outside random number generator called by
prodynstarterHP
# read from temp811, starting at a random place
srand(PROCINFO["pid"]); tester=rand()*1000
for (i=1;i<=tester;i++) getline < "temp811"
for (i=1;i<=numFreq;i++) {
  getline < "temp811"; randArr[i]=$1
  getline < "temp811"; randArrB[i]=$1
  getline < "temp811"; randArrC[i]=$1
}
if (rotationmode>0) {
  for (i=1;i<=6;i++) {
    getline < "temp811"; randArrR[i]=$1
  }
}

# for a QM distribution for a harmonic oscillator in its ground state, we want to generate a set of random numbers
#between -1 and 1 weighted such that numbers toward the center are properly more common
i=1
while (i<=numFreq) {
  if ((initialDis==2) || (disMode[i]==2)) {
    getline < "temp811"
    tempNum=2*($1-.5)
    prob=exp(-(tempNum^2))
    getline < "temp811"
    if ($1<prob) {
      randArrD[i]=tempNum
      i++
      }
    }
  if ((initialDis!=2) && (disMode[i]!=2)) i++
  }

# to start without normal modes or frequencies we need to just pick a random direction for the motion of each atom, requiring 3N
random numbers
for (i=1;i<=numAtoms;i++) {
  for (j=1;j<=3;j++) {
  getline < "temp811"
  if ($1>0.5) randArrE[i,j]=1
  if ($1<.5) randArrE[i,j]=-1
    }
  }

# determine energy in each normal mode
for (i=1;i<=numFreq;i++) {
  zpeJ[i]=0.5*h*c*freq[i]       #units J per molecule
#if classical, treat as modes spaced by classicalSpacing wavenumbers
  if (classical==1) zpeJ[i]=0.5*h*c*classicalSpacing  # the zpe is not used when classical but the spacing is used to calculate the
E in mode
  zpeK[i]=zpeJ[i]*avNum/4184    #units kcal/mol
```

```
  if (temp<10) vibN[i]=0        # avoids working with very small temperatures - if the temp is too low, it just acts like 0 K
  if (temp>=10) {
    zpeRat[i]=exp((-2*zpeK[i])/(RgasK*temp))
    if (zpeRat[i]==1) zpeRat[i]=.99999999999
    Q[i]=1/(1-zpeRat[i])
    newRand=randArr[i]
    vibN[i]=0
    tester=1/Q[i]
#    get up to 4000 excitations of low modes
    for (j=1;j<=(4000*zpeRat[i]+2);j++) {
      if (newRand>tester) vibN[i]++
      tester=tester+((zpeRat[i]^j)/Q[i])
      }
    }
  }

# figure out mode energies and maximum classical shift and then actual shift
# also calculated total energy desired for molecule
desiredModeEnK=0
for (i=1;i<=numFreq;i++) {
  modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i]+1) # units here are mDyne Ansgroms for compatability with Gaussian force constants
  if (classical==1) modeEn[i]=(zpeJ[i]*1E18)*2*vibN[i]    #no zpe when classical
  modeEnK[i]=zpeK[i]*(2*vibN[i]+1)
  if (classical==1) modeEnK[i]=zpeK[i]*2*vibN[i]          #no zpe when classical
  desiredModeEnK=desiredModeEnK + modeEnK[i]
# no 1/2 hv for imaginary frequencies
# treating modes with frequencies <10 as translations, ignoring their zero point energies
  if (freq[i]<10) modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i])
  maxShift[i]=(2*modeEn[i]/frc[i])^0.5
# new 2012 initialDis 3 means random phase of normal mode
  if (initialDis==3) shift[i]=maxShift[i]*sin(randArrC[i]*3.141592*2)
  if (initialDis==2) shift[i]=maxShift[i]*randArrD[i]
  if (initialDis==1) shift[i]=maxShift[i]*(2*(randArrC[i]-0.5))
  if (initialDis==0) shift[i]=0
# lines below allow for setting of displacement mode for individual modes
# It used to be necessary to use disMode 10 to turn off displacements for a mode, but hopefully that bug is killed and you can use
disMode 0
  if (disMode[i]==3) shift[i]=maxShift[i]*sin(randArrC[i]*3.141592*2)
  if (disMode[i]==2) shift[i]=maxShift[i]*randArrD[i]
  if (disMode[i]==1) shift[i]=maxShift[i]*(2*(randArrC[i]-0.5))
  if (disMode[i]==10) shift[i]=0 #kept for backward compatability
  if (disMode[i]==0) shift[i]=0
# no displacements along imaginary frequencies and very low ones - it is better to treat these
# as translations - employing a shift can give you initial weird geometries
  if (freq[i]<10) shift[i]=0
  if (numimag==1) shift[1]=0
  if (numimag==2) shift[2]=0
  }
for (i=1;i<=numFreq;i++) {
  if ((diag>1) && (i==1)) print "zpeJ[i],zpeK[i],zpeRat[i],Q[i],vibN[i],modeEn[i],maxShift[i],shift[i]" >> "diagnostics"
  if (diag>1) print zpeJ[i],zpeK[i],zpeRat[i],Q[i],vibN[i],modeEn[i],maxShift[i],shift[i] >> "diagnostics"
  }

# multiply each of the modes by its shift and add them up
# Do not do this if classical=2
if (classical!=2) {
  for (i=1;i<=numFreq;i++) {
    for (j=1;j<=numAtoms;j++) {
      for (k=1;k<=3;k++) {
        shiftMode[i,j,k]=mode[i,j,k]*shift[i]
        geoArr[j,k]=geoArr[j,k]+shiftMode[i,j,k]
        }
```

```
      }
    }
  }

#now start toward velocities
for (i=1;i<=numFreq;i++) {
  kinEn[i]=100000*(modeEn[i]-0.5*frc[i]*shift[i]^2)  # the 100000 converts to g angstrom^2 s^2
  vel[i]=(2*kinEn[i]/(redMass[i]/avNum))^0.5        # in angstrom / s
#use searchdir in progdyn.conf to control the direction for trajectories started from a saddle point
  if (numimag>1) numimag=1  #only the first freq can be sent in the searchdir direction, the rest go in a random direction
  if (i>numimag) {
    if (randArrB[i]<0.5) vel[i]=-vel[i]
    }
  if (i==numimag) {
    if (searchdir=="negative") vel[i]=-vel[i]
    }
  if ((diag>1) && (i==1)) print "vel[i]" >> "diagnostics"
  if (diag>1) print vel[i] >> "diagnostics"
  }

# if controlphase is being used, set the velocity on particular modes as positive or negative as requested
for (i=1;i<=numFreq;i++) {
  if ((controlPhase[i]=="positive") && (vel[i]<0)) vel[i]=-vel[i]
  if ((controlPhase[i]=="negative") && (vel[i]>0)) vel[i]=-vel[i]
  }

# multiply each of the modes by its velocity and add them up
# Do not do this if classical=2
if (classical!=2) {
  for (i=1;i<=numFreq;i++) {
    for (j=1;j<=numAtoms;j++) {
      for (k=1;k<=3;k++) {
        velMode[i,j,k]=mode[i,j,k]*vel[i]*timestep
        velArr[j,k]=velArr[j,k]+velMode[i,j,k]
        }
      }
    }
  }

# to start without normal modes or frequencies we figure out the energy per atom based on 1/2RT in degree of freedom
if (classical==2) {
# to avoid a bug with a box on, starts without modes should use the input geometry, not the standard
  do {
    getline < "tempinputgeos"
    if (oldline==$0) $0=""
    oldline=$0
    atom = $1
    geoArr[atom,1]=$4; geoArr[atom,2]=$5; geoArr[atom,3]=$6
    geoArrOrig[atom,1]=$4; geoArrOrig[atom,2]=$5; geoArrOrig[atom,3]=$6
    }
  while (length($0) > 0)
  degFreedomEnK=temp*RgasK
  degFreedomEnJ=degFreedomEnK/(avNum/4184)
  cartEn=degFreedomEnJ*1E18
  kinEnCart=100000*cartEn
#print degFreedomEnK, degFreedomEnJ, cartEn, kinEnCart
  for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
      velArr[i,j]=randArrE[i,j]*timestep*(2*kinEnCart/(atWeight[i]/avNum))^0.5
      if (DRP==1) velArr[i,j]=0
      }
    }
```

```
  }

# calculate the KE in the modes at this point
KEinitmodes=0
for (j=1;j<=numAtoms;j++) {
  KEinitmodes=KEinitmodes + 0.5*atWeight[j]*(velArr[j,1]^2 + velArr[j,2]^2 + velArr[j,3]^2)/((timestep^2)*conver1)
  }

# add molecular rotation if requested
if (rotationmode>0) {
#establish three rotation vectors
  for (j=1;j<=numAtoms;j++) {
    rotateX[j,1]=0
    rotateX[j,2]=-geoArrOrig[j,3]
    rotateX[j,3]=geoArrOrig[j,2]
    rotateY[j,1]=-geoArrOrig[j,3]
    rotateY[j,2]=0
    rotateY[j,3]=geoArrOrig[j,1]
    rotateZ[j,1]=-geoArrOrig[j,2]
    rotateZ[j,2]=geoArrOrig[j,1]
    rotateZ[j,3]=0
    }
#figure out how much energy is in the raw vectors
  eRotX=0;eRotY=0;eRotZ=0
  for (j=1;j<=numAtoms;j++) {
    for (k=1;k<=3;k++) {
      eRotX=eRotX + 0.5*atWeight[j]*(rotateX[j,k]^2)/((timestep^2)*conver1)
      eRotY=eRotY + 0.5*atWeight[j]*(rotateY[j,k]^2)/((timestep^2)*conver1)
      eRotZ=eRotZ + 0.5*atWeight[j]*(rotateZ[j,k]^2)/((timestep^2)*conver1)
      }
    }
#  print "rotation energies if raw vector used",eRotX,eRotY,eRotZ
#now deciie how much energy we want in each rotation
  keRx=-0.5*0.001987*temp*log(1-randArrR[1])
  keRy=-0.5*0.001987*temp*log(1-randArrR[2])
  keRz=-0.5*0.001987*temp*log(1-randArrR[3])
  if (eRotX<1) keRx=0;if (eRotY<1) keRy=0;if (eRotZ<1) keRz=0
  rotEdesired=keRx+keRy+keRz
  signX=1;signY=1;signZ=1
  if (randArrR[4]<.5) signX=-1
  if (randArrR[5]<.5) signY=-1
  if (randArrR[6]<.5) signZ=-1

#  print "desired energies",keRx,keRy,keRz,"and random numbers",randArrR[1],randArrR[2],randArrR[3]
#protect against zero rotations
  if (eRotX<1) eRotX=1;if (eRotY<1) eRotY=1;if (eRotZ<1) eRotZ=1
#now scale the rotational vectors
  scaleX=(keRx/eRotX)^.5
  scaleY=(keRy/eRotY)^.5
  scaleZ=(keRz/eRotZ)^.5
#  print "scaling factors" scaleX,scaleY,scaleZ
  for (j=1;j<=numAtoms;j++) {
    for (k=1;k<=3;k++) {
      rotateX[j,k]=rotateX[j,k]*scaleX*signX
      rotateY[j,k]=rotateY[j,k]*scaleY*signY
      rotateZ[j,k]=rotateZ[j,k]*scaleZ*signZ
      }
    }
  for (j=1;j<=numAtoms;j++) {
#     print rotateX[j,1],"    ",rotateX[j,2],"    ",rotateX[j,3]
    }
#  print ""
```

```
  for (j=1;j<=numAtoms;j++) {
#     print rotateY[j,1],"   ",rotateY[j,2],"   ",rotateY[j,3]
      }
#  print ""
  for (j=1;j<=numAtoms;j++) {
#     print rotateZ[j,1],"   ",rotateZ[j,2],"   ",rotateZ[j,3]
      }
# now add the rotational vectors  to velArr
  for (j=1;j<=numAtoms;j++) {
    for (k=1;k<=3;k++) {
      velArr[j,k]=velArr[j,k]+rotateX[j,k]+rotateY[j,k]+rotateZ[j,k]
      }
    }
  }

# if doing a cannonball, adjust multiplier until extra energy is correct
if (cannonball>0) {
  multiplier=1; tester=0; tolerance=.1
  while (tester==0) {
    KEinittotal=0
    for (j=1;j<=numAtoms;j++) {
      cannonvelArr[j,1]=velArr[j,1]+multiplier*cannonArr[j,1]; cannonvelArr[j,2]=velArr[j,2]+multiplier*cannonArr[j,2];
cannonvelArr[j,3]=velArr[j,3]+multiplier*cannonArr[j,3]
      KEinittotal=KEinittotal + 0.5*atWeight[j]*(cannonvelArr[j,1]^2 + cannonvelArr[j,2]^2 +
cannonvelArr[j,3]^2)/((timestep^2)*conver1)
      }
    if (KEinittotal>(KEinitmodes+cannonball+tolerance)) multiplier=multiplier*0.98901364
    if (KEinittotal<(KEinitmodes+cannonball-tolerance)) multiplier=multiplier*1.01
    if ((KEinittotal<(KEinitmodes+cannonball+tolerance)) && (KEinittotal>(KEinitmodes+cannonball-tolerance))) tester=1
    }
  for (j=1;j<=numAtoms;j++) {
    velArr[j,1]=velArr[j,1]+multiplier*cannonArr[j,1]; velArr[j,2]=velArr[j,2]+multiplier*cannonArr[j,2];
velArr[j,3]=velArr[j,3]+multiplier*cannonArr[j,3]
    }
  }

#output the new geometry.
# ****** this section changed for special experiment for cyclopentadiene.  do not use this for other cases
# atWeight[4]=140.0001
# ****** line below added for special experiment switching mass from 12 to 140, keeping momenta the same
#velArr[4,1]=velArr[4,1]/11.66667; velArr[4,2]=velArr[4,2]/11.66667; velArr[4,3]=velArr[4,3]/11.66667
for (j=1;j<=numAtoms;j++) {
  printf("%2s % .7f % .7f % .7f %9.5f \n",atSym[j],geoArr[j,1],geoArr[j,2],geoArr[j,3],atWeight[j])
  }

#output the velocities and calculate the total kinetic energy overall
KEinittotal=0
for (j=1;j<=numAtoms;j++) {
  KEinittotal=KEinittotal + 0.5*atWeight[j]*(velArr[j,1]^2 + velArr[j,2]^2 + velArr[j,3]^2)/((timestep^2)*conver1)
  printf("% .8f % .8f % .8f \n",velArr[j,1],velArr[j,2],velArr[j,3])
  }

#anything else I add to the file will not affect the trajectories but will keep a record and be good for analysis
if (classical!=2) {
  for (i=1;i<=numFreq;i++) {
    if (initialDis==0) printf("%.6f  % .6f   %4i   % 1.4e      % .6f %1i\n", randArr[i], randArrB[i], vibN[i], vel[i], shift[i],
disMode[i])
    if (initialDis==1) printf("%.6f  % .6f   %4i   % 1.4e      % .6f %1i\n", randArr[i], randArrC[i], vibN[i], vel[i], shift[i],
disMode[i])
    if (initialDis==2) printf("%.6f  % .6f   %4i   % 1.4e      % .6f %1i\n", randArr[i], randArrD[i], vibN[i], vel[i], shift[i],
disMode[i])
    if (initialDis==3) printf("%.6f  % .6f   %4i   % 1.4e      % .6f %1i % .6f\n", randArr[i], randArrC[i], vibN[i], vel[i], shift[i],
```

```
disMode[i], sin(randArrC[i]*3.141592*2))
     }
  }
print "temp ",temp
print "initialDis",initialDis
print "classical",classical
print "timestep",timestep
print "numimag",numimag
OFMT = "%.3f"
print "Total mode energy desired=",desiredModeEnK
print "KE initial from modes=",KEinitmodes,"   KE initial total=",KEinittotal,"   Rotational Energy desired=",rotEdesired
if (cannonball>0) print "cannonball",cannonball,"  cannon Energy=",KEinittotal-KEinitmodes
if (boxon>0) print "boxsize",boxsize
if (DRP>0) print "DRP",DRP,"   maxAtomMove",maxAtomMove
if (DRP>0) print maxAtomMove > "maxMove"
}  # End of BEGIN

/Zero-point correction/ {zpeGauss=$3}
/zero-point Energies/ {zpePlusE=$7}
END {
zpeGaussK=zpeGauss*627.509
potentialE=zpePlusE - zpeGauss
OFMT = "%.6f"
print "Gaussian zpe=",zpeGauss,"or",zpeGaussK,"kcal/mol  E + zpe=",zpePlusE,"  potential E=",potentialE
print "" #will use blank line to mark end of geoPlusVel file
}
```

Program prog1stpoint

```
BEGIN {
# 2014 added ONIOMcharge, more reliable convergence commands
# 2013 added multiple NMR calculations, molecular rotations
# 2012 added NMR calculations
# 2011 added linkatoms in ONIOM
# aug 2010 changed so that it is more careful in reading in from geoPlusVel
#     removed some default parameters that should always be defined
# Jan 2009 - a number of little changes to improve reporting, precision, etc
# aug 2008 added to atom list so handles H to Cl without change needed
# version Feb 2008 incorporates methodfile, boxon and boxsize, though this point unaffected by box
# version Jan 2008 - allows for ONIOM jobs, fixed atoms
# version Sept 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation
# this program creates the first input file for g09
# the title should be changed as appropriate
# the isomer number comes from a file isomernumber

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999; linkatoms=0
geometry="nonlinear";nonstandard=0
nmrtype=0;nmrevery=9999999
oniomcharge=0; oniommult=0

#initialization
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
```

```
numAtoms=0; atomnumber=0
getline < "runpointnumber"
runpointnum = $1

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="oniomchargemult") {
    oniomcharge=$2
    oniommult=$3
    }
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="timestep") timestep=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="method7") meth7=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="linkatoms") linkatoms=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="killcheck") killcheck=$2
  if ($1=="NMRmethod") nmrmethod=$2
  if ($1=="NMRmethod2") nmrmethod2=$2
  if ($1=="NMRmethod3") nmrmethod3=$2
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="NMRevery") nmrevery=$2
  if ($1=="nonstandard") nonstandard=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag==1) print "***************** starting prog1stpoint *****************" >> "diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print "processors,checkpoint,title" >> "diagnostics"
if (diag==1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

getline < "isomernumber"
isomernum = $1
#read in number of atoms, geometry, masses, and velocity from geoPlusVel
getline < "geoPlusVel"
numAtoms=$1
# geometry
for (i=1;i<=numAtoms;i++) {
```

```
  getline < "geoPlusVel"
  weight[i]=$5
  atSym[i]=$1
  for (j=1;j<=3;j++) {
    geoArr[i,j]=$(1+j)
    }
  }
#velocities not needed for 1st point
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  for (j=1;j<=3;j++) {
    velArr[i,j]=$j
    }
  }

print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
if (nonstandard==0) {
  print "# " method " force scf=(xqc,maxconven=55,fulllinear,nosym) "
  if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
  if (length(meth3)>2) print meth3
  if (length(meth4)>2) print meth4
  }
if (nonstandard==1) {
  print "# "
  print "nonstd"
  system("cat nonstandard")
  }
print ""
# make the title four words exactly, leaving out spaces if necessary
print title1,title2,title3,title4
print "runpoint ",runpointnum
print "runisomer ", isomernum
print ""
if (oniommult==0) print charge,multiplicity
if (oniommult>0) print charge,multiplicity,oniomcharge,oniommult
}

END {
for (i=1;i<=numAtoms;i++) {
  printf("%s %.7f %.7f %.7f",atSym[i],geoArr[i,1],geoArr[i,2],geoArr[i,3])
  if ((i>highlevel) && (i<=highlevel+linkatoms)) printf(" %s","M H")
  if (i>(highlevel+linkatoms)) printf(" %s","M")
  print ""
  }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
    }
  }
if ((nmrtype>0) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod " nmr=giao geom=check"
  if (nmrmethod==method) print "guess=tcheck"
```

```
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
if ((nmrtype>1) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod2 " nmr=giao geom=check"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
if ((nmrtype>2) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod3 " nmr=giao geom=check"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
}
```

Program prog2ndpoint

```
BEGIN {
# 2014 added ONIOMcharge, more reliable convergence commands
# aug 2013 includes molecular rotation, ability to do multiple NMR calculations, ONIOM with link atoms,
#nonstandard routes, checks more kinds of energies at point 2
#Aug 2010 added etolerance to make it controllable from progdyn.conf, made it so that DRP does not check energy
# aug 2008 added to atom list so handles 1 to 17 without change needed
# version Feb 2008 incorporates methodfile, boxon and boxsize, though this point unaffected by box
# version Jan 2008 - allows for ONIOM jobs, fixed atoms
# version Sept 9, 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation
# read progdyn.conf for configuration info

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
```

```
title3="a"; title4="progdyn.conf"; processors=1; highlevel=999; linkatoms=0
etolerance=1
geometry="nonlinear";nonstandard=0
NMRtype=none;NMRevery=9999999
oniomcharge=0; oniommult=0

#initialization
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447
numAtoms=0; atomnumber=0
getline < "runpointnumber"
runpointnum = $1

blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="oniomchargemult") {
    oniomcharge=$2
    oniommult=$3
    }
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="timestep") timestep=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="method7") meth7=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="linkatoms") linkatoms=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="DRP") DRP=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="killcheck") killcheck=$2
  if ($1=="etolerance") etolerance=$2
  if ($1=="reversetraj") reversetraj=$2
  if ($1=="NMRmethod") nmrmethod=$2
  if ($1=="NMRmethod2") nmrmethod2=$2
  if ($1=="NMRmethod3") nmrmethod3=$2
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="NMRevery") nmrevery=$2
  if ($1=="nonstandard") nonstandard=$2
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag>=1) print "***************** starting prog2ndpoint *****************" >> "diagnostics"
```

```
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag>=1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag>=1) print "processors,checkpoint,title" >> "diagnostics"
if (diag>=1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

#get the isomer number from file
getline < "isomernumber"
isomernum = $1

#get forward or reverse from skipstart if it exists
getline < "skipstart"
trajdirection = $1

print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
if (nonstandard==0) {
  print "# " method " force scf=(xqc,maxconven=55,fulllinear,nosym) "
  if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
  if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes faster, sometimes not
  if (length(meth3)>2) print meth3
  if (length(meth4)>2) print meth4
  }
if (nonstandard==1) {
  print "# "
  print "nonstd"
  system("cat nonstandard")
  }
print ""
print title1,title2,title3,title4
print "runpoint ",runpointnum
print "runisomer ", isomernum
print ""
if (oniommult==0) print charge,multiplicity
if (oniommult>0) print charge,multiplicity,oniomcharge,oniommult

# ok, now we have to figure the second point.  this should be
# x(t) = x + v*t + 1/2*F*t^2/m
# so we need to set up arrays for position, velocity, and force

#read in number of atoms, geometry, masses, and velocity from geoPlusVel
getline < "geoPlusVel"
numAtoms=$1
# geometry
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  weight[i]=$5
  atSym[i]=$1
  for (j=1;j<=3;j++) {
    geoArr[i,j]=$(1+j)
    }
  }
#velocities
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  for (j=1;j<=3;j++) {
    velArr[i,j]=$j
    }
  }

#now we go ahead and add the velocities
for (i=1;i<=numAtoms;i++) {
```

```
  for (j=1;j<=3;j++) {
    arr[i,j]=velArr[i,j]+geoArr[i,j]
    if (trajdirection=="reverserestart") arr[i,j]=geoArr[i,j]-velArr[i,j]
    }
  if ((diag>1) && (i==1)) print "geometry after adding velocities" >> "diagnostics"
  if (diag>1) print arr[i,1],arr[i,2],arr[i,3] >> "diagnostics"
  }

#pull out other information useful for testing whether total energy is right or bad
blankLineTester=10
while (blankLineTester>1) {
  getline < "geoPlusVel"
  if ($4=="desired=") desiredModeEnK=$5
  if ($4=="modes=") {
    KEinitmodes=$5
    KEinittotal=$9
    }
  if ($11=="potential") potentialE=$13
  blankLineTester=length($0)
  }
#get initial geometry into file traj
print numAtoms >> "traj"
print potentialE,title1,title2,title3,title4,"runpoint 1 ","runisomer ",isomernum >> "traj"
for (i=1;i<=numAtoms;i++) {
  print atSym[i],geoArr[i,1],geoArr[i,2],geoArr[i,3] >> "traj"
  }
#added by Samae on 102910
scfcount=0
} # end of BEGIN

#pull out the potential energy
/SCF Done/ || /EUMP2 =/ || / Energy=/ {
if (($1=="Energy=") && ($3=="NIter="))  newPotentialE=$2
if (($1=="SCF") && (scfcount==0)) newPotentialE=$5
if ($1=="E2") {
  tempstring=$6
  split(tempstring, arr10, "D")
  newPotentialE=arr10[1]*(10^arr10[2])
  }
newPotentialEK=(newPotentialE-potentialE)*627.509
if ($1=="SCF") {
  if (scfcount==0) {
    pddga=$5
    }
  if (scfcount==1) {
    qm=$5
    }
  if (scfcount==2) {
    pddgb=$5
    pddgc=(pddga-pddgb)
    newPotentialE=(qm+pddgc)
    newPotentialEK=(newPotentialE-potentialE)*627.509
    }
  scfcount++
  }
}

# now we go ahead and translate the forces and add them
(/      1   / || /      2   / || /      3   / || /      4   / || /      5   / || /      6   / || /      7   / || /      8   / || /      9   / || /      10   / || /
11   / || /      12   / || /      13   / || /      14   / || /      15   / || /      16   / || /      17   / || /      18   / || /      19   / || /      20   / || /
21   / || /      22   / || /      23   / || /      24   / || /      25   / || /      26   / || /      27   / || /      28   / || /      29   / || /      30   / || /
31   / || /      32   / || /      33   / || /      34   / || /      35   /) && length($3) > 9 {
```

```
i=$1
for (j=1;j<=3;j++) {
  forceArr[i,j]=$(2+j)    #the raw units of the forces are Hartree/Bohr
  }
if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
}

END {
#put out Echeck but only if not a DRP
if (DRP==0) {
  print "trajectory #",isomernum >> "Echeck"
  print "point 1 potential E=",newPotentialEK,"   point 1 kinetic E=",KEinitmodes,"  Total=",newPotentialEK+KEinitmodes >>
"Echeck"
  print "desired total energy=", desiredModeEnK >> "Echeck"
  if ((newPotentialEK+KEinitmodes)>(desiredModeEnK+etolerance)) print "XXXX bad total Energy" >> "Echeck"
  if ((newPotentialEK+KEinitmodes)<(desiredModeEnK-etolerance)) print "XXXX bad total Energy" >> "Echeck"
  }
# turn the forces into motion
for (i=1;i<=numAtoms;i++) {
  for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time (s^s) and divide by weight in kg
to get angstroms
    forceArr[i,j]=0.5*1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(avNum*1000))
# for simplicity, DRPs will throw away the forces at the second pont.  This means that if we are not at a saddlepoint, point 2 =
point 1 but this is a minor waste
    if (DRP==1) forceArr[i,j]=0
    arr[i,j]=arr[i,j]+forceArr[i,j]
# if atoms are fixed, replace calcd new position by original position
    if ((i==fixedatom1) || (i==fixedatom2) || (i==fixedatom3) || (i==fixedatom4)) arr[i,j]=geoArr[i,j]
    }
  if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
  if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
  printf("%s %.7f %.7f %.7f",atSym[i],arr[i,1],arr[i,2],arr[i,3])
  if ((i>highlevel) && (i<=highlevel+linkatoms)) printf(" %s","M H")
  if (i>(highlevel+linkatoms)) printf(" %s","M")
  print ""
  }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
    }
  }
if ((nmrtype>0) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod " nmr=giao geom=check"
  if (nmrmethod==method) print "guess=tcheck"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
```

```
print ""
if ((nmrtype>1) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod2 " nmr=giao geom=check"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
if ((nmrtype>2) && ((runpointnum % nmrevery)==0)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod3 " nmr=giao geom=check"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
#get second geometry into file traj
print numAtoms >> "traj"
print newPotentialE,title1,title2,title3,title4,"runpoint ",runpointnum,"runisomer ",isomernum >> "traj"
for (i=1;i<=numAtoms;i++) {
  print atSym[i],arr[i,1],arr[i,2],arr[i,3] >> "traj"
  }
}
```

Program progdynb

```
BEGIN { #this is the main routine for generating new .com files by the Verlet algorithym
# Oct 2015 added sanity check, elimiated dyn files and keepevery
# May 2015 added ability to force solvent into a sphere
# Feb 2015 added zeroatom ability to make solute centered in solvent
# Jan 2015 added applyforce to apply forces on motion of atoms and allow PMF calculations
# Dec 2014 added oniom charge specifications
# 2013 added multiple NMR calculations, molecular rotations, thermostat commands
# 2012 added NMR calculations
# 2011 added linkatoms in ONIOM
# Aug 2010 increased elements handled automatically but only up to bromine!
# Jan 2009 - a number of little changes to improve reporting, precision, etc
# Nov 2008 added ability to handle DRPs
# Aug 2008 added long list of atoms to handle 1-17 without change
# May 2008 added option to put out velocities in vellist - make diag=3
# version Feb 2008 incorporates methodfile, boxon and boxsize
# version Jan 2008 incorporates fixed atoms, oniom, and velocity damping
# version August 2007 incorporates keepevery to decrease size of dyn file
# version Sept 11, 2005 - incorportates meth3, meth4, meth5, meth6, but not yet rotation

# default parameters, including quassiclassical, no displacements, transition state, not a DRP
```

```
# do not change these - rather, change progdyn.conf to set the parameters
initialDis=0; timestep=1E-15; scaling=1.0; temp=298.15
classical=0; numimag=1; DRP=0; cannonball=0
memory=20000000
diag=1; checkpoint="g09.chk"; searchdir="positive"; boxon=0
boxsize=10; maxAtomMove=0.1; title1="you"; title2="need"
title3="a"; title4="progdyn.conf"; processors=1; highlevel=99999; linkatoms=0
damping=1;nonstandard=0
nmrtype=0;nmrevery=9999999;nmrcc=0;nmrrand=0;nmrdo=0
thermostat=0;thermostatemult=1.00
oniomcharge=0; oniommult=0
applyforce=0; applyforceB=0; applyforceC=0; zeroatomon=0
sphereon=0; spheresize=999; sphereforceK=0.01

#initialization
srand(PROCINFO["pid"])
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447; pi=3.14159265359
numAtoms=0; atomnumber=0
conver1=4.184E26 #dividing by this converts amu angs^2 /s^2 to kcal/mol
OFS="    "

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progdyn.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="oniomchargemult") {
    oniomcharge=$2
    oniommult=$3
    }
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="timestep") timestep=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="temperature") temp=$2
  if ($1=="thermostat") thermostat=$2
  if ($1=="thermostatmult") thermostatmult=$2
  if (thermostatmult>1) thermostatmult=1/thermostatmult
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="method7") meth7=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="linkatoms") linkatoms=$2
  if ($1=="fixedatom1") fixedatom1=$2
  if ($1=="fixedatom2") fixedatom2=$2
  if ($1=="fixedatom3") fixedatom3=$2
  if ($1=="fixedatom4") fixedatom4=$2
  if ($1=="boxon") boxon=$2
  if ($1=="boxsize") boxsize=$2
  if ($1=="sphereon") sphereon=$2
  if ($1=="spheresize") spheresize=$2
  if ($1=="sphereforce") sphereforceK=$2
  if ($1=="DRP") DRP=$2
  if ($1=="maxAtomMove") maxAtomMove=$2
```

```
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="killcheck") killcheck=$2
  if ($1=="damping") damping=$2
  if ($1=="NMRmethod") nmrmethod=$2
  if ($1=="NMRmethod2") nmrmethod2=$2
  if ($1=="NMRmethod3") nmrmethod3=$2
  if ($1=="NMRtype") nmrtype=$2
  if ($1=="NMRevery") nmrevery=$2
  if ($1=="NMRrand") nmrrand=$2
  if ($1=="loadlimit") loadlimit=$2
  if ($1=="NMRcc") nmrcc=$2
  if ($1=="nonstandard") nonstandard=$2
  if ($1=="applyforce") {
    applyforce=$2; apforce=$3; apforceX0=$4; apforce2=$5; apforce3=$6
    }
  if ($1=="applyforceB") {
    applyforceB=$2; apforceB=$3; apforceX0B=$4; apforce2B=$5; apforce3B=$6
    }
  if ($1=="applyforceC") {
    applyforceC=$2; apforceC=$3; apforceX0C=$4; apforce2C=$5; apforce3C=$6
    }
  if ($1=="afatoms") {
    for (i=1;i<8;i++) {
      if ($(i+1)>0) afatom[i]=$(i+1)
      }
    }
  if ($1=="afatomsB") {
    for (i=1;i<8;i++) {
      if ($(i+1)>0) afatomB[i]=$(i+1)
      }
    }
  if ($1=="afatomsC") {
    for (i=1;i<8;i++) {
      if ($(i+1)>0) afatomC[i]=$(i+1)
      }
    }
  if ($1=="zeroatom") {
    zeroatomon=1
    zeroatom=$2
    }
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

if (diag>=1) print "***************** starting progdynb *****************" >> "diagnostics"
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag>=1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag>=1) print "processors,checkpoint,title" >> "diagnostics"
if (diag>=1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

# get number of atoms and weights from geoPlusVel, and previous geometries from old and older
getline < "geoPlusVel"
numAtoms=$1
for (i=1;i<=numAtoms;i++) {
  getline < "geoPlusVel"
  weight[i]=$5; atSym[i]=$1
  }
```

```
blankLineTester=10
while (blankLineTester>1) {
  getline < "geoPlusVel"
  if ($11=="potential") potentialE=$13
  blankLineTester=length($0)
  }

for (at=1;at<=numAtoms;at++) {
  getline < "old"
  oldarr[at,1]=$4; oldarr[at,2]=$5; oldarr[at,3]=$6
  }

for (at=1;at<=numAtoms;at++) {
  getline < "older"
  olderarr[at,1]=$4; olderarr[at,2]=$5; olderarr[at,3]=$6
  }

#for DRPs read in oldAdjForces and maxAtomMove
if (DRP==1) {
  for (at=1;at<=numAtoms;at++) {
    getline < "oldAdjForces"
    oldForce[at,1]=$1; oldForce[at,2]=$2; oldForce[at,3]=$3
    }
  getline < "maxMove"
  if (($1<maxAtomMove) && ($1>0)) maxAtomMove=$1
  if (maxAtomMove<0.000001) maxAtomMove=0.000001
  }

# record atom velocities for IVR analysis.  This is actually the velocity in the previous run, which is the easiest to calculate.
getline < "isomernumber"
isomernum = $1
getline < "runpointnumber"
runpointnum = $1
# routine to control whether NMR calculations are done.
if ((nmrrand==0) && ((runpointnum % nmrevery)==0)) nmrdo=1
if ((nmrrand==1) && (rand()<(1/nmrevery))) nmrdo=1
getline < "uptimelist"
x=1.0001*substr($10,1,3);if (x<8) x=8
# turn of nmrs if load is too high - this is under control of loadlimit parameter in progdyn.conf and requires proganal to make
uptimelist
if ((nmrrand==1) && (x>loadlimit)) nmrdo=0

if (diag==3) print "runpoint ",runpointnum-1,"runisomer ",isomernum >> "vellist"
for (at=1;at<=numAtoms;at++) {
  atomVel=((oldarr[at,1]-olderarr[at,1])^2 + (oldarr[at,2]-olderarr[at,2])^2 +(oldarr[at,3]-olderarr[at,3])^2)^.5
  KEold=KEold+0.5*weight[at]*(atomVel^2)/((timestep^2)*conver1)
  if (diag==3) print atomVel >> "vellist"
  }
}

#pull out the potential energy
/SCF Done/ || /EUMP2 =/ || / Energy=/ || /ONIOM:/ {
if (($1=="Energy=") && ($3=="NIter="))  newPotentialE=$2
if ($1=="SCF") newPotentialE=$5
if ($2=="extrapolated")  newPotentialE=$5
if ($1=="E2") {
  tempstring=$6
  split(tempstring, arr10, "D")
  newPotentialE=arr10[1]*(10^arr10[2])
  }
newPotEK=(newPotentialE-potentialE)*627.509
}
```

```
#must adjust next line for weird atoms
(/ 1 / || / 2 / || / 3 / || / 4 / || / 5 / || / 6 / || / 7 / || / 8 / || / 9 / || / 10 / || /
11 / || / 12 / || / 13 / || / 14 / || / 15 / || / 16 / || / 17 / || / 18 / || / 19 / || / 20 / || /
21 / || / 22 / || / 23 / || / 24 / || / 25 / || / 26 / || / 27 / || / 28 / || / 29 / || / 30 / || /
31 / || / 32 / || / 33 / || / 34 / || / 35 /) && length($3) > 9 {
i=$1
for (j=1;j<=3;j++) {
  forceArr[i,j]=$(2+j)   #the raw units of the forces are Hartree/Bohr
  }
#if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
#if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
}

END {
# sanity check - avoids trajectory blow up
for (at=1;at<=numAtoms;at++) {
  if (((oldarr[at,1]-olderarr[at,1])^2)>1) exit
  }
#routine to apply a force to bring atoms within a sphere - note that if atoms are too far outside of a sphere then the force on them
will be very large
#unless sphereforce is turned down
if (sphereon==1) {
  sphereforcetotal=0; totalweight=0
  for (i=1;i<=numAtoms;i++) {
    distToOrig=((oldarr[i,1]^2+oldarr[i,2]^2+oldarr[i,3]^2)^.5)
    if (distToOrig>spheresize) {
#originally tried a harmonic restortation to the sphere but this is too big for atoms far outside the sphere
      sphereforce=sphereforceK*(distToOrig-spheresize)
      if (sphereforce>0.01) sphereforce=0.01
      sphereforcetotal=sphereforcetotal+sphereforce
# tried a constant force outside of sphere but am worried about what this means since the potential is discontinuous and steps are
discrete
#       sphereforce=sphereforceK

unitX=sphereforce*oldarr[i,1]/distToOrig;unitY=sphereforce*oldarr[i,2]/distToOrig;unitZ=sphereforce*oldarr[i,3]/distToOrig
      forceArr[i,1]=forceArr[i,1]-unitX;forceArr[i,2]=forceArr[i,2]-unitY;forceArr[i,3]=forceArr[i,3]-unitZ
      }
# calculate the density at 0.9*spheresize
    if (distToOrig<0.9*spheresize) {
      totalweight=totalweight+weight[i]
      }
    }
  density=(totalweight/avNum)/((4/3)*pi*(0.9*spheresize*1E-8)^3)
  }
# routine to apply forces between atoms, used for umbrella sampling
# the next few lines are a kludge to apply the force to one of a series of atoms, whichever is closest to afatom[1]
for (i=3;i<8;i++) {
  if (afatom[i]>0) {
    if(Distance(afatom[1],afatom[i])<Distance(afatom[1],afatom[2])) afatom[2]=afatom[i]
    }
  if (afatomB[i]>0) {
    if(Distance(afatomB[1],afatomB[i])<Distance(afatomB[1],afatomB[2])) afatomB[2]=afatomB[i]
    }
  if (afatomC[i]>0) {
    if(Distance(afatomC[1],afatomC[i])<Distance(afatomC[1],afatomC[2])) afatomC[2]=afatomC[i]
    }
  }
# applyforce 1 puts a linear constant force.
# applyforce 2 puts on a harmonic restoring force to apforceX0
if (applyforce>0) {
  delX=oldarr[afatom[1],1]-oldarr[afatom[2],1];delY=oldarr[afatom[1],2]-oldarr[afatom[2],2];delZ=oldarr[afatom[1],3]-
```

```
oldarr[afatom[2],3];
  distatoms=(delX^2+delY^2+delZ^2)^.5
  if (applyforce==2) apforce=apforce*(distatoms-apforceX0)
  if (applyforce==3) apforce=apforce*(distatoms-apforceX0) + apforce2*(distatoms-apforceX0)^2
  if (applyforce==4) apforce=apforce*(distatoms-apforceX0) + apforce2*(distatoms-apforceX0)^2 + apforce3*(distatoms-
apforceX0)^3
  unitX=apforce*delX/distatoms;unitY=apforce*delY/distatoms;;unitZ=apforce*delZ/distatoms;
  forceArr[afatom[1],1]=forceArr[afatom[1],1]-unitX;forceArr[afatom[1],2]=forceArr[afatom[1],2]-
unitY;forceArr[afatom[1],3]=forceArr[afatom[1],3]-unitZ

forceArr[afatom[2],1]=forceArr[afatom[2],1]+unitX;forceArr[afatom[2],2]=forceArr[afatom[2],2]+unitY;forceArr[afatom[2],3]=
forceArr[afatom[2],3]+unitZ
  }
if (applyforceB>0) {
  delX=oldarr[afatomB[1],1]-oldarr[afatomB[2],1];delY=oldarr[afatomB[1],2]-oldarr[afatomB[2],2];delZ=oldarr[afatomB[1],3]-
oldarr[afatomB[2],3];
  distatoms=(delX^2+delY^2+delZ^2)^.5
  if (applyforceB==2) apforceB=apforceB*(distatoms-apforceX0B)
  if (applyforceB==3) apforceB=apforceB*(distatoms-apforceX0B) + apforce2B*(distatoms-apforceX0B)^2
  if (applyforceB==4) apforceB=apforceB*(distatoms-apforceX0B) + apforce2B*(distatoms-apforceX0B)^2 +
apforce3B*(distatoms-apforceX0B)^3
  unitX=apforceB*delX/distatoms;unitY=apforceB*delY/distatoms;;unitZ=apforceB*delZ/distatoms;
  forceArr[afatomB[1],1]=forceArr[afatomB[1],1]-unitX;forceArr[afatomB[1],2]=forceArr[afatomB[1],2]-
unitY;forceArr[afatomB[1],3]=forceArr[afatomB[1],3]-unitZ

forceArr[afatomB[2],1]=forceArr[afatomB[2],1]+unitX;forceArr[afatomB[2],2]=forceArr[afatomB[2],2]+unitY;forceArr[afatom
B[2],3]=forceArr[afatomB[2],3]+unitZ
  }
if (applyforceC>0) {
  delX=oldarr[afatomC[1],1]-oldarr[afatomC[2],1];delY=oldarr[afatomC[1],2]-oldarr[afatomC[2],2];delZ=oldarr[afatomC[1],3]-
oldarr[afatomC[2],3];
  distatoms=(delX^2+delY^2+delZ^2)^.5
  if (applyforceC==2) apforceC=apforceC*(distatoms-apforceX0C)
  if (applyforceC==3) apforceC=apforceC*(distatoms-apforceX0C) + apforce2C*(distatoms-apforceX0C)^2
  if (applyforceC==4) apforceC=apforceC*(distatoms-apforceX0C) + apforce2C*(distatoms-apforceX0C)^2 +
apforce3C*(distatoms-apforceX0C)^3
  unitX=apforceC*delX/distatoms;unitY=apforceC*delY/distatoms;;unitZ=apforceC*delZ/distatoms;
  forceArr[afatomC[1],1]=forceArr[afatomC[1],1]-unitX;forceArr[afatomC[1],2]=forceArr[afatomC[1],2]-
unitY;forceArr[afatomC[1],3]=forceArr[afatomC[1],3]-unitZ

forceArr[afatomC[2],1]=forceArr[afatomC[2],1]+unitX;forceArr[afatomC[2],2]=forceArr[afatomC[2],2]+unitY;forceArr[afatom
C[2],3]=forceArr[afatomC[2],3]+unitZ
  }
#routine to slowly move an atom toward the origin as set by a harmonic potential
if (zeroatomon==1) {
  multiple=0.99996
  oldarr[zeroatom,1]=multiple*oldarr[zeroatom,1]
  oldarr[zeroatom,2]=multiple*oldarr[zeroatom,2]
  oldarr[zeroatom,3]=multiple*oldarr[zeroatom,3]
  }
#print out some things to vellist and do thermostat
apparentTemp=KEold*2/(3*RgasK*numAtoms)
# the damping in the thermostat is based on temperature based on old geo vs older geo
if (thermostat==1) {
  if (diag<4) print "KEold",KEold,"desired temperature",temp,"apparent Temperature",apparentTemp >> "vellist"
  if (apparentTemp>temp) damping=thermostatmult
  if (apparentTemp<temp) damping=1/thermostatmult
  }

#############routine for DRPs##############
if (DRP==1) {
  maxForce=0;oscillTest=0
```

```
  for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time (s^s) and divide by weight in kg
to get angstroms
      forceArr[i,j]=1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(avNum*1000))
      oscillTest=oscillTest+forceArr[i,j]*oldForce[i,j]
      if (forceArr[i,j]>maxForce) maxForce=forceArr[i,j]
      if ((0-forceArr[i,j])>maxForce) maxForce=-forceArr[i,j]
      }
    if (i==1) printf("% .8f % .8f % .8f \n",forceArr[1,1],forceArr[1,2],forceArr[1,3])  > "oldAdjForces"
    if (i>1) printf("% .8f % .8f % .8f \n",forceArr[i,1],forceArr[i,2],forceArr[i,3])  >> "oldAdjForces"
    }
  print "oscillTest ",oscillTest >> "oldAdjForces"
  if (oscillTest<0) {
    maxAtomMove = maxAtomMove*0.5
    print maxAtomMove > "maxMove"
    }
  if (oscillTest>0) {
    maxAtomMove = maxAtomMove*1.2
    print maxAtomMove > "maxMove"
    }
  print "maxAtomMove ",maxAtomMove >> "oldAdjForces"
  forceMult=maxAtomMove/maxForce
  for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
      newarr[i,j]=oldarr[i,j]+forceMult*forceArr[i,j]
      }
    }
  }
########

#############normal routine for Verlet ##############
if (DRP==0) {
  for (i=1;i<=numAtoms;i++) {
    for (j=1;j<=3;j++) {
# conversions here take force to J/angstrom, 1E20 converts to kg angstroms / s^2, then mult time (s^s) and divide by weight in kg
to get angstroms
      forceArr[i,j]=1E20*forceArr[i,j]*627.509*(4184/(0.529177*avNum))*(timestep^2)/(weight[i]/(avNum*1000))
#       if ((diag>1) && (i==1)) print "i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]" >> "diagnostics"
#       if (diag>1) print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3] >> "diagnostics"
      newarr[i,j]=oldarr[i,j]+damping*(oldarr[i,j]-olderarr[i,j])+forceArr[i,j]
      if ((i==fixedatom1) || (i==fixedatom2) || (i==fixedatom3) || (i==fixedatom4)) newarr[i,j]=oldarr[i,j]
#turn around atoms outside the box
      if (boxon==1) {
        if (newarr[i,j]>boxsize) if (oldarr[i,j]>olderarr[i,j]) newarr[i,j]=oldarr[i,j]+damping*(olderarr[i,j]-oldarr[i,j])+forceArr[i,j]
        if (newarr[i,j]<-1*boxsize) if (oldarr[i,j]<olderarr[i,j]) newarr[i,j]=oldarr[i,j]+damping*(olderarr[i,j]-
oldarr[i,j])+forceArr[i,j]
        }
      }
    }
  for (at=1;at<=numAtoms;at++) {
    atomVel=((oldarr[at,1]-newarr[at,1])^2 + (oldarr[at,2]-newarr[at,2])^2 +(oldarr[at,3]-newarr[at,3])^2)^.5
    KEnew=KEnew+0.5*weight[at]*(atomVel^2)/((timestep^2)*conver1)
    }
    KEave=0.5*KEold+0.5*KEnew
    Etotal=newPotEK+KEave
#still basing apparent Temperature on velocities from old vs older, even though the KE now represents an average of old and new
    if (diag==4) print runpointnum,"KEave",KEave,"apparent
Temperature",apparentTemp,"newPotEK",newPotEK,"Etotal",Etotal,"TotalSphereForce",sphereforcetotal,"density in
0.9r",density >> "vellist"
  }
########
```

```
print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
if (nonstandard==0) {
  print "#p " method " force scf=(xqc,maxconven=155,fulllinear,nosym) "
  if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
  if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes faster, sometimes not
  print "pop=none "
  if (length(meth3)>2) print meth3
  if (length(meth4)>2) print meth4
  }
if (nonstandard==1) {
  print "# "
  print "nonstd"
  system("cat nonstandard")
  }
print ""
print  title1,title2,title3,title4
print "runpoint ",runpointnum
print "runisomer ",isomernum
if (DRP==1) print "maxForce and forceMult and maxAtomMove",maxForce,forceMult,maxAtomMove
print ""
if (oniommult==0) print charge,multiplicity
if (oniommult>0) print charge,multiplicity,oniomcharge,oniommult
print numAtoms >> "traj"
print newPotentialE,title1,title2,title3,title4,"runpoint ",runpointnum,"runisomer ",isomernum >> "traj"
for (i=1;i<=numAtoms;i++) {
  printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3])
  printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3]) >> "traj"
  print "" >> "traj"
  if ((i>highlevel) && (i<=highlevel+linkatoms)) printf(" %s","M H")
  if (i>(highlevel+linkatoms)) printf(" %s","M")
  print ""
  }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
    }
  }
if ((nmrtype>0) && (nmrdo==1)) {
  print "--link1--"
  print "%nproc=" processors
  print "%mem=" memory
  print "%chk=" checkpoint
  print "# " nmrmethod " nmr=giao geom=check"
  if (nmrmethod==method) print "guess=tcheck"
  if (length(meth7)>2) print meth7
  print ""
  print title1,title2,title3,title4
  print "runpoint ",runpointnum
  print "runisomer ",isomernum
  print ""
  print charge,multiplicity
  }
print ""
if ((nmrtype>1) && (nmrdo==1)) {
  print "--link1--"
```

```
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod2 " nmr=giao geom=check"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""
if ((nmrtype>2) && (nmrdo==1)) {
   print "--link1--"
   print "%nproc=" processors
   print "%mem=" memory
   print "%chk=" checkpoint
   print "# " nmrmethod3 " nmr=giao geom=check"
   if (length(meth7)>2) print meth7
   print ""
   print title1,title2,title3,title4
   print "runpoint ",runpointnum
   print "runisomer ",isomernum
   print ""
   print charge,multiplicity
   }
print ""

if ((nmrcc==1) && (nmrdo==1)) {
   print "CCSD(T) NMR calculation" > "ZMAT"
   for (i=1;i<=numAtoms;i++) {
      printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3]) >> "ZMAT"
      print "" >> "ZMAT"
      }
   print "" >> "ZMAT"
   print "*ACES2(CALC=CCSD[T],PROP=NMR,BASIS=dzp" >> "ZMAT"
   print "ABCDTYPE=AOBASIS,TREAT_PERT=SEQUENTIAL,CC_PROG=ECC" >> "ZMAT"
   print "COORD=CARTESIAN" >> "ZMAT"
   print "MEM_UNIT=GB,MEMORY=2)" >> "ZMAT"
   print "" >> "ZMAT"
   }
}

function Distance(Atom1,Atom2) {
  return sqrt((oldarr[Atom1,1]-oldarr[Atom2,1])^2+(oldarr[Atom1,2]-oldarr[Atom2,2])^2+(oldarr[Atom1,3]-oldarr[Atom2,3])^2)
}
```

Program progcfour

This module calls an outside calculation with CFOUR but was not used for the current paper and its presense is not needed to reproduce the current work. Its listing was published in the SI for a previous paper: Biswas, B.; Singleton, D. A. *J. Am. Chem. Soc.* **2015**, *137*, 14244-14247.

Program randgen.c

This is compiled before use to give the service program *randgen*

```
#include <stdio.h>
#include <stdlib.h>
```

```
int a,b,c;
double d;

int product(int x, int y);

int main(void)
{
  int count=1;
  srand48(time (0));
  while (count<=100000)
  {
    d = drand48();
    printf ("%.20f\n", d);
    count++;
  }
  return 0;
}
```

Program proganal when collecting PMF data

```
BEGIN {
firsttitle=1
getline < "isomernumber"
isomer=$1
}
/ NO2/ {
  if (firsttitle==1) {
    printf("%s %s %s %s %s %s %s  ",$1,$2,$3,$4,$6,$7,$8)
    runpoint=$6
    }
  firsttitle++
  }
/Standard orientation/,/Rotational constants/ {
  if (($1>.5) && ($1<99)) {
    A[$1]=$4;B[$1]=$5;C[$1]=$6
    }
  }
#/before annihilation/ {
#   printf("%s %.5f ",$1,$6)
#   }

END {
  para=Distance(1,16)
  meta=Distance(2,16)
  if (Distance(6,16)<meta) meta=Distance(6,16)
  ortho=Distance(3,16)
  if (Distance(5,16)<ortho) ortho=Distance(5,16)
  ipso=Distance(4,16)
  Opara=Distance(1,17)
  if (Distance(1,18)<Opara) Opara=Distance(1,18)
  Ometa=Distance(2,17)
  if (Distance(2,18)<Ometa) Ometa=Distance(2,18)
  if (Distance(6,17)<Ometa) Ometa=Distance(6,17)
  if (Distance(6,18)<Ometa) Ometa=Distance(6,18)
  Oortho=Distance(3,17)
  if (Distance(3,18)<Oortho) Oortho=Distance(3,18)
  if (Distance(5,17)<Oortho) Oortho=Distance(5,17)
  if (Distance(5,18)<Oortho) Oortho=Distance(5,18)
  Oipso=Distance(4,17)
  if (Distance(4,18)<Oipso) Oipso=Distance(4,18)
  NitF=Distance(16,19)
  if (Distance(16,21)<NitF) NitF=Distance(16,21)
  if (Distance(16,22)<NitF) NitF=Distance(16,22)
```

```
  if (Distance(16,23)<NitF) NitF=Distance(16,23)
  BC=Distance(1,20)
  if (Distance(2,20)<BC) BC=Distance(2,20)
  if (Distance(3,20)<BC) BC=Distance(3,20)
  if (Distance(4,20)<BC) BC=Distance(4,20)
  if (Distance(5,20)<BC) BC=Distance(5,20)
  if (Distance(6,20)<BC) BC=Distance(6,20)
  choice=0
  if ((Opara<Ometa) && (Opara<Oortho) && (Opara<NitF)) choice=1
  if ((Ometa<Opara) && (Ometa<Oortho) && (Ometa<NitF)) choice=2
  if ((Oortho<Ometa) && (Oortho<Opara) && (Oortho<NitF)) choice=3
  if (Ometa<2) choice=2
  if (Oortho<2) choice=3
  if (choice==0) printf("%s %.3f %s %.3f %s %.3f %s %.2f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"NitForNO",NitF,"BC",BC)
  if (choice==1) printf("%s %.3f %s %.3f %s %.3f %s %.2f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"Opara",Opara,"BC",BC)
  if (choice==2) printf("%s %.3f %s %.3f %s %.3f %s %.2f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"Ometa",Ometa,"BC",BC)
  if (choice==3) printf("%s %.3f %s %.3f %s %.3f %s %.2f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"Oortho",Oortho,"BC",BC)
  if (runpoint>500000) {
     print "Too many points.  XXXXN"
#    system("date > nogo")
     }
  if (para<1.6) {
#    print "para product formed XXXX"
#    system("date > nogo")
     }
  if (meta<1.6) {
#    print "meta product formed XXXX"
#    system("date > nogo")
     }
  if (ortho<1.6) {
#    print "ortho product formed XXXX"
#    system("date > nogo")
     }
  if (ipso<1.6) {
#    print "ipso product formed XXXX"
#    system("date > nogo")
     }
  if (Opara<1.6) {
#    print "Opara product formed XXXX"
     }
  if (Ometa<1.6) {
#    print "Ometa product formed XXXX"
     }
  if (Oortho<1.6) {
#    print "Oortho product formed XXXX"
     }
  if (Oipso<1.6) {
#    print "Oipso product formed XXXX"
     }
# if (NitF<1.6) {
#    print "NitF product formed XXXX"
#    system("date > nogo")
#    }
  if ((para>5) && (meta>5) && (ortho>5)) {
#    if ((para<5.2) || (para>5.25)) print "Dissociated to SM XXXX"
     }

  system("date '+%b:%d:%Y %T'")
```

```
   system("tail -1 Echeck | grep XXXX")
   }

function Distance(Atom1,Atom2) {
  return sqrt((A[Atom1]-A[Atom2])^2 + (B[Atom1]-B[Atom2])^2 + (C[Atom1]-C[Atom2])^2)
}

function Angle(Atom1,Atom2,Atom3) {
   value=((-
Distance(Atom1,Atom3)^2+Distance(Atom1,Atom2)^2+Distance(Atom2,Atom3)^2)/(2*Distance(Atom1,Atom2)*Distance(Ato
m2,Atom3)))
   return acos(value)
}

function asin(x) { return (180/3.141592)*atan2(x, sqrt(1-x*x)) }

function acos(x) { return (180/3.141592)*atan2(sqrt(1-x*x), x) }

function atan(x) { return (180/3.141592)*atan2(x,1) }

function Dihedral(Atom1,Atom2,Atom3,Atom4) {
   B1x=A[Atom2]-A[Atom1]
   B1y=B[Atom2]-B[Atom1]
   B1z=C[Atom2]-C[Atom1]
   B2x=A[Atom3]-A[Atom2]
   B2y=B[Atom3]-B[Atom2]
   B2z=C[Atom3]-C[Atom2]
   B3x=A[Atom4]-A[Atom3]
   B3y=B[Atom4]-B[Atom3]
   B3z=C[Atom4]-C[Atom3]
   modB2=sqrt((B2x^2)+(B2y^2)+(B2z^2))
# yAx is x-coord. etc of modulus of B2 times B1
   yAx=modB2*(B1x)
   yAy=modB2*(B1y)
   yAz=modB2*(B1z)
# CP2 is the crossproduct of B2 and B3
   CP2x=(B2y*B3z)-(B2z*B3y)
   CP2y=(B2z*B3x)-(B2x*B3z)
   CP2z=(B2x*B3y)-(B2y*B3x)
   termY=((yAx*CP2x)+(yAy*CP2y)+(yAz*CP2z))
# CP is the crossproduct of B1 and B2
   CPx=(B1y*B2z)-(B1z*B2y)
   CPy=(B1z*B2x)-(B1x*B2z)
   CPz=(B1x*B2y)-(B1y*B2x)
   termX=((CPx*CP2x)+(CPy*CP2y)+(CPz*CP2z))
  dihed4=(180/3.141592)*atan2(termY,termX)
  return dihed4
}

function killdyn(isomer) {
   system("rm -f dyn")
}
```

Program proganal when running product-forming trajectories

```
BEGIN {
firsttitle=1
getline < "isomernumber"
isomer=$1
}
/ NO2/ {
```

```
  if (firsttitle==1) {
    printf("%s %s %s %s %s %s %s  ",$1,$2,$3,$4,$6,$7,$8)
    printf(" %s %s %s  ",$6,$7,$8) >> "fullDistList"
    runpoint=$6
    }
  firsttitle++
  }
/Standard orientation/,/Rotational constants/ {
  if (($1>.5) && ($1<99)) {
    A[$1]=$4;B[$1]=$5;C[$1]=$6
    }
  }
#/before annihilation/ {
#   printf("%s %.5f ",$1,$6)
#   }

END {
  para=Distance(1,16)
  meta=Distance(2,16)
  if (Distance(6,16)<meta) meta=Distance(6,16)
  ortho=Distance(3,16)
  if (Distance(5,16)<ortho) ortho=Distance(5,16)
  ipso=Distance(4,16)
  Opara=Distance(1,17)
  if (Distance(1,18)<Opara) Opara=Distance(1,18)
  Ometa=Distance(2,17)
  if (Distance(2,18)<Ometa) Ometa=Distance(2,18)
  if (Distance(6,17)<Ometa) Ometa=Distance(6,17)
  if (Distance(6,18)<Ometa) Ometa=Distance(6,18)
  Oortho=Distance(3,17)
  if (Distance(3,18)<Oortho) Oortho=Distance(3,18)
  if (Distance(5,17)<Oortho) Oortho=Distance(5,17)
  if (Distance(5,18)<Oortho) Oortho=Distance(5,18)
  Oipso=Distance(4,17)
  if (Distance(4,18)<Oipso) Oipso=Distance(4,18)
  NitF=Distance(16,19)
  if (Distance(16,21)<NitF) NitF=Distance(16,21)
  if (Distance(16,22)<NitF) NitF=Distance(16,22)
  if (Distance(16,23)<NitF) NitF=Distance(16,23)
  BC=Distance(1,20)
  if (Distance(2,20)<BC) BC=Distance(2,20)
  if (Distance(3,20)<BC) BC=Distance(3,20)
  if (Distance(4,20)<BC) BC=Distance(4,20)
  if (Distance(5,20)<BC) BC=Distance(5,20)
  if (Distance(6,20)<BC) BC=Distance(6,20)
  if (Distance(6,16)<meta) BC=-BC
  choice=0
  if ((Opara<Ometa) && (Opara<Oortho) && (Opara<NitF)) choice=1
  if ((Ometa<Opara) && (Ometa<Oortho) && (Ometa<NitF)) choice=2
  if ((Oortho<Ometa) && (Oortho<Opara) && (Oortho<NitF)) choice=3
  if (Ometa<2) choice=2
  if (Oortho<2) choice=3
  if (choice==0) printf("%s %.3f %s %.3f %s %.3f %s %.3f %s %.2f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"NitForNO",NitF,"BC",BC)
  if (choice==1) printf("%s %.3f %s %.3f %s %.3f %s %.3f %s %.2f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"Opara",Opara,"BC",BC)
  if (choice==2) printf("%s %.3f %s %.3f %s %.3f %s %.3f %s %.2f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"Ometa",Ometa,"BC",BC)
  if (choice==3) printf("%s %.3f %s %.3f %s %.3f %s %.3f %s %.2f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"Oortho",Oortho,"BC",BC)
  printf("%s %.3f %s %.3f %s %.3f %s %.3f %s %.3f %s %.3f
","p",para,"m1",Distance(2,16),"o1",Distance(3,16),"i",ipso,"o2",Distance(5,16),"m2",Distance(6,16)) >> "fullDistList"
```

```
  print "" >> "fullDistList"
  if (runpoint>500000) {
    print "Too many points.  XXXXN"
#    system("date > nogo")
    }
  if (para<1.5) {
    print "para product formed XXXX"
    }
  if (meta<1.5) {
    print "meta product formed XXXX"
    }
  if (ortho<1.5) {
    print "ortho product formed XXXX"
    }
  if (ipso<1.5) {
    print "ipso product formed XXXX"
    }
  if (Opara<1.6) {
    print "Opara product formed XXXX"
    }
  if (Ometa<1.6) {
    print "Ometa product formed XXXX"
    }
  if (Oortho<1.6) {
    print "Oortho product formed XXXX"
    }
  if (Oipso<1.6) {
    print "Oipso product formed XXXX"
    }
#  if (NitF<1.6) {
#    print "NitF product formed XXXX"
#    system("date > nogo")
#    }
  if ((para>5) && (meta>5) && (ortho>5)) {
    print "Dissociated to SM XXXX"
    }

  system("date '+%b:%d:%Y %T'")
  system("tail -1 Echeck | grep XXXX")
  }

function Distance(Atom1,Atom2) {
 return sqrt((A[Atom1]-A[Atom2])^2 + (B[Atom1]-B[Atom2])^2 + (C[Atom1]-C[Atom2])^2)
}

function Angle(Atom1,Atom2,Atom3) {
  value=((-
Distance(Atom1,Atom3)^2+Distance(Atom1,Atom2)^2+Distance(Atom2,Atom3)^2)/(2*Distance(Atom1,Atom2)*Distance(Ato
m2,Atom3)))
  return acos(value)
}

function asin(x) { return (180/3.141592)*atan2(x, sqrt(1-x*x)) }

function acos(x) { return (180/3.141592)*atan2(sqrt(1-x*x), x) }

function atan(x) { return (180/3.141592)*atan2(x,1) }

function Dihedral(Atom1,Atom2,Atom3,Atom4) {
  B1x=A[Atom2]-A[Atom1]
  B1y=B[Atom2]-B[Atom1]
  B1z=C[Atom2]-C[Atom1]
```

```
  B2x=A[Atom3]-A[Atom2]
  B2y=B[Atom3]-B[Atom2]
  B2z=C[Atom3]-C[Atom2]
  B3x=A[Atom4]-A[Atom3]
  B3y=B[Atom4]-B[Atom3]
  B3z=C[Atom4]-C[Atom3]
  modB2=sqrt((B2x^2)+(B2y^2)+(B2z^2))
# yAx is x-coord. etc of modulus of B2 times B1
  yAx=modB2*(B1x)
  yAy=modB2*(B1y)
  yAz=modB2*(B1z)
# CP2 is the crossproduct of B2 and B3
  CP2x=(B2y*B3z)-(B2z*B3y)
  CP2y=(B2z*B3x)-(B2x*B3z)
  CP2z=(B2x*B3y)-(B2y*B3x)
  termY=((yAx*CP2x)+(yAy*CP2y)+(yAz*CP2z))
# CP is the crossproduct of B1 and B2
  CPx=(B1y*B2z)-(B1z*B2y)
  CPy=(B1z*B2x)-(B1x*B2z)
  CPz=(B1x*B2y)-(B1y*B2x)
  termX=((CPx*CP2x)+(CPy*CP2y)+(CPz*CP2z))
 dihed4=(180/3.141592)*atan2(termY,termX)
 return dihed4
}

function killdyn(isomer) {
  system("rm -f dyn")
}
```

progdyn.conf for running product-forming trajectories after the release of constraints

```
#This is the configuration file for PROGDYN.  This file is read by progdynstarterHP and
# the awk programs proggenHP, prog1stpoint, prog2ndpoint, and progdynb.
#The programs won't read anything past the first blank line,
#and this file must end with a blank line.
#The program has a number of default values but they are unlikely to be what you want.
#Do not delete lines - rather, comment out lines for unwanted options.
#The values here are read repeatedly and most can be changed in the middle of running jobs
#***The keywords are case sensitive.  The following keywords should always be defined:***
#***method, charge, multiplicity, memory, processors, title
#*** method --The following word is copied exactly to the gaussian input file.
method ONIOM(M062X/6-311G*:PM3)
#To do a nonstandard route, make nonstandard 1.  For normal calcs, use nonstandard 0 or else leave it out.
#Then make a file called "nonstandard" containing the nonstandard route with no extra lines.
nonstandard 0
# NMRoptions As is NMRtype=1 will add a section for an NMR calc at every NMRevery intervals.  If you want to combine the
two use nonstandard
#NMRtype 1
#NMRmethod2 B97D/6-31G*
#NMRmethod LC-wPBE/6-31G*
#NMRmethod3 B3LYP/cc-pvtz
#NMRevery 4
#NMRrand 1
#NMRcc 1
#loadlimit 10.0
#geometry linear
rotationmode 0
#*** method2 --The options here are restricted, unrestricted, and read. restricted is the default
#If the method is U..., put unrestricted here and the .com files will have in them guess=mix.
```

```
#If you put read here, the .com files will contain guess=tcheck, which sometimes makes things faster, sometimes not.
#The use of read requires a specifically defined checkpoint file name using the keyword checkpoint.
method2 restricted
charge 0
multiplicity 1
oniomchargemult 1 1
processors 3
#*** memory --The following "word" is copied exactly to the gaussian input file after %mem=.
memory 7gb
#*** killcheck and checkpoint -- You can use a specifically defined checkpoint file name by putting
#the name after the keyword checkpoint.  This is necessary if you use the read option with method2.
#Defined checkpoint names are an unnecessary modest hastle and if you do not want to bother, use killcheck 1
killcheck 1
#checkpoint g09.chk
#*** diagnostics -- 0 prints out nothing extra, 1 (default) prints out extra stuff to a
#file "diagnostics", 2 adds more stuff, 3 adds velocities to a file "vellist"
#4 adds the apparent temperature to vellist, but this is meaningless with quasiclassical calculations
diagnostics 4
#*** title -- the title keyword must be followed by exactly four words
title NO2+Tol 101CH2Cl2IonP Oniom TrajFrom34
#*** initialdis -- 0 (default) turns off displacement of the normal modes, so that all trajectories start from the same place
# and only the energies and signs of the motion in the modes are randomized
# 1 gives a flat distribution of displacements where all of the possible values are equally likely
# 2 (recommended) gives a QM-like gaussian distribution of displacements, so that displacements in the middle are more likely
that
# those at the end by 1/e
initialdis 0
#*** timestep -- this is the time between points in the trajectory.  Typical values would be 1E-15 or 0.5E-15 or 0.25E-15
timestep 1E-15
#*** scaling -- this lets you scale the gaussian frequencies by a constant
scaling 1.0
temperature 298.15
#*** thermostat 1 puts in a damping factor so as to bring the classical temperature toward the desired temperature.
#*** use a thermostatmult between 0.95 and 1, typically 0.995, so the damping happens slowly - otherwise there will be
#*** overadjustment in response to random variation
#*** the thermostat is not exact.  The second traj point ignores this, so it only applies to later points handled by progdynb.
thermostat 1
thermostatmult 0.999
#*** method3, method4, method5, and method6 -- These keywords let you add extra lines to the gaussian input file.
#method3 and method4 add lines at the top of the input after the lines defining the method, and
#this is useful to implement things like the iop for mPW1k
#method5 and method6 add lines after the geometry, after a blank line of course
#only a single term with no spaces can be added, one per method line.  Here are some examples to uncomment if needed
#method3 IOp(3/76=0572004280)
#method3 scrf=(pcm,solvent=ethanol)
#method3 scrf=(pcm,Solvent=dichloromethane)
#add the line below with big structures to get it to put out the distance matrix and the input orientation
method4 iop(2/9=2000)
#method4 iop(3/124=3)
#method4 scrf=(pcm,solvent=dmso,read)
#method5 radii=bondi
#method6
#*** methodfile -- This keyword lets you add more complicated endings to gaussian input files
#such as a gen basis set.  Put after the keyword the number of lines in a file you create called
#methodfile that contains the test you want to add to the end of the gaussian input
methodfile 0
#*** numimag --This tells the program the number of imaginary frequencies in the starting structure.
#if 0, treats as ground state and direction of all modes is random
#if 1, motion along the reaction coordinate will start out in the direction defined by searchdir
#if 2, only lowest freq will go direction of searchdir and other imag mode will go in random direction
numimag 0
#*** searchdir -- This keyword says what direction to follow the mode associated with the imaginary frequency.
```

```
#The choices are "negative" and "positive".  Positive moves in the direction defined in the gaussian frequency calculation
#for the imaginary frequency, while negative moves in the opposite direction.  The correct choice can be made either
#by a careful inspection of the normal modes and standard orientation geometry, or by trial and error.
searchdir positive
#*** classical --  for quassiclassical dynamics, the default, use 0.  for classical dynamics, use 1
#if there are no normal modes and the velocities are to be generated from scratch, use classical 2
classical 2
#*** DRP, saddlepoint, and maxAtomMove --to run a DRP use 'DRP 1' in the line below, otherwise leave it at 0 or comment it
out
#the treatment of starting saddlepoints is not yet implemented so use saddlepoint no
#if DRP shows oscillations then decrease maxAtomMove
#DRP 1
#saddlepoint no
#maxAtomMove 0.01
#*** cannonball -- The program can "fire" a trajectory from a starting position toward a particular target, such as toward
#a ts.  To use this, make a file cannontraj with numAtom lines and three numbers per line that defines the vector
#for firing the trajectory, relative to the starting geometry's standard orientation.  The number following cannonball sets
#the extra energy being put into the structure in kcal/mol
#cannonball 10
#*** keepevery --This tells the program how often to write the gaussian output file to file dyn, after the first two points.
#Use 1 for most dynamics to start with, but use a higher number to save on disk space or molden loading time.
keepevery 99
#*** highlevel --For ONIOM jobs, the following line states the number of highlevel atoms,
#which must come before the medium level atoms.  Use some high value such as 999 if not using ONIOM
highlevel 18
#*** fixedatom1, fixedatom2, fixedatom3, and fixedatom4 - These fix atoms in space.
#Fixing one atom serves no useful purpose and messes things up, while fixing two atoms
#fixes one distance and fixing three has the effect of fixing three distances, not just two
#in current form fixed atoms only are meant to work with no displacements, that is, initialdis=0
#fixedatom1 16
#fixedatom2 1
#fixedatom3 4
#fixedatom4 20
#applyforce 1 lets one push atoms together or appart - a positive force pushes them together
#format is applyforce force    - with the units on force the same as in the Gaussian output file
#applyforce 2 or 3 or 4 applys a polynomical force centered at dist0.  2 is just harmonic, 3 is second order, 4 is third order
#format is applyforce 4 forcecoefficient dist0 forcecoefficient2 forcecoefficient3
#then use afatoms to chose the atoms with format afatoms firstatom secondatom [additional atoms]
#applyforce 2 0.1 2.1
#afatoms 16 1 2 3 4 5 6
#applyforceB 2 0.01 5.2
#afatomsB 8 15
#applyforceC 2 0.01 5.2
#afatomsC 8 15
#zeroatom pushes the numbered atom toward the origin with a small harmonic potential  - good with boxon when you want to
keep the reaction in the center
#zeroatom 16
#*** boxon and boxsize - With boxon 1, a cubic box is set such that atoms that reach the edge
#are reflected back toward the middle.  Useful for dynamics with solvent molecules.  This is a crude
#implementation that is ok for a few thousand femtoseconds but will not conserve energy long term.
#Set the box size so as to fit the entire initial molecule but not have too much extra room.
#The dimensions of the box are two times the boxsize, e.g. boxsize 7.5 leads to a box that is 15 x 15 x 15 angstroms
#boxon 1
#boxsize 11.2
#*** sphereon and spheresize and sphereforce - uses a force to push atoms within a sphere.  notice that if the atom is far outside
of
#the sphere then the force is large unless sphereforce is set small
sphereon 1
spheresize 12.9
sphereforce .01
#*** displacements -- This keyword lets you set the initialdis of particular modes by using a series of lines of the format
# displacements NumberOfMode InitialDisForThatMode, as in the example below. You should be able to do as many of these as
```

```
you like
# you might consider this for rotations where a straight-line displacement goes wrong at large displacements
# The choices for InitialDisForThatMode are 0, 1, 2, and 10, where 10 does the same thing as 0 but is maintained for now
because
# a previous version of the program had a bug that made 0 not work.
#displacements 2 0
#displacements 3 0
#displacements 4 0
#displacements 5 0
#displacements 6 0
#displacements 7 0
#displacements 8 0
#displacements 9 0
#displacements 10 0
#*** etolerance --This sets the allowable difference between the desired energy in a trajectory and the actual
#energy, known after point 1 from the potential energy + the kinetic energy in the initial velocities.
#The unit is kcal/mol and 1 is a normal value for mid-sized organic systems.  For very large and floppy molecules, a larger value
#may be needed, but the value must stay way below the average thermal energy in the molecule (not counting zpe).
#If initialdis is not 0 and few trajectories are being rejected, decrease the value.
etolerance 9999999
#*** controlphase --It is sometimes useful to set the phase of particular modes in the initialization of trajectories.
#The format is controlphase numberOfModeToControl positive or controlphase numberOfModeToControl negative.
#controlphase 2 positive
#*** damping -- The damping keyword lets you add or subtract energy from the system at each point, by multiplying the
velocities
#by the damping factor.  A damping of 1 has no effect, and since you mostly want to change the energy slowly, normal values
range
#from 0.95 to 1.05.  The use of damping lets one do simulated annealing - you add energy until the structure is moving enough
#to sample the kinds of possibilities you are interested in, then you take away the energy slowly.
damping 1.000
#at a damping of .9995, the energy is cut in half in 693 points
#*** reversetraj --This keyword sets the trajectories so that both directions from a transition state are explored.
reversetraj true


#updated Aug 9, 2007 to include the possibility of classical dynamics by the keyword classical
#updated Jan 2008 to include fixed atoms, ONIOM jobs, keepevery, and box size
#update Feb 2008 to include methodfile parameter
# updated Nov 2008 to allow for start without an initial freq calc using classical = 2
# update Aug 2010 to include etolerance, damping controlphase and reversetraj
```

progdyn.conf for molecular dynamics generation of the PMF

```
#In this example, the distance between the N of the nitronium and the aromatic carbons is held in the area of 3.1 Å by a harmonic
potential – see the keywords applyforce and afatoms.
#This is the configuration file for PROGDYN.  This file is read by progdynstarterHP and
# the awk programs proggenHP, prog1stpoint, prog2ndpoint, and progdynb.
#The programs won't read anything past the first blank line,
#and this file must end with a blank line.
#The program has a number of default values but they are unlikely to be what you want.
#Do not delete lines - rather, comment out lines for unwanted options.
#The values here are read repeatedly and most can be changed in the middle of running jobs
#***The keywords are case sensitive.  The following keywords should always be defined:***
#***method, charge, multiplicity, memory, processors, title
#*** method --The following word is copied exactly to the gaussian input file.
method ONIOM(M062X/6-311G*:PM3)
#To do a nonstandard route, make nonstandard 1.  For normal calcs, use nonstandard 0 or else leave it out.
#Then make a file called "nonstandard" containing the nonstandard route with no extra lines.
nonstandard 0
# NMRoptions As is NMRtype=1 will add a section for an NMR calc at every NMRevery intervals.  If you want to combine the
two use nonstandard
```

```
#NMRtype 1
#NMRmethod2 B97D/6-31G*
#NMRmethod LC-wPBE/6-31G*
#NMRmethod3 B3LYP/cc-pvtz
#NMRevery 4
#NMRrand 1
#NMRcc 1
#loadlimit 10.0
#geometry linear
rotationmode 0
#*** method2 --The options here are restricted, unrestricted, and read. restricted is the default
#If the method is U..., put unrestricted here and the .com files will have in them guess=mix.
#If you put read here, the .com files will contain guess=tcheck, which sometimes makes things faster, sometimes not.
#The use of read requires a specifically defined checkpoint file name using the keyword checkpoint.
method2 restricted
charge 0
multiplicity 1
oniomchargemult 1 1
processors 3
#*** memory --The following "word" is copied exactly to the gaussian input file after %mem=.
memory 7gb
#*** killcheck and checkpoint -- You can use a specifically defined checkpoint file name by putting
#the name after the keyword checkpoint.  This is necessary if you use the read option with method2.
#Defined checkpoint names are an unnecessary modest hastle and if you do not want to bother, use killcheck 1
killcheck 1
#checkpoint g09.chk
#*** diagnostics -- 0 prints out nothing extra, 1 (default) prints out extra stuff to a
#file "diagnostics", 2 adds more stuff, 3 adds velocities to a file "vellist"
#4 adds the apparent temperature to vellist, but this is meaningless with quasiclassical calculations
diagnostics 4
#*** title -- the title keyword must be followed by exactly four words
title NO2+Tol 101CH2Cl2IonP Oniom Eq
#*** initialdis -- 0 (default) turns off displacement of the normal modes, so that all trajectories start from the same place
# and only the energies and signs of the motion in the modes are randomized
# 1 gives a flat distribution of displacements where all of the possible values are equally likely
# 2 (recommended) gives a QM-like gaussian distribution of displacements, so that displacements in the middle are more likely
that
# those at the end by 1/e
initialdis 0
#*** timestep -- this is the time between points in the trajectory.  Typical values would be 1E-15 or 0.5E-15 or 0.25E-15
timestep 1E-15
#*** scaling -- this lets you scale the gaussian frequencies by a constant
scaling 1.0
temperature 298.15
#*** thermostat 1 puts in a damping factor so as to bring the classical temperature toward the desired temperature.
#*** use a thermostatmult between 0.95 and 1, typically 0.995, so the damping happens slowly - otherwise there will be
#*** overadjustment in response to random variation
#*** the thermostat is not exact.  The second traj point ignores this, so it only applies to later points handled by progdynb.
thermostat 1
thermostatmult 0.999
#*** method3, method4, method5, and method6 -- These keywords let you add extra lines to the gaussian input file.
#method3 and method4 add lines at the top of the input after the lines defining the method, and
#this is useful to implement things like the iop for mPW1k
#method5 and method6 add lines after the geometry, after a blank line of course
#only a single term with no spaces can be added, one per method line.  Here are some examples to uncomment if needed
#method3 IOp(3/76=0572004280)
method3 scf=(conver=5)
#method3 scrf=(pcm,Solvent=dichloromethane)
#add the line below with big structures to get it to put out the distance matrix and the input orientation
method4 iop(2/9=2000)
#method4 iop(3/124=3)
#method4 scrf=(pcm,solvent=dmso,read)
```

```
#method5 radii=bondi
#method6
#*** methodfile -- This keyword lets you add more complicated endings to gaussian input files
#such as a gen basis set.  Put after the keyword the number of lines in a file you create called
#methodfile that contains the test you want to add to the end of the gaussian input
methodfile 0
#*** numimag --This tells the program the number of imaginary frequencies in the starting structure.
#if 0, treats as ground state and direction of all modes is random
#if 1, motion along the reaction coordinate will start out in the direction defined by searchdir
#if 2, only lowest freq will go direction of searchdir and other imag mode will go in random direction
numimag 0
#*** searchdir -- This keyword says what direction to follow the mode associated with the imaginary frequency.
#The choices are "negative" and "positive".  Positive moves in the direction defined in the gaussian frequency calculation
#for the imaginary frequency, while negative moves in the opposite direction.  The correct choice can be made either
#by a careful inspection of the normal modes and standard orientation geometry, or by trial and error.
searchdir positive
#*** classical --  for quassiclassical dynamics, the default, use 0.  for classical dynamics, use 1
#if there are no normal modes and the velocities are to be generated from scratch, use classical 2
classical 2
#*** DRP, saddlepoint, and maxAtomMove --to run a DRP use 'DRP 1' in the line below, otherwise leave it at 0 or comment it
out
#the treatment of starting saddlepoints is not yet implemented so use saddlepoint no
#if DRP shows oscillations then decrease maxAtomMove
#DRP 1
#saddlepoint no
#maxAtomMove 0.01
#*** cannonball -- The program can "fire" a trajectory from a starting position toward a particular target, such as toward
#a ts.  To use this, make a file cannontraj with numAtom lines and three numbers per line that defines the vector
#for firing the trajectory, relative to the starting geometry's standard orientation.  The number following cannonball sets
#the extra energy being put into the structure in kcal/mol
#cannonball 10
#*** keepevery --This tells the program how often to write the gaussian output file to file dyn, after the first two points.
#Use 1 for most dynamics to start with, but use a higher number to save on disk space or molden loading time.
keepevery 99
#*** highlevel --For ONIOM jobs, the following line states the number of highlevel atoms,
#which must come before the medium level atoms.  Use some high value such as 999 if not using ONIOM
highlevel 18
#*** fixedatom1, fixedatom2, fixedatom3, and fixedatom4 - These fix atoms in space.
#Fixing one atom serves no useful purpose and messes things up, while fixing two atoms
#fixes one distance and fixing three has the effect of fixing three distances, not just two
#in current form fixed atoms only are meant to work with no displacements, that is, initialdis=0
#fixedatom1 16
#fixedatom2 1
#fixedatom3 4
#fixedatom4 20
#applyforce 1 lets one push atoms together or appart - a positive force pushes them together
#format is applyforce force    - with the units on force the same as in the Gaussian output file
#applyforce 2 or 3 or 4 applys a polynomical force centered at dist0.  2 is just harmonic, 3 is second order, 4 is third order
#format is applyforce 4 forcecoefficient dist0 forcecoefficient2 forcecoefficient3
#then use afatoms to chose the atoms with format afatoms firstatom secondatom [additional atoms]
applyforce 2 0.1 3.1
afatoms 16 1 2 3 4 5 6
#applyforceB 2 0.01 5.2
#afatomsB 8 15
#applyforceC 2 0.01 5.2
#afatomsC 8 15
#zeroatom pushes the numbered atom toward the origin with a small harmonic potential  - good with boxon when you want to
keep the reaction in the center
zeroatom 16
#*** boxon and boxsize - With boxon 1, a cubic box is set such that atoms that reach the edge
#are reflected back toward the middle.  Useful for dynamics with solvent molecules.  This is a crude
#implementation that is ok for a few thousand femtoseconds but will not conserve energy long term.
```

```
#Set the box size so as to fit the entire initial molecule but not have too much extra room.
#The dimensions of the box are two times the boxsize, e.g. boxsize 7.5 leads to a box that is 15 x 15 x 15 angstroms
#boxon 1
#boxsize 11.2
#*** sphereon and spheresize and sphereforce - uses a force to push atoms within a sphere.  notice that if the atom is far outside
of
#the sphere then the force is large unless sphereforce is set small
sphereon 1
spheresize 12.9
sphereforce .01
#*** displacements -- This keyword lets you set the initialdis of particular modes by using a series of lines of the format
# displacements NumberOfMode InitialDisForThatMode, as in the example below. You should be able to do as many of these as
you like
# you might consider this for rotations where a straight-line displacement goes wrong at large displacements
# The choices for InitialDisForThatMode are 0, 1, 2, and 10, where 10 does the same thing as 0 but is maintained for now
because
# a previous version of the program had a bug that made 0 not work.
#displacements 2 0
#displacements 3 0
#displacements 4 0
#displacements 5 0
#displacements 6 0
#displacements 7 0
#displacements 8 0
#displacements 9 0
#displacements 10 0
#*** etolerance --This sets the allowable difference between the desired energy in a trajectory and the actual
#energy, known after point 1 from the potential energy + the kinetic energy in the initial velocities.
#The unit is kcal/mol and 1 is a normal value for mid-sized organic systems.  For very large and floppy molecules, a larger value
#may be needed, but the value must stay way below the average thermal energy in the molecule (not counting zpe).
#If initialdis is not 0 and few trajectories are being rejected, decrease the value.
etolerance 9999999
#*** controlphase --It is sometimes useful to set the phase of particular modes in the initialization of trajectories.
#The format is controlphase numberOfModeToControl positive or controlphase numberOfModeToControl negative.
#controlphase 2 positive
#*** damping -- The damping keyword lets you add or subtract energy from the system at each point, by multiplying the
velocities
#by the damping factor.  A damping of 1 has no effect, and since you mostly want to change the energy slowly, normal values
range
#from 0.95 to 1.05.  The use of damping lets one do simulated annealing - you add energy until the structure is moving enough
#to sample the kinds of possibilities you are interested in, then you take away the energy slowly.
damping 1.000
#at a damping of .9995, the energy is cut in half in 693 points
#*** reversetraj --This keyword sets the trajectories so that both directions from a transition state are explored.
reversetraj false
```

progdyn.conf for quasiclassical trajectories started from a toluene / $NO_2^+BF_4^-$ PCM TS

Here, we are only showing the active keywords.

```
method ONIOM(M062X/6-311G*:PM3)
rotationmode 2
method2 restricted
charge 0
multiplicity 1
oniomchargemult 1 1
processors 3
memory 7gb
killcheck 1
diagnostics 0
title NO2+Tol PCMtsA Oniom 298dis2
initialdis 2
```

```
timestep 1E-15
scaling 1.0
temperature 298.15
method3 scrf=(pcm,Solvent=dichloromethane)
method4 iop(2/9=2000)
methodfile 0
numimag 1
searchdir positive
classical 0
keepevery 99999
highlevel 18
keep the reaction in the center
etolerance 1
damping 1.000
reversetraj true
```

progdynsam

```
BEGIN {
temp=298.15
if (pt<1) startpoint=6363
if (pt>1) startpoint=pt
line=0
printon=0
pointline=0
secondpoint=0
}

{
line++
if (line==1) numAtoms=$1
pointline++
if (printon==1) {
  if ($1=="H") atWeight[pointline]=1.00783
  if ($1=="C") atWeight[pointline]=12.0000
  if ($1=="B") atWeight[pointline]=10.81
  if ($1=="O") atWeight[pointline]=15.99940
  if ($1=="F") atWeight[pointline]=18.9984
  if ($1=="P") atWeight[pointline]=30.9738
  if ($1=="S") atWeight[pointline]=31.972
  if ($1=="N") atWeight[pointline]=14.0030740
  if ($1=="Al") atWeight[pointline]=26.981
  if ($1=="Cl") atWeight[pointline]=35.4527
  if (($1=="C") || ($1=="H") || ($1=="O") || ($1=="P") || ($1=="N") || ($1=="Cl")  || ($1=="B") || ($1=="F") || ($1=="S") ||
($1=="Al")) {
     Arr0[pointline,0]=$1
     Arr0[pointline,1]=$2
     Arr0[pointline,2]=$3
     Arr0[pointline,3]=$4
     Arr1[pointline,0]=$1
     Arr1[pointline,1]=$2
     Arr1[pointline,2]=$3
     Arr1[pointline,3]=$4
     }
  }
if (secondpoint==1) {
  if (($1=="C") || ($1=="H") || ($1=="O") || ($1=="P") || ($1=="N") || ($1=="Cl")  || ($1=="B") || ($1=="F") || ($1=="S") ||
($1=="Al")) {
     Arr1[pointline,1]=$2-Arr1[pointline,1]
     Arr1[pointline,2]=$3-Arr1[pointline,2]
```

```
      Arr1[pointline,3]=$4-Arr1[pointline,3]
      }
   }
if ($8=="runisomer") {
   pointline=0
   }
if ($7==startpoint) {
   pointline=0
   printon=1
   }
if ($7==startpoint+1) {
   secondpoint=1
   pointline=0
   printon=0
   }
if ($7>startpoint+1) {
   secondpoint=0
   printon=0
   }

}

END {
print numAtoms
for (i=1;i<=numAtoms;i++) {
   print Arr0[i,0],Arr0[i,1],Arr0[i,2],Arr0[i,3],atWeight[i]
   }
conver1=4.184E26
srand()
timestep=1E-15
for (i=1;i<=100;i++) {
   newRand=rand()
   newRand2=rand()
   randArr[i]=newRand
   sign[i]=1
   if (newRand2<0.5) sign[i]=-1
}
for (i=1;i<=numAtoms;i++) {
   if ((Arr1[i,1]==0) && (Arr1[i,2]==0) && (Arr1[i,3]==0)) {
      for (j=1;j<=3;j++) {
         KE=-0.001987*temp*log(1-randArr[3*i+j])
         Vel=sign[3*i+j]*timestep*(2*KE*conver1/atWeight[i])^0.5
         Arr1[i,j]=Vel
         }
      }
   print Arr1[i,1],Arr1[i,2],Arr1[i,3]
   }
printf("%s %i %i %s ","generated from points",startpoint,startpoint+1,"in a trajectory, so no modes to print out")
system("pwd")
print "Total mode energy desired=",0
for (i=1;i<=700;i++) {
   velsq= Arr1[i,1]^2+Arr1[i,2]^2+Arr1[i,3]^2
   KE=1E30*0.5*atWeight[i]*velsq/conver1
   KE=2.388E3*0.5*atWeight[i]*velsq
   #print i,KE
   }
print ""
}
```

Program progwhere

```
/ 1 run/ {
oldcurrent=""
finishtime=0;changetime=0;changedist=0
switches=0
shortestdistance=10;shortestpara=10;shortestmeta=10;shortestortho=10;shortestipso=10;short=10
oldshortestpara=10;oldshortestmeta=10;oldshortestortho=10;oldshortestipso=10
shortestrecent=10;reboundcount=0
olddist=10;
count18=0;count19=0;count2=0;count21=0;count22=0;count23=0;
}
/run/ {
olddist=dist
if (($9<$11) && ($9<$13) && ($9<$15)) {
  current="                para"
  dist=$9
  if (dist<shortestdistance) shortestdistance=dist
  if (dist<shortestpara) shortestpara=dist
  }
if (($11<$9) && ($11<$13) && ($11<$15)) {
  current="           meta"
  dist=$11
  if (dist<shortestdistance) shortestdistance=dist
  if (dist<shortestmeta) shortestmeta=dist
  }
if (($13<$9) && ($13<$11) && ($13<$15)) {
  current="     ortho"
  dist=$13
  if (dist<shortestdistance) shortestdistance=dist
  if (dist<shortestortho) shortestortho=dist
  }
if (($15<$9) && ($15<$11) && ($15<$13)) {
  current="ipso"
  dist=$15
  if (dist<shortestdistance) shortestdistance=dist
  if (dist<shortestipso) shortestipso=dist
  }
if ((olddist<2) && (dist>=2)) count2++
if (dist<shortestrecent) shortestrecent=dist
if ((dist>=2.3) && (shortestrecent<2)) {
  reboundcount++
  shortestrecent=10
  }
if (current!=oldcurrent) {
  changetime=$5
  changedist=dist
  startcurrent=""
  if ($5>4) switches++
  print oldcurrent,switches,shortestdistance
  shortestdistance=10
  }
oldcurrent=current
if ($5==4) startcurrent=current
}
/XXX/ {
  print "In XXX routine"
  print "final",current, switches, shortestdistance
  finishtime=$5
  if (startcurrent==current) print "No switch in this trajectory!!!!"
  print "data for last switch","finishtime",finishtime,"changetime",changetime,"difference",finishtime-
changetime,"changedist",changedist,"switches",switches
```

```
  if (current=="                  para") {
    short=shortestmeta;if (shortestortho<short) short=shortestortho; if (shortestipso<short) short=shortestipso
    print "shortestmeta",shortestmeta,"shortestortho",shortestortho,"shortestipso",shortestipso,"shortest overall",short
    }
  if (current=="           meta") {
    short=shortestpara; if (shortestortho<short) short=shortestortho; if (shortestipso<short) short=shortestipso
    print "shortestpara",shortestpara,"shortestortho",shortestortho,"shortestipso",shortestipso,"shortest overall",short
    }
  if (current==""      ortho") {
    short=shortestpara; if (shortestmeta<short) short=shortestmeta; if (shortestipso<short) short=shortestipso
    print "shortestpara",shortestpara,"shortestmeta",shortestmeta,"shortestipso",shortestipso,"shortest overall",short
    }
  if (current=="ipso") {
    short=shortestpara; if (shortestmeta<short) short=shortestmeta; if (shortestortho<short) short=shortestortho
    print "shortestpara",shortestpara,"shortestmeta",shortestmeta,"shortestortho",shortestortho,"shortest overall",short
    }
  print "count2   ",count2,"   reboundcount   ",reboundcount
  finishtime=0;changetime=0;changedist=0;switches=0
  shortestdistance=10
  print "ended XXX routine"
}
```

Program whamnit

```
cd ~
rm -f ~/regiocount
rm -f n8??/seriesfile*
awk -f ~/progseries n872/dynfollowfile n873/dynfollowfile n874/dynfollowfile n875/dynfollowfile n876/dynfollowfile
n837/dynfollowfile n838/dynfollowfile > n837/seriesfile
awk -f ~/progseries n800/dynfollowfile n810/dynfollowfile n819/dynfollowfile n820/dynfollowfile n821/dynfollowfile
n839/dynfollowfile > n800/seriesfile
awk -f ~/progseries n801/dynfollowfile n811/dynfollowfile n822/dynfollowfile n840/dynfollowfile n841/dynfollowfile
n86?/dynfollowfile > n801/seriesfile
awk -f ~/progseries n854/dynfollowfile n855/dynfollowfile n856/dynfollowfile n857/dynfollowfile n858/dynfollowfile
n859/dynfollowfile > n854/seriesfile
awk -f ~/progseries n802/dynfollowfile n812/dynfollowfile n823/dynfollowfile > n802/seriesfile
awk -f ~/progseries n803/dynfollowfile n813/dynfollowfile n824/dynfollowfile n842/dynfollowfile > n803/seriesfile
awk -f ~/progseries n804/dynfollowfile n814/dynfollowfile n825/dynfollowfile > n804/seriesfile
awk -f ~/progseries n805/dynfollowfile n815/dynfollowfile n826/dynfollowfile > n805/seriesfile
awk -f ~/progseries n806/dynfollowfile n816/dynfollowfile n827/dynfollowfile > n806/seriesfile
awk -f ~/progseries n807/dynfollowfile n817/dynfollowfile n828/dynfollowfile > n807/seriesfile
awk -f ~/progseries n808/dynfollowfile n829/dynfollowfile > n808/seriesfile
awk -f ~/progseries n809/dynfollowfile n830/dynfollowfile > n809/seriesfile
awk -f ~/progseries n831/dynfollowfile n832/dynfollowfile > n831/seriesfile
awk -f ~/progseries n833/dynfollowfile n834/dynfollowfile > n833/seriesfile
awk -f ~/progseries n835/dynfollowfile n836/dynfollowfile > n835/seriesfile
cd ~/wham/wham
./wham 1.475 5.675 84 0.000001 298.15 0 metadatafile.nitrations ~/output.nitrationfull 6 23
cd
cat output.nitrationfull
cat ~/regiocount
cat ~/wham/wham/metadatafile.nitrations
```

Program progseries

```
BEGIN {
countpara=0;countmeta=0;countortho=0;countipso=0;counttotal=0
oldfilename=""
switches=-1
current="";oldclosest=""
```

```
currentop=""
oldop=""
opswitches=-1
}
/run/ {
if (oldfilename!=FILENAME) {
  if (counttotal>0) {
    pp=int(.5+100*countpara/counttotal)
    pm=int(.5+100*countmeta/counttotal)
    po=int(.5+100*countortho/counttotal)
    pi=int(.5+100*countipso/counttotal)
    print oldfilename,"    ",countpara,countmeta,countortho,countipso,"    ",counttotal,"    ",pp,pm,po,pi,"
switches",switches,"   opswitches",opswitches >> "regiocount"
    }
  if (counttotal==0) print "" >> "regiocount"
  countpara=0;countmeta=0;countortho=0;countipso=0;counttotal=0;switches=-1;current="";oldclosest="";opswitches=-
1;oldop="";currentop=""
  }
oldfilename=FILENAME
counttotal++
if (($9<$11) && ($9<$13) && ($9<$15)) {
  countpara++
  current="para"
  currentop="para"
  }
if (($11<$9) && ($11<$13) && ($11<$15)) {
  countmeta++
  current="meta"
  }
if (($13<$9) && ($13<$11) && ($13<$15)) {
  countortho++
  current="ortho"
  currentop="ortho"
  }
if (($15<$9) && ($15<$11) && ($15<$13)) {
  countipso++
  current="ipso"
  }
if (current!=oldclosest) switches++
if (currentop!=oldop) opswitches++
oldclosest=current; oldop=currentop
dist=$9
if ($11<dist) dist=$11
if ($13<dist) dist=$13
if ($15<dist) dist=$15
printf("%.1f %.3f",$5,dist)
print ""
}
END {
if (counttotal>0) {
  pp=int(.5+100*countpara/counttotal)
  pm=int(.5+100*countmeta/counttotal)
  po=int(.5+100*countortho/counttotal)
  pi=int(.5+100*countipso/counttotal)
  }
print oldfilename,"    ",countpara,countmeta,countortho,countipso,"    ",counttotal,"    ",pp,pm,po,pi,"    switches",switches,"
opswitches",opswitches >> "regiocount"
}
```

Program prog3dpath

```
BEGIN {
A[1]=0.0;B[1]=-1.403;C[1]=-8
A[2]=1.198;B[2]=-.695;C[2]=-8
A[3]=1.198;B[3]=.695;C[3]=-8
A[4]=0.0;B[4]=1.403;C[4]=-8
A[5]=1.0;B[5]=0;C[5]=-5
A[6]=-1.198;B[6]=.695;C[6]=-8
A[7]=-1.198;B[7]=-.695;C[7]=-8
}
/run/ {
olderA=oldA;olderB=oldB;olderC=oldC
oldA=A[5];oldB=B[5];oldC=C[5]
delta=.1
optx=0;opty=0;optz=0
dp=$9;dm=$11;dor=$13;di=$15
if ((Error())^.5<delta) delta=(Error())^.5
#print "target distances",dp,dm,dor,di
#print "initial distances",Distance(1,5),Distance(2,5),Distance(3,5),Distance(4,5),"error",Error()
for (i=1;i<=14;i++) {
  olderror=Error()
  while (optz==0) {
    C[5]=C[5]+delta
    if (Error()>olderror) {
      optz=1
      }
    olderror=Error()
    }
  while (opty==0) {
    B[5]=B[5]+delta
    if (Error()>olderror) {
      opty=1
      }
    olderror=Error()
    }
  while (optx==0) {
    A[5]=A[5]+delta
    if (Error()>olderror) {
      optx=1
      }
    olderror=Error()
    }
  #print "x,y,z after passes",A[5],B[5],C[5]
#  print "intermediate distances",Distance(1,5),Distance(2,5),Distance(3,5),Distance(4,5),"error",Error(),i
  delta=-.5*delta
  optx=0;opty=0;optz=0
  }
countsinceflip++
secondderiv=olderA+A[5]-2*oldA
if ((secondderiv>.015) || (secondderiv<-.015)) {
  if ((A[5]<.05) && (A[5]>-.05) && (countsinceflip>10)) {
    A[2]=-A[2];A[3]=-A[3];A[6]=-A[6];A[7]=-A[7];
    A[5]=-A[5]
    countsinceflip=0
    print
"XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXX   flipped"
    }
  }
print "\t",A[5],"\t",B[5],"\t",C[5],"\t","error",Error()
printf("%.4f,",A[5]) > "tempA"
```

```
printf("%.4f,",B[5]) > "tempB"
printf("%.4f,",C[5]) > "tempC"
}
END {
for (i=1;i<=5;i++) {
  tA=A[5];tB=B[5];tC=C[5]
  A[5]=3*A[5]-3*oldA+olderA;B[5]=3*B[5]-3*oldB+olderB;C[5]=3*C[5]-3*oldC+olderC;
  olderA=oldA;olderB=oldB;olderC=oldC
  oldA=tA;oldB=tB;oldC=tC
  print "\t",A[5],"\t",B[5],"\t",C[5],"extrapolation"
  printf("%.4f,",A[5]) > "tempA"
  printf("%.4f,",B[5]) > "tempB"
  printf("%.4f,",C[5]) > "tempC"
  }
print "" >> "tempA"
print "" >> "tempB"
print "" >> "tempC"
}

function Distance(Atom1,Atom2) {
 return sqrt((A[Atom1]-A[Atom2])^2 + (B[Atom1]-B[Atom2])^2 + (C[Atom1]-C[Atom2])^2)
}

function Error() {
#  if (Distance(6,5)<Distance(3,5)) return (dp-Distance(1,5))^2+(dm-Distance(7,5))^2+(dor-Distance(6,5))^2+(di-
Distance(4,5))^2
  return (dp-Distance(1,5))^2+(dm-Distance(2,5))^2+(dor-Distance(3,5))^2+(di-Distance(4,5))^2
}
```

Program nitrationPara1.m

```
X6 =
[0.8444,0.8445,0.8427,0.8439,0.8385,0.8347,0.8275,0.8187,0.8101,0.7998,0.7895,0.7808,0.7736,0.7666,0.7644,0.7655,0.7695,0
.7788,0.7878,0.7973];
Y6 = [-0.6949,-0.6976,-0.7005,-0.7018,-0.7028,-0.7027,-0.7026,-0.7028,-0.7021,-0.7023,-0.7036,-0.7037,-0.7053,-0.7063,-
0.7089,-0.7109,-0.7120,-0.7151,-0.7163,-0.7199];
Z6 = [-4.3812,-4.3774,-4.3753,-4.3732,-4.3717,-4.3699,-4.3684,-4.3676,-4.3668,-4.3663,-4.3671,-4.3685,-4.3717,-4.3754,-
4.3814,-4.3874,-4.3956,-4.4040,-4.4127,-4.4219];


xorthoa = -1.198; xorthob = 1.198; ypara = -1.403; yipso = 1.403; yme = 2.96; ymeta = -.695; yortho = .695
dbmult=.75;
depth=-8;
X1 = [xorthoa,0,0,0,xorthob,xorthob,0,xorthoa,xorthoa];
Y1 = [yortho,yipso,yme,yipso,yortho,ymeta,ypara,ymeta,yortho];
Z1 = [depth,depth,depth,depth,depth,depth,depth,depth,depth];
X2 = [dbmult*xorthoa,0];
Y2 = [dbmult*yortho,dbmult*yipso];
Z2 = [depth,depth];
X3 = [dbmult*xorthob,dbmult*xorthob];
Y3 = [dbmult*yortho,dbmult*ymeta];
Z3 = [depth,depth];
X4 = [0,dbmult*xorthoa];
Y4 = [dbmult*ypara,dbmult*ymeta];
Z4 = [depth,depth];

figure(2216)
hFig = figure(2216);
colormap(hFig,'jet')
brighten(.7);
shading interp;
```

```
set(gca, 'LooseInset', get(gca,'TightInset'))
set(hFig, 'Position', [1 1 1056 1056],'color',[1 1 1])

plot3(X1,Y1,Z1,'b','LineWidth',8)
hold on;
plot3(X2,Y2,Z2,'b','LineWidth',8)
hold on;
plot3(X3,Y3,Z3,'b','LineWidth',8)
hold on;
plot3(X4,Y4,Z4,'b','LineWidth',8)
hold on;
plot3(X6,Y6,Z6,'r','LineWidth',4);
hold on;
axwidth=1;
Xi = -1.9; Xf = 2.5;
Yi = -3.2; Yf = yme+1.05*radiusc;
Zi = depth-radiuscz; Zf = -4.4;
fill3([Xi Xi Xf Xf],[Yi Yf Yf Yi],[Zi Zi Zi Zi],[1 1 .9]);
fill3([Xf Xf Xf Xf],[Yi Yf Yf Yi],[Zi Zi Zf Zf],[1 1 .9]);
fill3([Xi Xi Xf Xf],[Yf Yf Yf Yf],[Zi Zf Zf Zi],[1 1 .9]);
hold on;

[x y z]=sphere;
radiusc=.5;
radiuscz=.5;
ptalpha=.5;
salpha=.2;
surf(radiusc*x-1.21,radiusc*y+.7,radiuscz*z+depth,'facealpha',salpha,'edgealpha',ptalpha,'cdatamapping','direct','facecolor','k');
surf(radiusc*x,radiusc*y+1.4,radiuscz*z+depth,'facealpha',salpha,'edgealpha',ptalpha,'cdatamapping','direct','facecolor','k');
surf(radiusc*x+1.21,radiusc*y+.7,radiuscz*z+depth,'facealpha',salpha,'edgealpha',ptalpha,'cdatamapping','direct','facecolor','k');
surf(radiusc*x+1.21,radiusc*y-.7,radiuscz*z+depth,'facealpha',salpha,'edgealpha',ptalpha,'cdatamapping','direct','facecolor','k');
surf(radiusc*x,radiusc*y-1.4,radiuscz*z+depth,'facealpha',salpha,'edgealpha',ptalpha,'cdatamapping','direct','facecolor','k');
surf(radiusc*x-1.21,radiusc*y-.7,radiuscz*z+depth,'facealpha',salpha,'edgealpha',ptalpha,'cdatamapping','direct','facecolor','k');
surf(radiusc*x,radiusc*y+2.95,radiuscz*z+depth,'facealpha',salpha,'edgealpha',ptalpha,'cdatamapping','direct','facecolor','k');
%first and last point of arrays
radpt=.5;
radptz=.5;
numglobes = 100; numpts = numel(X6); oldpoint = 1;
for t=1:numglobes-2;
   thispt = 1+round((numpts-1)*(t/(numglobes-1)));
   if ((X6(thispt)-X6(oldpoint))^2 + (Y6(thispt)-Y6(oldpoint))^2 + (Z6(thispt)-Z6(oldpoint))^2)^.5 > .5;

surf(radpt*x+X6(thispt),radpt*y+Y6(thispt),radptz*z+Z6(thispt),'facealpha',.08,'edgealpha',.2,'cdatamapping','direct','facecolor','g'
);
      oldpoint = thispt;
   end;
end;
surf(radpt*x+X6(1),radpt*y+Y6(1),radptz*z+Z6(1),'facealpha',salpha/1.2,'edgealpha',ptalpha/1.2,'cdatamapping','direct','facecolo
r','g');
surf(radpt*x+X6(numel(X6)),radpt*y+Y6(numel(X6)),radptz*z+Z6(numel(X6)),'facealpha',.3,...
   'edgealpha',ptalpha,'cdatamapping','direct','facecolor','g');
plot3([X6(numel(X6)) 0],[Y6(numel(X6)) ypara],[Z6(numel(X6)) depth],'b','LineWidth',8);

view(-65,25)

axis('manual',[-2.5,2.5,-3.6,yme+1.1*radiusc,depth-1.1*radiuscz,-3.7])

set(gca,'XTick',[-2 -1 0 1 2],'xticklabel',{"","","","",""},'TickLength',[0.00 0.00])
set(gca,'YTick',[-2 -1 0 1 2 3],'yticklabel',{"","","","","",""},'TickLength',[0.00 0.00])
set(gca,'zTick',[-8 -6 -4 -2 0 2],'zticklabel',{"","","","","",""},'TickLength',[0.00 0.00])
set(gca,'LineWidth',axwidth)
set(gca,'xgrid','on','ygrid','on','zgrid','on')
```

```
set(gca,'FontSize',32)
set(gca,'PlotBoxAspectRatio',[.66 1 .64])
set(gca,'projection','perspective')
set(gca,'position',[.06 .06 .92 .92])
set(gca,'GridLineStyle',':')
set(gca,'color',[1 1 1])
set(gca,'XColor','w','YColor','w','ZColor','w')
```

Program Suite PROGMC

PROGMC is a new program created to run efficient Monte Carlo calculations on the system containing toluene / $NO_2^+BF_4^-$ / 101 CH_2Cl_2 system. Aspects of the program are recognizably *ad hoc*, but we envision that future modifications of the program will be usable on diverse systems.

A full listing of the subprograms of PROGMC is given below. To allow the reader to understand or make use of PROGMC, we describe here first the overall structure of the program.

The master control program for Monte Carlo, in the form of a Unix Shell Script, is called *progMC*. For a user to start to use *progMC*, some early lines in it that assign the scratch space and the location of the program files and input files would have to be modified for the local environment. These lines are between lines 12 and 21 and should be apparent. The location of the scratch space is usually passed to *progMC* as a parameter.

progMC takes as input files:

geo - This file contains the initial geometry at the beginning and later the current accepted geometry. Its format is line1: number of atoms; line 2: optional, often contains a title; line 3-end: the atoms and there positions in Cartesian coordinates. Here is an example:

```
18
  NO2+Tol  101CH2Cl2IonP  Oniom  MonteCarlo  runpoint  31398
C -1.2617403 0.1734595 1.7107956
C -0.2553121 -0.5054263 2.4640648
C 0.5521703 0.2290144 3.3654142
C 0.3782197 1.6373306 3.4257961
C -0.5518774 2.3254313 2.5924738
C -1.3446008 1.5460692 1.7229427
C 1.1698044 2.4529314 4.3843350
H -1.8962769 -0.4103785 1.0535189
H -0.2796489 -1.5907112 2.3450544
H 1.1595708 -0.3281763 4.1250153
H -0.6235700 3.3948345 2.5621955
H -2.1326424 1.9681938 1.0652780
H 1.2599393 2.0587910 5.4511793
H 0.9502583 3.4864759 4.4010777
H 2.2661395 2.3883560 4.0664127
N 0.1562194 0.6631665 -0.0922596
O 1.1591170 1.0349781 0.2849730
O -0.5782311 0.4442340 -0.9938770
```

progmc.conf – This is a file giving a variety of configuration options, called on by many of the subprograms. A progmc.conf example is listed below and contains explanations of the program options.

progMC calls the following programs:

progmcb - An awk program that takes random steps from geo and generates subsequent Gaussian input files

progEcheck – This awk program pulls the energy from Gaussian output files, adjusts the energy by any biasing potentials or the potential that holds the sphere of molecules together, and decides if the new energy and geometry should be accepted.

proganal – A program to analyze the latest point and extract data. This program must be redone for each new system. proganal creates the output to mcfollowfile

progMC has the following output files:

runpointnumber – a running tab of the point in the chain of geometries

Elist – a list of all accepted energies
energy – the latest energy
testgeo – the latest test geometry. If the energy of testgeo is accepted, testgeo is moved to geo
latestmcrun and latestmcrun2 – the Gaussian output file from the latest and previously accepted points
mcfollowfile – the output from proganal, records selected data from the successful points but not the unsuccessful points
traj – a file containing the full set of accepted geometries for a Monte Carlo run
vellist – output containing the density of the sphere and the amount of energy used to maintain the sphere, for each successful point
A number of files starting with '*temp*' are created then later erased.

The following helper programs were used for the current study.
whamnitmc – a shell script that extracts data from the mcfollowfile files, sets up and runs wham to calculate the PMF, and keeps track of some general aspects of trajectories
progseriesmc – an AWK script used by whamnitmv to extract data from the mcfollowfile files
wham – a program from Grossfield, Alan, "WHAM: the weighted histogram analysis method", version 2.0.9, http://membrane.urmc.rochester.edu/content/wham that performs the wham analysis

Program progMC

```
#!/bin/bash
#progMC started 12/21/2015
#                             OUTLINE
# A. initilize to perform Gaussian jobs, set the scratch, program, and other directores, remove errant control files
# B. use progmcb to read in the geometry from file geo.   progmcb then generates a new point and sets up g09.com
# C. progEcheck then checks to see if the new geometry is acceptable, based on new energy versus energy in file energy
#    If this is the first point, the energy is assigned as huge so the next point is accepted
#    If the new point is accepted then the new point is placed in file geo and the new energy is placed in file energy and proganal is run
# D. go to B
#
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
#origdir, randdir, scratchdir, g09root, logfile all may need varied from system to system and assigned here or by program calling this one
export LC_ALL=C
echo $1
scratchdir=$1
export g09root=/software/lms/g09_D01
. $g09root/g09/bsd/g09.profile
origdir=`pwd`
cd $origdir
logfile=docslog
randdir=~/bin
proggramdir=~/binmc
echo
echo ORIGDIR at the beginning of run:
echo $origdir
ls $origdir
echo
echo SCRATCHDIR at the beginning of run:
echo $scratchdir
ls $scratchdir
echo
echo PROGGRAMDIR at the beginning of run::
echo $proggramdir
ls $proggramdir

rm -f nogo    # assume that if someone is starting a job, they want it to go.
rm -f diagnostics goingwell tempdone # diagnostics contains extra info from previous runs, other two files are from older versions of progdyn
```

```
cd $origdir
if (test -s runpointnumber) then
  echo "skipping start and continuing from previous runs"
else
  echo 1 > runpointnumber
fi
if (test -f energy) then
  echo "we have an energy in place"
  cat energy
else
  echo 9999999999999 > energy
fi
if (test -s progmc.conf) then
  echo "we have a progmc.conf"
else
  echo "no progmc.conf"
  exit 9
fi
if (test -s g09.com) then
  sed -i '/guess=tcheck/d' g09.com      # no chk file on first point
fi
rm -f latestmcrun   # just using this as a signal that we are on the first point of submission

while (true)
do
#
BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB
BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB
  rm -f $scratchdir/goingwell $scratchdir/goodenergy
  cd $origdir
  if (test -s latestmcrun) then
    awk -f $proggramdir/progmcb geo > g09.com
  else
    awk -f $proggramdir/progmcb geo > g09.com
    sed -i '/guess=tcheck/d' g09.com      # no chk file on first point
  fi
  if (test -s g09.com) then
    cd $scratchdir
    cp $origdir/g09.com $scratchdir/g09.com
    $g09root/g09/g09 $scratchdir/g09.com > $scratchdir/g09.log
    cd $origdir
    grep 'Normal termination' $scratchdir/g09.log > $scratchdir/goingwell
  else
    echo "g09.com not generated"
    break
  fi
  if (test -s $scratchdir/goingwell) then
    cp $scratchdir/g09.log latestmcrun
  else
    echo "some problem in middle of gaussian job"
    cp $scratchdir/g09.log $origdir/g09.log
    break
  fi
#
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
  rm -f goodenergy
  awk -f $proggramdir/progEcheck latestmcrun
  if (test -s goodenergy) then
    awk -f $proggramdir/proganal latestmcrun >> mcfollowfile
    cat testgeo >> traj
```

```
    cp testgeo geo
    cp latestmcrun latestmcrun2
    cat energy >> Elist
    cp goodenergy energy
  fi
  cp runpointnumber $scratchdir/temp533
  awk 'BEGIN {getline;i=$1+1;print i}' $scratchdir/temp533 > runpointnumber
  rm $scratchdir/temp533

# here is a cool link that lets you interupt the dynamics with a short job, then
# it automatically goes back to the dynamics  just make the file 'detour' and it
# will delete detour, run run.com, then go back to dynamics
  if (test  -f detour) then
    rm detour
    date >> $logfile
    cat run.com >> $logfile
    cp run.log temp.log
    cd $scratchdir
    $g09root/g09/g09 $origdir/run.com > $origdir/run.log
    cd $origdir
  fi

#stop it all nicely by creating a nogo file
    if (test  -f nogo) then
      break
    fi

#no obvious reason to have an mc run quit on its own if everything is working ok
#
END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_Loop____END_of_C_L
oop____
done
exit 0
```

Program progmcb

```
BEGIN {
#Dec 21 2015
#This main routine for generating .com files by Monti-Carlo
#setting values for parameters such that program fails if there are no parameters
# do not change these - rather, change progmc.conf to set the parameters
temp=0.0;memory=20000000;
diag=1; checkpoint="g09.chk"; boxon=0
boxsize=10; title1="you"; title2="need"
title3="a"; title4="progmc.conf"; processors=1; highlevel=99999; linkatoms=0
nonstandard=0
oniomcharge=0; oniommult=0
applypotential=0; zeroatomon=0
sphereon=0; spheresize=999; sphereforceK=0.01
moleculecount=0

#initialization
srand(PROCINFO["pid"])
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447; pi=3.14159265359
numAtoms=0; atomnumber=0
conver1=4.184E26 #dividing by this converts amu angs^2 /s^2 to kcal/mol
OFS="   "

# read progdyn.conf for configuration info
```

```
blankLineTester=10
while (blankLineTester>1) {
  getline < "progmc.conf"
  if ($1=="method") method=$2
  if ($1=="method2") meth2=$2
  if ($1=="charge") charge=$2
  if ($1=="multiplicity") multiplicity=$2
  if ($1=="oniomchargemult") {
    oniomcharge=$2
    oniommult=$3
    }
  if ($1=="memory") memory=$2
  if ($1=="processors") processors=$2
  if ($1=="checkpoint") checkpoint=$2
  if ($1=="diagnostics") diag=$2
  if ($1=="temperature") temp=$2
  if ($1=="mcstepsize") mcstep=$2
  if ($1=="lengthstep") lengthstep=$2
  if ($1=="anglestep") anglestep=$2
  if ($1=="mcmolrotangle") mcmolrotangle=$2
  if ($1=="molecule") {
    moleculecount++
    molAtoms[moleculecount]=NF-2
    for (i=1;i<NF-1;i++) {
      molecule[moleculecount,i]=$(i+1)
      }
    molStep[moleculecount]=$NF
    }
  if ($1=="method3") meth3=$2
  if ($1=="method4") meth4=$2
  if ($1=="method5") meth5=$2
  if ($1=="method6") meth6=$2
  if ($1=="method7") meth7=$2
  if ($1=="highlevel") highlevel=$2
  if ($1=="linkatoms") linkatoms=$2
  if ($1=="boxon") boxon=$2
  if ($1=="boxsize") boxsize=$2
  if ($1=="sphereon") sphereon=$2
  if ($1=="spheresize") spheresize=$2
  if ($1=="sphereforce") sphereforceK=$2
  if ($1=="methodfile") methodfilelines=$2
  if ($1=="killcheck") killcheck=$2
  if ($1=="nonstandard") nonstandard=$2
  if ($1=="applypotential") {
    apforce=$2; apforceX0=$3
    }
  if ($1=="apatoms") {
    for (i=1;i<8;i++) {
      if ($(i+1)>0) apatom[i]=$(i+1)
      }
    }
  if ($1=="applypotentialplane") {
    apforceplane=$2; apforceplaneX0=$3
    }
  if ($1=="applaneatoms") {
    for (i=1;i<8;i++) {
      if ($(i+1)>0) afplaneatoms[i]=$(i+1)
      }
    }
  if ($1=="zeroatom") {
    zeroatomon=1
    zeroatom=$2
```

```
    zeroatompotential=$3
    }
  if ($1=="title") {
    title1=$2
    title2=$3
    title3=$4
    title4=$5
    }
  blankLineTester=length($0)
  }

#for (i=1;i<=moleculecount;i++) {
#   for (j=1;j<=molAtoms[i];j++) {
#      print molecule[i,j]
#     }
#   print molStep[i]
#   }

if (diag>=1) print "***************** starting progdynb *****************" >> "diagnostics"
if (diag>=1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag>=1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag>=1) print "processors,checkpoint,title" >> "diagnostics"
if (diag>=1) print processors,checkpoint,title1,title2,title3,title4 >> "diagnostics"

# get number of atoms and geometry from file geo
getline <  "geo"
numAtoms=$1
getline < "geo"
for (i=1;i<=numAtoms;i++) {
  getline < "geo"
  atSym[i]=$1
  oldarr[i,1]=$2; oldarr[i,2]=$3; oldarr[i,3]=$4
  if (atSym[i]=="H") atRadius[i]=1.2
  if (atSym[i]=="B") atRadius[i]=1.8
  if (atSym[i]=="C") atRadius[i]=1.7
  if (atSym[i]=="N") atRadius[i]=1.55
  if (atSym[i]=="O") atRadius[i]=1.52
  if (atSym[i]=="F") atRadius[i]=1.47
  if (atSym[i]=="Cl") atRadius[i]=1.75
  }

# record atom velocities for IVR analysis.  This is actually the velocity in the previous run, which is the easiest to calculate.
getline < "runpointnumber"
runpointnum = $1
}

#pull out the potential energy
/SCF Done/ || /EUMP2 =/ || / Energy=/ || /ONIOM:/ {
  if (($1=="Energy=") && ($3=="NIter="))  newPotentialE=$2
  if ($1=="SCF") newPotentialE=$5
  if ($2=="extrapolated")  newPotentialE=$5
  if ($1=="E2") {
    tempstring=$6
    split(tempstring, arr10, "D")
    newPotentialE=arr10[1]*(10^arr10[2])
    }
  newPotEK=(newPotentialE-potentialE)*627.509
  }

END {
# idea for moving atoms within molecules - define each atom by a vector vs its nearest neighbor, displace by changing
# the length of the vector and by moving it in two orthogonal directions
```

```
for (k=1;k<=moleculecount;k++) {
#  print atSym[molecule[k,1]]
  for (i=2;i<=molAtoms[k];i++) {
    atCon[i]=i-1
    for (m=1;m<i-1;m++) {
      if (Distance(molecule[k,m],molecule[k,i])<Distance(molecule[k,atCon[i]],molecule[k,i])) atCon[i]=m
      }
    vector[i,1]=oldarr[molecule[k,i],1]-oldarr[molecule[k,atCon[i]],1]
    vector[i,2]=oldarr[molecule[k,i],2]-oldarr[molecule[k,atCon[i]],2]
    vector[i,3]=oldarr[molecule[k,i],3]-oldarr[molecule[k,atCon[i]],3]
#     print atSym[molecule[k,i]],atCon[i],vector[i,1],vector[i,2],vector[i,3]
# now make one unit vector that is perpendicular to the first vector
    pervector1[i,1]=vector[i,2]/((vector[i,1]^2+vector[i,2]^2)^.5)
    pervector1[i,2]=-vector[i,1]/((vector[i,1]^2+vector[i,2]^2)^.5)
    pervector1[i,3]=0
#     print "perpendicular unit vector",pervector1[i,1],pervector1[i,2],pervector1[i,3]`
# now make another unit vector perpendicular to both
    pervector2[i,1]=vector[i,2]*pervector1[i,3]-vector[i,3]*pervector1[i,2]
    pervector2[i,2]=vector[i,3]*pervector1[i,1]-vector[i,1]*pervector1[i,3]
    pervector2[i,3]=vector[i,1]*pervector1[i,2]-vector[i,2]*pervector1[i,1]
    norm=(pervector2[i,1]^2+pervector2[i,2]^2+pervector2[i,3]^2)^.5
    pervector2[i,1]=pervector2[i,1]/norm;pervector2[i,2]=pervector2[i,2]/norm;pervector2[i,3]=pervector2[i,3]/norm;
#     print "2nd perpendicular unit vector",pervector2[i,1],pervector2[i,2],pervector2[i,3]`
    stepL=2*(rand()-.5)*lengthstep
    step1=2*(rand()-.5)*anglestep
    step2=2*(rand()-.5)*anglestep
    if (molecule[k,i]<7) {
      step1=step1/5;step2=step2/5;stepL=stepL/5
      }

vector[i,1]=vector[i,1]+step1*pervector1[i,1]+step2*pervector2[i,1]+stepL*vector[i,1]/Distance(molecule[k,atCon[i]],molecule[k
,i])

vector[i,2]=vector[i,2]+step1*pervector1[i,2]+step2*pervector2[i,2]+stepL*vector[i,2]/Distance(molecule[k,atCon[i]],molecule[k
,i])

vector[i,3]=vector[i,3]+step1*pervector1[i,3]+step2*pervector2[i,3]+stepL*vector[i,3]/Distance(molecule[k,atCon[i]],molecule[k
,i])
#     print "newvector",atSym[molecule[k,i]],atCon[i],vector[i,1],vector[i,2],vector[i,3]
    }
# now we convert back to exteranl cartesian coordinates
# atom 1 is just at its original position
#  print atSym[molecule[k,1]],oldarr[molecule[k,1],1],oldarr[molecule[k,1],2],oldarr[molecule[k,1],3]
  for (i=2;i<=molAtoms[k];i++) {
    oldarr[molecule[k,i],1]=oldarr[molecule[k,atCon[i]],1]+vector[i,1]
    oldarr[molecule[k,i],2]=oldarr[molecule[k,atCon[i]],2]+vector[i,2]
    oldarr[molecule[k,i],3]=oldarr[molecule[k,atCon[i]],3]+vector[i,3]
#     print atSym[molecule[k,i]],oldarr[molecule[k,i],1],oldarr[molecule[k,i],2],oldarr[molecule[k,i],3]
    }
  }


############# monte Carlo motion of atoms ##############
# treat motion as steps of molecules and steps within molecules
# move each molecule by delX,delY,delZ - these are relatively big steps defined by molStep
# move all atoms but the first in a molecule, relatively, by mcstep
for (k=1;k<=moleculecount;k++) {
  delX=2*(rand()-.5)*molStep[k];delY=2*(rand()-.5)*molStep[k];delZ=2*(rand()-.5)*molStep[k]
  for (i=1;i<=molAtoms[k];i++) {
    delAtX=0;delAtY=0;delAtZ=0
    if (i>1) {
      delAtX=2*(rand()-.5)*mcstep;delAtY=2*(rand()-.5)*mcstep;delAtZ=2*(rand()-.5)*mcstep
```

```
      }
    newarr[molecule[k,i],1]=oldarr[molecule[k,i],1]+delX+delAtX;
    newarr[molecule[k,i],2]=oldarr[molecule[k,i],2]+delY+delAtY;
    newarr[molecule[k,i],3]=oldarr[molecule[k,i],3]+delZ+delAtZ;
    }
  }

#Rotating molecules
#Originally tried rotating about center of mass but that give lopsided motion for things like CH2Cl2
#So switched to weighting by vdw radius
# now figure out the center of mass of each molecule and the coordinates of each molecule relative to the CM
for (k=1;k<=moleculecount;k++) {
  for (i=1;i<=molAtoms[k];i++) {
    CM[k,1]=CM[k,1]+newarr[molecule[k,i],1]*atRadius[molecule[k,i]]
    CM[k,2]=CM[k,2]+newarr[molecule[k,i],2]*atRadius[molecule[k,i]]
    CM[k,3]=CM[k,3]+newarr[molecule[k,i],3]*atRadius[molecule[k,i]]
    totalradius[k]=totalradius[k]+atRadius[molecule[k,i]]
    }
  CM[k,1]=CM[k,1]/totalradius[k];CM[k,2]=CM[k,2]/totalradius[k];CM[k,3]=CM[k,3]/totalradius[k];
#  print "center of mass coordinates and totalradius",CM[k,1],CM[k,2],CM[k,3],totalradius[k] > "tempradius"
# figure out the angle to rotate around x, y, and z axes, in radians
  angleX=pi*mcmolrotangle*2*(rand()-.5)/180
  angleY=pi*mcmolrotangle*2*(rand()-.5)/180
  angleZ=pi*mcmolrotangle*2*(rand()-.5)/180
  maxDistToX=0;maxDistToY=0;maxDistToZ=0
  for (i=1;i<=molAtoms[k];i++) {
# change coordinates to center of mass
    CMgeo[k,i,1]=newarr[molecule[k,i],1]-CM[k,1]
    CMgeo[k,i,2]=newarr[molecule[k,i],2]-CM[k,2]
    CMgeo[k,i,3]=newarr[molecule[k,i],3]-CM[k,3]
    if ((CMgeo[k,i,2]^2+CMgeo[k,i,3]^2)^.5>maxDistToX) maxDistToX=(CMgeo[k,i,2]^2+CMgeo[k,i,3]^2)^.5
    if ((CMgeo[k,i,1]^2+CMgeo[k,i,3]^2)^.5>maxDistToY) maxDistToY=(CMgeo[k,i,1]^2+CMgeo[k,i,3]^2)^.5
    if ((CMgeo[k,i,1]^2+CMgeo[k,i,2]^2)^.5>maxDistToZ) maxDistToZ=(CMgeo[k,i,1]^2+CMgeo[k,i,2]^2)^.5
# figure out how big the molecule is.  We will rotate big molecules less and small ones more.
    }
#  print maxDistToX,maxDistToY,maxDistToZ > "tempradius"
#cut rotation angle if molecule is bigger to 2 angs radius
  if (maxDistToX>1.6) angleX=angleX*1.6/maxDistToX
  if (maxDistToY>1.6) angleY=angleY*1.6/maxDistToY
  if (maxDistToZ>1.6) angleZ=angleZ*1.6/maxDistToZ
#now apply the rotation
  for (i=1;i<=molAtoms[k];i++) {
# first x
    tempvar=CMgeo[k,i,2]*cos(angleX)-CMgeo[k,i,3]*sin(angleX)
    CMgeo[k,i,3]=CMgeo[k,i,2]*sin(angleX)+CMgeo[k,i,3]*cos(angleX)
    CMgeo[k,i,2]=tempvar
# then y
    tempvar=CMgeo[k,i,1]*cos(angleY)+CMgeo[k,i,3]*sin(angleY)
    CMgeo[k,i,3]=-CMgeo[k,i,1]*sin(angleY)+CMgeo[k,i,3]*cos(angleY)
    CMgeo[k,i,1]=tempvar
# then z
    tempvar=CMgeo[k,i,1]*cos(angleZ)-CMgeo[k,i,2]*sin(angleZ)
    CMgeo[k,i,2]=CMgeo[k,i,1]*sin(angleZ)+CMgeo[k,i,2]*cos(angleZ)
    CMgeo[k,i,1]=tempvar
#now restore to external coordinates
    newarr[molecule[k,i],1]=CMgeo[k,i,1]+CM[k,1]
    newarr[molecule[k,i],2]=CMgeo[k,i,2]+CM[k,2]
    newarr[molecule[k,i],3]=CMgeo[k,i,3]+CM[k,3]
    #print newarr[molecule[k,i],1],newarr[molecule[k,i],2],newarr[molecule[k,i],3]
    }
  }
```

```
print "%nproc=" processors
print "%mem=" memory
if (killcheck!=1) print "%chk=" checkpoint
if (nonstandard==0) {
  print "#p " method " scf=(xqc,maxconven=155,fulllinear,nosym) "
  if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
  if (meth2=="read") print "guess=tcheck" #for reading orbitals from check, sometimes faster, sometimes not
  print "pop=none "
  if (length(meth3)>2) print meth3
  if (length(meth4)>2) print meth4
  }
if (nonstandard==1) {
  print "# "
  print "nonstd"
  system("cat nonstandard")
  }
print ""
print  title1,title2,title3,title4
print "runpoint ",runpointnum
print ""
if (oniommult==0) print charge,multiplicity
if (oniommult>0) print charge,multiplicity,oniomcharge,oniommult
print numAtoms > "testgeo"
print newPotentialE,title1,title2,title3,title4,"runpoint ",runpointnum >> "testgeo"
for (i=1;i<=numAtoms;i++) {
  printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3])
  printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3]) >> "testgeo"
  print "" >> "testgeo"
  if ((i>highlevel) && (i<=highlevel+linkatoms)) printf(" %s","M H")
  if (i>(highlevel+linkatoms)) printf(" %s","M")
  print ""
  }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
if (methodfilelines>=1) {
  for (i=1;i<=methodfilelines;i++) {
    getline < "methodfile"
    print $0
    }
  }
}

function Distance(Atom1,Atom2) {
 return sqrt((oldarr[Atom1,1]-oldarr[Atom2,1])^2+(oldarr[Atom1,2]-oldarr[Atom2,2])^2+(oldarr[Atom1,3]-oldarr[Atom2,3])^2)
}

function Angle(Atom1,Atom2,Atom3) {
  value=((-
Distance(Atom1,Atom3)^2+Distance(Atom1,Atom2)^2+Distance(Atom2,Atom3)^2)/(2*Distance(Atom1,Atom2)*Distance(Ato
m2,Atom3)))
  return acos(value)
}

function asin(x) { return (180/3.141592)*atan2(x, sqrt(1-x*x)) }

function acos(x) { return (180/3.141592)*atan2(sqrt(1-x*x), x) }

function atan(x) { return (180/3.141592)*atan2(x,1) }

function Dihedral(Atom1,Atom2,Atom3,Atom4) {
  B1x=oldarr[Atom2,1]-oldarr[Atom1,1]
```

```
  B1y=oldarr[Atom2,2]-oldarr[Atom1,2]
  B1z=oldarr[Atom2,3]-oldarr[Atom1,3]
  B2x=oldarr[Atom3,1]-oldarr[Atom2,1]
  B2y=oldarr[Atom3,2]-oldarr[Atom2,2]
  B2z=oldarr[Atom3,3]-oldarr[Atom2,3]
  B3x=oldarr[Atom4,1]-oldarr[Atom3,1]
  B3y=oldarr[Atom4,2]-oldarr[Atom3,2]
  B3z=oldarr[Atom4,3]-oldarr[Atom3,3]
  modB2=sqrt((B2x^2)+(B2y^2)+(B2z^2))
# yAx is x-coord. etc of modulus of B2 times B1
  yAx=modB2*(B1x)
  yAy=modB2*(B1y)
  yAz=modB2*(B1z)
# CP2 is the crossproduct of B2 and B3
  CP2x=(B2y*B3z)-(B2z*B3y)
  CP2y=(B2z*B3x)-(B2x*B3z)
  CP2z=(B2x*B3y)-(B2y*B3x)
  termY=((yAx*CP2x)+(yAy*CP2y)+(yAz*CP2z))
# CP is the crossproduct of B1 and B2
  CPx=(B1y*B2z)-(B1z*B2y)
  CPy=(B1z*B2x)-(B1x*B2z)
  CPz=(B1x*B2y)-(B1y*B2x)
  termX=((CPx*CP2x)+(CPy*CP2y)+(CPz*CP2z))
 dihed4=(180/3.141592)*atan2(termY,termX)
 return dihed4
}
```

Program progEcheck

```
BEGIN {
#Dec 21 2015
#This program pulls out the energy from latestmcrun and it pulls the energy from file energy
#and it applies the Monte Carlo test to see if the new point is accepted.  If so, it makes a file "goodenergy"

#some default parameters
apforce[1]=0;apatom[1,1]=0;apatom[1,2]=0;
sphereon=0;spheresize=99999;sphereforce=0
zeroatom=0;zeroatomforceK=0.1
potentialcount=0; planeradius=1.4

#initialization
srand(PROCINFO["pid"])
i=1;j=1;k=1
c=29979245800; h=6.626075E-34; avNum=6.0221415E23
RgasK=0.00198588; RgasJ=8.31447; pi=3.14159265359
pi=3.141592
numAtoms=0; atomnumber=0
conver1=4.184E26 #dividing by this converts amu angs^2 /s^2 to kcal/mol
OFS="   "

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
  getline < "progmc.conf"
  if ($1=="temperature") temp=$2
  if ($1=="zeroatom") {
    zeroatomon=1
    zeroatom=$2
    zeroatomforceK=$3
    }
  if ($1=="sphereon") sphereon=$2
```

```
  if ($1=="spheresize") spheresize=$2
  if ($1=="sphereforce") sphereforceK=$2
  if ($1=="applypotential") {
    potentialcount++
    apforce[potentialcount]=$2; apforceX0[potentialcount]=$3
    }
  if ($1=="apatoms") {
    potatoms[potentialcount]=NF-1
    for (i=1;i<=potatoms[potentialcount];i++) {
      if ($(i+1)>0) apatom[potentialcount,i]=$(i+1)
      }
    }
  if ($1=="applypotentialplane") {
    appotentialplane=$2; appotentialplaneX0=$3; planeradius=$4
    }
  if ($1=="applaneatoms") {
    applaneatomnum=NF-1
    if ((appotentialplane>0) && (applaneatomnum<4)) {
      print "you need at least three atoms to define a plane"
      exit
      }
    for (i=1;i<=applaneatomnum;i++) {
      if ($(i+1)>0) applaneatoms[i]=$(i+1)
      }
    }
  blankLineTester=length($0)
  }

#get the old energy
getline < "energy"
oldenergy=$1
close("energy")

# get runpointnumber
getline < "runpointnumber"
runpointnum = $1

# get number of atoms and geometry from file testgeo
getline <  "testgeo"
numAtoms=$1
getline < "testgeo"
for (i=1;i<=numAtoms;i++) {
  getline < "testgeo"
  atSym[i]=$1
  oldarr[i,1]=$2; oldarr[i,2]=$3; oldarr[i,3]=$4
  if (atSym[i]=="H") atWeight[i]=1.00783
  if (atSym[i]=="B") atWeight[i]=10.811
  if (atSym[i]=="C") atWeight[i]=12.
  if (atSym[i]=="N") atWeight[i]=14.007
  if (atSym[i]=="O") atWeight[i]=15.9994
  if (atSym[i]=="F") atWeight[i]=18.9984
  if (atSym[i]=="Cl") atWeight[i]=35.4527
  }
}

#pull out the potential energy
/SCF Done/ || /EUMP2 =/ || / Energy=/ || /ONIOM:/ {
  if (($1=="Energy=") && ($3=="NIter="))  newPotentialE=$2
  if ($1=="SCF") newPotentialE=$5
  if ($2=="extrapolated")  newPotentialE=$5
  if ($1=="E2") {
    tempstring=$6
```

```
    split(tempstring, arr10, "D")
    newPotentialE=arr10[1]*(10^arr10[2])
    }
  newPotEK=(newPotentialE)*627.509
  }

END {
#Now we have to add in an energy based on the testgeo and the various biasing potentials
#First, we work with a sphere
if (sphereon==1) {
  biasE=0;totalweight=0
  for (i=1;i<=numAtoms;i++) {
    distToOrig=((oldarr[i,1]^2+oldarr[i,2]^2+oldarr[i,3]^2)^.5)
    if (distToOrig>spheresize) {
      biasE=biasE+0.5*sphereforceK*(distToOrig-spheresize)^2
      }
    if (distToOrig<0.9*spheresize) {
      totalweight=totalweight+atWeight[i]
      }
    }
  density=(totalweight/avNum)/((4/3)*pi*(0.9*spheresize*1E-8)^3)
  print "density",density,"sphere biasing energy",biasE >> "vellist"
  newPotEK=newPotEK+biasE
  }

#Now work on zeroatom bias
if (zeroatomon==1) {
  newPotEK=newPotEK+0.5*zeroatomforceK*(oldarr[zeroatom,1]^2+oldarr[zeroatom,2]^2+oldarr[zeroatom,3]^2)
  }

#Next, specific biasing potentials between atoms
for (k=1;k<=potentialcount;k++) {
  if ((apforce[k]!=0) && (apatom[k,1]>0) && (apatom[k,2]>0)) {
#first figure out which atom is closest to apatom[1] and put it into apatom[2]
    for (i=3;i<=potatoms[k];i++) {
      if(Distance(apatom[k,1],apatom[k,i])<Distance(apatom[k,1],apatom[k,2])) apatom[k,2]=apatom[k,i]
      }
#now add an energy to the molecule based on the biasing potential
    biasE=0.5*apforce[k]*(Distance(apatom[k,1],apatom[k,2])-apforceX0[k])^2
    newPotEK=newPotEK+biasE
    }
  }

#routine for adding a potential based on an atoms distance from a plane defined by other atoms.  The plane should have
#a limited radius so we should really consider it as a disk
if (appotentialplane>0) {
#first figure out the center of the plane atoms and move all of the atoms to put that center at the origin
  for (i=2;i<=applaneatomnum;i++) {
    k=applaneatoms[i]
    cmass[1]=cmass[1]+oldarr[k,1];cmass[2]=cmass[2]+oldarr[k,2];cmass[3]=cmass[3]+oldarr[k,3];
    }
  numplaneatoms=applaneatomnum-1
  cmass[1]=cmass[1]/numplaneatoms;cmass[2]=cmass[2]/numplaneatoms;cmass[3]=cmass[3]/numplaneatoms
  for (i=1;i<=applaneatomnum;i++) {
    k=applaneatoms[i]
    newarr[k,1]=oldarr[k,1]-cmass[1];newarr[k,2]=oldarr[k,2]-cmass[2];newarr[k,3]=oldarr[k,3]-cmass[3];
    }
#expect that bugs in process arise when plane is nearly vertical.  To avoid this, want to pick the z dimension as the one
#that has the smallest range.  since plane is centered, can use sum of absolute values as surrogate for range
  for (i=2;i<=applaneatomnum;i++) {
    k=applaneatoms[i]
    for (m=1;m<=3;m++) {
```

```
      if (newarr[k,m]>0) sum[m]=sum[m]+newarr[k,m];if (newarr[k,m]<0) sum[m]=sum[m]-newarr[k,m]
      }
    }
  if (sum[1]<sum[3]) {
    for (i=1;i<=applaneatomnum;i++) {
      k=applaneatoms[i]
      tempvar=newarr[k,1];newarr[k,1]=newarr[k,3];newarr[k,3]=tempvar
      }
    tempvar=sum[1];sum[1]=sum[3];sum[3]=tempvar
    }
  if (sum[2]<sum[3]) {
    for (i=1;i<=applaneatomnum;i++) {
      k=applaneatoms[i]
      tempvar=newarr[k,2];newarr[k,2]=newarr[k,3];newarr[k,3]=tempvar
      }
    tempvar=sum[2];sum[2]=sum[3];sum[3]=tempvar
    }
#now lets find the best plane
  for (i=2;i<=applaneatomnum;i++) {
    k=applaneatoms[i]
    A[1,1]=A[1,1]+newarr[k,1]^2;A[1,2]=A[1,2]+newarr[k,1]*newarr[k,2];A[1,3]=A[1,3]+newarr[k,1]
    A[2,1]=A[2,1]+newarr[k,1]*newarr[k,2];A[2,2]=A[2,2]+newarr[k,2]^2;A[2,3]=A[2,3]+newarr[k,2]
    A[3,1]=A[3,1]+newarr[k,1];A[3,2]=A[3,2]+newarr[k,2]
    b[1]=b[1]+newarr[k,1]*newarr[k,3];b[2]=b[2]+newarr[k,2]*newarr[k,3];b[3]=b[3]+newarr[k,3]
    }
  A[3,3]=numplaneatoms
  Det=A[1,1]*A[2,2]*A[3,3]+A[1,2]*A[2,3]*A[3,1]+A[1,3]*A[2,1]*A[3,2]-A[1,3]*A[2,2]*A[3,1]-A[1,2]*A[2,1]*A[3,3]-
A[1,1]*A[2,3]*A[3,2]
  E=(b[1]*A[2,2]*A[3,3]+A[1,2]*A[2,3]*b[3]+A[1,3]*b[2]*A[3,2]-A[1,3]*A[2,2]*b[3]-A[1,2]*b[2]*A[3,3]-
b[1]*A[2,3]*A[3,2])/Det
  F=(A[1,1]*b[2]*A[3,3]+b[1]*A[2,3]*A[3,1]+A[1,3]*A[2,1]*b[3]-A[1,3]*b[2]*A[3,1]-b[1]*A[2,1]*A[3,3]-
A[1,1]*A[2,3]*b[3])/Det
  G=(A[1,1]*A[2,2]*b[3]+A[1,2]*b[2]*A[3,1]+b[1]*A[2,1]*A[3,2]-b[1]*A[2,2]*A[3,1]-A[1,2]*A[2,1]*b[3]-
A[1,1]*b[2]*A[3,2])/Det
#  E, F, and G are the coefficients in the plane z=Ex+Fy+G - if the zeroing of the plane has worked G = 0
  print "E, F, and G are the coefficients in the plane z=Ex+Fy+G",E,F,G >> "diagnostics"
  conatom=applaneatoms[1]
  distplane=(-newarr[conatom,1]*E-newarr[conatom,2]*F+newarr[conatom,3]-G)/(E^2+F^2+1)^.5
  if (distplane<0) distplane=-distplane
  t=(newarr[conatom,1]*E+newarr[conatom,2]*F-newarr[conatom,3]+G)/(E^2+F^2+1)
  planepoint[1]=newarr[conatom,1]-t*E;planepoint[2]=newarr[conatom,2]-t*F;planepoint[3]=newarr[conatom,3]+t
  distcmass=((planepoint[1])^2+(planepoint[2])^2+(planepoint[3])^2)^.5
  print "distplane",distplane,"t",t,"planepoint",planepoint[1],planepoint[2],planepoint[3],"distcmass",distcmass  >> "diagnostics"
  if (distcmass>planeradius) {
    planepoint[1]=(planeradius/distcmass)*planepoint[1];
    planepoint[2]=(planeradius/distcmass)*planepoint[2];
    planepoint[3]=(planeradius/distcmass)*planepoint[3];
    distcmass=((planepoint[1])^2+(planepoint[2])^2+(planepoint[3])^2)^.5
    distplane=((planepoint[1]-newarr[conatom,1])^2+(planepoint[2]-newarr[conatom,2])^2+(planepoint[3]-
newarr[conatom,3])^2)^.5
    print "new distplane",distplane,"newplanepoint",planepoint[1],planepoint[2],planepoint[3],"newdistcmass",distcmass >>
"diagnostics"
    }
#finally add an energy to the molecule based on the biasing potential and distance from plane
    biasE=0.5*appotentialplane*(distplane-appotentialplaneX0)^2
    print "biasE from plane potential",biasE >> "diagnostics"
    newPotEK=newPotEK+biasE

  }

#now we decide whether or not to accept the new geometry
printon=0
```

```
if (newPotEK<oldenergy) printon=1
Ediff=newPotEK-oldenergy
if (Ediff>10) Ediff=10
if (Ediff<-10) Ediff=-10
AcceptProb=exp(-(Ediff)/(0.001987*temp))
randtest=rand()
if (randtest<AcceptProb) printon=1
printf("%i   %s %.4f %s %.4f %s %.5f %s %.6f        %i",runpointnum,"oldE",oldenergy,"new total
E",newPotEK,"AcceptProb",AcceptProb,"randomNum",randtest,printon) >> "testlist"
print "" >> "testlist"
#print runpointnum,"oldenergy",oldenergy,"new total energy",newPotEK,"AcceptProb",AcceptProb,"randomNum",randtest,"
",printon >> "testlist"
if (printon==1) {
   printf("%.5f",newPotEK) > "goodenergy"
   print "" >> "goodenergy"
   }
}


function Distance(Atom1,Atom2) {
  return sqrt((oldarr[Atom1,1]-oldarr[Atom2,1])^2+(oldarr[Atom1,2]-oldarr[Atom2,2])^2+(oldarr[Atom1,3]-oldarr[Atom2,3])^2)
}
```

Program proganal

```
BEGIN {
firsttitle=1
getline < "isomernumber"
isomer=$1
# read progdyn.conf for information on the plane potential atoms, if present
blankLineTester=10
while (blankLineTester>1) {
   getline < "progmc.conf"
   if ($1=="applypotentialplane") {
      appotentialplane=$2; appotentialplaneX0=$3; planeradius=$4
      }
   if ($1=="applaneatoms") {
      applaneatomnum=NF-1
      for (i=1;i<=applaneatomnum;i++) {
         if ($(i+1)>0) applaneatoms[i]=$(i+1)
         }
      }
   blankLineTester=length($0)
   }

}
/ NO2/ {
   if (firsttitle==1) {
      printf("%s %s %s %s %s %s %s  ",$1,$2,$3,$4,$6,$7,$8)
      runpoint=$6
      }
   firsttitle++
   }
/Input orientation/,/Stoichiometry/ {
   if (($1>.5) && ($1<99) && ($3=="0")) {
      A[$1]=$4;B[$1]=$5;C[$1]=$6
      i=$1
      oldarr[i,1]=$4; oldarr[i,2]=$5; oldarr[i,3]=$6
      }
   }
#/before annihilation/ {
```

```
#   printf("%s %.5f ",$1,$6)
#   }

END {
  para=Distance(1,16)
  meta=Distance(2,16)
  if (Distance(6,16)<meta) meta=Distance(6,16)
  ortho=Distance(3,16)
  if (Distance(5,16)<ortho) ortho=Distance(5,16)
  ipso=Distance(4,16)
  Opara=Distance(1,17)
  if (Distance(1,18)<Opara) Opara=Distance(1,18)
  Ometa=Distance(2,17)
  if (Distance(2,18)<Ometa) Ometa=Distance(2,18)
  if (Distance(6,17)<Ometa) Ometa=Distance(6,17)
  if (Distance(6,18)<Ometa) Ometa=Distance(6,18)
  Oortho=Distance(3,17)
  if (Distance(3,18)<Oortho) Oortho=Distance(3,18)
  if (Distance(5,17)<Oortho) Oortho=Distance(5,17)
  if (Distance(5,18)<Oortho) Oortho=Distance(5,18)
  Oipso=Distance(4,17)
  if (Distance(4,18)<Oipso) Oipso=Distance(4,18)
  NitF=Distance(16,19)
  if (Distance(16,21)<NitF) NitF=Distance(16,21)
  if (Distance(16,22)<NitF) NitF=Distance(16,22)
  if (Distance(16,23)<NitF) NitF=Distance(16,23)
  NtoPlane=Planedist(16,1,3,5,2,4,6)
  if (appotentialplane>0) NtoPlane=Planedist2()
  BC=Distance(1,20)
  if (Distance(2,20)<BC) BC=Distance(2,20)
  if (Distance(3,20)<BC) BC=Distance(3,20)
  if (Distance(4,20)<BC) BC=Distance(4,20)
  if (Distance(5,20)<BC) BC=Distance(5,20)
  if (Distance(6,20)<BC) BC=Distance(6,20)
  choice=0
  if ((Opara<Ometa) && (Opara<Oortho) && (Opara<NitF)) choice=1
  if ((Ometa<Opara) && (Ometa<Oortho) && (Ometa<NitF)) choice=2
  if ((Oortho<Ometa) && (Oortho<Opara) && (Oortho<NitF)) choice=3
  if (Ometa<2) choice=2
  if (Oortho<2) choice=3
  if (choice==0) printf("%s %.3f %s %.3f %s %.3f %s %.3f %s %.3f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"NtoPlane",NtoPlane,"BC",BC)
  if (choice==1) printf("%s %.3f %s %.3f %s %.3f %s %.3f %s %.3f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"NtoPlane",NtoPlane,"BC",BC)
  if (choice==2) printf("%s %.3f %s %.3f %s %.3f %s %.3f %s %.3f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"NtoPlane",NtoPlane,"BC",BC)
  if (choice==3) printf("%s %.3f %s %.3f %s %.3f %s %.3f %s %.3f %s %.2f
","p",para,"m",meta,"o",ortho,"i",ipso,"NtoPlane",NtoPlane,"BC",BC)
  if (runpoint>500000) {
    print "Too many points.  XXXXN"
#   system("date > nogo")
    }
  if (para<1.6) {
#   print "para product formed XXXX"
#   system("date > nogo")
    }
  if (meta<1.6) {
#   print "meta product formed XXXX"
#   system("date > nogo")
    }
  if (ortho<1.6) {
#   print "ortho product formed XXXX"
```

```
#     system("date > nogo")
      }
   if (ipso<1.6) {
#     print "ipso product formed XXXX"
#     system("date > nogo")
      }
   if (Opara<1.6) {
#     print "Opara product formed XXXX"
      }
   if (Ometa<1.6) {
#     print "Ometa product formed XXXX"
      }
   if (Oortho<1.6) {
#     print "Oortho product formed XXXX"
      }
   if (Oipso<1.6) {
#     print "Oipso product formed XXXX"
      }
#  if (NitF<1.6) {
#     print "NitF product formed XXXX"
#     system("date > nogo")
#     }
   if ((para>5) && (meta>5) && (ortho>5)) {
#     if ((para<5.2) || (para>5.25)) print "Dissociated to SM XXXX"
      }

   system("date '+%b:%d:%Y %T'")
   }

function Distance(Atom1,Atom2) {
  return sqrt((A[Atom1]-A[Atom2])^2 + (B[Atom1]-B[Atom2])^2 + (C[Atom1]-C[Atom2])^2)
}

function Angle(Atom1,Atom2,Atom3) {
   value=((-
Distance(Atom1,Atom3)^2+Distance(Atom1,Atom2)^2+Distance(Atom2,Atom3)^2)/(2*Distance(Atom1,Atom2)*Distance(Ato
m2,Atom3)))
   return acos(value)
}

function Planedist2() {
#first figure out the center of the plane atoms and move all of the atoms to put that center at the origin
   cmass[1]=0;cmass[2]=0;cmass[3]=0
   for (i=2;i<=applaneatomnum;i++) {
      k=applaneatoms[i]
      cmass[1]=cmass[1]+oldarr[k,1];cmass[2]=cmass[2]+oldarr[k,2];cmass[3]=cmass[3]+oldarr[k,3];
      }
   numplaneatoms=applaneatomnum-1
   cmass[1]=cmass[1]/numplaneatoms;cmass[2]=cmass[2]/numplaneatoms;cmass[3]=cmass[3]/numplaneatoms
#  print "center of masse",cmass[1],cmass[2],cmass[3]
   for (i=1;i<=applaneatomnum;i++) {
      k=applaneatoms[i]
#     print k,oldarr[k,1],oldarr[k,2],oldarr[k,3]
      newarr[k,1]=oldarr[k,1]-cmass[1];newarr[k,2]=oldarr[k,2]-cmass[2];newarr[k,3]=oldarr[k,3]-cmass[3];
#     print "             new",k,newarr[k,1],newarr[k,2],newarr[k,3]
      }
#expect that bugs in process arise when plane is nearly vertical.  To avoid this, want to pick the z dimension as the one
#that has the smallest range.  since plane is centered, can use sum of absolute values as surrogate for range
   for (i=2;i<=applaneatomnum;i++) {
      k=applaneatoms[i]
      for (m=1;m<=3;m++) {
         if (newarr[k,m]>0) sum[m]=sum[m]+newarr[k,m];if (newarr[k,m]<0) sum[m]=sum[m]-newarr[k,m]
```

```
      }
    }
  if (sum[1]<sum[3]) {
    for (i=1;i<=applaneatomnum;i++) {
      k=applaneatoms[i]
      tempvar=newarr[k,1];newarr[k,1]=newarr[k,3];newarr[k,3]=tempvar
      }
    tempvar=sum[1];sum[1]=sum[3];sum[3]=tempvar
    }
  if (sum[2]<sum[3]) {
    for (i=1;i<=applaneatomnum;i++) {
      k=applaneatoms[i]
      tempvar=newarr[k,2];newarr[k,2]=newarr[k,3];newarr[k,3]=tempvar
      }
    tempvar=sum[2];sum[2]=sum[3];sum[3]=tempvar
    }
#now lets find the best plane
  A[1,1]=0;A[1,2]=0;A[1,3]=0;A[2,1]=0;A[2,2]=0;A[2,3]=0;A[3,1]=0;A[3,2]=0;A[3,3]=0;b[1]=0;b[2]=0;b[3]=0
  for (i=2;i<=applaneatomnum;i++) {
    k=applaneatoms[i]
    A[1,1]=A[1,1]+newarr[k,1]^2;A[1,2]=A[1,2]+newarr[k,1]*newarr[k,2];A[1,3]=A[1,3]+newarr[k,1]
    A[2,1]=A[2,1]+newarr[k,1]*newarr[k,2];A[2,2]=A[2,2]+newarr[k,2]^2;A[2,3]=A[2,3]+newarr[k,2]
    A[3,1]=A[3,1]+newarr[k,1];A[3,2]=A[3,2]+newarr[k,2]
    b[1]=b[1]+newarr[k,1]*newarr[k,3];b[2]=b[2]+newarr[k,2]*newarr[k,3];b[3]=b[3]+newarr[k,3]
    }
  A[3,3]=numplaneatoms
  Det=A[1,1]*A[2,2]*A[3,3]+A[1,2]*A[2,3]*A[3,1]+A[1,3]*A[2,1]*A[3,2]-A[1,3]*A[2,2]*A[3,1]-A[1,2]*A[2,1]*A[3,3]-
A[1,1]*A[2,3]*A[3,2]
  E=(b[1]*A[2,2]*A[3,3]+A[1,2]*A[2,3]*b[3]+A[1,3]*b[2]*A[3,2]-A[1,3]*A[2,2]*b[3]-A[1,2]*b[2]*A[3,3]-
b[1]*A[2,3]*A[3,2])/Det
  F=(A[1,1]*b[2]*A[3,3]+b[1]*A[2,3]*A[3,1]+A[1,3]*A[2,1]*b[3]-A[1,3]*b[2]*A[3,1]-b[1]*A[2,1]*A[3,3]-
A[1,1]*A[2,3]*b[3])/Det
  G=(A[1,1]*A[2,2]*b[3]+A[1,2]*b[2]*A[3,1]+b[1]*A[2,1]*A[3,2]-b[1]*A[2,2]*A[3,1]-A[1,2]*A[2,1]*b[3]-
A[1,1]*b[2]*A[3,2])/Det
#  E, F, and G are the coefficients in the plane z=Ex+Fy+G - if the zeroing of the plane has worked G = 0
#  print "E, F, and G are the coefficients in the plane z=Ex+Fy+G",E,F,G
  conatom=applaneatoms[1]
  distplane=(-newarr[conatom,1]*E-newarr[conatom,2]*F+newarr[conatom,3]-G)/(E^2+F^2+1)^.5
  if (distplane<0) distplane=-distplane
  t=(newarr[conatom,1]*E+newarr[conatom,2]*F-newarr[conatom,3]+G)/(E^2+F^2+1)
  planepoint[1]=newarr[conatom,1]-t*E;planepoint[2]=newarr[conatom,2]-t*F;planepoint[3]=newarr[conatom,3]+t
  distcmass=((planepoint[1])^2+(planepoint[2])^2+(planepoint[3])^2)^.5
#  print "distplane",distplane,"t",t,"planepoint",planepoint[1],planepoint[2],planepoint[3],"distcmass",distcmass
  if (distcmass>planeradius) {
    planepoint[1]=(planeradius/distcmass)*planepoint[1];
    planepoint[2]=(planeradius/distcmass)*planepoint[2];
    planepoint[3]=(planeradius/distcmass)*planepoint[3];
    distcmass=((planepoint[1])^2+(planepoint[2])^2+(planepoint[3])^2)^.5
    distplane=((planepoint[1]-newarr[conatom,1])^2+(planepoint[2]-newarr[conatom,2])^2+(planepoint[3]-
newarr[conatom,3])^2)^.5
#     print "new distplane",distplane,"newplanepoint",planepoint[1],planepoint[2],planepoint[3],"newdistcmass",distcmass
    }
  return distplane
  }

function Planedist(Atom1,Atom2,Atom3,Atom4,Atom5,Atom6,Atom7) {

afplaneatoms[1]=Atom1;afplaneatoms[2]=Atom2;afplaneatoms[3]=Atom3;afplaneatoms[4]=Atom4;afplaneatoms[5]=Atom5;afp
laneatoms[6]=Atom6;afplaneatoms[7]=Atom7
  for (i=2;i<8;i++) {
    if (afplaneatoms[i]>.5) {
      k=afplaneatoms[i]
```

```
        A[1,1]=A[1,1]+A[k]^2;A[1,2]=A[1,2]+A[k]*B[k];A[1,3]=A[1,3]+A[k]
        A[2,1]=A[2,1]+A[k]*B[k];A[2,2]=A[2,2]+B[k]^2;A[2,3]=A[2,3]+B[k]
        A[3,1]=A[3,1]+A[k];A[3,2]=A[3,2]+B[k];A[3,3]++
        b[1]=b[1]+A[k]*C[k];b[2]=b[2]+B[k]*C[k];b[3]=b[3]+C[k]
# find center of mass assuming all atoms same weight
        cmass[1]=cmass[1]+A[k];cmass[2]=cmass[2]+B[k];cmass[3]=cmass[3]+C[k];
        }
      }
   cmass[1]=cmass[1]/A[3,3];cmass[2]=cmass[2]/A[3,3];cmass[3]=cmass[3]/A[3,3]
#  print "matrix A"
#  for (i=1;i<=3;i++) {
#     print A[i,1],A[i,2],A[i,3]
#     }
#  print "matrix b"
#  print b[1],b[2],b[3]

   Det=A[1,1]*A[2,2]*A[3,3]+A[1,2]*A[2,3]*A[3,1]+A[1,3]*A[2,1]*A[3,2]-A[1,3]*A[2,2]*A[3,1]-A[1,2]*A[2,1]*A[3,3]-
A[1,1]*A[2,3]*A[3,2]
   E=(b[1]*A[2,2]*A[3,3]+A[1,2]*A[2,3]*b[3]+A[1,3]*b[2]*A[3,2]-A[1,3]*A[2,2]*b[3]-A[1,2]*b[2]*A[3,3]-
b[1]*A[2,3]*A[3,2])/Det
   F=(A[1,1]*b[2]*A[3,3]+b[1]*A[2,3]*A[3,1]+A[1,3]*A[2,1]*b[3]-A[1,3]*b[2]*A[3,1]-b[1]*A[2,1]*A[3,3]-
A[1,1]*A[2,3]*b[3])/Det
   G=(A[1,1]*A[2,2]*b[3]+A[1,2]*b[2]*A[3,1]+b[1]*A[2,1]*A[3,2]-b[1]*A[2,2]*A[3,1]-A[1,2]*A[2,1]*b[3]-
A[1,1]*b[2]*A[3,2])/Det
#  E, F, and G are the coefficients in the plane z=Ex+Fy+G"
# make a function that tests the fit
   for (i=2;i<8;i++) {
     if (afplaneatoms[i]>.5) {
       k=afplaneatoms[i]
       distplane=(-A[k]*E-B[k]*F+C[k]-G)/(E^2+F^2+1)^.5;if (distplane<0) distplane=-distplane
       aberror=aberror+distplane
       }
     }
# if the fit is bad, as can happen, decrease to 3 atoms in plane, using only the first three atoms in list after the conatom
   if (aberror>2) {
     print "proganal original aberror",aberror >> "diagnostics"
     A[1,1]=0;A[1,2]=0;A[1,3]=0;A[2,1]=0;A[2,2]=0;A[2,3]=0;A[3,1]=0;A[3,2]=0;A[3,3]=0
     for (i=2;i<5;i++) {
       k=afplaneatoms[i]
       A[1,1]=A[1,1]+A[k]^2;A[1,2]=A[1,2]+A[k]*B[k];A[1,3]=A[1,3]+A[k]
       A[2,1]=A[2,1]+A[k]*B[k];A[2,2]=A[2,2]+B[k]^2;A[2,3]=A[2,3]+B[k]
       A[3,1]=A[3,1]+A[k];A[3,2]=A[3,2]+B[k];A[3,3]++
       b[1]=b[1]+A[k]*C[k];b[2]=b[2]+B[k]*C[k];b[3]=b[3]+C[k]
       }
     Det=A[1,1]*A[2,2]*A[3,3]+A[1,2]*A[2,3]*A[3,1]+A[1,3]*A[2,1]*A[3,2]-A[1,3]*A[2,2]*A[3,1]-A[1,2]*A[2,1]*A[3,3]-
A[1,1]*A[2,3]*A[3,2]
     E=(b[1]*A[2,2]*A[3,3]+A[1,2]*A[2,3]*b[3]+A[1,3]*b[2]*A[3,2]-A[1,3]*A[2,2]*b[3]-A[1,2]*b[2]*A[3,3]-
b[1]*A[2,3]*A[3,2])/Det
     F=(A[1,1]*b[2]*A[3,3]+b[1]*A[2,3]*A[3,1]+A[1,3]*A[2,1]*b[3]-A[1,3]*b[2]*A[3,1]-b[1]*A[2,1]*A[3,3]-
A[1,1]*A[2,3]*b[3])/Det
     G=(A[1,1]*A[2,2]*b[3]+A[1,2]*b[2]*A[3,1]+b[1]*A[2,1]*A[3,2]-b[1]*A[2,2]*A[3,1]-A[1,2]*A[2,1]*b[3]-
A[1,1]*b[2]*A[3,2])/Det
     aberror=0
     for (i=2;i<5;i++) {
       k=afplaneatoms[i]
       distplane=(-A[k]*E-B[k]*F+C[k]-G)/(E^2+F^2+1)^.5;if (distplane<0) distplane=-distplane
       aberror=aberror+distplane
       }
     }
   if (aberror>2) {
#      printf("%s %.2f ","aberror",aberror)
      return 99999999
```

```
    }
  conatom=afplaneatoms[1]
  distplane=(-A[conatom]*E-B[conatom]*F+C[conatom]-G)/(E^2+F^2+1)^.5
  if (distplane<0) distplane=-distplane
  t=(A[conatom]*E+B[conatom]*F-C[conatom]+G)/(E^2+F^2+1)
  planepoint[1]=A[conatom]-t*E;planepoint[2]=B[conatom]-t*F;planepoint[3]=C[conatom]+t
  distcmass=((planepoint[1]-cmass[1])^2+(planepoint[2]-cmass[2])^2+(planepoint[3]-cmass[3])^2)^.5
  if (distcmass>1.4) {
    vector[1]=planepoint[1]-cmass[1];vector[2]=planepoint[2]-cmass[2];vector[3]=planepoint[3]-cmass[3]
    vector[1]=vector[1]*1.4/distcmass;vector[2]=vector[2]*1.4/distcmass;vector[3]=vector[3]*1.4/distcmass
    planepoint[1]=cmass[1]+vector[1];planepoint[2]=cmass[2]+vector[2];planepoint[3]=cmass[3]+vector[3];
    distcmass=((planepoint[1]-cmass[1])^2+(planepoint[2]-cmass[2])^2+(planepoint[3]-cmass[3])^2)^.5
    distplane=((planepoint[1]-A[conatom])^2+(planepoint[2]-B[conatom])^2+(planepoint[3]-C[conatom])^2)^.5
#    print "new distplane",distplane,"newplanepoint",planepoint[1],planepoint[2],planepoint[3],"newdistcmass",distcmass >>
"diagnostics"
    }

  return distplane
  }

function asin(x) { return (180/3.141592)*atan2(x, sqrt(1-x*x)) }

function acos(x) { return (180/3.141592)*atan2(sqrt(1-x*x), x) }

function atan(x) { return (180/3.141592)*atan2(x,1) }

function Dihedral(Atom1,Atom2,Atom3,Atom4) {
  B1x=A[Atom2]-A[Atom1]
  B1y=B[Atom2]-B[Atom1]
  B1z=C[Atom2]-C[Atom1]
  B2x=A[Atom3]-A[Atom2]
  B2y=B[Atom3]-B[Atom2]
  B2z=C[Atom3]-C[Atom2]
  B3x=A[Atom4]-A[Atom3]
  B3y=B[Atom4]-B[Atom3]
  B3z=C[Atom4]-C[Atom3]
  modB2=sqrt((B2x^2)+(B2y^2)+(B2z^2))
# yAx is x-coord. etc of modulus of B2 times B1
  yAx=modB2*(B1x)
  yAy=modB2*(B1y)
  yAz=modB2*(B1z)
# CP2 is the crossproduct of B2 and B3
  CP2x=(B2y*B3z)-(B2z*B3y)
  CP2y=(B2z*B3x)-(B2x*B3z)
  CP2z=(B2x*B3y)-(B2y*B3x)
  termY=((yAx*CP2x)+(yAy*CP2y)+(yAz*CP2z))
# CP is the crossproduct of B1 and B2
  CPx=(B1y*B2z)-(B1z*B2y)
  CPy=(B1z*B2x)-(B1x*B2z)
  CPz=(B1x*B2y)-(B1y*B2x)
  termX=((CPx*CP2x)+(CPy*CP2y)+(CPz*CP2z))
 dihed4=(180/3.141592)*atan2(termY,termX)
 return dihed4
}

function killdyn(isomer) {
  system("rm -f dyn")
}
```

Program progmc.conf

```
#This is the configuration file for PROGMC.  This file is read by progMC and
# the awk programs progmcb and progEcheck
#The programs won't read anything past the first blank line,
#and this file must end with a blank line.
#Do not delete lines - rather, comment out lines for unwanted options.
#The values here are read repeatedly and most can be changed in the middle of running jobs
#***The keywords are case sensitive.  The following keywords should always be defined:***
#***method, charge, multiplicity, memory, processors, title
#*** method --The following word is copied exactly to the gaussian input file.
method ONIOM(M062X/6-311G*:PM3)
#*** method2 --The options here are restricted, unrestricted, and read. restricted is the default
#If the method is U..., put unrestricted here and the .com files will have in them guess=mix.
#If you put read here, the .com files will contain guess=tcheck, which sometimes makes things faster, sometimes not.
#The use of read requires a specifically defined checkpoint file name using the keyword checkpoint.
method2 read
charge 0
multiplicity 1
oniomchargemult 1 1
processors 3
#*** memory --The following "word" is copied exactly to the gaussian input file after %mem=.
memory 7gb
#*** killcheck and checkpoint -- You can use a specifically defined checkpoint file name by putting
#the name after the keyword checkpoint.  This is necessary if you use the read option with method2.
#Defined checkpoint names are an unnecessary modest hastle and if you do not want to bother, use killcheck 0
killcheck 0
checkpoint g09.chk
#*** diagnostics -- 0 prints out nothing extra, 1 (default) prints out extra stuff to a
#file "diagnostics"
diagnostics 0
#*** title -- the title keyword must be followed by exactly four words
title NO2+Tol 101CH2Cl2IonP Oniom MonteCarlo
temperature 298.15
#SPECIFIC MONTE CARLO OPTIONS ****
#*** mcstepsize sets the maximum distance in each dimension that atoms can be moved for each new point and is applied to all
atoms
mcstepsize 0.0010
lengthstep 0.001
anglestep 0.005
#mcmolrotangle sets the maximum angle in degrees for rotation of molecules about X, Y, Z axes through molecule center of
mass
mcmolrotangle 1.00
# molecule specifications - divides system into molecules and allows a separate stepsize for each molecule.  This is in addition to
the step above.
molecule 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 0.02
molecule 16 17 18 0.02
molecule 19 20 21 22 23 0.02
molecule 24 25 26 27 28 0.02
molecule 29 30 31 32 33 0.02
molecule 34 35 36 37 38 0.02
molecule 39 40 41 42 43 0.02
molecule 44 45 46 47 48 0.02
molecule 49 50 51 52 53 0.02
molecule 54 55 56 57 58 0.02
molecule 59 60 61 62 63 0.02
molecule 64 65 66 67 68 0.02
molecule 69 70 71 72 73 0.02
molecule 74 75 76 77 78 0.02
molecule 79 80 81 82 83 0.02
molecule 84 85 86 87 88 0.02
molecule 89 90 91 92 93 0.02
```

molecule 94 95 96 97 98 0.02
molecule 99 100 101 102 103 0.02
molecule 104 105 106 107 108 0.02
molecule 109 110 111 112 113 0.02
molecule 114 115 116 117 118 0.02
molecule 119 120 121 122 123 0.02
molecule 124 125 126 127 128 0.02
molecule 129 130 131 132 133 0.02
molecule 134 135 136 137 138 0.02
molecule 139 140 141 142 143 0.02
molecule 144 145 146 147 148 0.02
molecule 149 150 151 152 153 0.02
molecule 154 155 156 157 158 0.02
molecule 159 160 161 162 163 0.02
molecule 164 165 166 167 168 0.02
molecule 169 170 171 172 173 0.02
molecule 174 175 176 177 178 0.02
molecule 179 180 181 182 183 0.02
molecule 184 185 186 187 188 0.02
molecule 189 190 191 192 193 0.02
molecule 194 195 196 197 198 0.02
molecule 199 200 201 202 203 0.02
molecule 204 205 206 207 208 0.02
molecule 209 210 211 212 213 0.02
molecule 214 215 216 217 218 0.02
molecule 219 220 221 222 223 0.02
molecule 224 225 226 227 228 0.02
molecule 229 230 231 232 233 0.02
molecule 234 235 236 237 238 0.02
molecule 239 240 241 242 243 0.02
molecule 244 245 246 247 248 0.02
molecule 249 250 251 252 253 0.02
molecule 254 255 256 257 258 0.02
molecule 259 260 261 262 263 0.02
molecule 264 265 266 267 268 0.02
molecule 269 270 271 272 273 0.02
molecule 274 275 276 277 278 0.02
molecule 279 280 281 282 283 0.02
molecule 284 285 286 287 288 0.02
molecule 289 290 291 292 293 0.02
molecule 294 295 296 297 298 0.02
molecule 299 300 301 302 303 0.02
molecule 304 305 306 307 308 0.02
molecule 309 310 311 312 313 0.02
molecule 314 315 316 317 318 0.02
molecule 319 320 321 322 323 0.02
molecule 324 325 326 327 328 0.02
molecule 329 330 331 332 333 0.02
molecule 334 335 336 337 338 0.02
molecule 339 340 341 342 343 0.02
molecule 344 345 346 347 348 0.02
molecule 349 350 351 352 353 0.02
molecule 354 355 356 357 358 0.02
molecule 359 360 361 362 363 0.02
molecule 364 365 366 367 368 0.02
molecule 369 370 371 372 373 0.02
molecule 374 375 376 377 378 0.02
molecule 379 380 381 382 383 0.02
molecule 384 385 386 387 388 0.02
molecule 389 390 391 392 393 0.02
molecule 394 395 396 397 398 0.02
molecule 399 400 401 402 403 0.02

```
molecule 404 405 406 407 408 0.02
molecule 409 410 411 412 413 0.02
molecule 414 415 416 417 418 0.02
molecule 419 420 421 422 423 0.02
molecule 424 425 426 427 428 0.02
molecule 429 430 431 432 433 0.02
molecule 434 435 436 437 438 0.02
molecule 439 440 441 442 443 0.02
molecule 444 445 446 447 448 0.02
molecule 449 450 451 452 453 0.02
molecule 454 455 456 457 458 0.02
molecule 459 460 461 462 463 0.02
molecule 464 465 466 467 468 0.02
molecule 469 470 471 472 473 0.02
molecule 474 475 476 477 478 0.02
molecule 479 480 481 482 483 0.02
molecule 484 485 486 487 488 0.02
molecule 489 490 491 492 493 0.02
molecule 494 495 496 497 498 0.02
molecule 499 500 501 502 503 0.02
molecule 504 505 506 507 508 0.02
molecule 509 510 511 512 513 0.02
molecule 514 515 516 517 518 0.02
molecule 519 520 521 522 523 0.02
molecule 524 525 526 527 528 0.02
#*** method3, method4, method5, and method6 -- These keywords let you add extra lines to the gaussian input file.
#method3 and method4 add lines at the top of the input after the lines defining the method, and
#this is useful to implement things like the iop for mPW1k
#method5 and method6 add lines after the geometry, after a blank line of course
#only a single term with no spaces can be added, one per method line.  Here are some examples to uncomment if needed
#method3 IOp(3/76=0572004280)
method3 scf=(conver=5)
#method3 scrf=(pcm,Solvent=dichloromethane)
#add the line below with big structures to get it to put out the distance matrix and the input orientation
method4 iop(2/9=2000)
#method4 iop(3/124=3)
#method4 scrf=(pcm,solvent=dmso,read)
#method5 radii=bondi
#method6
#*** methodfile -- This keyword lets you add more complicated endings to gaussian input files
#such as a gen basis set.  Put after the keyword the number of lines in a file you create called
#methodfile that contains the test you want to add to the end of the gaussian input
methodfile 0
#*** highlevel --For ONIOM jobs, the following line states the number of highlevel atoms,
#which must come before the medium level atoms.  Use some high value such as 999 if not using ONIOM
highlevel 18
#applypotential adds energy to bias the MC.  Format is applypotential forceConstant(E=.5k(x-x0)^2) x0
#the force constant is in kcal/mol/ang^2
#apatoms choses the atoms with format apatoms firstatom secondatom [additional atoms]
applypotential 118.56 2.35
apatoms 16 1 2 3 4 5 6
#applypotentialplane sets a energy addition to constrain an atom to a distance from a plane defined by other atoms.
#if the number of atoms defining the plane is >3, the plane is a
#least squares best fit  keyword applaneatoms is followed first by the atom being set and then by the series of atoms, up to 6, that
define the plane
#first number is forceConstant  kcal/mol/ang^2, second is distance in angstroms
#applypotentialplane 100 2.1
#applaneatoms 16 1 3 5 2 4 6
#zeroatom pushes the numbered atom toward the origin with a harmonic potential set by second number in  kcal/mol/ang^2
zeroatom 16 1
#*** boxon and boxsize - With boxon 1, a cubic box is set such that atoms that reach the edge
#are reflected back toward the middle.  Useful for dynamics with solvent molecules.  This is a crude
```

```
#implementation that is ok for a few thousand femtoseconds but will not conserve energy long term.
#Set the box size so as to fit the entire initial molecule but not have too much extra room.
#The dimensions of the box are two times the boxsize, e.g. boxsize 7.5 leads to a box that is 15 x 15 x 15 angstroms
#boxon 1
#boxsize 11.2
#*** sphereon and spheresize and sphereforce - uses a force to push atoms within a sphere.  notice that if the atom is far outside
of
#the sphere then the force is large unless sphereforce is set small
sphereon 1
spheresize 12.9
sphereforce 11.85


#created Dec 21, 2015
```

Program whamnitmc

```
cd ~
rm -f ~/regiocount
rm -f n1??/seriesfile*
awk -v pt=3000 -f ~/progseriesmc n16?/mcfollowfile > n160/seriesfile
awk -v pt=3000 -f ~/progseriesmc n154/mcfollowfile n155/mcfollowfile n156/mcfollowfile n157/mcfollowfile
n158/mcfollowfile n159/mcfollowfile > n154/seriesfile
awk -v pt=4000 -f ~/progseriesmc n112/mcfollowfile n142/mcfollowfile n143/mcfollowfile n144/mcfollowfile
n145/mcfollowfile> n112/seriesfile
awk -f ~/progseriesmc n106/mcfollowfile n107/mcfollowfile n108/mcfollowfile n109/mcfollowfile n110/mcfollowfile
n111/mcfollowfile > n106/seriesfile
awk -f ~/progseriesmc n100/mcfollowfile n101/mcfollowfile n102/mcfollowfile n103/mcfollowfile n104/mcfollowfile
n105/mcfollowfile > n100/seriesfile
awk -f ~/progseriesmc n113/mcfollowfile n114/mcfollowfile > n113/seriesfile
awk -f ~/progseriesmc n115//mcfollowfile n146/mcfollowfile > n115/seriesfile
awk -f ~/progseriesmc n116/mcfollowfile n117/mcfollowfile n118/mcfollowfile > n116/seriesfile
awk -f ~/progseriesmc n119/mcfollowfile n120/mcfollowfile > n119/seriesfile
awk -f ~/progseriesmc n121/mcfollowfile n122/mcfollowfile > n121/seriesfile
awk -f ~/progseriesmc n123/mcfollowfile n124/mcfollowfile > n123/seriesfile
awk -f ~/progseriesmc n125/mcfollowfile n126/mcfollowfile > n125/seriesfile
awk -f ~/progseriesmc n127/mcfollowfile n128/mcfollowfile > n127/seriesfile
awk -f ~/progseriesmc n129/mcfollowfile n147/mcfollowfile > n129/seriesfile
cd ~/wham/wham
./wham 1.475 5.675 84 0.000001 298.15 0 metadatafile.nitrationmc ~/output.nitrationfull 6 23
cd
cat output.nitrationfull
cat ~/regiocount
cat ~/wham/wham/metadatafile.nitrationmc
```

Program progseriesmc

```
BEGIN {
if (pt<1) startfile=100
if (pt>1) startfile=pt
countpara=0;countmeta=0;countortho=0;countipso=0;counttotal=0
oldfilename=""
switches=-1
current="";oldclosest=""
currentop=""
oldop=""
opswitches=-1
}
/NO2/ {
if (oldfilename!=FILENAME) {
```

```
   if (counttotal>0) {
      pp=int(.5+100*countpara/counttotal)
      pm=int(.5+100*countmeta/counttotal)
      po=int(.5+100*countortho/counttotal)
      pi=int(.5+100*countipso/counttotal)
      print oldfilename,"     ",countpara,countmeta,countortho,countipso,"    ",counttotal,"     ",pp,pm,po,pi,"
switches",switches,"   opswitches",opswitches >> "regiocount"
      }
   if (counttotal==0) print "" >> "regiocount"
   countpara=0;countmeta=0;countortho=0;countipso=0;counttotal=0;switches=-1;current="";oldclosest="";opswitches=-
1;oldop=""
   fileline=0
   }
oldfilename=FILENAME
fileline++
if (fileline>startfile) {
   counttotal++
   if (($7<$9) && ($7<$11) && ($7<$13)) {
      countpara++
      current="para"
      currentop="para"
      }
   if (($9<$7) && ($9<$11) && ($9<$13)) {
      countmeta++
      current="meta"
      }
   if (($11<$7) && ($11<$9) && ($11<$13)) {
      countortho++
      current="ortho"
      currentop="ortho"
      }
   if (($13<$7) && ($13<$9) && ($13<$11)) {
      countipso++
      current="ipso"
      }
   if (current!=oldclosest) switches++
   if (currentop!=oldop) opswitches++
   oldclosest=current; oldop=currentop
   dist=$7
   if ($9<dist) dist=$9
   if ($11<dist) dist=$11
   if ($13<dist) dist=$13
   printf("%.1f %.3f",$5,dist)
   print ""
   }
}
END {
if (counttotal>0) {
   pp=int(.5+100*countpara/counttotal)
   pm=int(.5+100*countmeta/counttotal)
   po=int(.5+100*countortho/counttotal)
   pi=int(.5+100*countipso/counttotal)
   }
print oldfilename,"     ",countpara,countmeta,countortho,countipso,"    ",counttotal,"     ",pp,pm,po,pi,"      switches",switches,"
opswitches",opswitches >> "regiocount"
}
```

Computational Methods Evaluation Studies

For our purposes here, we sought to identify a DFT method that would be practical for trajectories reasonably accurate on the relative and absolute energies for the complexes of NO_2^+ with toluene, and closely accurate in the area of the energy surface where the selectivity is determined. A problem is that DFT methods tend to overestimate the proton affinity of benzene and to a larger extent overestimate the affinity of aromatics for NO_2^+. This overestimation is unlikely to matter to the study of selectivity in the reaction since the energy surface is closely accurate in the critical portion where the selectivity is set, but we sought to minimize the errors.

Benzene proton affinity

Table S4 shows potential energies for benzene versus benzenium ions for various methods and basis sets. All of the energies are based on optimized structures with the exception of the CCSD(T) energies, which use M06-2X/6-311G* structures in single-point calculations. Considering the G3B3, G4, and CCSD(T) results as standards, it can be seen that most methods with the exception of M06-2X and M11 overestimate the proton affinity.

Table S4. Potential energies for benzene versus benzenium ion for various methods / bases sets.

	G3B3	G4	CCSD(T) aug-cc-pvtz	CCSD(T) cc-pvqz	B3LYP 6-31G*	
C6H7+	-232.446453	-232.485091	-232.114897	-232.165936	-232.555624	
C6H6	-232.153910	-232.192698	-231.820193	-231.871714	-232.248659	
Ediff (kcal/mol)	183.6	183.5	184.9	184.6	193.0	

	BP86 6-31G*	BPW91 6-31G*	PBE0 6-31G*	M06L 6-31G*	M11 6-31G*	wB97XD 6-31G*	M062X 6-31G*
C6H7+	-232.545356	-232.522170	-232.268032	-232.515650	-232.382321	-232.471561	-232.431806
C6H6	-232.238232	-232.213239	-231.964089	-232.208701	-232.086900	-232.164329	-232.136450
Ediff (kcal/mol)	192.7	193.9	190.7	192.6	185.4	192.8	185.3

	BP86 6-311G*	BPW91 6-311G*	PBE0 6-311G*	M06L 6-311G*	M11 6-311G*	wB97XD 6-311G*	M062X 6-311G*
C6H7+	-232.588069	-232.563072	-232.305809	-232.556019	-232.425979	-232.510480	-232.478495
C6H6	-232.287205	-232.259976	-232.006696	-232.254016	-232.136073	-232.208675	-232.187864
Ediff (kcal/mol)	188.8	190.2	187.7	189.5	181.9	189.4	182.4

	BP86 6-311+G**	BPW91 6-311+G**	PBE0 6-311+G**	M06L 6-311+G**	M11 6-311+G**	wB97XD 6-311+G**	M062X 6-311+G**
C6H7+	-232.599849	-232.575118	-232.318087	-232.571711	-232.436198	-232.521959	-232.488282
C6H6	-232.299970	-232.272828	-232.019721	-232.269721	-232.146204	-232.220834	-232.198336
Ediff (kcal/mol)	188.2	189.7	187.2	189.5	182.0	189.0	181.9

	revTPSS 6-311+G**	VSXC 6-311+G**	B97D 6-311+G**	B3P86 6-311+G**	APFD 6-311+G**	B98 6-311+G**	LC-wPBE 6-311+G**
C6H7+	-232.590042	-232.716083	-232.435907	-233.361656	-232.403993	-232.510985	-232.423149
C6H6	-232.286856	-232.411864	-232.128749	-233.062288	-232.103840	-232.209049	-232.125794
Ediff (kcal/mol)	190.3	190.9	192.7	187.9	188.3	189.5	186.6

	BP86	BPW91	PBE0	M06L	M11	wB97XD	M062X
	6-311++G(2df,2p)	6-311++G(2df,2p)	6-311++G(2df,2p)	6-311++G(2df,2p)	6-311++G(2df,2p)	6-311++G(2df,2p)	6-311++G(2df,2p)
C6H7+	-232.61386	-232.58895	-232.33251	-232.58540	-232.45793	-232.53685	-232.50405
C6H6	-232.31418	-232.28679	-232.03418	-232.28290	-232.16717	-232.23542	-232.21451
Ediff (kcal/mol)	188.1	189.6	187.2	189.8	182.5	189.1	181.7

The experimental proton affinity of benzene is 178.0 ± 2.2 kcal/mol (Chong, S. –L.; Franklin, J. L. *J. Am. Chem. Soc.* **1972**, *94*, 6630.) The expected difference between the potential energy and the enthalpy is about 6.4 kcal/mol. This places the computational standards with the experimental error of the experimental value.

Toluene + NO_2^+

Table S5 shows potential energies for toluene, NO_2^+, and adducts of the two in the para, meta, ortho, and ipso positions. In some computational methods such as B3LYP, additional minima are locatable for adducts in the meta and ipso positions in which the C-N distance is 1.9 – 2.2 Å – these minima are usually absent in qualitatively better calculations and they were ignored overall. Only the M06-2X and M11 results are shown here; exploratory studies using other DFT methods suggests the same trend that was seen in the proton affinities of too high of binding energy. The M06-2X/6-311G* results are themselves still too high in binding energy but the relative energies of of the complexes are very close to those seen in the G3B3 and CCSD(T) results.

Table S5. Potential energies for toluene + NO_2^+ .

	G3B3	E vs NO_2^+ + toluene	relative E	CCSD(T) 6-31+G**	E vs NO_2^+ + toluene	relative E
toluene	-271.457270			-270.797567		
NO2+	-204.644943			-204.242147		
para	-476.156827	-34.3	0.0	-475.101758	-38.9	0.0
meta	-476.148239	-28.9	5.4	-475.093278	-33.6	5.3
ortho	-476.153003	-31.9	2.4	-475.097989	-36.6	2.4
ipso	-476.148914	-29.3	5.0	-475.095107	-34.8	4.2
					MAD	***0.2***

	M06-2X 6-31+G**	E vs NO_2^+ + toluene	relative E	M06-2X 6-311G*	E vs NO_2^+ + toluene	relative E
toluene	-271.451006			-271.492905		
NO2+	-204.627399			-204.684513		
para	-476.154788	-47.9	0.0	-476.248544	-44.6	0.0
meta	-476.145124	-41.9	6.1	-476.239089	-38.7	5.9
ortho	-476.150080	-45.0	3.0	-476.245375	-42.6	2.0
ipso	-476.145421	-42.1	5.9	-476.240076	-39.3	5.3
		MAD	***0.5***		MAD	***0.3***

	M06-2X 6-311+G**	E vs NO_2^+ + toluene	relative E	M06-2X 6-311G**	E vs NO_2^+ + toluene	relative E
toluene	-271.504880			-271.502483		
NO2+	-204.685003			-204.682183		
para	-476.263290	-46.1	0.0	-476.256565	-45.1	0.0
meta	-476.253410	-39.9	6.2	-476.246814	-39.0	6.1
ortho	-476.259368	-43.6	2.5	-476.252838	-42.8	2.3
ipso	-476.253979	-40.2	5.8	-476.247714	-39.6	5.6
		MAD	***0.4***		MAD	***0.3***

	M06-2X 6-31G*	E vs NO_2^+ + toluene	relative E	M11/6-311G*	E vs NO_2^+ + toluene	relative E
toluene	-271.433102			-271.432396		
NO2+	-204.622943			-204.697027		
para	-476.133152	-48.4	0.0	-476.198950	-43.6	0.0
meta	-476.123756	-42.5	5.9	-476.189197	-37.5	6.1
ortho	-476.129481	-46.1	2.3	-476.195673	-41.6	2.1
ipso	-476.124093	-42.7	5.7	-476.190691	-38.4	5.2

	B3LYP/6-31G*	E vs NO_2^+ + toluene	relative E	B3LYP/6-311+G**		relative E
toluene	-271.5666482			-2.71E+02		
NO2+	-204.7118274			-2.04E+02		
para	-476.354632	-47.8	0.0	-4.75E+02	-33.6	0.0
meta	-476.3460622	-42.4	5.4	-4.75E+02	-28.3	5.3
ortho	-476.3506832	-45.3	2.5	-4.75E+02	-31.4	2.3
ipso	-476.3427837	-40.4	7.4	-4.75E+02	-29.5	4.1
		MAD	***0.6***			***0.3***

MP2/6-311G*	Pot E			B3LYP/6-311++G(2d,2p) GD3		
toluene	-2.71E+02			-271.6579217		
NO2+	-2.04E+02			-204.7832824		
para	-4.75E+02	-19.1	0.0	-476.5140227	#VALUE!	0.0
meta	-	-	-	-476.5048891	-299011.1	5.7
ortho	-4.75E+02	-17.5	1.6	-476.5089966	-299013.7	3.2
ipso	-	-	-	-476.5030528	-299010.0	6.9

The Energy Surface as NO_2^+ Approaches Toluene

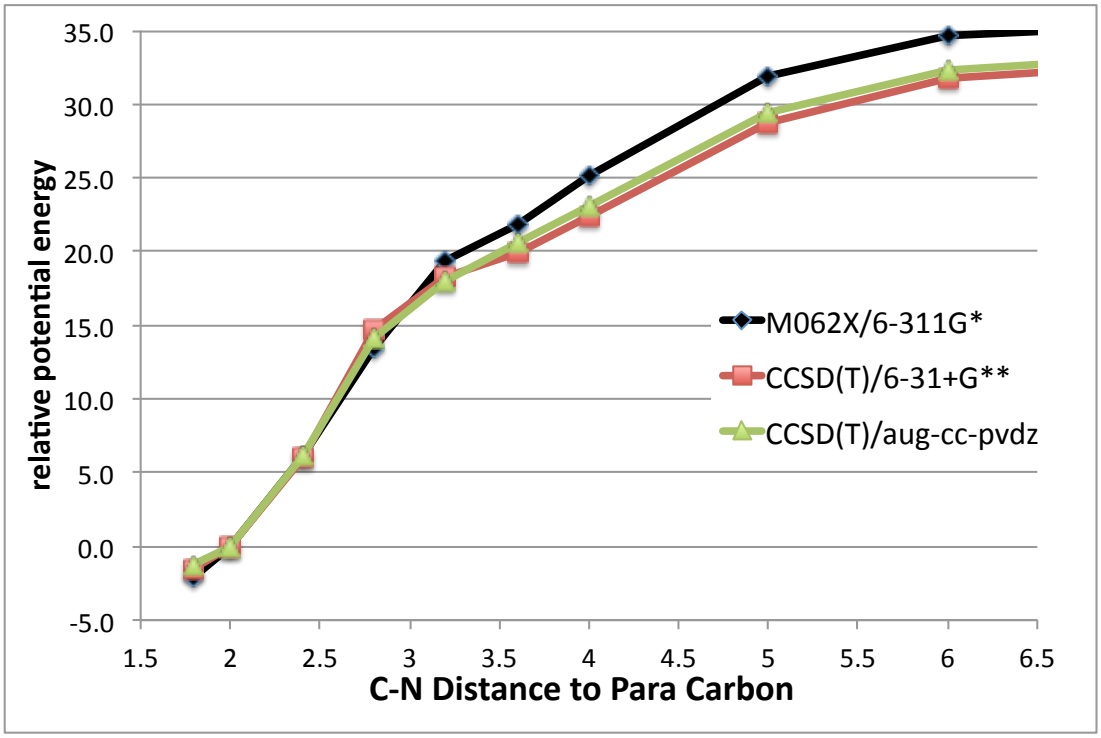
The table below shows potential energies for along a series of geometries as the NO_2^+ approaches the para position of toluene. For these geometries, the C-N distance was fixed at the value shown in the table, the angle to the meta carbon (N-para C-meta C) was set at 90°, and the dihedral angle to the ortho carbon (N-para C-meta C-ortho C) was set at 90°. For the 1.8 Å C-N distance, the angle to the meta carbon was not fixed since the distortion of the ring makes this constraint unnatural versus the normal attack angle.

The graph below the table shows a plot of the M06-2X potential energies versus

CCSD(T) single-point energies. The key result is that the relative energies track very closely in the key region where the C-N distance is between 2.0 and 3.2 Å. (It should be noted that the energy comparison Table S6 and the graph below has set the zero of energy at a C-N distance of 2.0 Å. This arbitrary choice is ok because it is the slope of the energy versus distance, not the absolute energy, that is important in deciding the shape of the energy surface in this area.) From this, we concluded that the M06-2X/6-311G* energies would be adequate for the study.

Table S6. Potential energies as NO_2^+ Approaches Toluene, M06-2X/6-311G* vs CCSD(T)

C-N dist.	M062X/6-311G*	rel E	CCSD(T)/6-31+G**	rel E	CCSD(T)/aug-cc-pvdz	rel E
1.8 Å	-476.241300	-2.1	-475.094510	-1.5	-475.186643	-1.0
2 Å	-476.237969	0.0	-475.092113	0.0	-475.185021	0.0
2.4 Å	-476.228126	6.2	-475.082409	6.1	-475.175199	6.2
2.8 Å	-476.216525	13.5	-475.068768	14.6	-475.162416	14.2
3.2 Å	-476.207179	19.3	-475.062964	18.3	-475.156380	18.0
3.6 Å	-476.203234	21.8	-475.060262	20.0	-475.152208	20.6
4 Å	-476.197929	25.1	-475.056327	22.5	-475.148288	23.1
5 Å	-476.187026	32.0	-475.046326	28.7	-475.138043	29.5
6 Å	-476.182830	34.6	-475.041421	31.8	-475.133430	32.4
NO2+	-204.684513		-204.237150		-204.302711	
toluene	-271.492905	38.0	-270.797002	36.4	-270.823600	36.8



The NO_2^+ - BF_4 Interaction

Exploratory computational studies on $NO_2^+BF_4^-$ encountered decomposition to afford

$NO_2F + BF_3$. Since this is counter to the experimental observation that $NO_2^+BF_4^-$ is obtained from $NO_2F + BF_3$, this reaction was examined carefully.

A series of structures along an approximate $NO_2^+BF_4^-$ to NO_2F / BF_3 gas phase pathway were obtained by optimizing each (as complexes) and optimizing structures with a B-F interatomic distance constrained at 1.5, 1.6, 1.7, 1.8, 1.9, 2.0, 2.2, 2.4, and 2.6 Å, in M062X/6-31+G** calculations. The structures obtained are listed below. The following Table S6 shows the calculated energies of these structures at a series of computational levels.

It may be noted from Table S6 that M06-2X calculations generally underestimate the stability of $NO_2^+BF_4^-$ versus NO_2F / BF_3, relative to CCSD(T) calculations. The highest level CCSD(T) calculations place the barrier for decomposition of $NO_2^+BF_4^-$ in the gas phase at 3.3 kcal/mol, compared to only 0.2 kcal/mol in M06-2X/6-311G*. Larger basis sets come closer with M06-2X, but they underestimate the barrier and place the NO_2F / BF_3 at 3 kcal/mol too stable versus the CCSD(T) results. PM3 calculations in contrast greatly overestimate the stability of the $NO_2^+BF_4^-$.

In solution, the ionic structure is stabilized. CCSD(T)/jun-cc-pvtz calculations including a PCM estimate place the $NO_2^+BF_4^-$ as more stable than the NO_2F / BF_3 by 14 kcal/mol, as fits with the experimental observation. On this basis it was judged that the overstabilization of $NO_2^+BF_4^-$ by the PM3 calculations was acceptable. It should be noted that we have made this comparison with PM3 instead of the ONIOM(M06-2X/6-311G*:PM3) used for the actual modeling because the ONIOM calculation fails as the atom transfer occurs. The PM3 part of the ONIOM calculation is the part that dominates the $NO_2^+BF_4^-$ interaction since it is part that contains both ions. See below for a direct measurement of the ONIOM energies outside of the context of the F transfer.

$NO_2^+BF_4^-$ optimized
N,0,-0.022319944,-0.0029035981,0.6020011006
O,0,0.8959765174,0.6378858721,0.5940170116
O,0,-1.0408605484,-0.4640447783,0.5224527331
F,0,0.5700340065,-1.1977733821,2.3900375434
B,0,1.5944950494,-1.9175546725,1.6551417477
F,0,1.0645114001,-1.9305547694,0.3039510007
F,0,1.7577203971,-3.1750387776,2.13569363
F,0,2.732149122,-1.1325228942,1.6491662329

B---F 1.5
N,0,-0.017444,-0.01891,0.636823
O,0,0.890343,0.638022,0.60259
O,0,-1.030554,-0.489376,0.531911
F,0,0.584343,-1.179712,2.345214
B,0,1.640719,-1.944471,1.604126
F,0,1.114298,-1.954237,0.267388
F,0,1.762859,-3.188862,2.119797
F,0,2.776162,-1.167321,1.62604

B---F 1.6
N,0,-0.0051631862,-0.0920951565,0.8159755109
O,0,0.8091398438,0.6831751727,0.6177411295
O,0,-1.0427317163,-0.516653794,0.5981578317
F,0,0.6148274245,-1.0947475218,2.1160202206
B,0,1.7559979801,-2.0164048625,1.4770549797
F,0,1.3117874952,-2.0694552011,0.1664084691
F,0,1.6715159015,-3.1676866073,2.1673553267
F,0,2.8835672573,-1.2804990295,1.6325405319

B---F 2.0
N,0,0.061651,-0.206496,0.909102
O,0,0.822225,0.610563,0.57027
O,0,-1.028229,-0.549447,0.675384
F,0,0.668367,-1.082456,1.983521
B,0,2.093159,-2.284777,1.259371
F,0,1.580426,-2.245116,0.026896
F,0,1.801043,-3.302036,2.049766
F,0,3.113167,-1.4926,1.546398

B---F 2.2
N,0,0.08738,-0.245572,0.908685
O,0,0.865704,0.53582,0.514434
O,0,-1.024824,-0.542556,0.694299
F,0,0.668208,-1.087182,1.975806
B,0,2.241359,-2.404697,1.182488
F,0,1.689249,-2.311617,-0.02134
F,0,1.91113,-3.400761,1.977986
F,0,3.230039,-1.594801,1.503076

B---F 2.4
N,0,0.1191221211,-0.2813409529,0.9030886757
O,0,0.8997504999,0.4937531268,0.49397702
O,0,-0.9882456338,-0.5880304693,0.6654499697
F,0,0.6720261052,-1.0712198189,2.0009059884
B,0,2.3694818934,-2.5152969054,1.1102394798
F,0,1.7517688,-2.3489242473,-0.0497008719
F,0,2.0320536432,-3.5162956538,1.8933153544
F,0,3.368719571,-1.7230100793,1.4328853839

B---F 1.7 N,0,0.0120379944,-0.1303437117,0.8551360326 O,0,0.7978244436,0.6715642226,0.6050831369 O,0,-1.0405457893,-0.5339990736,0.6259678996 F,0,0.6366218478,-1.0788826779,2.0625820976 B,0,1.8455862705,-2.0825002843,1.4136181325 F,0,1.3971885629,-2.1153036438,0.12334003 F,0,1.6802099981,-3.1919148854,2.142284238 F,0,2.9482326721,-1.3424859457,1.6206054328	B---F 2.6 N,0,0.123677,-0.346353,0.855384 O,0,0.777015,0.54421,0.454345 O,0,-0.888309,-0.861403,0.554706 F,0,0.719678,-0.968173,2.024171 B,0,2.508952,-2.600422,1.078514 F,0,1.839943,-2.321167,-0.028958 F,0,2.157547,-3.633982,1.810118 F,0,3.54261,-1.862075,1.416609
B---F 1.8 N,0,0.02454,-0.163116,0.878316 O,0,0.772261,0.663628,0.568513 O,0,-1.036309,-0.572667,0.665475 F,0,0.68131,-1.044964,2.030338 B,0,1.933703,-2.149608,1.35857 F,0,1.477161,-2.131897,0.085025 F,0,1.675263,-3.224053,2.100573 F,0,3.027448,-1.43069,1.61917	NO_2F / BF_3 optimized N,0,0.1472631518,-0.3686395546,0.8592591372 O,0,0.7710290149,0.5394206139,0.4535398093 O,0,-0.8694484471,-0.8925379889,0.5960145524 F,0,0.8085900878,-1.0131920582,1.9886974492 B,0,2.4732315258,-2.5703641874,1.0789656983 F,0,1.8677680127,-2.3223345198,-0.0724994903 F,0,2.0837769337,-3.5877475263,1.8148803041 F,0,3.4989027204,-1.8339697788,1.4460315397
B---F 1.9 N,0,0.050719,-0.186403,0.896569 O,0,0.826207,0.623231,0.589223 O,0,-1.031482,-0.532953,0.652855 F,0,0.645878,-1.091422,1.998952 B,0,2.011546,-2.217028,1.307605 F,0,1.515919,-2.219268,0.059813 F,0,1.769088,-3.254951,2.094826 F,0,3.045718,-1.424071,1.563501	

Table S6. Relative energies for structures in the decomposition of $NO_2^+ BF_4^-$

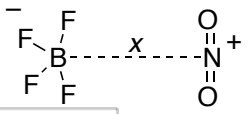
	CCSD(T)		CCSD(T)		CCSD(T)	
	aug-cc-pvdz	Erel	cc-pvtz	Erel	jun-cc-pvtz	Erel
$NO_2^+ BF_4^-$	-628.21720	0.0	-628.69569	0.0	-628.72372	0.0
1.5	-628.21690	0.2	-628.69481	0.6	-628.72280	0.6
1.6	-628.21179	3.4	-628.69241	2.1	-628.71845	3.3
1.7	-628.21148	3.6	-628.69300	1.7	-628.71851	3.3
1.8	-628.21182	3.4	-628.69415	1.0	-628.71939	2.7
1.9	-628.21266	2.9	-628.69558	0.1	-628.72076	1.9
2	-628.21371	2.2	-628.69724	-1.0	-628.72241	0.8
2.2	-628.21571	0.9	-628.69999	-2.7	-628.72525	-1.0
2.4	-628.21656	0.4	-628.70140	-3.6	-628.72673	-1.9
2.6	-628.21634	0.5	-628.70165	-3.7	-628.72705	-2.1
NO_2F BF_3	-628.21666	0.3	-628.70164	-3.7	-628.72698	-2.1
	M06-2X		M06-2X		M06-2X	
	6-31+G**	Erel	6-311G*	Erel	aug-cc-pvtz	Erel
$NO_2^+ BF_4^-$	-629.23780	0.0	-629.3995962	0.0	-629.4981163	0.0
1.5	-629.23723	0.4	-629.3993008	0.2	-629.4972818	0.5
1.6	-629.23710	0.4	-629.39987	-0.2	-629.4951584	1.9
1.7	-629.23834	-0.3	-629.4012319	-1.0	-629.4956709	1.5
1.8	-629.23990	-1.3	-629.4030977	-2.2	-629.4969063	0.8
1.9	-629.24194	-2.6	-629.4053221	-3.6	-629.4987515	-0.4

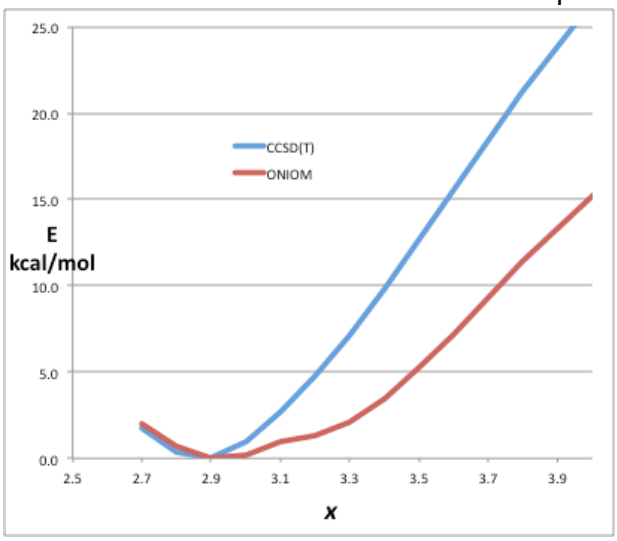
2	-629.24426	-4.1	-629.4077262	-5.1	-629.5009719	-1.8
2.2	-629.24786	-6.3	-629.4110628	-7.2	-629.5045536	-4.0
2.4	-629.24923	-7.2	-629.4120594	-7.8	-629.5061669	-5.1
2.6	-629.24909	-7.1	-629.4115213	-7.5	-629.5061913	-5.1
NO_2F BF_3	-629.24930	-7.2	-629.4120478	-7.8	-629.5062855	-5.1

	M06-2X/PCM 6-31+G**	Erel	PM3	Erel
NO2+ BF4-	-629.427384	0.0	-0.469309867	0.0
1.5	-629.4255249	1.2	-0.467750082	1.0
1.6	-629.4133525	8.8	-0.464537377	3.0
1.7	-629.4103337	10.7	-0.456245746	8.2
1.8	-629.4094253	11.3	-0.451351991	11.3
1.9	-629.4099826	10.9	-0.449115832	12.7
2	-629.4114811	10.0	-0.448821348	12.9
2.2	-629.4141471	8.3	-0.449866933	12.2
2.4	-629.4148851	7.8	-0.450117622	12.0
2.6	-629.4141815	8.3	-0.448763219	12.9
NO2F BF3	-629.4147793	7.9	-0.449721036	12.3

A second issue with regard to the $NO_2^+BF_4^-$ is the general energetic attraction of the two ions. To explore this issue, we obtained a series of structures optimized in the ONIOM calculations in which the B and N atoms were set at fixed distances *x* with *x* being 2.7, 2.8, 2.9, 3.0, 3.1, 3.2, 3.3, 3.4, 3.5, 3.6, 3.8, 4.0, 4.5, 5, 6, 8, 10, 12, 15, and 20 Å, then calculated CCSD(T)/jun-cc-pvtz single point energies for these structures. This process was complicated by the observation that the NO_2^+ may approach the BF_4^- in two ways, one that is symmetrical with respect to a pair of BF bonds and one in which the N approaches a single F; in each case we chose the lowest energy of the two possibilities. The absolute and relative energies obtained are shown in Table S7. The graphs below shows plots of the energies in the relavent area of the energy surface (left) and the overall surface out to 20 Å (right). Energies at shorter distances could not be obtained from the ONIOM calculation. The CCSD(T) calculation failed for the 3.0 Å structure for unknown reasons.

The ONIOM calculations underestimate the gas-phase attraction of the ions by 17 kcal/mole. The curves at long distances are identical because the energy is dominated by simple electrostatic interaction. At short diestances, however, there there is a degree of electron transfer between the ions that is underestimated in the underlying PM3 calculations of the ONIOM. The effect of the error in the ONIOM calculations is that the BF_4^- ion will tend to adopt a longer distance from the NO_2^+ than it would in reality. In this way, the BF_4^- should act like a larger anion. Experimentally, the choice of counterion has very little effect on the selectivity experimentally (see Table 8 in ref 14). In toluene solvent, NO_2BF_4, NO_2PF_6, NO_2ClO_4, $NO_2Cl/TiCl_4$, $NO_2Cl/SnCl_4$, NO_2Cl/BF_3, and NO_2Cl/PF_5 all provide product ratios that are within experimental error of each other. For this reason, it was viewed that the tightness of counterion to the NO_2^+ is not a major factor in the reaction's selectivity, so the error in the ONIOM surface was considered acceptable.





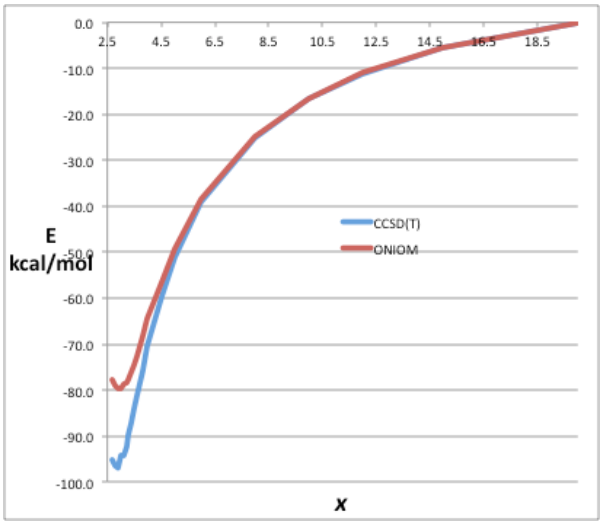


Table S7.

	CCSD(T)		ONIOM	
	jun-cc-pvtz	Erel		Erel
2.7	-628.716699	1.8	-205.490359	2.0
2.8	-628.718872	0.4	-205.492503	0.7
2.9	-628.719513	0.0	-205.493599	0.0
3			-205.493268	0.2
3.1	-628.715203	2.7	-205.492045	1.0
3.2	-628.711965	4.7	-205.491569	1.3
3.3	-628.708135	7.1	-205.490231	2.1
3.4	-628.703843	9.8	-205.488038	3.5
3.5	-628.699288	12.7	-205.485174	5.3
3.6	-628.694660	15.6	-205.482086	7.2
3.8	-628.685665	21.2	-205.475378	11.4
4	-628.677344	26.5	-205.469391	15.2
4.5	-628.659918	37.4	-205.456273	23.4
5	-628.646589	45.8	-205.445056	30.5
6	-628.627561	57.7	-205.427762	41.3
8	-628.604911	71.9	-205.405945	55.0
10	-628.591549	80.3	-205.392807	63.2
12	-628.582692	85.9	-205.384032	68.8
15	-628.573856	91.4	-205.375245	74.3
20	-628.565032	96.9	-205.366448	79.8

Calculated Structures and Complete Energies

Guide to Structures, Structure Titles and Their Organization

The sections below are divided into systems (e.g. toluene + NO_2^+, toluene + $NO_2^+BF_4^-$, toluene + NO_2^+ + H_2SO_4) then subdivided by type of structure (e.g. transition structures, pi complexes, product). Individual structures are then given a specific descriptive title. When dealing with large classes of structures, the structures are given a code number that makes them uniquely identifiable. The code is associated with a number in the original calculation file, so that this file can always be located even if the file title changes.

The structure titles contain some short descriptive words. Here is what those words mean in a longer format:

PCM – means that a PCM implicit model was employed. With no other description, this would be for CH_2Cl_2 using default procedures in Gaussian 09.

ONIOM – means a 2-layer ONIOM calculation with M06-2X/6-311G* used for the toluene and NO_2^+ and PM3 used for all other atoms.

para, meta, ortho, and ipso – refers to the closest aromatic carbon to the NO_2^+, with no other implication.

O-Pi or N-Pi – The O-Pi complexes have the an oxygen of NO_2^+ near the center of the ring, while the N-Pi complexes have the N of NO_2^+ closest to the arene carbons. Some pictures of structures are included to make the distinction clear. The N-Pi complexes tend to be lower in energy.

In cases some of the located structures are very similar to each other, often differing by only by the rotation of the methyl group of the toluene. When two nearly identical structures were located and recognized as such, only the lower energy of the two structures is presented.

Toluene M062X/6-311G*/PCM(CH_2Cl_2)

M062X/6-311G*
E(RM062X) = -271.495957959

Zero-point correction= 0.128768 (Hartree/Particle)
Thermal correction to Energy= 0.134919
Thermal correction to Enthalpy= 0.135863
Thermal correction to Gibbs Free Energy= 0.098498
Sum of electronic and ZPE= -271.367190
Sum of electronic and thermal Energies= -271.361039
Sum of electronic and thermal Enthalpies= -271.360095
Sum of electronic and thermal Free Energies= -271.397460

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	84.663	23.067	78.640

C,0,0.9255051816,1.9370543762,0.0057654806
C,0,1.0098007575,1.2375724004,1.2064981383
C,0,1.1869602,-0.1419972957,1.199941624
C,0,1.284754455,-0.8481474363,-0.0010834637
C,0,1.1963030969,-0.1355138276,-1.1978033889
C,0,1.0190097515,1.2451366148,-1.1975078481
C,0,1.5061423469,-2.3389391059,-0.0002698899
H,0,0.7844816855,3.0119095013,0.0085174978
H,0,0.9338148302,1.767208922,2.1498296396
H,0,1.2484042735,-0.6817083439,2.1403208093
H,0,1.2648270094,-0.6689711516,-2.1410921768
H,0,0.9503454097,1.7799882021,-2.1384493338
H,0,1.1685149351,-2.7912053875,-0.933916141
H,0,0.9746972721,-2.8180741361,0.8238800437
H,0,2.5680077949,-2.5733583322,0.115225009

NO_2^+ M062X/6-311G*/PCM(CH_2Cl_2)

M062X/6-311G*
E(RM062X) = -204.788876622

Zero-point correction= 0.012555 (Hartree/Particle)
Thermal correction to Energy= 0.015140
Thermal correction to Enthalpy= 0.016085
Thermal correction to Gibbs Free Energy= -0.008096
Sum of electronic and ZPE= -204.776322
Sum of electronic and thermal Energies= -204.773736
Sum of electronic and thermal Enthalpies= -204.772792
Sum of electronic and thermal Free Energies= -204.796972

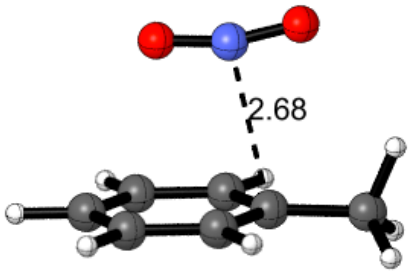
	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	9.501	6.672	50.892

N,0,0.,0.,0.

O,0,0.,0.,1.1050096647
O,0,0.,0.,-1.1050096647

TSs for Toluene + NO_2^+ M062X/6-311G*/PCM(CH_2Cl_2)

TS Toluene + NO2+ ipso 190031



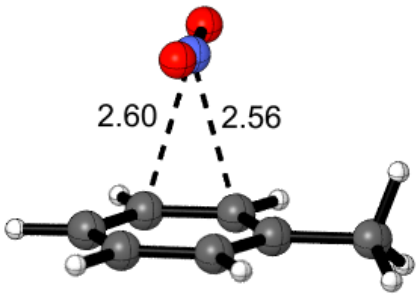
M062X/6-311G*
E(RM062X) = -476.296115891

Zero-point correction= 0.141325 (Hartree/Particle)
Thermal correction to Energy= 0.150604
Thermal correction to Enthalpy= 0.151548
Thermal correction to Gibbs Free Energy= 0.106085
Sum of electronic and ZPE= -476.154791
Sum of electronic and thermal Energies= -476.145512
Sum of electronic and thermal Enthalpies= -476.144567
Sum of electronic and thermal Free Energies= -476.190031

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.506	33.264	95.686

C,0,2.1672683791,0.2486907575,-0.0004712612
C,0,1.5625348931,-0.0974844662,1.2081640532
C,0,0.3528173158,-0.7780810616,1.2088488719
C,0,-0.2726812838,-1.1334771936,-0.0002270444
C,0,0.3518313009,-0.7767183139,-1.2094310257
C,0,1.5615584322,-0.0961373784,-1.2089937919
C,0,-1.5482229909,-1.92620715,-0.0002035311
H,0,3.1109815205,0.7810412512,-0.0005534484
H,0,2.0368034317,0.1634132127,2.1466030878
H,0,-0.1103170428,-1.0632187373,2.1477619935
H,0,-0.1121037368,-1.0607846902,-2.1482740695
H,0,2.0350421274,0.16583767,-2.1475302639
H,0,-2.4330309543,-1.279601995,-0.0004969304
H,0,-1.6138415968,-2.5570191297,0.886310191
H,0,-1.6135964559,-2.5573480016,-0.8865091068
N,0,-1.1032373006,1.4195320168,0.0007037226
O,0,-0.1516379665,2.0013528584,0.0011227659
O,0,-2.1768570722,1.102142351,0.0004667874

TS Toluene + NO2+ ortho 187860



M062X/6-311G*
E(RM062X) = -476.294517695

Zero-point correction= 0.141530 (Hartree/Particle)
Thermal correction to Energy= 0.150793
Thermal correction to Enthalpy= 0.151737
Thermal correction to Gibbs Free Energy= 0.106658
Sum of electronic and ZPE= -476.152987
Sum of electronic and thermal Energies= -476.143725
Sum of electronic and thermal Enthalpies= -476.142781
Sum of electronic and thermal Free Energies= -476.187860

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.624	33.285	94.876

C,0,-0.5370453891,1.6439196992,-0.3417689813
C,0,0.3000637444,1.62370211,0.770636242
C,0,1.3745771267,0.7145044368,0.8312402415
C,0,1.6384611575,-0.1693810902,-0.2244298334
C,0,0.7695380963,-0.1536089411,-1.3108920962
C,0,-0.3082690004,0.7394096259,-1.3699189916
C,0,2.7927172121,-1.1306323004,-0.150534918
H,0,-1.3587472313,2.3467319397,-0.3966609169
H,0,0.1439539419,2.3202021322,1.5873903479
H,0,2.0347425662,0.7297203351,1.6934500313
H,0,0.9323034965,-0.842482785,-2.1330428887
H,0,-0.9624323514,0.726329728,-2.2337266311
H,0,3.6561540251,-0.6707058127,0.3312374874
H,0,3.0888765539,-1.4657179193,-1.1441972936
H,0,2.5196327958,-2.0144126616,0.432365723
N,0,-0.6052259966,-0.5593893368,1.8464850176
O,0,-1.027666461,-1.049203666,0.932046291
O,0,-0.4143452866,-0.3235974938,2.9288431692

TS Toluene + NO2+ ortho 188821

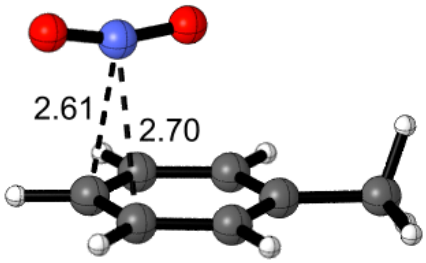
M062X/6-311G*
E(RM062X) = -476.294566581

Zero-point correction= 0.141190 (Hartree/Particle)
Thermal correction to Energy= 0.150618
Thermal correction to Enthalpy= 0.151562
Thermal correction to Gibbs Free Energy= 0.105746
Sum of electronic and ZPE= -476.153376
Sum of electronic and thermal Energies= -476.143948
Sum of electronic and thermal Enthalpies= -476.143004
Sum of electronic and thermal Free Energies= -476.188821

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 94.514 33.406 96.429

C,0,1.1834182488,-1.8213603392,-0.0074468132
C,0,0.9036265049,-1.102631014,-1.1637612621
C,0,0.8259477107,0.2938919668,-1.1352153998
C,0,1.0259422288,1.0087213506,0.0438879169
C,0,1.3547508915,0.2826590341,1.194334319
C,0,1.4244269157,-1.1267622855,1.173141158
C,0,0.9117097384,2.5081850653,0.0656010201
H,0,1.2264246262,-2.902957644,-0.0262113719
H,0,0.7369076795,-1.625649349,-2.0980560501
H,0,0.5995344072,0.832506658,-2.0497745405
H,0,1.5201075769,0.8068040156,2.1307018113
H,0,1.6469561262,-1.6628552483,2.0894211457
H,0,1.5979451274,2.9618720438,-0.6523402558
H,0,1.1313160887,2.9108719742,1.0539170941
H,0,-0.098847885,2.8158046412,-0.2101700001
N,0,3.7803704251,-0.2366731594,0.5802599905
O,0,3.715183174,-0.2623974668,-0.5381135981
O,0,4.2269824149,-0.1963352435,1.6116498359

TS Toluene + NO2+ para 189331



M062X/6-311G*
E(RM062X) = -476.295678690

Zero-point correction= 0.141612 (Hartree/Particle)
Thermal correction to Energy= 0.150949
Thermal correction to Enthalpy= 0.151893
Thermal correction to Gibbs Free Energy= 0.106347
Sum of electronic and ZPE= -476.154067
Sum of electronic and thermal Energies= -476.144729
Sum of electronic and thermal Enthalpies= -476.143785
Sum of electronic and thermal Free Energies= -476.189331

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 94.722 33.253 95.860

C,0,-0.5435533055,1.6133674884,-0.3083296762
C,0,0.3318768929,1.6372581043,0.7809606653
C,0,1.3936532979,0.7494258262,0.8254657678
C,0,1.6309136573,-0.1586602508,-0.2229857734
C,0,0.777579219,-0.1452924296,-1.3266777776
C,0,-0.3073665484,0.724622953,-1.3710041813
C,0,2.7751687066,-1.1264478982,-0.1321259101
H,0,-1.376263163,2.3065628837,-0.354950136
H,0,0.1703229618,2.3373176015,1.5918387775
H,0,2.062570149,0.7529677609,1.6798062069
H,0,0.9552977155,-0.8253658824,-2.1524845045
H,0,-0.965379832,0.7289997335,-2.2329649359
H,0,3.6727159558,-0.6350459515,0.2466695322
H,0,3.0017548639,-1.5700743604,-1.1009643816
H,0,2.5301109804,-1.9359216135,0.5613325559
N,0,-1.8065947214,-0.5303172071,0.4876200744
O,0,-0.9554220161,-1.081052024,0.956302857
O,0,-2.8312568138,-0.2131517339,0.1622928397

TS Toluene + NO2+ para 189465

M062X/6-311G*
E(RM062X) = -476.295695036

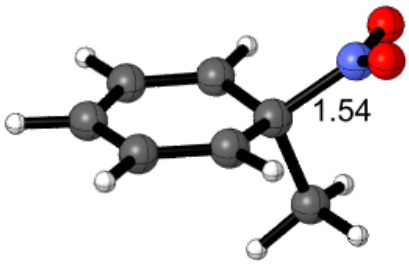
Zero-point correction= 0.141612 (Hartree/Particle)
Thermal correction to Energy= 0.150957
Thermal correction to Enthalpy= 0.151901
Thermal correction to Gibbs Free Energy= 0.106230
Sum of electronic and ZPE= -476.154083
Sum of electronic and thermal Energies= -476.144738
Sum of electronic and thermal Enthalpies= -476.143794
Sum of electronic and thermal Free Energies= -476.189465

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 94.727 33.262 96.123

C,0,1.2371176234,-1.8033976043,-0.0727628045
C,0,1.0643492992,-1.0837595813,-1.2588237738
C,0,0.9829704918,0.2975163754,-1.2154069276
C,0,1.0367001984,0.9948047667,0.0061344534
C,0,1.1685482115,0.2660518842,1.1877953072
C,0,1.2766097832,-1.1213122454,1.1546614612
C,0,0.9480607965,2.4937237333,0.0128894923
H,0,1.2989703182,-2.8859238401,-0.0951762409
H,0,1.0105049196,-1.605076008,-2.2070036433
H,0,0.8693324356,0.8596753922,-2.1366152781
H,0,1.1964176281,0.7844498648,2.1398327963
H,0,1.3772231459,-1.6802446042,2.0784899098
H,0,0.0432919158,2.8261028619,-0.500587567
H,0,1.7989605335,2.9301513584,-0.5161251439
H,0,0.9350811516,2.8899775451,1.0273550526
N,0,3.7789779476,-1.234438154,0.152308798
O,0,3.771553092,-0.1998956799,-0.2680767254
O,0,4.104723508,-2.2297850648,0.5512668336

Product Structures for Toluene + NO_2^+ M062X/6-311G*/PCM(CH_2Cl_2)

ipso Product 206704



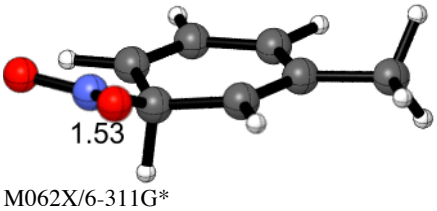
M062X/6-311G*
E(RM062X) = -476.316372222

Zero-point correction= 0.143680 (Hartree/Particle)
Thermal correction to Energy= 0.152373
Thermal correction to Enthalpy= 0.153317
Thermal correction to Gibbs Free Energy= 0.109668
Sum of electronic and ZPE= -476.172692
Sum of electronic and thermal Energies= -476.163999
Sum of electronic and thermal Enthalpies= -476.163055
Sum of electronic and thermal Free Energies= -476.206704

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.615	32.893	91.867

C,0,2.506597,0.004363,-0.35746
C,0,1.821609,1.235953,-0.366006
C,0,0.47896,1.246062,-0.150502
C,0,-0.222044,0.01277,0.247585
C,0,0.522533,-1.248143,0.090584
C,0,1.864563,-1.229623,-0.126688
C,0,-0.507674,0.15364,1.802645
H,0,3.571186,0.00263,-0.565688
H,0,2.354653,2.150549,-0.586194
H,0,-0.104587,2.158665,-0.19314
H,0,-0.019763,-2.174855,0.236525
H,0,2.43285,-2.148781,-0.161972
H,0,-1.080621,1.065581,1.957271
H,0,0.433726,0.199061,2.345977
H,0,-1.083665,-0.714579,2.118651
N,0,-1.621983,-0.053778,-0.384001
O,0,-2.212164,0.990342,-0.471944
O,0,-2.029981,-1.141836,-0.691102

meta Product 209211



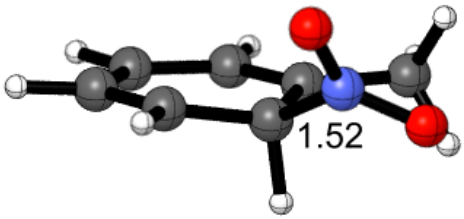
M062X/6-311G*
E(RM062X) = -476.317016634

Zero-point correction= 0.142484 (Hartree/Particle)
Thermal correction to Energy= 0.151453
Thermal correction to Enthalpy= 0.152398
Thermal correction to Gibbs Free Energy= 0.107805
Sum of electronic and ZPE= -476.174532
Sum of electronic and thermal Energies= -476.165563
Sum of electronic and thermal Enthalpies= -476.164619
Sum of electronic and thermal Free Energies= -476.209211

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.038	33.084	93.852

C,0,0.6875660452,-0.9364256012,-0.9367337752
C,0,1.3651837913,-2.0179307942,-0.4642351184
C,0,1.0332425181,-2.5417915931,0.7991123413
C,0,0.0131984715,-2.0266758448,1.6373168672
C,0,-0.6810987093,-0.9433043686,1.1807802261
C,0,-0.47358629,-0.4478800693,-0.1859691639
C,0,-0.2312838456,-2.6380690569,2.9859509581
H,0,0.9255971391,-0.4616764054,-1.880511529
H,0,2.1837123664,-2.4467666137,-1.0260582439
H,0,1.616551419,-3.3806323103,1.1688235704
H,0,-1.4504463492,-0.4634519897,1.7750905966
H,0,-1.3267598862,-0.9068428154,-0.7440467929
H,0,-0.9925709358,-2.0857612344,3.5334029514
H,0,0.6876332382,-2.6431063251,3.5740878912
H,0,-0.5645612667,-3.6712126057,2.8742500394
N,0,-0.7395716363,1.0490398443,-0.3573132393
O,0,-1.4159341394,1.572198211,0.4857827191
O,0,-0.2836009304,1.5618415724,-1.3430902979

ortho Product 212984



M062X/6-311G*
E(RM062X) = -476.321390301

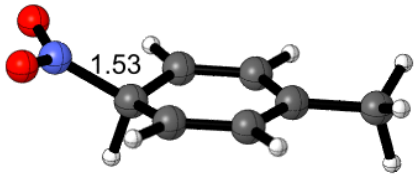
Zero-point correction= 0.142993 (Hartree/Particle)
Thermal correction to Energy= 0.151863
Thermal correction to Enthalpy= 0.152808
Thermal correction to Gibbs Free Energy= 0.108406
Sum of electronic and ZPE= -476.178398
Sum of electronic and thermal Energies= -476.169527
Sum of electronic and thermal Enthalpies= -476.168583
Sum of electronic and thermal Free Energies= -476.212984

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.296	32.771	93.451

C,0,0.650428293,-1.1992474621,-1.795157402

C,0,1.5325085093,-2.1117890349,-1.1643259315
C,0,1.7226048612,-2.1671676253,0.2185232456
C,0,1.0450435924,-1.3166595151,1.0610808633
C,0,-0.0227372038,-0.4747224968,0.4450134691
C,0,-0.0549840997,-0.3402510706,-1.0252190145
C,0,1.2929319815,-1.2931890461,2.5216796779
H,0,0.5797483773,-1.1722367306,-2.8736400517
H,0,2.1145662045,-2.7813270832,-1.7887074913
H,0,2.4506172289,-2.8553839476,0.6287653644
H,0,-0.9433448888,-1.0532509394,0.6763450913
H,0,-0.7193435995,0.4041219837,-1.4474785467
H,0,1.654117331,-0.3045206563,2.8226938318
H,0,2.0326571462,-2.0413783639,2.7943975211
H,0,0.3688602558,-1.4622969597,3.0784768328
N,0,-0.2266439519,0.8506886157,1.1539514622
O,0,0.0610957192,1.8443606703,0.5390414736
O,0,-0.6520597569,0.7957206618,2.2797696049

para Product 218203



M062X/6-311G*
E(RM062X) = -476.325950643

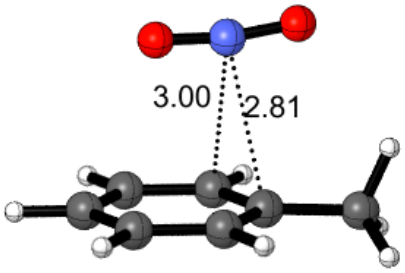
Zero-point correction= 0.142396 (Hartree/Particle)
Thermal correction to Energy= 0.151304
Thermal correction to Enthalpy= 0.152248
Thermal correction to Gibbs Free Energy= 0.107747
Sum of electronic and ZPE= -476.183555
Sum of electronic and thermal Energies= -476.174647
Sum of electronic and thermal Enthalpies= -476.173702
Sum of electronic and thermal Free Energies= -476.218203

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.945	32.968	93.660

C,0,0.7360771244,-0.0002709661,0.469881242
C,0,0.0164015985,1.2589692412,0.2082599022
C,0,-1.321469905,1.2404089282,0.0097718584
C,0,-2.0203607344,0.0034402296,-0.0896358402
C,0,-1.3250793597,-1.2348623369,0.0071751287
C,0,0.0134388178,-1.2567114434,0.2043274759
C,0,-3.4813133516,0.0101271303,-0.2967286415
H,0,0.8821685472,-0.002735125,1.5728435287
H,0,0.5800106178,2.182728102,0.2494004641
H,0,-1.8684945708,2.1661756168,-0.1173216544
H,0,-1.8737530075,-2.1590676372,-0.1224074629
H,0,0.5751813784,-2.1818354006,0.2409845196
H,0,-3.8064567059,0.8783877945,-0.869231685
H,0,-3.9407247489,0.0955409055,0.6994154673
H,0,-3.8415112524,-0.9139319814,-0.7445300402
N,0,2.1747266763,-0.0015604569,-0.0497654389
O,0,2.685314064,-1.0774286123,-0.2104573187
O,0,2.6876478118,1.0733580117,-0.2091555052

Pi Complexes for Toluene + NO_2^+ M062X/6-311G*/PCM(CH_2Cl_2)

ipso N-Pi complex 191410



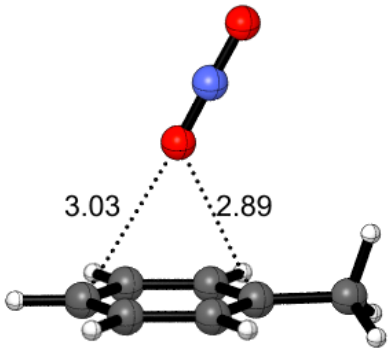
M062X/6-311G*
E(RM062X) = -476.296104866

Zero-point correction= 0.141850 (Hartree/Particle)
Thermal correction to Energy= 0.151978
Thermal correction to Enthalpy= 0.152922
Thermal correction to Gibbs Free Energy= 0.104695
Sum of electronic and ZPE= -476.154255
Sum of electronic and thermal Energies= -476.144127
Sum of electronic and thermal Enthalpies= -476.143183
Sum of electronic and thermal Free Energies= -476.191410

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.367	35.073	101.502

C,0,2.1495738018,-0.342989473,0.0010760284
C,0,1.5634500941,0.0367593582,-1.205514675
C,0,0.3929824921,0.7871233338,-1.2055983562
C,0,-0.2085796583,1.1803138549,0.0003221646
C,0,0.3912230097,0.7854893348,1.206645806
C,0,1.5616892812,0.0351389838,1.2073112094
C,0,-1.4461688013,2.0353549772,0.0001138875
H,0,3.0626734946,-0.9263808186,0.0013425784
H,0,2.020695139,-0.2498637761,-2.1451980265
H,0,-0.0513773844,1.0974455012,-2.1458353572
H,0,-0.0546069085,1.0945482965,2.1466102715
H,0,2.0174540454,-0.252898714,2.147284871
H,0,-2.3622220767,1.4342907718,0.0019340372
H,0,-1.4814434913,2.668908275,-0.8863188681
H,0,-1.4798039232,2.6715282648,0.884751737
N,0,-1.1925076611,-1.4507996971,-0.0017056564
O,0,-0.243491035,-2.0266656288,-0.0011828152
O,0,-2.2254434184,-1.0339338445,-0.0021618366

ipso O-Pi complex 186028



M062X/6-311G*
E(RM062X) = -476.291663427

Zero-point correction= 0.142539 (Hartree/Particle)
Thermal correction to Energy= 0.152465
Thermal correction to Enthalpy= 0.153409
Thermal correction to Gibbs Free Energy= 0.105636
Sum of electronic and ZPE= -476.149124
Sum of electronic and thermal Energies= -476.139199
Sum of electronic and thermal Enthalpies= -476.138255
Sum of electronic and thermal Free Energies= -476.186028

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.673	34.509	100.547

C,0,-1.48808,-1.699732,0.000349
C,0,-1.356044,-1.010326,1.202963
C,0,-1.089886,0.356829,1.200512
C,0,-0.948409,1.060087,0.00026
C,0,-1.09165,0.357085,-1.199934
C,0,-1.357813,-1.010066,-1.202307
C,0,-0.607395,2.527007,0.000153
H,0,-1.700661,-2.762387,0.000391
H,0,-1.467367,-1.534712,2.145302
H,0,-0.9948,0.887147,2.143069
H,0,-0.997926,0.887629,-2.142499
H,0,-1.470543,-1.534213,-2.144611
H,0,-1.003142,3.02686,0.884942
H,0,-1.003616,3.02686,-0.884413
H,0,0.477968,2.668915,-0.000126
N,0,2.426069,-0.358906,-0.000576
O,0,1.365184,-0.67207,-0.001319
O,0,3.486474,-0.032813,0.000069

meta N-Pi complex 189935

M062X/6-311G*
E(RM062X) = -476.295961987

Zero-point correction= 0.142018 (Hartree/Particle)
Thermal correction to Energy= 0.151977
Thermal correction to Enthalpy= 0.152922
Thermal correction to Gibbs Free Energy= 0.106027
Sum of electronic and ZPE= -476.153944
Sum of electronic and thermal Energies= -476.143985
Sum of electronic and thermal Enthalpies= -476.143040
Sum of electronic and thermal Free Energies= -476.189935

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.367	34.945	98.698

C,0,-0.566614,1.648636,-0.150145
C,0,0.231864,1.514868,0.98521
C,0,1.2888,0.612055,0.988483
C,0,1.581413,-0.167274,-0.139716
C,0,0.785221,-0.0152,-1.274862
C,0,-0.283342,0.881319,-1.283076
C,0,2.725979,-1.14336,-0.113405
H,0,-1.387225,2.357201,-0.16302
H,0,0.027435,2.11257,1.865867
H,0,1.903554,0.5082,1.877152
H,0,1.002174,-0.599212,-2.163031
H,0,-0.886114,0.993253,-2.178069
H,0,2.856685,-1.628261,-1.080674
H,0,2.558038,-1.91948,0.637275
H,0,3.658998,-0.63851,0.144967
N,0,-1.904649,-0.889763,0.289032
O,0,-1.051926,-1.255747,0.893449
O,0,-2.82069,-0.612213,-0.273277

meta N-Pi complex 190153

M062X/6-311G*
E(RM062X) = -476.295477416

Zero-point correction= 0.141922 (Hartree/Particle)
Thermal correction to Energy= 0.151957
Thermal correction to Enthalpy= 0.152901
Thermal correction to Gibbs Free Energy= 0.105325
Sum of electronic and ZPE= -476.153555
Sum of electronic and thermal Energies= -476.143521
Sum of electronic and thermal Enthalpies= -476.142577
Sum of electronic and thermal Free Energies= -476.190153

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.354	34.932	100.132

C,0,0.354336,-1.781366,-0.365589
C,0,-0.528191,-1.723467,0.710543
C,0,-1.432964,-0.670576,0.816742
C,0,-1.484007,0.342912,-0.147074
C,0,-0.59152,0.279199,-1.218414
C,0,0.320365,-0.773966,-1.329731
C,0,-2.495812,1.452365,-0.045294
H,0,1.054198,-2.603415,-0.458484
H,0,-0.512272,-2.498297,1.468294
H,0,-2.115987,-0.634645,1.659596
H,0,-0.616137,1.049107,-1.983131
H,0,0.993707,-0.812982,-2.179655
H,0,-2.619596,1.784181,0.98658
H,0,-3.471004,1.107455,-0.398329
H,0,-2.207638,2.310542,-0.653011
N,0,1.918909,0.744044,0.459462
O,0,1.2209,0.687871,1.316574

O,0,2.680241,0.854522,-0.339724

meta N-Pi complex 190249

M062X/6-311G*
E(RM062X) = -476.295601518

Zero-point correction= 0.142032 (Hartree/Particle)
Thermal correction to Energy= 0.152141
Thermal correction to Enthalpy= 0.153085
Thermal correction to Gibbs Free Energy= 0.105353
Sum of electronic and ZPE= -476.153569
Sum of electronic and thermal Energies= -476.143461
Sum of electronic and thermal Enthalpies= -476.142517
Sum of electronic and thermal Free Energies= -476.190249

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.470	34.945	100.460

C,0,-0.136271,1.886722,-0.423211
C,0,0.772256,1.747752,0.623788
C,0,1.516614,0.578944,0.755274
C,0,1.376206,-0.477198,-0.151636
C,0,0.451762,-0.334854,-1.188327
C,0,-0.297207,0.839693,-1.327328
C,0,2.22012,-1.715703,-0.013173
H,0,-0.709923,2.799001,-0.535028
H,0,0.903263,2.551506,1.338924
H,0,2.225324,0.484091,1.571946
H,0,0.327116,-1.136455,-1.910156
H,0,-0.995145,0.9356,-2.152353
H,0,1.892094,-2.501416,-0.693542
H,0,2.185926,-2.104003,1.006613
H,0,3.264786,-1.489324,-0.239542
N,0,-1.909878,-0.623969,0.497401
O,0,-1.321272,-0.34124,1.391216
O,0,-2.571875,-0.94918,-0.331339

ortho N-Pi complex 189508

M062X/6-311G*
E(RM062X) = -476.295731534

Zero-point correction= 0.142352 (Hartree/Particle)
Thermal correction to Energy= 0.152324
Thermal correction to Enthalpy= 0.153268
Thermal correction to Gibbs Free Energy= 0.106224
Sum of electronic and ZPE= -476.153379
Sum of electronic and thermal Energies= -476.143408
Sum of electronic and thermal Enthalpies= -476.142463
Sum of electronic and thermal Free Energies= -476.189508

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.585	34.846	99.013

C,0,0.5562375542,1.6434878112,-0.167642926
C,0,0.2819617716,0.8575819862,-1.283383631
C,0,-0.7800371484,-0.053803273,-1.2570078873
C,0,-1.5880070585,-0.1874728055,-0.123999319
C,0,-1.2911580689,0.6016141734,0.9908897339
C,0,-0.2328371165,1.507272347,0.9719751166
C,0,-2.7649896336,-1.1257340309,-0.1110253199
H,0,1.3746199511,2.3532347205,-0.1864402328
H,0,0.8825659986,0.9568113219,-2.1811772917
H,0,-0.9962526403,-0.6494174421,-2.1391459789
H,0,-1.9008788738,0.5092648754,1.8839176639
H,0,-0.0247322701,2.1082354862,1.8496539776
H,0,-3.6864467213,-0.5754907572,-0.3174859129
H,0,-2.8806086296,-1.6034846318,0.8629653303
H,0,-2.666114218,-1.9027765478,-0.8696093477
N,0,1.3983159958,-1.5303244135,-0.0990032039
O,0,1.1979329044,-1.1561507012,0.9234101686
O,0,1.6671312034,-1.9776111189,-1.0783369397

ortho O-Pi complex 187442

M062X/6-311G*
E(RM062X) = -476.292124312

Zero-point correction= 0.142162 (Hartree/Particle)
Thermal correction to Energy= 0.152268
Thermal correction to Enthalpy= 0.153212
Thermal correction to Gibbs Free Energy= 0.104683
Sum of electronic and ZPE= -476.149962
Sum of electronic and thermal Energies= -476.139856
Sum of electronic and thermal Enthalpies= -476.138912
Sum of electronic and thermal Free Energies= -476.187442

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.550	34.690	102.139

C,0,-0.921954,1.93888,0.014999
C,0,-1.034305,1.250841,-1.19041
C,0,-1.208317,-0.131338,-1.193721
C,0,-1.275962,-0.850605,0.002837
C,0,-1.15797,-0.147722,1.206129
C,0,-0.984065,1.233882,1.21506
C,0,-1.509356,-2.338373,0.000606
H,0,-0.790806,3.014693,0.019528
H,0,-0.989538,1.790129,-2.129895
H,0,-1.299263,-0.658938,-2.13814
H,0,-1.209644,-0.689369,2.145702
H,0,-0.900236,1.759866,2.159474
H,0,-2.575877,-2.556187,0.102334
H,0,-0.997005,-2.823538,0.832923
H,0,-1.167918,-2.794483,-0.929531
N,0,2.542212,-0.118414,-0.017595
O,0,1.482637,0.199607,-0.03503
O,0,3.60316,-0.44294,0.001002

ortho O-Pi complex 187803

M062X/6-311G*
E(RM062X) = -476.292122761

Zero-point correction= 0.142106 (Hartree/Particle)
Thermal correction to Energy= 0.152247

Thermal correction to Enthalpy= 0.153192
Thermal correction to Gibbs Free Energy= 0.104320
Sum of electronic and ZPE= -476.150017
Sum of electronic and thermal Energies= -476.139875
Sum of electronic and thermal Enthalpies= -476.138931
Sum of electronic and thermal Free Energies= -476.187803

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.537	34.703	102.859

C,0,0.925866,1.938147,-0.005811
C,0,1.019102,1.245465,1.19851
C,0,1.19051,-0.1372,1.199127
C,0,1.274434,-0.852125,0.000982
C,0,1.175587,-0.144407,-1.201281
C,0,1.00459,1.237494,-1.207466
C,0,1.504895,-2.340377,0.000501
H,0,0.796481,3.014158,-0.008471
H,0,0.961436,1.781097,2.139407
H,0,1.266672,-0.6686,2.142707
H,0,1.240265,-0.68247,-2.14212
H,0,0.935772,1.767394,-2.150873
H,0,1.157842,-2.798258,0.927657
H,0,2.57145,-2.560157,-0.09658
H,0,0.995683,-2.822263,-0.835676
N,0,-2.542843,-0.115552,0.005189
O,0,-1.483369,0.203211,0.010074
O,0,-3.603581,-0.441213,-0.000042

para N-Pi complex 189915

M062X/6-311G*
E(RM062X) = -476.295984404

Zero-point correction= 0.141599 (Hartree/Particle)
Thermal correction to Energy= 0.150964
Thermal correction to Enthalpy= 0.151908
Thermal correction to Gibbs Free Energy= 0.106069
Sum of electronic and ZPE= -476.154386
Sum of electronic and thermal Energies= -476.145020
Sum of electronic and thermal Enthalpies= -476.144076
Sum of electronic and thermal Free Energies= -476.189915

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.731	33.128	96.476

C,0,-0.619284,1.588824,-0.108409
C,0,0.122251,1.410011,1.059896
C,0,1.217505,0.555026,1.061082
C,0,1.607116,-0.125408,-0.100793
C,0,0.864963,0.070472,-1.266805
C,0,-0.241909,0.91691,-1.274702
C,0,2.812738,-1.024983,-0.085461
H,0,-1.472228,2.258462,-0.117617
H,0,-0.158698,1.933239,1.966463
H,0,1.785167,0.410662,1.974851
H,0,1.154056,-0.442251,-2.178002
H,0,-0.800719,1.067728,-2.191798
H,0,3.728312,-0.430252,-0.034428
H,0,2.862371,-1.640641,-0.983509
H,0,2.802914,-1.68262,0.785654
N,0,-1.910165,-0.912844,0.208883
O,0,-1.021153,-1.413786,0.640268
O,0,-2.867633,-0.514905,-0.189349

para N-Pi complex 190032

M062X/6-311G*
E(RM062X) = -476.295972760

Zero-point correction= 0.142122 (Hartree/Particle)
Thermal correction to Energy= 0.152111
Thermal correction to Enthalpy= 0.153055
Thermal correction to Gibbs Free Energy= 0.105940
Sum of electronic and ZPE= -476.153851
Sum of electronic and thermal Energies= -476.143862
Sum of electronic and thermal Enthalpies= -476.142918
Sum of electronic and thermal Free Energies= -476.190032

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.451	34.938	99.161

C,0,-0.6388762601,1.5696736671,0.0040454767
C,0,-0.0753284116,1.1544719318,1.2115852809
C,0,1.0486367875,0.3329302965,1.2087953706
C,0,1.6320799698,-0.0824679734,0.008746454
C,0,1.0636843333,0.3505731406,-1.1956402649
C,0,-0.058387267,1.1699312136,-1.2033017963
C,0,2.8365655878,-0.9836878909,-0.0024101185
H,0,-1.5068904481,2.2202134349,0.0023552685
H,0,-0.5077693008,1.4781275452,2.1516031391
H,0,1.4816088099,0.0128507689,2.1507130514
H,0,1.512174078,0.0430889002,-2.1349790515
H,0,-0.4785841039,1.5064611117,-2.1443282528
H,0,2.5620655248,-1.9892016494,-0.332142453
H,0,3.28319924,-1.0645790799,0.9884021472
H,0,3.5945166451,-0.6108323663,-0.6935576987
N,0,-1.9270525762,-0.9506410492,-0.0075061625
O,0,-0.9967805058,-1.5515576504,-0.0110505825
O,0,-2.9179141027,-0.4497263512,-0.0051978077

para N-Pi complex 190293

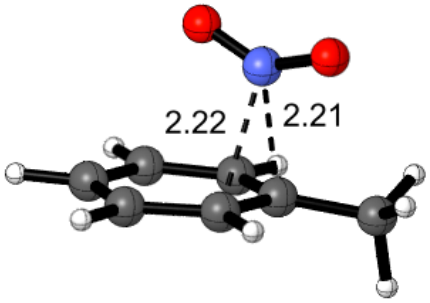
M062X/6-311G*
E(RM062X) = -476.296006510

Zero-point correction= 0.141913 (Hartree/Particle)
Thermal correction to Energy= 0.151943
Thermal correction to Enthalpy= 0.152887
Thermal correction to Gibbs Free Energy= 0.105714
Sum of electronic and ZPE= -476.154094
Sum of electronic and thermal Energies= -476.144064
Sum of electronic and thermal Enthalpies= -476.143120
Sum of electronic and thermal Free Energies= -476.190293

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	95.346	35.032	99.284

C,0,0.629224,1.59598,-0.101083
C,0,0.247736,0.933174,-1.272232
C,0,-0.863614,0.094234,-1.269694
C,0,-1.605615,-0.107229,-0.103331
C,0,-1.215589,0.567167,1.060689
C,0,-0.114641,1.416387,1.064602
C,0,-2.78129,-1.045524,-0.087993
H,0,1.484514,2.262593,-0.106933
H,0,0.805993,1.089298,-2.188768
H,0,-1.158993,-0.408296,-2.184742
H,0,-1.786958,0.425674,1.972382
H,0,0.16511,1.937224,1.972899
H,0,-3.550929,-0.701861,0.603923
H,0,-2.46936,-2.04276,0.235063
H,0,-3.224149,-1.142186,-1.07961
N,0,1.888091,-0.926765,0.207504
O,0,0.990675,-1.418441,0.632198
O,0,2.851934,-0.538742,-0.18501

TS for the migration of NO_2^+ from *ipso* to *ortho*



Scrf=(solvent=dichloromethane)
m062x/6-311G*
E(RM062X) = -476.302669724

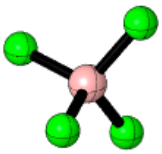
Zero-point correction= 0.141605 (Hartree/Particle)
Thermal correction to Energy= 0.150243
Thermal correction to Enthalpy= 0.151188
Thermal correction to Gibbs Free Energy= 0.108239
Sum of electronic and ZPE= -476.161065
Sum of electronic and thermal Energies= -476.152426
Sum of electronic and thermal Enthalpies= -476.151482
Sum of electronic and thermal Free Energies= -476.194431

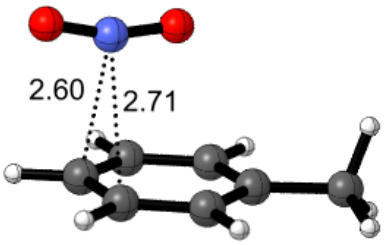
	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	94.279	32.609	90.393

C,0,0.1719202161,0.5186216559,0.1194991911
C,0,0.2052091644,0.2401799303,1.5321778975
C,0,1.3908187831,-0.1438193477,2.1649975075
C,0,2.5164779705,-0.3391461263,1.3975337687
C,0,2.5006535919,-0.0849774777,-0.000500622
C,0,1.3645681283,0.361755791,-0.6235817863
H,0,-0.7024120498,0.3902473263,2.1078705062
H,0,1.3997029568,-0.3266375682,3.2312600527
H,0,3.4346139323,-0.6834264978,1.8580302445
H,0,3.4087890605,-0.2357292737,-0.5711589485
C,0,-1.048645912,1.1112253491,-0.4940469319
N,0,-0.3763519628,-1.5945512614,0.4350723136
H,0,-1.9554269383,0.8305419608,0.0417133385
H,0,-0.9591030465,2.2008131442,-0.4238118605
H,0,-1.1397541357,0.8469332254,-1.5469306938
O,0,-1.5347204034,-1.6216534966,0.3596449594
O,0,0.5334658982,-2.3052120233,0.3816892307
H,0,1.3583977465,0.5825146898,-1.6841041673

TSs and CVTSs for Toluene + $NO_2^+BF_4^-$ ONIOM(M062X/6-311G*:PM3)/PCM(CH_2Cl_2)

TS NO2BF4 PCM ONIOM 2.596_94018





ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276289546170

Zero-point correction= 0.156550 (Hartree/Particle)
Thermal correction to Energy= 0.173208
Thermal correction to Enthalpy= 0.174153
Thermal correction to Gibbs Free Energy= 0.105710
Sum of electronic and ZPE= -476.889342
Sum of electronic and thermal Energies= -476.872684
Sum of electronic and thermal Enthalpies= -476.871740
Sum of electronic and thermal Free Energies= -476.940182

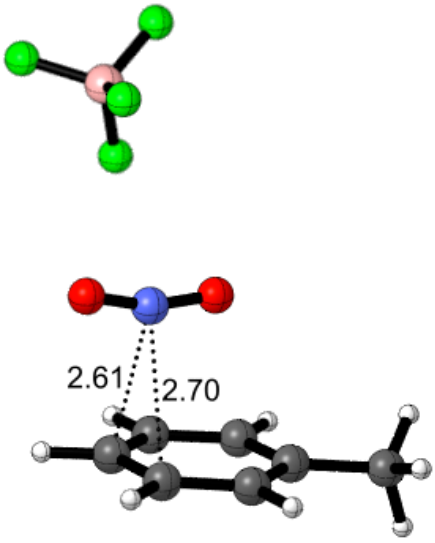
	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.690	54.241	144.049

C,0,-2.6750868221,-1.4450653026,0.9828832779
C,0,-2.5040158475,-0.2625959191,1.7089629213
C,0,-2.9659197248,0.9336015956,1.1861691486
C,0,-3.6356270313,0.978620074,-0.0500217921
C,0,-3.8424005293,-0.2139864295,-0.7457798979
C,0,-3.3616106466,-1.4175909998,-0.2431453722
C,0,-4.0944536161,2.2940543599,-0.6092199975
H,0,-2.3182803499,-2.3878800668,1.3827134923
H,0,-1.9966904161,-0.2824724102,2.6660905215

H,0,-2.8128539199,1.8566838461,1.7354393182
H,0,-4.3738275336,-0.1990210904,-1.6908384857
H,0,-3.5249027646,-2.3403893541,-0.7885766553
H,0,-3.2536472815,2.8199896921,-1.0710205756
H,0,-4.48886255,2.9384181701,0.1775894623
H,0,-4.8626986396,2.1584178923,-1.3699058876
N,0,-0.7230961856,-0.9221129588,-0.6475052607
O,0,-0.8577705552,0.1797627829,-0.7745931324
O,0,-0.3091521567,-1.9636809271,-0.689433912
F,0,3.6345058339,-0.678394182,-0.6012902021
B,0,4.4043348073,0.2674850522,0.0445426799
F,0,5.3512354381,-0.3638945191,0.823102373
F,0,5.0284029508,1.0664143303,-0.8904072038
F,0,3.5940685401,1.044987364,0.84647118

H,0,-1.5805447968,2.2903776473,0.9206664874
H,0,-4.5882807817,-0.1478398962,-0.926440983
H,0,-3.8313156484,-2.086678476,0.4091663052
H,0,-4.203258574,3.0430821593,-0.2811859366
H,0,-4.1677465731,2.0953466686,-1.7699655222
H,0,-2.7278383181,2.9837593653,-1.2389958367
N,0,-1.0127362199,-1.5370397775,-0.8012895032
O,0,-0.8466721162,-2.625438221,-0.5878976788
O,0,-0.9788531623,-0.521766717,-1.2654073403
F,0,3.0720407201,-0.3664111865,-0.7720125981
B,0,4.0123538479,0.2706131387,0.0118743057
F,0,4.7894432063,-0.6727870397,0.6508763568
F,0,4.8097315258,1.0663826949,-0.7834376731
F,0,3.3710968969,1.0517912867,0.950912163

TS NO2BF4 PCM ONIOM 2.605_94107



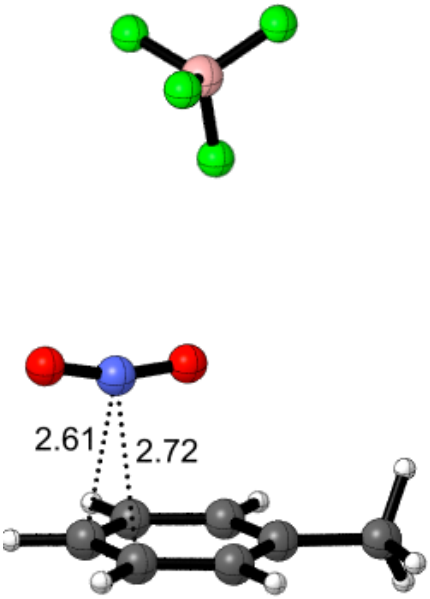
ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276199237599

Zero-point correction= 0.156724 (Hartree/Particle)
Thermal correction to Energy= 0.173431
Thermal correction to Enthalpy= 0.174375
Thermal correction to Gibbs Free Energy= 0.104649
Sum of electronic and ZPE= -476.889068
Sum of electronic and thermal Energies= -476.872361
Sum of electronic and thermal Enthalpies= -476.871417
Sum of electronic and thermal Free Energies= -476.941143

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.830	54.230	146.751

C,0,-2.2669844045,-0.9912855138,1.4162855093
C,0,-1.6531620259,0.2539137337,1.5801027024
C,0,-2.0729649762,1.3292075432,0.8146072886
C,0,-3.131470379,1.2026068148,-0.103427409
C,0,-3.7648748462,-0.0345772069,-0.2302321635
C,0,-3.3363489235,-1.1276544078,0.5148664178
C,0,-3.5805488844,2.3926487205,-0.9015632609
H,0,-1.947642179,-1.8409397423,2.0097141152
H,0,-0.8417093879,0.3702544115,2.288543254

TS NO2BF4 PCM ONIOM 2.607_93956



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.275743056438

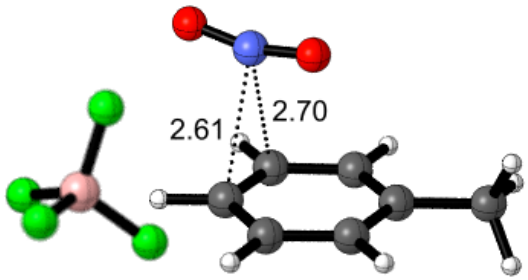
Zero-point correction= 0.157050 (Hartree/Particle)
Thermal correction to Energy= 0.173587
Thermal correction to Enthalpy= 0.174531
Thermal correction to Gibbs Free Energy= 0.106233
Sum of electronic and ZPE= -476.888744
Sum of electronic and thermal Energies= -476.872207
Sum of electronic and thermal Enthalpies= -476.871263
Sum of electronic and thermal Free Energies= -476.939561

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.928	54.104	143.745

C,0,-2.9533365588,-1.2001956215,1.0391206817
C,0,-2.346265656,-0.1367943783,1.7150542644
C,0,-2.3306145992,1.1212256158,1.1377236552
C,0,-2.9433287343,1.3604463597,-0.1063746993
C,0,-3.5839209018,0.3023921787,-0.7526108366
C,0,-3.5866730989,-0.9707455506,-0.1932185255

C,0,-2.8942365383,2.7328469908,-0.7130966515
H,0,-2.9734796907,-2.1896378522,1.4822446976
H,0,-1.8763771925,-0.3024566631,2.6772381666
H,0,-1.8384622263,1.9425286337,1.6488192907
H,0,-4.0734021437,0.4721701504,-1.7051098672
H,0,-4.0865760538,-1.7875678505,-0.7018994828
H,0,-3.2753171097,3.4773956171,-0.0111303028
H,0,-3.4818277691,2.7863768581,-1.6287471509
H,0,-1.8632627115,3.0085621276,-0.9499014719
N,0,-0.9498472462,-1.5123785781,-0.6003474817
O,0,-0.6727150649,-0.4448722443,-0.7733649719
O,0,-0.9562858454,-2.6335296065,-0.5919091797
F,0,3.1203605941,0.8314416412,0.8176231126
B,0,4.0735292224,0.2099035439,0.0373069546
F,0,4.8451401581,1.1616151532,-0.5953012429
F,0,4.8740321896,-0.5806311744,0.8352334436
F,0,3.4481169769,-0.5787903508,-0.9067994022

TS NO2BF4 PCM ONIOM 2.609_93861



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276187286919

Zero-point correction= 0.156846 (Hartree/Particle)
Thermal correction to Energy= 0.173315
Thermal correction to Enthalpy= 0.174259
Thermal correction to Gibbs Free Energy= 0.107775
Sum of electronic and ZPE= -476.889544
Sum of electronic and thermal Energies= -476.873075
Sum of electronic and thermal Enthalpies= -476.872131
Sum of electronic and thermal Free Energies= -476.938616

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.757	54.156	139.928

C,0,-1.141141,0.34911,1.435769
C,0,-2.446576,0.859763,1.34469
C,0,-3.412049,0.181075,0.607708
C,0,-3.092585,-1.000356,-0.060814
C,0,-1.784618,-1.507821,0.050302
C,0,-0.822272,-0.855222,0.801951
C,0,-4.108618,-1.731236,-0.890524
H,0,-0.395888,0.868413,2.028154
H,0,-2.702367,1.77737,1.862753
H,0,-4.4185,0.579074,0.544542
H,0,-1.532957,-2.430206,-0.462876
H,0,0.179544,-1.263401,0.883707
H,0,-3.826679,-1.709787,-1.946517
H,0,-5.099355,-1.289388,-0.791559
H,0,-4.164384,-2.780222,-0.592394
N,0,-1.006739,1.76587,-0.75135
O,0,-1.407796,1.024254,-1.484012
O,0,-0.539607,2.674689,-0.290257
F,0,3.485517,0.469511,1.079387
B,0,3.54916,-0.329812,-0.043275
F,0,4.799774,-0.90264,-0.136114
F,0,2.593724,-1.321434,0.042984
F,0,3.308576,0.440417,-1.162959

CVTS NO2BF4 PCM ONIOM 940511

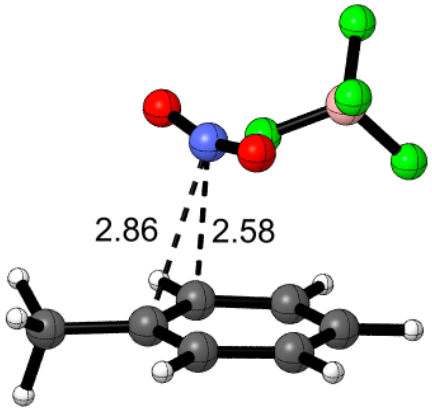
ONIOM(M062X/6-311G*:PM3)

Zero-point correction= 0.157810 (Hartree/Particle)
Thermal correction to Energy= 0.173570
Thermal correction to Enthalpy= 0.174514
Thermal correction to Gibbs Free Energy= 0.113420
Sum of electronic and ZPE= -476.896120
Sum of electronic and thermal Energies= -476.880361
Sum of electronic and thermal Enthalpies= -476.879417
Sum of electronic and thermal Free Energies= -476.940511

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.917	53.889	128.583

C,0,1.7726430496,2.5274859545,0.240607936
C,0,2.8292589405,1.7903559498,0.7792647208
C,0,3.0323207689,0.4751898159,0.3877278275
C,0,2.1811200223,-0.1324809068,-0.5511615161
C,0,1.120903404,0.6232021886,-1.0843309495
C,0,0.923467677,1.9435074253,-0.6962544567
C,0,2.4119857903,-1.5483440568,-0.995604446
H,0,1.6124348637,3.5519354883,0.5533989076
H,0,3.4883825545,2.2441521946,1.5090553414
H,0,3.8559738788,-0.0947654829,0.8035006892
H,0,0.4372075869,0.1578963808,-1.7922498013
H,0,0.0971893364,2.5085782374,-1.1099938065
H,0,1.4849672211,-2.0258494483,-1.3219437276
H,0,2.8623115577,-2.1502267662,-0.2048005008
H,0,3.0975054607,-1.5611752144,-1.8470008158
N,0,0.3927626694,-0.5153161317,1.4621973487
O,0,0.3748899157,-1.616734835,1.2706915126
O,0,0.2697508018,0.5154684258,1.8694208377
F,0,-1.118223307,-1.9341451047,-1.1353371699
B,0,-2.1167102286,-0.9863438358,-1.0458060102
F,0,-1.8222726,-0.1757559868,0.0408847399
F,0,-2.1543965771,-0.2286247,-2.1938722023
F,0,-3.3316067866,-1.5998445914,-0.8441094589

CVTS NO2BF4 PCM ONIOM 940237 (6c‡)



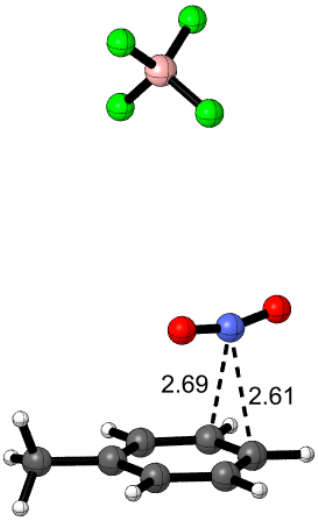
ONIOM(M062X/6-311G*:PM3)

Zero-point correction= 0.157445 (Hartree/Particle)
Thermal correction to Energy= 0.173403
Thermal correction to Enthalpy= 0.174347
Thermal correction to Gibbs Free Energy= 0.111801
Sum of electronic and ZPE= -476.894592
Sum of electronic and thermal Energies= -476.878634
Sum of electronic and thermal Enthalpies= -476.877690
Sum of electronic and thermal Free Energies= -476.940237

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.812	53.944	131.641

6 1.162594 2.052032 0.027483
6 2.420896 1.786859 0.576235
6 3.108754 0.618414 0.257979
6 2.547968 -0.327074 -0.597824
6 1.260489 -0.067365 -1.114869
6 0.587322 1.128557 -0.829996
6 3.299343 -1.563081 -1.003210
1 0.639542 2.965705 0.279393
1 2.869039 2.501467 1.255678
1 4.089707 0.439999 0.683566
1 0.798385 -0.791333 -1.780470
1 -0.401359 1.298649 -1.247357
1 3.868666 -1.363493 -1.914962
1 2.623925 -2.392726 -1.217956
1 4.004169 -1.872292 -0.231650
7 0.364926 -1.033384 1.101319
8 -0.067757 -1.971783 0.658998
8 0.662400 -0.255219 1.849836
9 -1.977631 0.248247 0.949054
5 -2.747493 0.067043 -0.189773
9 -3.948033 -0.510810 0.152936
9 -2.966927 1.277723 -0.805782
9 -2.039679 -0.775329 -1.024216

TS NO2BF4 PCM ONIOM 2.609_94138



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276337070450

Zero-point correction= 0.156436 (Hartree/Particle)
Thermal correction to Energy= 0.173186
Thermal correction to Enthalpy= 0.174131
Thermal correction to Gibbs Free Energy= 0.104413
Sum of electronic and ZPE= -476.889365
Sum of electronic and thermal Energies= -476.872614
Sum of electronic and thermal Enthalpies= -476.871670
Sum of electronic and thermal Free Energies= -476.941388

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.676	54.278	146.734

C,0,-3.3094513666,-1.5601810401,0.1154391825
C,0,-3.5151836577,-0.7721911543,1.2507907225
C,0,-3.513809622,0.6076734124,1.1349944023
C,0,-3.3416619794,1.2365624301,-0.1126472721
C,0,-3.1801378907,0.4411558921,-1.2466085333
C,0,-3.1538260358,-0.9458405401,-1.1389322494
C,0,-3.3200758338,2.7353197005,-0.199059069
H,0,-3.3109278073,-2.641589153,0.192155557
H,0,-3.6584003652,-1.2395436347,2.2175987841
H,0,-3.6502059683,1.2220787223,2.0190580771
H,0,-3.0604484662,0.9070135916,-2.2185508049
H,0,-3.0261785813,-1.5572296931,-2.0256699005
H,0,-3.3873947169,3.0776907173,-1.2310299378
H,0,-2.3922981684,3.1260518242,0.2281196268
H,0,-4.1457446974,3.1692413714,0.3675634328
N,0,-0.7360338145,-1.1364852696,0.0225442567
O,0,-0.4392952885,-2.1639976787,-0.3153149728
O,0,-0.7072313714,-0.0867064979,0.4035093715
F,0,5.3613674993,-0.5403606028,-0.6226608844
B,0,4.4151476502,0.2310319945,0.0187303481
F,0,5.0405289368,1.1714819982,0.8099468911
F,0,3.6281475548,0.8676444416,-0.919099954
F,0,3.6219869904,-0.5781068319,0.8065769258

TS NO2BF4 PCM ONIOM 2.611_93953

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276799127793

Zero-point correction= 0.157066 (Hartree/Particle)
Thermal correction to Energy= 0.173641
Thermal correction to Enthalpy= 0.174585
Thermal correction to Gibbs Free Energy= 0.106473
Sum of electronic and ZPE= -476.888948
Sum of electronic and thermal Energies= -476.872372
Sum of electronic and thermal Enthalpies= -476.871428
Sum of electronic and thermal Free Energies= -476.939540

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.961	54.150	143.354

C,0,-3.1851351685,-1.1370697472,-0.7819697525
C,0,-3.8692077091,-0.4981942687,0.2547543425
C,0,-3.5169693561,0.7922826011,0.6136403913
C,0,-2.5048364517,1.4918553414,-0.070406071
C,0,-1.8587510044,0.8629613648,-1.1344348395
C,0,-2.1831507088,-0.4442963687,-1.4846742468
C,0,-2.12610192,2.8795255219,0.3597490167
H,0,-3.4523393173,-2.1465603433,-1.0737960739
H,0,-4.6591283282,-1.0167380018,0.7843872428
H,0,-4.0309511305,1.2817616621,1.4343353411
H,0,-1.0866655126,1.3912550156,-1.6832062639
H,0,-1.6737569836,-0.9277320913,-2.3112885881
H,0,-1.495644503,2.83937431,1.2527257306
H,0,-3.0105892945,3.4661881024,0.6122874393
H,0,-1.570948711,3.4002711952,-0.4198908877
N,0,-1.0412025106,-1.6306214756,0.6241130087
O,0,-1.0628013505,-0.7450107001,1.3054428202
O,0,-0.7869000475,-2.6215025142,0.1634609924
F,0,4.6525434942,0.793887154,-0.9694176894
B,0,3.8683055771,0.1565381417,-0.0313856429
F,0,4.6582035447,-0.6441683714,0.7670079786
F,0,3.2279972937,1.0950580464,0.7514038404
F,0,2.926630098,-0.6233975742,-0.671230089

TS NO2BF4 PCM ONIOM 2.610_94049

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276300266484

Zero-point correction= 0.156770 (Hartree/Particle)
Thermal correction to Energy= 0.173457
Thermal correction to Enthalpy= 0.174401
Thermal correction to Gibbs Free Energy= 0.105311
Sum of electronic and ZPE= -476.889033
Sum of electronic and thermal Energies= -476.872347
Sum of electronic and thermal Enthalpies= -476.871402
Sum of electronic and thermal Free Energies= -476.940492

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.846	54.161	145.412

C,0,3.3198182545,-1.5280803069,-0.1132524094
C,0,2.9719067116,-0.8256111231,-1.27927259
C,0,2.9397899672,0.565484325,-1.2741872659
C,0,3.2337573345,1.2761887374,-0.1108854678
C,0,3.5977537962,0.5603397676,1.0453403394
C,0,3.6577222184,-0.8229786235,1.0453922282
C,0,3.1586997358,2.7752383753,-0.0700338292
H,0,3.3641322821,-2.6112761288,-0.1270582991
H,0,2.7395505925,-1.3719831021,-2.1868802698
H,0,2.6721567015,1.1012645203,-2.1780927975
H,0,3.8371293035,1.110319138,1.9495903835
H,0,3.9477123575,-1.3585818856,1.9412153786
H,0,4.0673341382,3.1959436059,0.3646703164
H,0,2.3207966775,3.0969390806,0.5544206629
H,0,3.0215844359,3.1964107474,-1.0653830767
N,0,0.7468147841,-1.2027818039,0.1870762578
O,0,0.7419680947,-0.1834310153,0.6433888391
O,0,0.4388144602,-2.2171296846,-0.1787256487
F,0,-3.5420724644,1.0300567449,0.7932016532
B,0,-4.3410304182,0.2264406419,0.0059425192
F,0,-4.960182619,-0.7186799977,0.7970727562
F,0,-5.2920386999,0.9997334224,-0.6255031877
F,0,-3.5604406448,-0.4078154351,-0.9389304927

TS NO2BF4 PCM ONIOM 2.611_94056

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276280398458

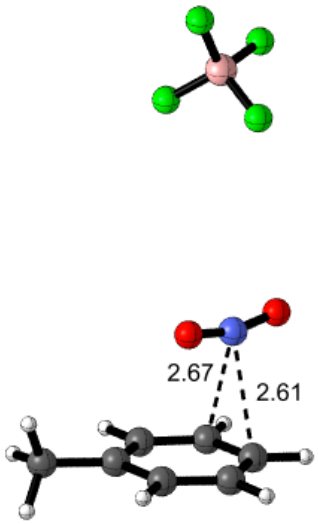
Zero-point correction= 0.156771 (Hartree/Particle)
Thermal correction to Energy= 0.173463
Thermal correction to Enthalpy= 0.174407
Thermal correction to Gibbs Free Energy= 0.105258
Sum of electronic and ZPE= -476.889047
Sum of electronic and thermal Energies= -476.872355
Sum of electronic and thermal Enthalpies= -476.871411
Sum of electronic and thermal Free Energies= -476.940560

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.849	54.163	145.536

C,0,-3.3290279452,-1.5307805045,0.1109179366
C,0,-2.982488655,-0.8286420044,1.2774981483
C,0,-2.9548030649,0.5626025638,1.274172895
C,0,-3.2517515046,1.2738220973,0.1119851672
C,0,-3.613932981,0.5582178572,-1.0449453384
C,0,-3.6695157217,-0.8253226567,-1.0466754257
C,0,-3.1822493898,2.7732113941,0.073111299
H,0,-3.3699318259,-2.6141156485,0.1233957854
H,0,-2.7479811535,-1.3753672985,2.1843378835
H,0,-2.6883904254,1.0980587989,2.1786313333
H,0,-3.855491916,1.1085382395,-1.9484150347
H,0,-3.9581645092,-1.3607136306,-1.9430598035
H,0,-3.042489102,3.193381995,1.0685144297
H,0,-4.094399018,3.1911624245,-0.3569107881
H,0,-2.3483899329,3.0990593793,-0.5545460943
N,0,-0.7558730041,-1.196076506,-0.1878797579
O,0,-0.75550337,-0.1777439524,-0.6463786961
O,0,-0.444127893,-2.2082912874,0.1804683732
F,0,4.9888115223,-0.5668055179,0.9356586827
B,0,4.3664399762,0.2256925513,-0.0061192261
F,0,5.3150634384,0.8757263133,-0.7668816158

F,0,3.5836674784,-0.5642269493,-0.8232907877
F,0,3.568896997,1.1541833421,0.6308886345

TS NO2BF4 PCM ONIOM 2.612_94115



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276652314278

Zero-point correction= 0.156617 (Hartree/Particle)
Thermal correction to Energy= 0.173321
Thermal correction to Enthalpy= 0.174265
Thermal correction to Gibbs Free Energy= 0.104690
Sum of electronic and ZPE= -476.889231
Sum of electronic and thermal Energies= -476.872527
Sum of electronic and thermal Enthalpies= -476.871583
Sum of electronic and thermal Free Energies= -476.941158

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.761	54.240	146.433

C,0,3.1418573429,-1.6764251096,-0.1081662376
C,0,3.4765349531,-0.93414199,-1.2437926861
C,0,3.6761454128,0.4316301192,-1.1330827351
C,0,3.582661498,1.0870951755,0.1095264695
C,0,3.2897424431,0.3317740025,1.2438264442
C,0,3.0591833782,-1.03731418,1.140597703
C,0,3.7890541861,2.5723331009,0.1886468296
H,0,2.9858722967,-2.7471281749,-0.1798575458
H,0,3.5633500173,-1.4229373963,-2.2066265805
H,0,3.9143567299,1.0140456437,-2.0172183854
H,0,3.2256547884,0.8158436477,2.2120069836
H,0,2.8267880735,-1.6171314342,2.0272383772
H,0,2.9750389555,3.0969529478,-0.3188163622
H,0,4.7180151685,2.8603608466,-0.3072769205
H,0,3.8249377421,2.917257244,1.2212984227
N,0,0.6595530302,-0.8680306126,-0.0142666734
O,0,0.7883237896,0.1594232039,-0.434262599
O,0,0.209586049,-1.8249010913,0.3598425383
F,0,-5.13036512,-0.7037884801,0.76761482
B,0,-4.5066046067,0.2391749289,-0.0222856253
F,0,-5.45402977,1.0160925799,-0.6547432312
F,0,-3.7061051096,1.0402010708,0.766297609
F,0,-3.7270442487,-0.3972010425,-0.9665236153

TS NO2BF4 PCM ONIOM 2.613_94064

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276431719226

Zero-point correction= 0.156537 (Hartree/Particle)
Thermal correction to Energy= 0.173222
Thermal correction to Enthalpy= 0.174166
Thermal correction to Gibbs Free Energy= 0.105269
Sum of electronic and ZPE= -476.889376
Sum of electronic and thermal Energies= -476.872691
Sum of electronic and thermal Enthalpies= -476.871747
Sum of electronic and thermal Free Energies= -476.940644

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.699	54.249	145.007

C,0,3.2075474601,-1.4794373705,0.5093753733
C,0,3.8406053965,-0.9263825442,-0.6068713694
C,0,3.7939571153,0.4423344726,-0.8111089998
C,0,3.1484185883,1.2964345822,0.1028102457
C,0,2.5554472671,0.7399803946,1.2351603782
C,0,2.5734037352,-0.6370250963,1.4377876942
C,0,3.1088966202,2.7750493447,-0.1554458275
H,0,3.238018329,-2.5494212882,0.6819221738
H,0,4.3496681382,-1.5681664432,-1.3155594877
H,0,4.2638578757,0.8728234762,-1.68941124
H,0,2.0644795358,1.3832600652,1.956913858
H,0,2.1092324719,-1.0624600785,2.3208426915
H,0,2.5598435044,2.9884712958,-1.0759538043
H,0,4.1190889244,3.1698193104,-0.2826941763
H,0,2.6283385073,3.3111673902,0.6621312335
N,0,0.7947262402,-1.2669586805,-0.4726651369
O,0,0.9199778838,-0.3304075092,-1.068463059
O,0,0.3891444682,-2.2203315048,-0.0438823771
F,0,-5.2100460273,-0.3964140215,0.7994704299
B,0,-4.2641704022,0.2311505713,0.0165443892
F,0,-4.8895509495,1.0300480945,-0.9174885275
F,0,-3.4490426321,1.0076869634,0.8145121064
F,0,-3.4992510506,-0.7181564244,-0.6301275681

TS NO2BF4 PCM ONIOM 2.613_94071

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276821454218

Zero-point correction= 0.156423 (Hartree/Particle)
Thermal correction to Energy= 0.173140
Thermal correction to Enthalpy= 0.174084
Thermal correction to Gibbs Free Energy= 0.105191
Sum of electronic and ZPE= -476.889491
Sum of electronic and thermal Energies= -476.872774
Sum of electronic and thermal Enthalpies= -476.871830
Sum of electronic and thermal Free Energies= -476.940723

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 108.647 54.310 144.997

C,0,3.0224903345,-1.4263357801,0.7635508635
C,0,3.8550301339,-0.9749464128,-0.2633723677
C,0,3.8578583074,0.3679425871,-0.601687913
C,0,3.0627826395,1.2994864119,0.0923279105
C,0,2.2658275823,0.8465190361,1.142191704
C,0,2.2327955965,-0.5056392688,1.4725750561
C,0,3.0801712193,2.7463679762,-0.3087432271
H,0,3.0126219705,-2.4747817078,1.040055968
H,0,4.4816700033,-1.6751251481,-0.8021412307
H,0,4.486547015,0.7161517913,-1.4146770705
H,0,1.6556380442,1.5498835791,1.6979545513
H,0,1.6073290036,-0.8486781569,2.2896445963
H,0,2.5151111891,3.3614915846,0.3906382766
H,0,2.6438797503,2.8717747903,-1.3032447731
H,0,4.1040149503,3.1224806015,-0.3546812017
N,0,0.82391867,-1.3146699784,-0.6456226419
O,0,1.0829337801,-0.4590288523,-1.3157535668
O,0,0.3198220076,-2.2083923599,-0.1930486656
F,0,-3.3319368184,1.0327271952,0.8168214364
B,0,-4.1424033843,0.2393501755,0.0307931039
F,0,-5.0903237922,1.023613844,-0.5917835974
F,0,-3.372674073,-0.3964201888,-0.9219640871
F,0,-4.7653561295,-0.7043137187,0.8204098761

TS NO2BF4 PCM ONIOM 2.615_93981

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276549001638

Zero-point correction= 0.157000 (Hartree/Particle)
Thermal correction to Energy= 0.173600
Thermal correction to Enthalpy= 0.174545
Thermal correction to Gibbs Free Energy= 0.106270
Sum of electronic and ZPE= -476.889079
Sum of electronic and thermal Energies= -476.872479
Sum of electronic and thermal Enthalpies= -476.871534
Sum of electronic and thermal Free Energies= -476.939809

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 108.936 54.169 143.695

C,0,3.1196291982,-1.0808566656,0.8080661191
C,0,3.7985115228,-0.4226485134,-0.2204279618
C,0,3.4026591545,0.8498516611,-0.5967407263
C,0,2.3489746754,1.5137491368,0.0605114995
C,0,1.7029568685,0.8647695748,1.111529413
C,0,2.0736508322,-0.4257038764,1.4803448496
C,0,1.941791196,2.8910005313,-0.3778143084
H,0,3.4219625001,-2.075619746,1.1152601751
H,0,4.6189361356,-0.9131240327,-0.7300387553
H,0,3.9145381098,1.3539158729,-1.4100582988
H,0,0.8965857839,1.363629141,1.6379740843
H,0,1.5654742515,-0.9230810774,2.2994573387
H,0,2.807601422,3.5552922789,-0.4131860066
H,0,1.2015711975,3.3214271574,0.2957237416
H,0,1.5143785617,2.8611657411,-1.3834551806
N,0,1.0219673041,-1.6849087066,-0.6318777582
O,0,1.0275033153,-0.8113089123,-1.3282589771
O,0,0.7981750005,-2.6756490282,-0.1561079368
F,0,-2.927252812,-0.4902361943,0.9725884872
B,0,-3.7106899216,0.147416636,0.0323470408
F,0,-4.3258879968,-0.7956109265,-0.7646074416
F,0,-4.6649648154,0.9126932271,0.6684029762
F,0,-2.9148494839,0.9583627209,-0.7504803736

TS NO2BF4 PCM ONIOM 2.622_94034

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276107961845

Zero-point correction= 0.156649 (Hartree/Particle)
Thermal correction to Energy= 0.173357
Thermal correction to Enthalpy= 0.174302
Thermal correction to Gibbs Free Energy= 0.105680
Sum of electronic and ZPE= -476.889379
Sum of electronic and thermal Energies= -476.872670
Sum of electronic and thermal Enthalpies= -476.871726
Sum of electronic and thermal Free Energies= -476.940348

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 108.783 54.263 144.427

C,0,3.3948242133,-0.8389460343,0.6037496846
C,0,3.7721539307,-0.0666775372,-0.4973071118
C,0,3.1079355413,1.1198846919,-0.7606445035
C,0,2.0777848345,1.5844757159,0.0785899169
C,0,1.7346063819,0.8267338107,1.1973900247
C,0,2.3772500919,-0.3810001995,1.4572450621
C,0,1.3734327192,2.8710879859,-0.2434363144
H,0,3.907835837,-1.7686402366,0.8224163757
H,0,4.5691274989,-0.4031991637,-1.149044871
H,0,3.3853369834,1.7098321009,-1.6282818991
H,0,0.9522513046,1.173543422,1.8634870744
H,0,2.1027057769,-0.9649724716,2.3291172233
H,0,0.6774999295,3.1545490591,0.5452056759
H,0,0.8137067586,2.7774017282,-1.1776059465
H,0,2.094095311,3.6801577302,-0.3782249101
N,0,1.2120651589,-1.777031207,-0.5071644015
O,0,1.2381728141,-2.7932986149,-0.0347681514
O,0,0.9631084816,-0.9062733554,-1.1598973717
F,0,-4.6528966211,0.6911334075,0.7842058976
B,0,-3.7002073634,0.0495005246,0.0214102305
F,0,-2.9064324461,0.9844139664,-0.6102517746
F,0,-2.9147686012,-0.7413766948,0.83530138
F,0,-4.3180095353,-0.7416496284,-0.9247892903

TS NO2BF4 PCM ONIOM 2.629_93709

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276064279501

Zero-point correction= 0.157132 (Hartree/Particle)
Thermal correction to Energy= 0.173324
Thermal correction to Enthalpy= 0.174268
Thermal correction to Gibbs Free Energy= 0.110282
Sum of electronic and ZPE= -476.890187

Sum of electronic and thermal Energies= -476.873995
Sum of electronic and thermal Enthalpies= -476.873051
Sum of electronic and thermal Free Energies= -476.937037

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.763	54.005	134.671

C,0,-2.7170462734,-0.2931307136,1.263782627
C,0,-1.3163721188,-0.340497541,1.3670979738
C,0,-0.5317036628,0.6062740058,0.7137601153
C,0,-1.1237923323,1.5997194367,-0.0645095098
C,0,-2.5277503934,1.6427183476,-0.1488893955
C,0,-3.3189955139,0.7204780963,0.5166900268
C,0,-0.2952446922,2.6204416713,-0.7904444944
H,0,-3.3235841378,-1.0217112166,1.7895297544
H,0,-0.8459819185,-1.1120653305,1.9670876845
H,0,0.5531532266,0.5528335885,0.7890910265
H,0,-2.9939689007,2.4170263624,-0.7491131178
H,0,-4.3983331205,0.7744119775,0.4444080357
H,0,-0.3744829626,3.5911683855,-0.2941882526
H,0,-0.6449522602,2.7496387761,-1.816178538
H,0,0.7573828297,2.336167493,-0.8134878494
N,0,-1.9630654861,-1.729572798,-0.8059289005
O,0,-1.8408432789,-0.9069040518,-1.5506837675
O,0,-2.0689855834,-2.7368849573,-0.3255847113
F,0,3.1532528531,0.7755089808,1.0269810754
B,0,3.1026883565,-0.2014699505,0.054469445
F,0,4.3854656577,-0.5713058083,-0.2926584696
F,0,2.4277354348,-1.3034037357,0.5407803481
F,0,2.451556277,0.2823699818,-1.0621381061

TS NO2BF4 PCM ONIOM 2.635_93808

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.275285670989

Zero-point correction= 0.157062 (Hartree/Particle)
Thermal correction to Energy= 0.173401
Thermal correction to Enthalpy= 0.174345
Thermal correction to Gibbs Free Energy= 0.108630
Sum of electronic and ZPE= -476.889651
Sum of electronic and thermal Energies= -476.873312
Sum of electronic and thermal Enthalpies= -476.872368
Sum of electronic and thermal Free Energies= -476.938082

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.811	54.069	138.308

C,0,-1.368715425,0.663147184,1.4948294022
C,0,-2.765110848,0.6942260621,1.4473503522
C,0,-3.4439236979,-0.2140282207,0.6519093833
C,0,-2.7562304148,-1.1916017019,-0.0893704684
C,0,-1.3648433836,-1.2366447511,-0.0078228458
C,0,-0.6704801596,-0.3146936256,0.7699612437
C,0,-3.5210641608,-2.1574289553,-0.9483776656
H,0,-0.825940152,1.3665601541,2.1162379102
H,0,-3.3110081344,1.4342093866,2.0197650272
H,0,-4.5271540055,-0.1793620431,0.5992941311
H,0,-0.8171913522,-1.9917697755,-0.5609707996
H,0,0.4151440785,-0.3581138695,0.823231277
H,0,-4.0171823936,-1.631651269,-1.7681181132
H,0,-4.2985913736,-2.6575619327,-0.3675714794
H,0,-2.8663557281,-2.9160867434,-1.3756685536
N,0,-1.0708340577,1.8293555623,-0.8501019731
O,0,-0.1976994675,2.4632723305,-0.5533856607
O,0,-1.9367653842,1.3738866243,-1.3860390643
F,0,2.8100212727,0.4685828514,0.937681276
B,0,3.4187055443,-0.3436897351,0.0031481093
F,0,4.2003192678,-1.2811119331,0.6447433902
F,0,2.4567070139,-0.9832214934,-0.7516714197
F,0,4.2074949614,0.428416894,-0.824636459

TS NO2BF4 PCM ONIOM 2.677_94011

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.277990728277

Zero-point correction= 0.157761 (Hartree/Particle)
Thermal correction to Energy= 0.173818
Thermal correction to Enthalpy= 0.174763
Thermal correction to Gibbs Free Energy= 0.111701
Sum of electronic and ZPE= -476.894037
Sum of electronic and thermal Energies= -476.877980
Sum of electronic and thermal Enthalpies= -476.877036
Sum of electronic and thermal Free Energies= -476.940097

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.073	53.859	132.724

C,0,-1.0167931141,0.6546539756,1.52626604
C,0,-2.2990088058,1.0955655399,1.1690867471
C,0,-3.1170585723,0.2913891123,0.3855843569
C,0,-2.6766441813,-0.9592999878,-0.0591211476
C,0,-1.3973484339,-1.3933992,0.3152810796
C,0,-0.5750966505,-0.6028718646,1.1071760951
C,0,-3.5430288791,-1.8106946082,-0.9437312266
H,0,-0.3811942374,1.2760124438,2.1475500179
H,0,-2.6542185414,2.0591747718,1.5157718749
H,0,-4.1081653425,0.6364115615,0.1125184195
H,0,-1.0453509355,-2.361810367,-0.0238930574
H,0,0.4224270008,-0.9448522609,1.370964448
H,0,-3.3321439386,-1.5997566066,-1.9962107429
H,0,-4.6009209354,-1.6119900618,-0.7715251193
H,0,-3.3547284525,-2.8715408394,-0.7768710517
N,0,-0.408345002,1.6853649948,-0.8696071573
O,0,0.0884334374,2.5856723793,-0.4331813499
O,0,-0.8312157186,0.887663773,-1.5200562673
F,0,2.4643425372,-1.7621210008,-0.1613232214
B,0,2.8234332436,-0.4402276232,-0.0176409319
F,0,2.9676520273,-0.1341389008,1.3177089518
F,0,4.0078924533,-0.2078779038,-0.6812561056
F,0,1.8363940412,0.3665336728,-0.5652726519

TS NO2BF4 PCM ONIOM 2.682_93941

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.277735092828

Zero-point correction= 0.158019 (Hartree/Particle)
Thermal correction to Energy= 0.173952
Thermal correction to Enthalpy= 0.174897
Thermal correction to Gibbs Free Energy= 0.112396
Sum of electronic and ZPE= -476.893796
Sum of electronic and thermal Energies= -476.877863
Sum of electronic and thermal Enthalpies= -476.876919
Sum of electronic and thermal Free Energies= -476.939419

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.157	53.774	131.543

C,0,-1.0207411657,0.6534675118,1.5263236065
C,0,-2.2994375449,1.0973039372,1.1654703933
C,0,-3.117590623,0.2953410304,0.3770750003
C,0,-2.6788048175,-0.9542082167,-0.0673439985
C,0,-1.3997246597,-1.3911406695,0.3095809906
C,0,-0.579285103,-0.6046811057,1.1052253285
C,0,-3.5440513631,-1.8218325778,-0.9372420806
H,0,-0.3853208824,1.2728916106,2.1497339728
H,0,-2.6537458569,2.0616602361,1.5110485606
H,0,-4.1063061267,0.6437191132,0.1006015769
H,0,-1.0483100067,-2.3587783708,-0.0332194102
H,0,0.4177655663,-0.9476179631,1.3695793122
H,0,-4.5305260858,-1.3830793431,-1.0834829269
H,0,-3.6682801604,-2.8108144532,-0.4913803389
H,0,-3.0834922845,-1.9645120946,-1.9179770629
N,0,-0.4032232657,1.6936065265,-0.8701806119
O,0,0.0906409865,2.592535309,-0.4281434221
O,0,-0.8223463573,0.8953343874,-1.5219544042
F,0,4.0091640572,-0.211715705,-0.6754599702
B,0,2.8224784046,-0.4421480664,-0.0151514308
F,0,2.4577728085,-1.7616615465,-0.1664147733
F,0,2.9657560083,-0.1437782211,1.3220459733
F,0,1.8400964721,0.3719026714,-0.5603382845

TS NO2BF4 PCM ONIOM 2.684_93988

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.277678376338

Zero-point correction= 0.157775 (Hartree/Particle)
Thermal correction to Energy= 0.173751
Thermal correction to Enthalpy= 0.174696
Thermal correction to Gibbs Free Energy= 0.111918
Sum of electronic and ZPE= -476.894012
Sum of electronic and thermal Energies= -476.878036
Sum of electronic and thermal Enthalpies= -476.877092
Sum of electronic and thermal Free Energies= -476.939870

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.031	53.837	132.127

C,0,-1.0149183164,0.6485224514,1.5297841378
C,0,-2.2944213392,1.094042334,1.1724346355
C,0,-3.1149385925,0.2938705021,0.3855385963
C,0,-2.6781717096,-0.9559204435,-0.0618921704
C,0,-1.3998088571,-1.3950904181,0.3127645785
C,0,-0.5762896707,-0.6095674403,1.1071728457
C,0,-3.5425641648,-1.8097925219,-0.9460411757
H,0,-0.3775723186,1.2666285275,2.1525242999
H,0,-2.6472572039,2.0580184107,1.5205826672
H,0,-4.104436673,0.643068586,0.1125816311
H,0,-1.0506451487,-2.3635641831,-0.0297675655
H,0,0.4204241034,-0.9545317226,1.3701481197
H,0,-3.5062986754,-2.8550430398,-0.6353981227
H,0,-3.1901909069,-1.7647239458,-1.9802922249
H,0,-4.5801883673,-1.4775282543,-0.9298705636
N,0,-0.4075657098,1.6882032406,-0.873354704
O,0,0.0854516011,2.5883823289,-0.4333203468
O,0,-0.8280881043,0.8876088521,-1.5211790391
F,0,1.8359087115,0.368621953,-0.5644665109
B,0,2.8222728194,-0.4385707053,-0.0162447601
F,0,2.4638958027,-1.7604313923,-0.162030013
F,0,4.0077098316,-0.2051368112,-0.6777531851
F,0,2.9643388885,-0.1339953082,1.31967987

TS NO2BF4 PCM ONIOM 2.693_94047

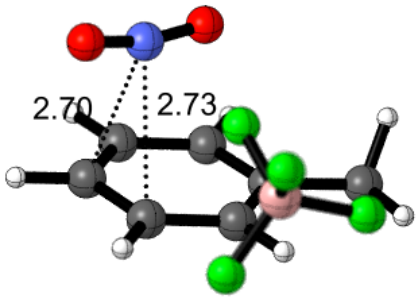
ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.278733764858

Zero-point correction= 0.157605 (Hartree/Particle)
Thermal correction to Energy= 0.173752
Thermal correction to Enthalpy= 0.174697
Thermal correction to Gibbs Free Energy= 0.110995
Sum of electronic and ZPE= -476.893866
Sum of electronic and thermal Energies= -476.877718
Sum of electronic and thermal Enthalpies= -476.876774
Sum of electronic and thermal Free Energies= -476.940476

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.031	53.909	134.071

C,0,-1.9710484295,-1.1388058593,-1.2792846128
C,0,-3.1092259835,-0.7678585052,-0.5612491217
C,0,-3.1486081812,0.4616202217,0.0795415164
C,0,-2.0688343092,1.3564459554,0.0061755954
C,0,-0.9478050077,0.9894850043,-0.7403880898
C,0,-0.8917428627,-0.2479391618,-1.374923141
C,0,-2.1209628474,2.6672139285,0.7386932447
H,0,-1.9308322235,-2.0964383566,-1.7857098687
H,0,-3.9545498644,-1.4421040755,-0.4986009583
H,0,-4.0276472368,0.7422789257,0.6500516451
H,0,-0.0955227686,1.6598748122,-0.8035738181
H,0,-0.0057241961,-0.5256650632,-1.9369433534
H,0,-1.3784764944,3.3668556811,0.3556763072
H,0,-1.9222663533,2.5150758191,1.803258911
H,0,-3.1078240187,3.1242039094,0.652305364
N,0,-0.5299459837,-1.6993452272,0.9264021151
O,0,-0.9406385848,-0.9067382833,1.5918059868
O,0,-0.0243222606,-2.5923275535,0.4834354033
F,0,1.632626258,-0.3080600916,0.4256453401
B,0,2.7692503742,0.3130130217,-0.0702201201
F,0,3.2144796789,-0.3814783983,-1.1736185876
F,0,2.4728009674,1.6109391124,-0.422367258
F,0,3.7419973274,0.3077401841,0.9057085004

TS NO2BF4 PCM ONIOM 2.701_94088



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.278953217307

Zero-point correction= 0.157420 (Hartree/Particle)
Thermal correction to Energy= 0.173557
Thermal correction to Enthalpy= 0.174501
Thermal correction to Gibbs Free Energy= 0.110945
Sum of electronic and ZPE= -476.894402
Sum of electronic and thermal Energies= -476.878265
Sum of electronic and thermal Enthalpies= -476.877321
Sum of electronic and thermal Free Energies= -476.940877

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.909	53.925	133.764

C,0,1.9765542662,-1.0795331913,1.2912844969
C,0,3.0913080629,-0.6243938626,0.5854724117
C,0,3.0405650283,0.5963925347,-0.0703197674
C,0,1.8901834759,1.402719156,-0.0250441598
C,0,0.7907174647,0.9514768017,0.7041431096
C,0,0.8260611657,-0.2797700687,1.3544350618
C,0,1.8632781214,2.7182666793,-0.7502434448
H,0,2.0061095431,-2.0318374001,1.8080714397
H,0,3.9893211564,-1.2284939134,0.5425322621
H,0,3.9026233158,0.9400344144,-0.6326083896
H,0,-0.1210671873,1.5426124855,0.7390806288
H,0,-0.0486638354,-0.6208284268,1.9010953363
H,0,2.6391965208,3.3831178385,-0.3643454733
H,0,0.9001434398,3.2150698863,-0.6378957523
H,0,2.0567570382,2.577105315,-1.8159137816
N,0,0.5794721697,-1.762734616,-0.9185829284
O,0,0.9777948632,-0.9749079694,-1.5971888283
O,0,0.0986779013,-2.6637438864,-0.4640688699
F,0,-2.5057061004,0.2193259369,1.4408649788
B,0,-2.6579664105,0.2875306978,0.0734703039
F,0,-2.5456307729,1.5937726518,-0.3490189358
F,0,-1.6750884126,-0.4780040949,-0.537532773
F,0,-3.8928848142,-0.2106219683,-0.2795919255

TS NO2BF4 PCM ONIOM 2.704_94050

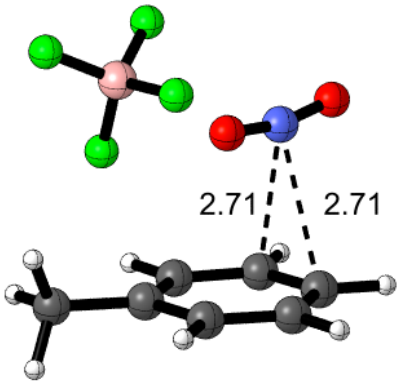
ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.278838719430

Zero-point correction= 0.157559 (Hartree/Particle)
Thermal correction to Energy= 0.173652
Thermal correction to Enthalpy= 0.174597
Thermal correction to Gibbs Free Energy= 0.111322
Sum of electronic and ZPE= -476.894264
Sum of electronic and thermal Energies= -476.878170
Sum of electronic and thermal Enthalpies= -476.877226
Sum of electronic and thermal Free Energies= -476.940501

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.969	53.894	133.174

C,0,1.9715952026,-1.0799432063,-1.2941516224
C,0,0.8229693975,-0.2773893443,-1.3561354884
C,0,0.7915618952,0.9540926975,-0.7064387747
C,0,1.8932394482,1.4030311879,0.0212537759
C,0,3.0416054174,0.594147815,0.0650867954
C,0,3.0883277884,-0.6272858636,-0.5900710785
C,0,1.8651580401,2.7132307959,0.7561970318
H,0,1.9985481718,-2.0320030507,-1.8115216483
H,0,-0.0528564376,-0.6161938028,-1.9024086211
H,0,-0.1183115953,1.5481562199,-0.7414009548
H,0,3.9059405518,0.9365139214,0.6245620208
H,0,3.9854395915,-1.2328732011,-0.5492166902
H,0,1.8869622149,2.5482353827,1.8363951944
H,0,0.9686034973,3.2844495215,0.5172825847
H,0,2.7382705583,3.3170470902,0.5017316922
N,0,0.5806384726,-1.7596743155,0.9228404845
O,0,0.9788379699,-0.9684788417,1.5973835391
O,0,0.1010570164,-2.6621227139,0.4703235097
F,0,-1.6736620529,-0.4775328617,0.5364412099
B,0,-2.6579110368,0.2868604786,-0.0737736271
F,0,-2.5459789371,1.5933942414,0.3478953663
F,0,-2.5075163205,0.2182343619,-1.4413443418
F,0,-3.8919528537,-0.2121695124,0.2811446426

TS NO2BF4 PCM ONIOM 2.707_94118 (6b‡)



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.279306447119

Zero-point correction= 0.157378 (Hartree/Particle)
Thermal correction to Energy= 0.173583
Thermal correction to Enthalpy= 0.174528
Thermal correction to Gibbs Free Energy= 0.110257
Sum of electronic and ZPE= -476.894062
Sum of electronic and thermal Energies= -476.877857
Sum of electronic and thermal Enthalpies= -476.876912
Sum of electronic and thermal Free Energies= -476.941183

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 108.925 54.011 135.269

C,0,2.3215255531,-1.0762211587,1.1383689184
C,0,3.270536233,-0.5009921066,0.2930659736
C,0,3.02550623,0.7417530586,-0.2725311943
C,0,1.8456986966,1.4524578568,0.0066482872
C,0,0.9168480258,0.8833693305,0.8768664558
C,0,1.1432523001,-0.3739016818,1.4333679999
C,0,1.6019405633,2.7902196422,-0.6328861843
H,0,2.5007259598,-2.0473157729,1.5854871041
H,0,4.1892151072,-1.0289619709,0.0688546777
H,0,3.7559535961,1.1782534454,-0.9457960294
H,0,-0.0103779224,1.4045641726,1.0974265787
H,0,0.4027608163,-0.8093525217,2.0960194833
H,0,2.4276919562,3.4734350406,-0.4243457612
H,0,0.6800288602,3.2426982856,-0.2690482559
H,0,1.5290206364,2.6899341734,-1.7186168035
N,0,0.6044614291,-1.7295835898,-0.8495629621
O,0,0.8948576018,-0.9166578677,-1.5533535414
O,0,0.2023369755,-2.6541150058,-0.3657284551
F,0,-2.5797991112,0.9922755677,1.1987205634
B,0,-2.7654216009,0.2255606728,0.0696923816
F,0,-3.8118480238,-0.6477883708,0.2697760571
F,0,-3.0388137881,1.0400672759,-1.0073135994
F,0,-1.6147580941,-0.5019934753,-0.1941886943

TS NO2BF4 PCM ONIOM 2.712_94072

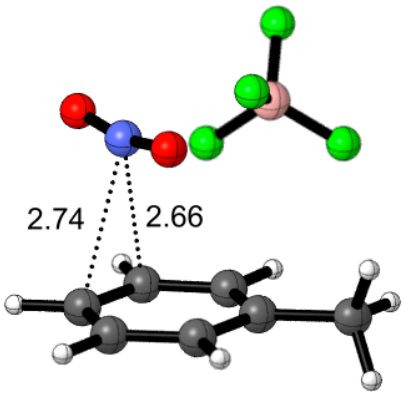
ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.278797036640

Zero-point correction= 0.157425 (Hartree/Particle)
Thermal correction to Energy= 0.173604
Thermal correction to Enthalpy= 0.174548
Thermal correction to Gibbs Free Energy= 0.110732
Sum of electronic and ZPE= -476.894027
Sum of electronic and thermal Energies= -476.877848
Sum of electronic and thermal Enthalpies= -476.876903
Sum of electronic and thermal Free Energies= -476.940720

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 108.938 54.006 134.313

C,0,2.3119519558,-1.0678310163,1.1438175581
C,0,3.2595746539,-0.4955513001,0.2946029718
C,0,3.0137744648,0.7452071681,-0.2750341343
C,0,1.8340765867,1.4560464413,0.0029561804
C,0,0.9058595774,0.8889566528,0.8754882816
C,0,1.1339407858,-0.3653769983,1.437618523
C,0,1.5894094139,2.7921754403,-0.6397962513
H,0,2.4923478007,-2.0373372449,1.5939597731
H,0,4.1780695789,-1.0242134344,0.0710904125
H,0,3.743472686,1.1796570861,-0.9504489327
H,0,-0.0214957061,1.4103700631,1.0949319694
H,0,0.3938313763,-0.7990118418,2.1019190504
H,0,0.6678055408,3.2454375343,-0.2761421307
H,0,1.515540271,2.6894497892,-1.7252318993
H,0,2.415203635,3.4760541964,-0.4335486222
N,0,0.6033066316,-1.7392391212,-0.8517826992
O,0,0.878079132,-0.9151886295,-1.5481504066
O,0,0.2208354099,-2.6711890063,-0.3675434193
F,0,-3.8458304912,-0.5965395241,0.2368745085
B,0,-2.7518393751,0.2240322034,0.0704776734
F,0,-2.5887958203,1.0111160547,1.1889303439
F,0,-1.6239478751,-0.5606739833,-0.1171657801
F,0,-2.9328202325,1.0212974705,-1.0385899706

TS NO2BF4 PCM ONIOM 2.742_94075



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.281649295723

Zero-point correction= 0.157282 (Hartree/Particle)
Thermal correction to Energy= 0.173358
Thermal correction to Enthalpy= 0.174302
Thermal correction to Gibbs Free Energy= 0.111129
Sum of electronic and ZPE= -476.894598
Sum of electronic and thermal Energies= -476.878522
Sum of electronic and thermal Enthalpies= -476.877578
Sum of electronic and thermal Free Energies= -476.940751

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 108.784 53.994 132.960

C,0,-2.1758758775,-1.1605793379,1.1659709875
C,0,-1.0036682114,-0.4225299404,1.3900926485
C,0,-0.8454798091,0.8435373145,0.8243591998
C,0,-1.8385385901,1.384336082,0.0111163724
C,0,-3.0089259289,0.6364570947,-0.2001872126
C,0,-3.1849938244,-0.6146508683,0.3763634323
C,0,-1.6752957276,2.7267264907,-0.6444584712
H,0,-2.2985541947,-2.1361610845,1.6219081051
H,0,-0.211501113,-0.8342483285,2.0086050299
H,0,0.0819794638,1.3865097724,0.9896497199
H,0,-3.7891397156,1.04995284,-0.8306392372
H,0,-4.0990257105,-1.1683914424,0.2013396595
H,0,-1.6456284619,2.6213676374,-1.7317241379
H,0,-0.7573414661,3.2178462159,-0.3236922597
H,0,-2.5181584396,3.3774968311,-0.4036317123
N,0,-0.4320162787,-1.6586770531,-0.8911414942
O,0,-0.9201033941,-0.9533677078,-1.6030754113
O,0,0.160840161,-2.4826399997,-0.4198615699
F,0,1.6785127479,-0.0832303557,-0.8760443011

B,0,2.6101072289,0.2807360038,0.0856367947
F,0,3.8635838047,-0.1078006484,-0.3304456661
F,0,2.5797682523,1.6446201609,0.2695127468
F,0,2.2866250845,-0.3641566768,1.2604547769

TS NO2BF4 PCM ONIOM 2.776_93985

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.281369632739

Zero-point correction= 0.157929 (Hartree/Particle)
Thermal correction to Energy= 0.173892
Thermal correction to Enthalpy= 0.174836
Thermal correction to Gibbs Free Energy= 0.112232
Sum of electronic and ZPE= -476.894156
Sum of electronic and thermal Energies= -476.878194
Sum of electronic and thermal Enthalpies= -476.877249
Sum of electronic and thermal Free Energies= -476.939853

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.119	53.794	131.760

C,0,-2.1592162888,-1.2691328579,1.0968431457
C,0,-1.0647400636,-0.4548409042,1.4254238728
C,0,-0.9600667674,0.8339133152,0.90252836
C,0,-1.931724389,1.3270626062,0.0323801525
C,0,-3.0262369922,0.505289644,-0.2793599879
C,0,-3.1472747848,-0.7739488307,0.2504821682
C,0,-1.8022711025,2.6893226631,-0.5891385618
H,0,-2.2425900724,-2.2634510131,1.519587532
H,0,-0.2929961084,-0.8277041222,2.092210775
H,0,-0.0936751127,1.441126681,1.1512616263
H,0,-3.7915001786,0.8808657368,-0.9504644224
H,0,-4.0042341865,-1.3860200902,-0.0026815437
H,0,-2.7752052678,3.17325231,-0.6815672184
H,0,-1.3792871148,2.6079344008,-1.5944806738
H,0,-1.1465436485,3.3320372856,-0.0021235174
N,0,-0.2353581887,-1.5673033644,-0.8832901832
O,0,-0.750379684,-0.8741413085,-1.5866986848
O,0,0.3882131071,-2.356687437,-0.397231002
F,0,2.0839242704,-0.5744424092,1.0235325738
B,0,2.5690190161,0.3206601807,0.0904948053
F,0,2.4754403533,1.6057498744,0.572404079
F,0,3.876349794,0.0220457672,-0.2152541088
F,0,1.7837514099,0.1811148724,-1.0434231863

TS NO2BF4 PCM ONIOM 2.967_93897

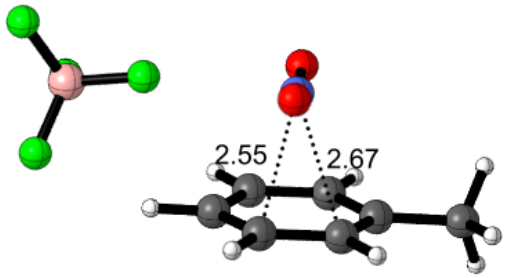
ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.286733098719

Zero-point correction= 0.157529 (Hartree/Particle)
Thermal correction to Energy= 0.173441
Thermal correction to Enthalpy= 0.174385
Thermal correction to Gibbs Free Energy= 0.112496
Sum of electronic and ZPE= -476.893942
Sum of electronic and thermal Energies= -476.878030
Sum of electronic and thermal Enthalpies= -476.877086
Sum of electronic and thermal Free Energies= -476.938974

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.836	53.968	130.255

C,0,0.5150953323,1.3864896702,0.5293945678
C,0,0.9150109798,0.3146227384,1.3312595361
C,0,2.1716666343,-0.2921581852,1.1422732745
C,0,3.0321170754,0.1514104175,0.1417984112
C,0,2.6001162069,1.2043081384,-0.6721943744
C,0,1.3609377491,1.8197301208,-0.4823093835
C,0,4.3803656685,-0.4783994172,-0.0768821301
H,0,-0.461218166,1.8382681677,0.6749470812
H,0,0.2584363433,-0.0442841529,2.1179149498
H,0,2.4708265221,-1.107663799,1.7921439811
H,0,3.2474870895,1.5525823865,-1.4703359001
H,0,1.0606404219,2.6324605526,-1.1321854404
H,0,5.1723197943,0.2623806827,0.0491047078
H,0,4.4638432378,-0.8769383567,-1.090056717
H,0,4.5581142136,-1.2898977019,0.6279722
N,0,0.2567097919,-1.3998875899,-0.4586812227
O,0,0.6532860251,-0.929133621,-1.3933778436
O,0,-0.2547338205,-2.1184359992,0.2360694752
F,0,-2.0450437022,-0.1703730071,-1.1002249315
B,0,-2.8339244033,0.1696770229,-0.0120586857
F,0,-4.0556286177,-0.4539421713,-0.1130910553
F,0,-2.1696181306,-0.2732395659,1.1154112349
F,0,-3.0003012455,1.5340456693,0.0400682647

TS NO2BF4 PCM ONIOM 2.998_94196 (6a‡)



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.285542011062

Zero-point correction= 0.157344 (Hartree/Particle)
Thermal correction to Energy= 0.173485
Thermal correction to Enthalpy= 0.174429
Thermal correction to Gibbs Free Energy= 0.109301
Sum of electronic and ZPE= -476.893257
Sum of electronic and thermal Energies= -476.877116
Sum of electronic and thermal Enthalpies= -476.876172
Sum of electronic and thermal Free Energies= -476.941300

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.863	53.951	137.074

C,0,0.3947296521,-1.1883715728,0.6862498997
C,0,1.1040211645,-1.7910502132,-0.3440539161
C,0,2.4065960889,-1.3801134014,-0.6409877201
C,0,3.0368291717,-0.3627020573,0.0798424992

C,0,2.3083297344,0.2610990745,1.0920428013
C,0,0.9921223037,-0.144354218,1.3929849978
C,0,4.4496317367,0.0439271191,-0.2376442475
H,0,-0.6259904464,-1.4859349479,0.9081100116
H,0,0.6470993888,-2.5814317025,-0.9272966141
H,0,2.9423011255,-1.8646935455,-1.4507270029
H,0,2.7618781328,1.0591778526,1.6710342903
H,0,0.4544898883,0.3482034576,2.1960341571
H,0,5.1382466032,-0.7757707321,-0.0227544029
H,0,4.7565250617,0.907269529,0.3522041183
H,0,4.5565695618,0.2924298118,-1.2952358331
N,0,0.5713564188,1.5858066627,-0.4372626633
O,0,0.716085983,0.9861807251,-1.371218658
O,0,0.3088265442,2.4378858596,0.2468897907
F,0,-3.0694977601,-0.5760204515,1.2779384867
B,0,-2.954745117,-0.1764248109,-0.0352918729
F,0,-2.7376305123,-1.2724252236,-0.8412449412
F,0,-4.1072111267,0.4663268963,-0.4304621832
F,0,-1.8864165977,0.6999918882,-0.1584209976

TS NO2BF4 PCM ONIOM 3.076_93756

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.285711715731

Zero-point correction= 0.158386 (Hartree/Particle)
Thermal correction to Energy= 0.173688
Thermal correction to Enthalpy= 0.174633
Thermal correction to Gibbs Free Energy= 0.114875
Sum of electronic and ZPE= -476.894053
Sum of electronic and thermal Energies= -476.878750
Sum of electronic and thermal Enthalpies= -476.877806
Sum of electronic and thermal Free Energies= -476.937563

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.991	53.385	125.770

C,0,-3.2547581362,-0.6243801209,0.3870708919
C,0,-2.1705069763,-0.6130023114,1.2651373096
C,0,-1.183492014,0.3822556807,1.1604210931
C,0,-1.2618157108,1.379338248,0.1803338293
C,0,-2.3346118501,1.3290216903,-0.7074760857
C,0,-3.3218475058,0.3405602225,-0.6064224011
C,0,-0.2109138543,2.4496910932,0.1007971388
H,0,-4.0214984837,-1.3833562729,0.4753522742
H,0,-2.0933817816,-1.3599635944,2.0474379093
H,0,-0.3502279043,0.3837170879,1.8592900893
H,0,-2.4110520295,2.0741178498,-1.4918926883
H,0,-4.1435904222,0.3364673427,-1.31225482
H,0,-0.2289312769,3.0655663939,1.0023267477
H,0,-0.3731445985,3.1010088961,-0.7567849371
H,0,0.807218023,2.0169905486,0.0233614652
N,0,-0.4656414518,-1.6250596029,-0.4423968186
O,0,-0.8558205681,-1.1824418475,-1.3919697122
O,0,0.0730068675,-2.2825523226,0.2892455239
F,0,1.9891051138,-0.4175918161,1.1360055462
B,0,2.5716178752,0.0796740249,-0.0125017901
F,0,2.5123649356,1.4572321756,-0.0067490859
F,0,3.8752202029,-0.3446573073,-0.1082981308
F,0,1.8351885461,-0.406081058,-1.0813093488

TS NO2BF4 PCM ONIOM 3.092_93919

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.284342827126

Zero-point correction= 0.157445 (Hartree/Particle)
Thermal correction to Energy= 0.173463
Thermal correction to Enthalpy= 0.174407
Thermal correction to Gibbs Free Energy= 0.111649
Sum of electronic and ZPE= -476.893404
Sum of electronic and thermal Energies= -476.877387
Sum of electronic and thermal Enthalpies= -476.876442
Sum of electronic and thermal Free Energies= -476.939200

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.849	53.908	132.084

C,0,-0.3795939688,-1.4128422029,0.286873647
C,0,-0.7152745902,-0.3940532377,1.1745072438
C,0,-2.0064182075,0.1686041654,1.1561314904
C,0,-2.9764871084,-0.2854556067,0.2575536827
C,0,-2.610720037,-1.2867892962,-0.6409069363
C,0,-1.3287022079,-1.8443143649,-0.6313826168
C,0,-4.3561222921,0.3133778652,0.2299328849
H,0,0.6239628991,-1.8269392216,0.2929014336
H,0,0.0236483572,-0.0305342689,1.8827228224
H,0,-2.25697092,0.9482536844,1.8686563984
H,0,-3.3383645882,-1.6435330999,-1.362189019
H,0,-1.0792811721,-2.6192711861,-1.3462091543
H,0,-5.1123812431,-0.4595754217,0.0897150093
H,0,-4.4520186253,1.0201508931,-0.598338607
H,0,-4.5749722658,0.8468561712,1.154456599
N,0,-0.5800444188,1.5573616385,-0.5512308751
O,0,-0.8265071674,0.9985121712,-1.4875727226
O,0,-0.2381864625,2.3606992115,0.1541117855
F,0,2.6634010048,-0.3570590805,1.3798020907
B,0,2.9065303573,-0.1415516925,0.0409134836
F,0,3.037714,-1.3455968099,-0.6152553628
F,0,1.8455491821,0.5660898923,-0.5055932651
F,0,4.0590884745,0.5975667968,-0.1095530123

TS NO2BF4 PCM ONIOM 3.093_93956

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.284309011817

Zero-point correction= 0.157296 (Hartree/Particle)
Thermal correction to Energy= 0.173338
Thermal correction to Enthalpy= 0.174282
Thermal correction to Gibbs Free Energy= 0.111305
Sum of electronic and ZPE= -476.893601
Sum of electronic and thermal Energies= -476.877560
Sum of electronic and thermal Enthalpies= -476.876616
Sum of electronic and thermal Free Energies= -476.939593

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.771	53.938	132.546

C,0,-0.3832312917,-1.4105449184,0.2744952036
C,0,-0.7133255809,-0.3904961179,1.1627920811
C,0,-2.0012939002,0.1786873449,1.1449605429
C,0,-2.9764551172,-0.2737788828,0.2501982099
C,0,-2.6142390738,-1.271608824,-0.653117491
C,0,-1.3341408289,-1.8344503537,-0.6452025729
C,0,-4.3704610904,0.2901643285,0.2683835113
H,0,0.6193531522,-1.8270278056,0.2772592881
H,0,0.0291661311,-0.0269229174,1.8673326189
H,0,-2.2458815012,0.9633770474,1.8540607132
H,0,-3.3413221987,-1.6203657171,-1.378764421
H,0,-1.0868702215,-2.6051440893,-1.3654056931
H,0,-5.0281704068,-0.3565670774,0.8540934602
H,0,-4.7834977232,0.3558582171,-0.7386348114
H,0,-4.3936948923,1.2818451073,0.7204896141
N,0,-0.5751533764,1.5615209707,-0.5631707861
O,0,-0.8130065843,1.0000538006,-1.500150192
O,0,-0.238558675,2.3674095238,0.1420195206
F,0,2.6586765388,-0.3710460261,1.3858832886
B,0,2.9075173277,-0.1465133455,0.0495287922
F,0,3.040921174,-1.3461165369,-0.6142942914
F,0,1.8494395781,0.5652103173,-0.4973702448
F,0,4.0612595605,0.5928329545,-0.0904983411

TS NO2BF4 PCM ONIOM 3.099_93450

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.280523634869

Zero-point correction= 0.157616 (Hartree/Particle)
Thermal correction to Energy= 0.173566
Thermal correction to Enthalpy= 0.174510
Thermal correction to Gibbs Free Energy= 0.111767
Sum of electronic and ZPE= -476.888642
Sum of electronic and thermal Energies= -476.872693
Sum of electronic and thermal Enthalpies= -476.871749
Sum of electronic and thermal Free Energies= -476.934492

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.914	53.904	132.055

C,0,-3.7681847838,-0.1030048406,-0.3098101657
C,0,-3.5359779163,0.8542355079,0.6677436454
C,0,-2.3207823696,1.5500349973,0.7132864373
C,0,-1.3103497574,1.3051413901,-0.2115702732
C,0,-1.5339878119,0.3040930866,-1.1678227678
C,0,-2.7566846225,-0.3899381435,-1.2236599099
C,0,-0.01794227,2.0727860165,-0.2025933301
H,0,-4.7120525223,-0.6312239421,-0.3543214266
H,0,-4.3010440225,1.0726827111,1.4033418995
H,0,-2.168857994,2.2993440945,1.4827204439
H,0,-0.7640581473,0.0864973646,-1.9029222078
H,0,-2.9100798601,-1.1371323689,-1.9945572094
H,0,0.0542158849,2.7006299523,-1.0935170328
H,0,0.8467554937,1.4005444738,-0.207492069
H,0,0.0536847157,2.7176210075,0.6725233632
N,0,-1.2335159649,-1.7348745911,0.4127942417
O,0,-1.55028369,-1.2703593437,1.3800864734
O,0,-0.7962810479,-2.4567910853,-0.3278258066
F,0,3.5641318571,1.306858997,-0.2747360345
B,0,3.2374410406,0.0018281682,0.0259924562
F,0,4.3908393548,-0.7327182984,0.2090092329
F,0,2.4866886022,-0.03926299,1.1839562506
F,0,2.5113818314,-0.5479591639,-1.0115632109

TS NO2BF4 PCM ONIOM 3.107_93658

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.280227926471

Zero-point correction= 0.157041 (Hartree/Particle)
Thermal correction to Energy= 0.173317
Thermal correction to Enthalpy= 0.174261
Thermal correction to Gibbs Free Energy= 0.109510
Sum of electronic and ZPE= -476.889055
Sum of electronic and thermal Energies= -476.872780
Sum of electronic and thermal Enthalpies= -476.871836
Sum of electronic and thermal Free Energies= -476.936587

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.758	54.046	136.280

C,0,-0.2478575519,-1.063655345,-0.0783260366
C,0,-1.1334577255,-1.6805471471,0.7954031736
C,0,-2.512691603,-1.4687107564,0.680769267
C,0,-3.0404607341,-0.6386917455,-0.3041463934
C,0,-2.1393217414,0.014786356,-1.1545178678
C,0,-0.7516049734,-0.2041567798,-1.0502045603
C,0,-4.5243256209,-0.4511421198,-0.4591840538
H,0,0.8240186074,-1.2217578758,0.0053728004
H,0,-0.7584947342,-2.3341935239,1.574015726
H,0,-3.1837805033,-1.9647328726,1.3736836748
H,0,-2.5167744919,0.6744757399,-1.9299117267
H,0,-0.0735773334,0.297529259,-1.7336007378
H,0,-5.0429934722,-0.6092335389,0.4863487763
H,0,-4.9196100954,-1.1705103562,-1.1805629795
H,0,-4.7635333244,0.5475369468,-0.8261515489
N,0,-1.3359857955,1.7825479794,0.5300425108
O,0,-1.4521504821,1.2200019329,1.4908635209
O,0,-1.193563156,2.6338670075,-0.1896156183
F,0,3.3462878065,-1.3106915217,-0.7483193231
B,0,3.3414289906,-0.1149126975,-0.0606677133
F,0,4.6175755966,0.4082195215,-0.0354166846
F,0,2.4988386103,0.779287158,-0.6902751322
F,0,2.9087887271,-0.3214096208,1.2335289265

TS NO2BF4 PCM ONIOM 3.119_93855

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.283232372106

Zero-point correction= 0.158157 (Hartree/Particle)
Thermal correction to Energy= 0.173706
Thermal correction to Enthalpy= 0.174650
Thermal correction to Gibbs Free Energy= 0.113100
Sum of electronic and ZPE= -476.893479
Sum of electronic and thermal Energies= -476.877931
Sum of electronic and thermal Enthalpies= -476.876987

Sum of electronic and thermal Free Energies= -476.938536

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.002	53.516	129.542

C,0,3.4948409159,0.2701610057,-0.2827532036
C,0,2.8168147608,0.4945654408,0.9115465642
C,0,1.7035879115,-0.296875606,1.2547915087
C,0,1.2646266756,-1.3294766482,0.4183103945
C,0,1.9413748645,-1.5174136267,-0.7868653265
C,0,3.0412986384,-0.7287940504,-1.1361102332
C,0,0.0766743639,-2.1727473908,0.7792766376
H,0,4.3564224429,0.8709788386,-0.544812752
H,0,3.1535844776,1.2658475952,1.5953276172
H,0,1.1996651773,-0.1235251859,2.2008487915
H,0,1.6092079035,-2.2963201574,-1.4651131297
H,0,3.5447755877,-0.9051984177,-2.0790494532
H,0,-0.1064937723,-2.1598705204,1.8533344998
H,0,0.2238598019,-3.2067198591,0.4667408471
H,0,-0.839736399,-1.8025090133,0.2732519466
N,0,0.7310765548,1.708395222,-0.1370565899
O,0,0.7524128189,1.2425874241,-1.152383538
O,0,0.5242732296,2.4036457241,0.7183641595
F,0,-1.7108360574,0.7768957335,0.1766128492
B,0,-2.8003103231,-0.0286700252,-0.1170053868
F,0,-2.3426783943,-1.2648971012,-0.5281743491
F,0,-3.5808230947,-0.1708358061,1.007847343
F,0,-3.5336840839,0.5543994247,-1.1260911969

TS NO2BF4 PCM ONIOM 3.119_93935

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.284974969347

Zero-point correction= 0.157584 (Hartree/Particle)
Thermal correction to Energy= 0.173458
Thermal correction to Enthalpy= 0.174402
Thermal correction to Gibbs Free Energy= 0.112713
Sum of electronic and ZPE= -476.894480
Sum of electronic and thermal Energies= -476.878606
Sum of electronic and thermal Enthalpies= -476.877662
Sum of electronic and thermal Free Energies= -476.939352

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.847	53.944	129.837

C,0,-3.3021454725,-0.7248114187,0.3588455249
C,0,-2.2380908749,-0.6681815587,1.257912484
C,0,-1.2938527201,0.3680635734,1.1704369387
C,0,-1.3972857567,1.3623313538,0.1889140065
C,0,-2.4522118164,1.2725529258,-0.7154266065
C,0,-3.3951288085,0.2404835947,-0.6335208041
C,0,-0.3754934517,2.4636173572,0.1206900624
H,0,-4.035539406,-1.5179544007,0.4289189923
H,0,-2.1422389875,-1.4134856101,2.0397750139
H,0,-0.4735149614,0.4055635043,1.8837804999
H,0,-2.54736967,2.0163221534,-1.4989749988
H,0,-4.2037064779,0.2008332721,-1.3535157121
H,0,-0.5672062101,3.1334985279,-0.7162438163
H,0,0.6330803907,2.0506643086,0.006979562
H,0,-0.3829712247,3.0513469474,1.0406753392
N,0,-0.4019599373,-1.5563306484,-0.4324882499
O,0,-0.8435892795,-1.1698838553,-1.3830492586
O,0,0.1925975886,-2.1429020321,0.3143236405
F,0,3.1474863882,1.3811552349,-0.0923456203
B,0,2.658438859,0.0981847026,-0.0160883511
F,0,1.7852748263,-0.149863002,-1.0645781328
F,0,3.6961063469,-0.8046349996,-0.069412343
F,0,1.9459236553,-0.0829949306,1.1527528292

TS NO2BF4 PCM ONIOM 3.125_93949

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.283497076933

Zero-point correction= 0.157586 (Hartree/Particle)
Thermal correction to Energy= 0.173581
Thermal correction to Enthalpy= 0.174525
Thermal correction to Gibbs Free Energy= 0.111589
Sum of electronic and ZPE= -476.893496
Sum of electronic and thermal Energies= -476.877502
Sum of electronic and thermal Enthalpies= -476.876558
Sum of electronic and thermal Free Energies= -476.939494

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.924	53.955	132.460

C,0,-3.5106872231,-0.3059477972,-0.3260345591
C,0,-2.8598944005,-0.5149651651,0.8863693476
C,0,-1.7656462627,0.2919453025,1.2506518874
C,0,-1.319812659,1.327060102,0.4193817859
C,0,-1.9672922366,1.499557085,-0.8022911633
C,0,-3.0477575726,0.6925382385,-1.1741939158
C,0,-0.1561875222,2.1919525353,0.8177615518
H,0,-4.3581301776,-0.9188690051,-0.6057240094
H,0,-3.2034101843,-1.2857176176,1.5674493486
H,0,-1.2823178495,0.1302331014,2.2097442285
H,0,-1.6302523757,2.2795360548,-1.4766784715
H,0,-3.5292875776,0.8564537443,-2.1309054025
H,0,-0.1042226303,2.3080327568,1.9004866524
H,0,-0.2316182332,3.1808203727,0.3658234538
H,0,0.7901922845,1.7482821864,0.4851063744
N,0,-0.7171387762,-1.6907998611,-0.103671641
O,0,-0.4878031396,-2.3592822083,0.7675538645
O,0,-0.7545418245,-1.2520213936,-1.1306987941
F,0,3.8423083218,-0.8456937962,-0.4570604309
B,0,2.8395065915,0.0385420048,-0.1240468969
F,0,2.5848577758,0.8684671106,-1.1940631054
F,0,1.6924331952,-0.6788945848,0.1817192364
F,0,3.2219694763,0.7831488338,0.9697266588

TS NO2BF4 PCM ONIOM 3.130_93945

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.283803815230

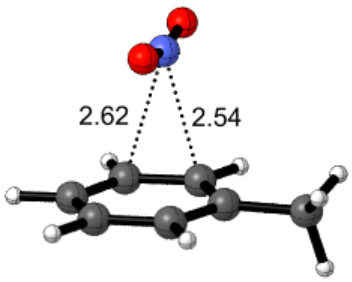
Zero-point correction= 0.157378 (Hartree/Particle)
Thermal correction to Energy= 0.173421

Thermal correction to Enthalpy= 0.174365
Thermal correction to Gibbs Free Energy= 0.111440
Sum of electronic and ZPE= -476.893528
Sum of electronic and thermal Energies= -476.877484
Sum of electronic and thermal Enthalpies= -476.876540
Sum of electronic and thermal Free Energies= -476.939465

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.823	53.937	132.437

C,0,-0.3827288153,-1.4610221546,0.1860600006
C,0,-0.6513585541,-0.4550868045,1.1088562922
C,0,-1.9239847498,0.1455550433,1.1531613278
C,0,-2.9482795031,-0.2675261064,0.2925640323
C,0,-2.6495167988,-1.256817626,-0.6416041543
C,0,-1.3830608543,-1.8469487593,-0.6985263663
C,0,-4.3253387828,0.3305942357,0.3801615901
H,0,0.6096287635,-1.8981210547,0.1368708035
H,0,0.1287841251,-0.1200936112,1.7866270022
H,0,-2.1204096856,0.920030997,1.8882922977
H,0,-3.4151456216,-1.5764082995,-1.3404266038
H,0,-1.1850234924,-2.6093653903,-1.442478374
H,0,-4.3022813081,1.3172879667,0.8432682057
H,0,-4.972229746,-0.3060910697,0.9884778382
H,0,-4.7812831559,0.4189436895,-0.6064310288
N,0,-0.617653682,1.560350888,-0.5984585371
O,0,-0.820713415,0.9756908177,-1.5291548209
O,0,-0.3193111032,2.3866609268,0.0997403972
F,0,2.7209804267,-0.4954340705,1.3831726791
B,0,2.9074428062,-0.1298280611,0.0681636818
F,0,3.008173531,-1.2539936698,-0.7219384011
F,0,1.8291347589,0.6335817597,-0.3547038125
F,0,4.0567338565,0.6210913532,-0.0462400498

TS NO2BF4 PCM ONIOM 3.138_94010



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.280523313130

Zero-point correction= 0.156402 (Hartree/Particle)
Thermal correction to Energy= 0.173090
Thermal correction to Enthalpy= 0.174034
Thermal correction to Gibbs Free Energy= 0.104549
Sum of electronic and ZPE= -476.888255
Sum of electronic and thermal Energies= -476.871567
Sum of electronic and thermal Enthalpies= -476.870623
Sum of electronic and thermal Free Energies= -476.940108

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.616	54.288	146.245

C,0,-2.95621,-1.965957,0.224333
C,0,-2.943216,-1.029008,1.250913
C,0,-3.250011,0.320777,0.980886
C,0,-3.602886,0.742775,-0.308982
C,0,-3.574924,-0.205569,-1.326573
C,0,-3.253709,-1.543082,-1.066063
C,0,-4.001371,2.167369,-0.575858
H,0,-2.720651,-3.0035,0.425229
H,0,-2.70719,-1.327685,2.266471
H,0,-3.256643,1.036737,1.797443
H,0,-3.809304,0.095037,-2.342362
H,0,-3.241616,-2.254206,-1.883756
H,0,-5.088353,2.267056,-0.521953
H,0,-3.68933,2.48585,-1.570782
H,0,-3.570825,2.847353,0.159722
N,0,-0.743892,0.229963,0.588546
O,0,-0.692354,-0.083251,-0.486151
O,0,-0.414449,0.607074,1.596045
F,0,3.533152,0.65596,-0.938277
B,0,4.480576,0.027604,-0.15624
F,0,5.278164,-0.768239,-0.951292
F,0,5.255887,0.976531,0.476423
F,0,3.847983,-0.754118,0.788731

TS NO2BF4 PCM ONIOM 3.139_93772

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.280226078977

Zero-point correction= 0.157220 (Hartree/Particle)
Thermal correction to Energy= 0.173691
Thermal correction to Enthalpy= 0.174635
Thermal correction to Gibbs Free Energy= 0.107388
Sum of electronic and ZPE= -476.887891
Sum of electronic and thermal Energies= -476.871420
Sum of electronic and thermal Enthalpies= -476.870476
Sum of electronic and thermal Free Energies= -476.937723

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.993	54.093	141.534

C,0,-1.319303,1.607591,0.685691
C,0,-2.102119,1.954466,-0.409645
C,0,-3.237448,1.20703,-0.743209
C,0,-3.617479,0.095922,0.004192
C,0,-2.795213,-0.278644,1.075673
C,0,-1.659132,0.479431,1.424391

C,0,-4.869053,-0.672238,-0.318656
H,0,-0.447581,2.193537,0.949457
H,0,-1.835655,2.81467,-1.012676
H,0,-3.834149,1.502269,-1.599815
H,0,-3.060504,-1.143505,1.676582
H,0,-1.06128,0.181569,2.279062
H,0,-5.059757,-0.684678,-1.392082
H,0,-5.729473,-0.20302,0.164834
H,0,-4.80983,-1.700581,0.038273
N,0,-0.950084,-1.3368,-0.337819
O,0,-0.979226,-0.691052,-1.252005
O,0,-0.706508,-2.194339,0.346731
F,0,4.925431,-0.482174,0.803191
B,0,3.991965,0.076864,-0.044034
F,0,2.986034,0.658574,0.700477
F,0,4.593989,1.03433,-0.832925
F,0,3.451585,-0.906862,-0.847096

TS NO2BF4 PCM ONIOM 3.146_93865

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.279983587293

Zero-point correction= 0.156982 (Hartree/Particle)
Thermal correction to Energy= 0.173553
Thermal correction to Enthalpy= 0.174497
Thermal correction to Gibbs Free Energy= 0.106381
Sum of electronic and ZPE= -476.888056
Sum of electronic and thermal Energies= -476.871486
Sum of electronic and thermal Enthalpies= -476.870542
Sum of electronic and thermal Free Energies= -476.938658

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.906	54.128	143.362

C,0,-1.568092,1.776682,0.451435
C,0,-2.54018,1.93872,-0.528878
C,0,-3.580674,1.012298,-0.665832
C,0,-3.674246,-0.098298,0.166994
C,0,-2.663083,-0.28221,1.121047
C,0,-1.623068,0.656115,1.27353
C,0,-4.817839,-1.068314,0.057302
H,0,-0.771132,2.501018,0.564292
H,0,-2.498975,2.793312,-1.193979
H,0,-4.32981,1.166667,-1.43505
H,0,-2.704812,-1.141087,1.78422
H,0,-0.872954,0.500807,2.041573
H,0,-4.518785,-2.072476,0.359428
H,0,-5.204596,-1.111201,-0.960952
H,0,-5.636573,-0.757078,0.710765
N,0,-0.884306,-1.146529,-0.49187
O,0,-1.135551,-0.575225,-1.421562
O,0,-0.42251,-1.911287,0.190056
F,0,4.877063,1.017677,-0.611263
B,0,4.099137,0.059828,0.004276
F,0,3.478706,-0.71494,-0.954507
F,0,4.891964,-0.741487,0.798668
F,0,3.141121,0.675277,0.783754

TS NO2BF4 PCM ONIOM 3.182_93693

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.283532272052

Zero-point correction= 0.157814 (Hartree/Particle)
Thermal correction to Energy= 0.173702
Thermal correction to Enthalpy= 0.174647
Thermal correction to Gibbs Free Energy= 0.112236
Sum of electronic and ZPE= -476.891358
Sum of electronic and thermal Energies= -476.875469
Sum of electronic and thermal Enthalpies= -476.874525
Sum of electronic and thermal Free Energies= -476.936936

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.000	53.827	131.355

C,0,0.869728,1.840317,-0.086325
C,0,2.051368,1.859372,0.646381
C,0,3.015822,0.861411,0.471833
C,0,2.821829,-0.179212,-0.431552
C,0,1.610064,-0.214012,-1.136783
C,0,0.645044,0.796086,-0.977356
C,0,3.873244,-1.229633,-0.662165
H,0,0.11815,2.607175,0.054118
H,0,2.22952,2.652118,1.363059
H,0,3.930564,0.899372,1.052942
H,0,1.42673,-1.018669,-1.842448
H,0,-0.28859,0.742605,-1.532729
H,0,4.470107,-0.974814,-1.541352
H,0,3.425287,-2.207942,-0.842251
H,0,4.549518,-1.306874,0.188886
N,0,0.19155,-1.119438,0.868088
O,0,-0.411148,-1.843825,0.263601
O,0,0.655733,-0.56242,1.720992
F,0,-2.143484,-1.045484,-0.649591
B,0,-2.760882,0.087827,-0.148865
F,0,-1.928274,0.573804,0.847119
F,0,-2.907,1.025727,-1.143805
F,0,-3.985352,-0.237608,0.384782

TS NO2BF4 PCM ONIOM 3.341_93662

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.281527933861

Zero-point correction= 0.157834 (Hartree/Particle)
Thermal correction to Energy= 0.173687
Thermal correction to Enthalpy= 0.174631
Thermal correction to Gibbs Free Energy= 0.112712
Sum of electronic and ZPE= -476.891431
Sum of electronic and thermal Energies= -476.875578
Sum of electronic and thermal Enthalpies= -476.874634
Sum of electronic and thermal Free Energies= -476.936553

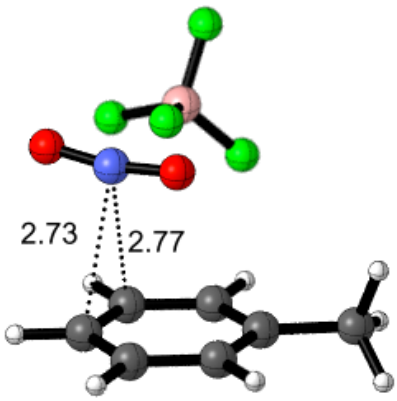
	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.990	53.810	130.318

C,0,1.1925142962,2.0209814205,-0.0626052304
C,0,2.4179528437,1.7784993049,0.5580469855

C,0,3.1166354993,0.5956471237,0.3194253928
C,0,2.6053642051,-0.3778583479,-0.5359148493
C,0,1.3568263337,-0.135020221,-1.1353614835
C,0,0.6624017372,1.0619857621,-0.915252695
C,0,3.3703558879,-1.6374970087,-0.8354166172
H,0,0.6548625998,2.9409276166,0.1293491737
H,0,2.8328447913,2.51575558,1.2351412447
H,0,4.0696525594,0.4285809059,0.8090472676
H,0,0.9300012401,-0.8822024324,-1.7986317292
H,0,-0.305730639,1.214178878,-1.3852122752
H,0,4.0011298506,-1.4906021477,-1.7158175371
H,0,2.7002012488,-2.4714129538,-1.0493196199
H,0,4.0191059872,-1.9141237035,-0.004296111
N,0,0.1906914861,-0.9559005745,1.0780010733
O,0,-0.3635076842,-1.7751955651,0.5587049054
O,0,0.6187281238,-0.2470038306,1.8273412336
F,0,-1.9512120614,-0.986894728,-0.6451485094
B,0,-2.7155832503,0.072259934,-0.1848121496
F,0,-2.0019267598,0.6322853106,0.8632245527
F,0,-2.8987501667,0.9982631414,-1.1843998396
F,0,-3.9300651287,-0.3848564646,0.2686428171

Pi Complexes for Toluene / $NO_2^+BF_4^-$ ONIOM(M062X/6-311G*:PM3)/PCM(CH_2Cl_2)

Pi Complex NO2BF4 PCM ONIOM 2.727_94123



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.277319186051

Zero-point correction= 0.157909 (Hartree/Particle)
Thermal correction to Energy= 0.174806
Thermal correction to Enthalpy= 0.175751
Thermal correction to Gibbs Free Energy= 0.110238
Sum of electronic and ZPE= -476.893568
Sum of electronic and thermal Energies= -476.876670
Sum of electronic and thermal Enthalpies= -476.875726
Sum of electronic and thermal Free Energies= -476.941238

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.693	55.813	137.883

C,0,2.0243110462,-1.1198338361,-1.2361097836
C,0,0.9237187983,-0.261719388,-1.3653063835
C,0,0.9343670649,0.9870599447,-0.7503421204
C,0,2.0317817943,1.3987786419,0.0084284194
C,0,3.1324000593,0.535138849,0.117631817
C,0,3.1367467403,-0.7068679903,-0.5015778393
C,0,2.0351339021,2.7245979483,0.7162011028
H,0,2.0200468404,-2.0865279526,-1.7266708772
H,0,0.0556473451,-0.5721357543,-1.9381463024
H,0,0.0651546775,1.6323434211,-0.8400670706
H,0,3.9934542015,0.8489090961,0.6983134749
H,0,3.9984873981,-1.3568468226,-0.4110019521
H,0,1.8207997292,2.5885718158,1.7798688004
H,0,1.2815676458,3.3963897177,0.3057825866
H,0,3.0106355006,3.2068111431,0.6381683703
N,0,0.5464302646,-1.6808939886,0.9866215372
O,0,0.9318424854,-0.8588596325,1.6283541808
O,0,0.0784531361,-2.5902563669,0.5401311422
F,0,-2.5076498748,1.5285181873,-0.5064847311
B,0,-2.7743416203,0.2314361905,-0.1283938447
F,0,-3.1826965483,-0.5004014606,-1.2218708245
F,0,-1.6297273853,-0.3467885189,0.3998629116
F,0,-3.7623212012,0.222309756,0.8321183862

Pi Complex NO2BF4 PCM ONIOM 2.731_94156

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.275835792227

Zero-point correction= 0.158085 (Hartree/Particle)
Thermal correction to Energy= 0.174956
Thermal correction to Enthalpy= 0.175900
Thermal correction to Gibbs Free Energy= 0.109954
Sum of electronic and ZPE= -476.893430
Sum of electronic and thermal Energies= -476.876559
Sum of electronic and thermal Enthalpies= -476.875615
Sum of electronic and thermal Free Energies= -476.941561

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.786	55.764	138.795

C,0,-2.7526799987,-3.2822077645,-0.5237856215
C,0,-3.7168170082,-2.9617021087,-1.4871374555
C,0,-3.4138564705,-3.0727555219,-2.8409388706
C,0,-2.1492491674,-3.492992918,-3.257407313
C,0,-1.1936607732,-3.814752487,-2.2818607745
C,0,-1.4903509322,-3.7224208487,-0.929035911
C,0,-1.800914383,-3.5972160511,-4.7159635405
H,0,-2.9913243822,-3.2077210482,0.5314188011
H,0,-4.7051315343,-2.6419946115,-1.1768870659
H,0,-4.1663230025,-2.8261091741,-3.5818076776
H,0,-0.2073445043,-4.141366856,-2.5948114047
H,0,-0.7362163279,-3.9638440473,-0.1862393024
H,0,-2.6749267096,-3.4374056538,-5.3465884272
H,0,-1.38563567,-4.5808317214,-4.9438433899
H,0,-1.0448351507,-2.8555731293,-4.9856037385
N,0,-2.0685680996,-0.6836914865,-1.0168195253
O,0,-2.5553819302,-0.3191541654,-0.0826821915
O,0,-1.5233869155,-0.8511953567,-1.9700062745
F,0,1.3794214955,-0.9445783826,2.105780924

B,0,1.1823587158,-1.7872517893,1.0339931238
F,0,2.2368678065,-1.6754631829,0.1544564462
F,0,1.0805428465,-3.087689755,1.4760644311
F,0,0.0118732954,-1.42627814,0.3837912579

Pi Complex NO2BF4 PCM ONIOM 2.750_94123

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.275463893129

Zero-point correction= 0.158040 (Hartree/Particle)
Thermal correction to Energy= 0.174847
Thermal correction to Enthalpy= 0.175791
Thermal correction to Gibbs Free Energy= 0.110262
Sum of electronic and ZPE= -476.893452
Sum of electronic and thermal Energies= -476.876646
Sum of electronic and thermal Enthalpies= -476.875701
Sum of electronic and thermal Free Energies= -476.941230

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.718	55.756	137.917

C,0,-1.3542900963,-0.957284536,1.3924321068
C,0,-0.9517617727,0.3747870075,1.2660824863
C,0,-1.7057838568,1.254239155,0.5010209439
C,0,-2.8831104377,0.8347977899,-0.1356706858
C,0,-3.282975175,-0.4951835944,0.0088757669
C,0,-2.5269544952,-1.388519579,0.7621469735
C,0,-3.6869510619,1.8131561631,-0.9461448302
H,0,-0.7695390938,-1.6495774174,1.9880289592
H,0,-0.0366126111,0.7135481094,1.7421987087
H,0,-1.3824881422,2.2842660478,0.391052719
H,0,-4.1920380861,-0.8361416429,-0.4742170844
H,0,-2.8523426845,-2.4168023538,0.870784776
H,0,-4.5398553098,1.3325527781,-1.423952779
H,0,-3.0707047742,2.2740842225,-1.721335919
H,0,-4.0604732241,2.6179062565,-0.3087173432
N,0,-0.3178322503,-1.5008319031,-1.096176228
O,0,0.167104222,-2.4366465528,-0.7349601101
O,0,-0.7200362836,-0.6105302001,-1.6234512444
F,0,3.1381463412,1.561208126,-0.5900821345
B,0,2.8239116312,0.5576290366,0.2997863688
F,0,3.8956983854,-0.2971772124,0.435127625
F,0,2.5075457227,1.101718914,1.5250915272
F,0,1.7367060527,-0.1547796146,-0.1832936026

Pi Complex NO2BF4 PCM ONIOM 2.750_94145

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276758808342

Zero-point correction= 0.157889 (Hartree/Particle)
Thermal correction to Energy= 0.174751
Thermal correction to Enthalpy= 0.175695
Thermal correction to Gibbs Free Energy= 0.110402
Sum of electronic and ZPE= -476.893966
Sum of electronic and thermal Energies= -476.877105
Sum of electronic and thermal Enthalpies= -476.876161
Sum of electronic and thermal Free Energies= -476.941454

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.658	55.760	137.421

C,0,0.0883681213,-1.5282565367,-0.3839513117
C,0,-1.1443820513,-1.0645989768,-0.8611158729
C,0,-1.2003556734,0.0558516397,-1.686939576
C,0,-0.0365030615,0.7355809432,-2.0467953649
C,0,1.1930285935,0.2542120977,-1.569269543
C,0,1.2600671874,-0.8671268523,-0.7545149194
C,0,-0.0811450378,1.9548302944,-2.9246014497
H,0,0.1316582705,-2.4065105815,0.2498150055
H,0,-2.065350787,-1.5682226883,-0.5809207645
H,0,-2.1691711078,0.4181852941,-2.0219845939
H,0,2.1054727793,0.773291037,-1.8440457486
H,0,2.2193339695,-1.2250730886,-0.4007372123
H,0,-1.1045114703,2.2116338672,-3.1967034003
H,0,0.485100401,1.7859837355,-3.8431536072
H,0,0.3669349051,2.8134465043,-2.4196051155
N,0,-0.6413911065,0.3900824665,1.4463390135
O,0,-0.2191888005,1.2594192574,0.8979017559
O,0,-1.0710499946,-0.3454775614,2.1662488367
F,0,-3.0831652049,0.8922532035,0.6330929634
B,0,-4.2812859844,0.8313023519,-0.0642206828
F,0,-5.3144993488,1.1132538618,0.8023390884
F,0,-4.2630811234,1.75889895,-1.0824156464
F,0,-4.4452247756,-0.4344443184,-0.5824140543

Pi Complex NO2BF4 PCM ONIOM 2.754_94188

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.275832663268

Zero-point correction= 0.157975 (Hartree/Particle)
Thermal correction to Energy= 0.174817
Thermal correction to Enthalpy= 0.175762
Thermal correction to Gibbs Free Energy= 0.109972
Sum of electronic and ZPE= -476.893882
Sum of electronic and thermal Energies= -476.877039
Sum of electronic and thermal Enthalpies= -476.876095
Sum of electronic and thermal Free Energies= -476.941885

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.700	55.768	138.467

C,0,0.6484210141,0.0548256445,1.4246063295
C,0,0.576774373,-1.0858450623,0.6265568603
C,0,1.6763817423,-1.4720778693,-0.1309907103
C,0,2.8733311266,-0.7444165712,-0.0928279513
C,0,2.9397932494,0.3883728763,0.7218994546
C,0,1.8391825742,0.7927034487,1.4712657631
C,0,4.068728052,-1.1913893963,-0.8879386482
H,0,-0.2179645712,0.3658310946,2.0009667594
H,0,-0.3527793388,-1.6460085456,0.5731282287
H,0,1.609877126,-2.3495700526,-0.7652356576
H,0,3.8590679097,0.9621420723,0.7653337297

H,0,1.9053133145,1.673540542,2.1000926967
H,0,4.691141829,-1.8579397226,-0.2849470145
H,0,4.6866526395,-0.3438595285,-1.1860561599
H,0,3.7702908737,-1.7381915779,-1.7827462759
N,0,0.3737714708,1.7637747488,-0.7175227834
O,0,0.857157424,1.0910607023,-1.4571226283
O,0,-0.1552223856,2.552679057,-0.1350064751
F,0,-2.6990885913,-0.4454847688,1.3163937799
B,0,-2.8393762995,-0.4272221369,-0.053936167
F,0,-2.7485555596,-1.7069878791,-0.5553045257
F,0,-4.0604636975,0.1160946627,-0.3879552552
F,0,-1.8351032751,0.354018262,-0.6073163494

Pi Complex NO2BF4 PCM ONIOM 2.763_94064

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.274782288346

Zero-point correction= 0.158015 (Hartree/Particle)
Thermal correction to Energy= 0.174810
Thermal correction to Enthalpy= 0.175754
Thermal correction to Gibbs Free Energy= 0.110746
Sum of electronic and ZPE= -476.893373
Sum of electronic and thermal Energies= -476.876578
Sum of electronic and thermal Enthalpies= -476.875634
Sum of electronic and thermal Free Energies= -476.940641

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.695	55.730	136.820

C,0,-1.3305096692,0.6246798162,1.7183039599
C,0,-2.6215812971,0.9402745364,1.2834924297
C,0,-3.2795795229,0.0986236824,0.3939265035
C,0,-2.6684531357,-1.068096806,-0.0765769715
C,0,-1.3811675004,-1.3806580423,0.3786465806
C,0,-0.7159466804,-0.5483719149,1.2699805992
C,0,-3.3599159245,-1.9576873963,-1.07184155
H,0,-0.8163856445,1.2750953182,2.4171792285
H,0,-3.1101338729,1.8371959221,1.6459543221
H,0,-4.2803464694,0.3478134125,0.0579393665
H,0,-0.8973637382,-2.2847722131,0.0240929822
H,0,0.2881542985,-0.7975628075,1.6004363663
H,0,-4.4348378863,-1.7787520047,-1.0856530589
H,0,-3.184708929,-3.0103355059,-0.8454817307
H,0,-2.9764425028,-1.7713564822,-2.0791625333
N,0,-0.5436955526,1.7728782412,-0.6692212219
O,0,-0.039534421,2.6067366163,-0.1302585548
O,0,-0.9964712766,1.0268228573,-1.3545997299
F,0,2.7838075074,-0.9457494638,0.9670968215
B,0,2.7991020786,-0.3882176067,-0.2921562064
F,0,2.8336708458,-1.3832792828,-1.2441014758
F,0,1.6555908028,0.3749407516,-0.476187582
F,0,3.9037654904,0.423644372,-0.4282355448

Pi Complex NO2BF4 PCM ONIOM 2.765_93840

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.269314072713

Zero-point correction= 0.158372 (Hartree/Particle)
Thermal correction to Energy= 0.174965
Thermal correction to Enthalpy= 0.175909
Thermal correction to Gibbs Free Energy= 0.110873
Sum of electronic and ZPE= -476.890907
Sum of electronic and thermal Energies= -476.874314
Sum of electronic and thermal Enthalpies= -476.873370
Sum of electronic and thermal Free Energies= -476.938406

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.792	55.407	136.879

C,0,-1.2151308202,0.6288312051,1.2999564902
C,0,-2.5689066913,0.9632149359,1.1936019162
C,0,-3.4382906609,0.1370886099,0.4865960128
C,0,-2.9742334923,-1.027562861,-0.1274679026
C,0,-1.6154697885,-1.352802616,-0.0067269952
C,0,-0.7403078472,-0.5414274677,0.7031228915
C,0,-3.8986911294,-1.928346949,-0.8991632547
H,0,-0.5410887181,1.265261516,1.8626909118
H,0,-2.9435404288,1.8597042355,1.6744467667
H,0,-4.4869568825,0.4020402826,0.4095246248
H,0,-1.2448601327,-2.25665729,-0.4793980801
H,0,0.3250869279,-0.8128541544,0.7876422834
H,0,-3.526022879,-2.0922918314,-1.9127567513
H,0,-4.9023829195,-1.5095827838,-0.9650371871
H,0,-3.9684007972,-2.9064675259,-0.41772505
N,0,-1.2033431051,1.9352278478,-1.1375795281
O,0,-1.6228771859,1.09969079,-1.7341285314
O,0,-0.760601548,2.8520996427,-0.6888388316
F,0,2.6428407548,0.1953583873,-0.6961039669
B,0,3.0867133555,-0.521987459,0.3953436374
F,0,3.568359213,0.3475818259,1.3504690871
F,0,2.0345277517,-1.2481104392,0.923478247
F,0,4.0872850237,-1.3850629011,0.0040922101

Pi Complex NO2BF4 PCM ONIOM 2.768_94165

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.274298805200

Zero-point correction= 0.157883 (Hartree/Particle)
Thermal correction to Energy= 0.174813
Thermal correction to Enthalpy= 0.175757
Thermal correction to Gibbs Free Energy= 0.109751
Sum of electronic and ZPE= -476.893523
Sum of electronic and thermal Energies= -476.876592
Sum of electronic and thermal Enthalpies= -476.875648
Sum of electronic and thermal Free Energies= -476.941655

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.697	55.769	138.923

C,0,-1.8085554837,2.0886892327,1.6905850152
C,0,-1.9632011711,2.6919178773,0.4376302692
C,0,-2.7137650807,2.0628214832,-0.5454888973

C,0,-3.3341921216,0.8296688184,-0.3021757839
C,0,-3.1863626774,0.2453924064,0.9587109152
C,0,-2.4318357643,0.8655807672,1.9505467575
C,0,-4.1475301839,0.1650088323,-1.3780240051
H,0,-1.2262091833,2.5781167312,2.4633064818
H,0,-1.496294967,3.6488961598,0.23701982
H,0,-2.8245392585,2.5290593649,-1.5191075439
H,0,-3.6577158185,-0.7098227315,1.1629666621
H,0,-2.3128700674,0.3869385904,2.9185854221
H,0,-3.58511137,0.1031015272,-2.3118762822
H,0,-5.0529686703,0.7416634667,-1.5819865746
H,0,-4.4457595479,-0.8418738845,-1.0871773309
N,0,0.1623715847,0.5029685731,0.5665679692
O,0,-0.4483559553,0.072921305,-0.2539745481
O,0,0.910271627,0.854687273,1.3123964218
F,0,-0.3823956847,-1.4319010115,2.2603891697
B,0,-0.5215161356,-2.1917400705,3.4120342712
F,0,0.5093685691,-1.8917354944,4.2754769211
F,0,-1.727756526,-1.9031717334,4.0111301753
F,0,-0.4753605136,-3.5270334831,3.0767858949

Pi Complex NO2BF4 PCM ONIOM 2.770_94103

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.269841120227

Zero-point correction= 0.158274 (Hartree/Particle)
Thermal correction to Energy= 0.175059
Thermal correction to Enthalpy= 0.176003
Thermal correction to Gibbs Free Energy= 0.108264
Sum of electronic and ZPE= -476.891026
Sum of electronic and thermal Energies= -476.874242
Sum of electronic and thermal Enthalpies= -476.873297
Sum of electronic and thermal Free Energies= -476.941036

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.851	55.436	142.568

C,0,-2.381805155,-3.6461105929,-0.7101818265
C,0,-3.3944953505,-4.1429224965,-1.5320349979
C,0,-3.2569487544,-4.0811816589,-2.9115937368
C,0,-2.1046940739,-3.5415337029,-3.5021593123
C,0,-1.0901880918,-3.0667652176,-2.670259719
C,0,-1.2239469849,-3.1090384281,-1.2841163166
C,0,-1.9848592183,-3.468822124,-4.999109442
H,0,-2.4784508006,-3.697321984,0.3684319125
H,0,-4.287037887,-4.5736393596,-1.0943861994
H,0,-4.0496468482,-4.4595241538,-3.5485896434
H,0,-0.1869301299,-2.6548421066,-3.1074151066
H,0,-0.4129864941,-2.7318026484,-0.6388400167
H,0,-0.9746827592,-3.1968474879,-5.3042142197
H,0,-2.6736511229,-2.7225674602,-5.4037461898
H,0,-2.2383687867,-4.4265492355,-5.4570846445
N,0,-3.0778011849,-1.0051881626,-1.178212652
O,0,-2.8516241651,-0.6897546217,-0.1353167419
O,0,-3.3848892843,-1.1565743058,-2.2339808555
F,0,2.6157525667,-1.1681255451,-0.600885921
B,0,1.7695188088,-1.0706159708,0.4826736237
F,0,0.8316866103,-2.0863512175,0.4284144674
F,0,2.4914521913,-1.1799034308,1.6512572975
F,0,1.1196901146,0.1455055112,0.4502443406

Pi Complex NO2BF4 PCM ONIOM 2.782_93989

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.274781462191

Zero-point correction= 0.158187 (Hartree/Particle)
Thermal correction to Energy= 0.174943
Thermal correction to Enthalpy= 0.175887
Thermal correction to Gibbs Free Energy= 0.110415
Sum of electronic and ZPE= -476.892121
Sum of electronic and thermal Energies= -476.875365
Sum of electronic and thermal Enthalpies= -476.874421
Sum of electronic and thermal Free Energies= -476.939893

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.778	55.625	137.798

C,0,2.4503276908,-1.3334665444,0.9658425561
C,0,3.330018558,-0.9003847672,-0.0274534545
C,0,3.266139398,0.4090513684,-0.483799244
C,0,2.3403381176,1.3201017553,0.048238561
C,0,1.4814653176,0.8832855088,1.0576611443
C,0,1.5272575376,-0.4337247452,1.5110673628
C,0,2.285131852,2.7298578678,-0.4717245886
H,0,2.4965616091,-2.3530960006,1.3315059885
H,0,4.0567893031,-1.5868988017,-0.4452725818
H,0,3.9424873933,0.7398879017,-1.265423794
H,0,0.761760211,1.5736050432,1.4851950337
H,0,0.8537412019,-0.7589521959,2.2967450302
H,0,3.2595596594,3.2138101645,-0.377647259
H,0,1.551819859,3.3262393852,0.0703552723
H,0,2.0181625991,2.7403370126,-1.5313583354
N,0,0.3222945209,-1.5135008382,-0.8185408221
O,0,0.6424896312,-0.6553543387,-1.445254477
O,0,-0.1057004082,-2.4149199452,-0.3241465846
F,0,-2.0432433691,-0.3352939185,-0.6220138399
B,0,-3.0636398249,0.3073150743,0.0616269134
F,0,-3.874016629,0.961773689,-0.8392969159
F,0,-3.7968004428,-0.6274632158,0.7588502173
F,0,-2.5100497856,1.2133815404,0.9395408172

Pi Complex NO2BF4 PCM ONIOM 2.788_93809

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.268745628951

Zero-point correction= 0.157810 (Hartree/Particle)
Thermal correction to Energy= 0.174777
Thermal correction to Enthalpy= 0.175721
Thermal correction to Gibbs Free Energy= 0.109249
Sum of electronic and ZPE= -476.889532
Sum of electronic and thermal Energies= -476.872565
Sum of electronic and thermal Enthalpies= -476.871621
Sum of electronic and thermal Free Energies= -476.938093

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 109.674 55.744 139.903

C,0,0.9354279697,-0.410030922,1.4317404439
C,0,2.31784071,-0.6127072306,1.4792365674
C,0,3.1697010641,0.2130904951,0.7500657915
C,0,2.6607154837,1.2462294525,-0.0391128238
C,0,1.2727948786,1.4426676169,-0.0719321035
C,0,0.4154224886,0.6305780037,0.6584354003
C,0,3.565973485,2.1318411211,-0.8502289298
H,0,0.2721844789,-1.0424511539,2.0118418376
H,0,2.7276111924,-1.4041367091,2.0966980814
H,0,4.2413384322,0.0523637711,0.7945148922
H,0,0.8659915266,2.2447538818,-0.6794720902
H,0,-0.6595388213,0.7943335746,0.6205470144
H,0,3.3680176706,3.1843553648,-0.6384546215
H,0,3.3969805341,1.9787928851,-1.9191875094
H,0,4.6158285826,1.929826802,-0.6398310147
N,0,1.2774352222,-2.0043377281,-0.8299597963
O,0,0.8702160668,-2.8960344209,-0.3052410517
O,0,1.6848191742,-1.2033389198,-1.4793396838
F,0,-4.5999356621,0.0375245079,-0.3577496832
B,0,-3.2776753874,0.2793765244,-0.0489339485
F,0,-3.1259130519,0.3199385126,1.3214423266
F,0,-2.4988679234,-0.7326941682,-0.5743723401
F,0,-2.8932491142,1.4854527392,-0.5978617587

Pi Complex NO2BF4 PCM ONIOM 2.789_94125

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.275819250827

Zero-point correction= 0.157993 (Hartree/Particle)
Thermal correction to Energy= 0.174880
Thermal correction to Enthalpy= 0.175824
Thermal correction to Gibbs Free Energy= 0.110130
Sum of electronic and ZPE= -476.893392
Sum of electronic and thermal Energies= -476.876504
Sum of electronic and thermal Enthalpies= -476.875560
Sum of electronic and thermal Free Energies= -476.941254

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 109.739 55.802 138.265

C,0,-0.5997583627,-5.0760376813,3.2579206179
C,0,-0.0905813002,-5.8020675744,2.1841753194
C,0,-0.9305564685,-6.6290421181,1.4453519975
C,0,-2.2930087883,-6.7388902043,1.7499477731
C,0,-2.7986772994,-5.9896880467,2.8165781645
C,0,-1.9640388103,-5.1695541705,3.5687013902
C,0,-3.1933439423,-7.6564326882,0.969845457
H,0,0.0463704508,-4.4264348595,3.8372456818
H,0,0.9591393893,-5.7279575041,1.9272296749
H,0,-0.5251775161,-7.2003757629,0.6171480676
H,0,-3.8498439,-6.069291875,3.081368176
H,0,-2.3726880672,-4.6033720609,4.399026112
H,0,-4.1551315111,-7.1817776796,0.769954714
H,0,-3.3920253356,-8.5699937031,1.5369665223
H,0,-2.7433946958,-7.9429639874,0.0197173884
N,0,-0.7854343704,-7.3103841237,4.9168391832
O,0,-0.9540716304,-8.033128443,4.0914479069
O,0,-0.5736135396,-6.7375568559,5.8484440617
F,0,-4.940124909,-7.3887159653,7.1462168667
B,0,-4.6810560777,-7.4514590846,5.7945988752
F,0,-5.3968332425,-6.4738382264,5.139708079
F,0,-3.324140581,-7.2561027165,5.5859012503
F,0,-5.034790392,-8.6920552684,5.3105896203

Pi Complex NO2BF4 PCM ONIOM 2.795_93851

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.268316105542

Zero-point correction= 0.157802 (Hartree/Particle)
Thermal correction to Energy= 0.174782
Thermal correction to Enthalpy= 0.175726
Thermal correction to Gibbs Free Energy= 0.108435
Sum of electronic and ZPE= -476.889149
Sum of electronic and thermal Energies= -476.872169
Sum of electronic and thermal Enthalpies= -476.871224
Sum of electronic and thermal Free Energies= -476.938516

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 109.678 55.717 141.627

C,0,1.347760806,-0.5762478335,1.5557316277
C,0,2.7425629374,-0.5942989719,1.487052328
C,0,3.4064418514,0.3005184172,0.6587833783
C,0,2.7003101839,1.2387581225,-0.1072292925
C,0,1.3071376516,1.2574268087,-0.0190653006
C,0,0.6314423836,0.3574772357,0.8013047783
C,0,3.438373884,2.1916035123,-1.0063327401
H,0,0.8235860863,-1.2653170008,2.2087304888
H,0,3.305643287,-1.3057284057,2.0794609682
H,0,4.4900662466,0.2798199451,0.6032264239
H,0,0.7426696782,1.9818396914,-0.5965909224
H,0,-0.4540764753,0.3900656671,0.8615675164
H,0,2.7694937155,2.9448551827,-1.4218984795
H,0,3.9044816951,1.655536923,-1.8371113743
H,0,4.2351940836,2.701263885,-0.4613565095
N,0,1.1786610847,-1.9395106045,-0.8790110929
O,0,0.3864596141,-2.6141824957,-0.4879993878
O,0,1.9737157124,-1.3592421635,-1.3894902906
F,0,-2.80662585,-0.6395619191,0.7695927324
B,0,-3.4256650692,0.3159077503,-0.0100319235
F,0,-2.4749889724,1.0465617617,-0.6925512263
F,0,-4.2557959631,-0.3069791767,-0.919230792
F,0,-4.1669685712,1.1562336685,0.7935110902

Pi Complex NO2BF4 PCM ONIOM 2.805_94148

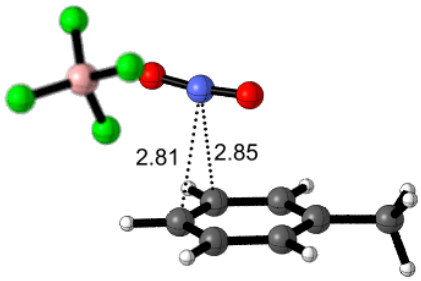
ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.273196595396

Zero-point correction= 0.157623 (Hartree/Particle)
Thermal correction to Energy= 0.174656
Thermal correction to Enthalpy= 0.175600
Thermal correction to Gibbs Free Energy= 0.108064
Sum of electronic and ZPE= -476.891929
Sum of electronic and thermal Energies= -476.874896
Sum of electronic and thermal Enthalpies= -476.873952
Sum of electronic and thermal Free Energies= -476.941488

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.598	55.835	142.142

C,0,2.4450375713,-2.3021044858,-0.220467116
C,0,3.224269275,-1.3603091138,-0.8940048413
C,0,4.466557246,-1.0017681909,-0.3878025232
C,0,4.9661254448,-1.5795419436,0.788870782
C,0,4.1864810941,-2.5334036288,1.4445607904
C,0,2.9338527521,-2.8914302653,0.9502211594
C,0,6.3079115558,-1.1609826268,1.3233338292
H,0,1.4762951271,-2.5921743628,-0.6121571215
H,0,2.8598567198,-0.9077086017,-1.8087304075
H,0,5.0665725593,-0.2633892673,-0.9101774215
H,0,4.5570841345,-2.9975660853,2.3523069948
H,0,2.3416583977,-3.637249014,1.4694086814
H,0,7.0767558479,-1.2522769419,0.5535528641
H,0,6.6041235488,-1.767692277,2.1785963556
H,0,6.2878520969,-0.1146547896,1.6389523262
N,0,1.7079839606,-0.4563817864,1.7599557816
O,0,0.6833509713,-0.8799334321,1.8539801683
O,0,2.6787423046,0.0800234823,1.748496263
F,0,1.4890201512,1.8847465083,5.6364305397
B,0,0.689060757,2.2545335404,4.5768400737
F,0,-0.636961972,2.1567534386,4.9376337251
F,0,0.9781176393,3.5498513216,4.2067720124
F,0,0.9317649171,1.4082190218,3.5076030841

Pi Complex NO2BF4 PCM ONIOM 2.807_94201



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.268383408515

Zero-point correction= 0.157436 (Hartree/Particle)
Thermal correction to Energy= 0.174783
Thermal correction to Enthalpy= 0.175727
Thermal correction to Gibbs Free Energy= 0.104068
Sum of electronic and ZPE= -476.888647
Sum of electronic and thermal Energies= -476.871301
Sum of electronic and thermal Enthalpies= -476.870357
Sum of electronic and thermal Free Energies= -476.942016

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.678	55.878	150.819

C,0,1.873814788,0.5117575716,-1.7021996179
C,0,2.9561232409,1.2134945715,-1.1610525461
C,0,3.7835373517,0.6064681601,-0.2187959318
C,0,3.543657847,-0.7022145376,0.2042091516
C,0,2.4545638927,-1.3930415524,-0.3448411546
C,0,1.6313275716,-0.8002125816,-1.2941861857
C,0,4.4420531758,-1.3753020171,1.2052965178
H,0,1.2381952537,0.9793060764,-2.4464061252
H,0,3.159689679,2.2283105123,-1.48537368
H,0,4.6234478746,1.1569032465,0.1913046573
H,0,2.2560535838,-2.4099979211,-0.0216549767
H,0,0.7982698074,-1.3541459128,-1.7113606633
H,0,5.0560754068,-0.6513018856,1.7408820684
H,0,5.1125937686,-2.0744119395,0.6987083924
H,0,3.8639333214,-1.9474548916,1.9328608197
N,0,0.7846749666,1.5886001548,0.6512397611
O,0,0.363553945,2.4660497058,0.1142947457
O,0,1.1277937306,0.7609272015,1.3038684196
F,0,-2.7251870558,-0.7365030981,-0.4729179318
B,0,-3.9606345522,-0.5534506728,0.1138996211
F,0,-4.1564035647,-1.5160388928,1.082116977
F,0,-4.0079490864,0.6967276832,0.6963718115
F,0,-4.9442719461,-0.6551569811,-0.8470331303

Pi Complex NO2BF4 PCM ONIOM 2.813_93970

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266398676533

Zero-point correction= 0.157694 (Hartree/Particle)
Thermal correction to Energy= 0.174883
Thermal correction to Enthalpy= 0.175828
Thermal correction to Gibbs Free Energy= 0.106798
Sum of electronic and ZPE= -476.888807
Sum of electronic and thermal Energies= -476.871617
Sum of electronic and thermal Enthalpies= -476.870673
Sum of electronic and thermal Free Energies= -476.939703

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.741	55.760	145.286

C,0,-1.3811038169,-4.2686842653,4.6316795158
C,0,-0.0715271929,-4.5105334915,4.2050757943
C,0,0.7370011936,-5.3907133941,4.9124893438
C,0,0.2613162061,-6.0495065892,6.0535232375
C,0,-1.0515766272,-5.8054621194,6.4648398038
C,0,-1.8704447064,-4.9264889573,5.7608446593
C,0,1.1529181978,-6.9998117506,6.804681916
H,0,-2.0194156132,-3.5905392072,4.0759453304
H,0,0.3097891837,-4.0147734153,3.3198373176
H,0,1.7538967059,-5.5731744219,4.5800668683
H,0,-1.4391657594,-6.3030328213,7.3494658783
H,0,-2.8892176797,-4.7547012789,6.0944124127
H,0,0.6657846625,-7.3795337909,7.7024011079

H,0,2.0836437477,-6.5099968645,7.0989940149
H,0,1.4193785124,-7.8521288597,6.1753702084
N,0,-0.2422505678,-2.4729287383,6.4745034811
O,0,0.3970156857,-3.2144421271,6.99264606
O,0,-0.82948522,-1.6392426891,6.033498154
F,0,-2.870880678,-5.7078614558,9.4944408483
B,0,-4.1651132415,-5.2465790242,9.3677683727
F,0,-5.0167306629,-6.3119680973,9.1650054047
F,0,-4.524984347,-4.5788567831,10.5202050536
F,0,-4.2456150826,-4.3805312581,8.2961575167

Pi Complex NO2BF4 PCM ONIOM 2.814_93946 file
E(RPM3) = 0.267813568592

Zero-point correction= 0.157317 (Hartree/Particle)
Thermal correction to Energy= 0.173840
Thermal correction to Enthalpy= 0.174784
Thermal correction to Gibbs Free Energy= 0.106756
Sum of electronic and ZPE= -476.888899
Sum of electronic and thermal Energies= -476.872376
Sum of electronic and thermal Enthalpies= -476.871432
Sum of electronic and thermal Free Energies= -476.939460

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.086	53.899	143.177

Pi Complex NO2BF4 PCM ONIOM 2.815_94069

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267668627983

Zero-point correction= 0.157398 (Hartree/Particle)
Thermal correction to Energy= 0.174685
Thermal correction to Enthalpy= 0.175629
Thermal correction to Gibbs Free Energy= 0.105358
Sum of electronic and ZPE= -476.888658
Sum of electronic and thermal Energies= -476.871371
Sum of electronic and thermal Enthalpies= -476.870427
Sum of electronic and thermal Free Energies= -476.940698

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.617	55.909	147.898

C,0,4.3896506802,0.1122259262,-3.1759287026
C,0,4.4906212256,1.3444832472,-2.522007904
C,0,4.9880967259,1.4083878875,-1.2224096389
C,0,5.3838045163,0.2503839446,-0.5506908931
C,0,5.2852086509,-0.9769607026,-1.221242538
C,0,4.7997362678,-1.0490068879,-2.521109208
C,0,5.8833757421,0.3060796078,0.866715993
H,0,4.0163588666,0.0632116878,-4.1927630134
H,0,4.1949120624,2.2540824567,-3.0335954836
H,0,5.0676947261,2.3696224836,-0.7258729185
H,0,5.594811672,-1.8843284125,-0.7123360169
H,0,4.7374789786,-2.0072230798,-3.0235163258
H,0,6.1575575769,1.3219892695,1.1511419596
H,0,6.7529344966,-0.3388878933,1.0018995338
H,0,5.1102221743,-0.0393487786,1.5586015152
N,0,1.9857774073,0.2635020379,-1.7171203884
O,0,2.4166545191,-0.1848234216,-0.7999902789
O,0,1.4280073491,0.6972830062,-2.5752332235
F,0,-2.1621417887,-3.0959941737,1.053236947
B,0,-1.2992678299,-2.3429683171,1.8220409637
F,0,-0.053430436,-2.9357038152,1.8260940751
F,0,-1.2003165579,-1.0741318711,1.2883649683
F,0,-1.7762275254,-2.2636247016,3.113345778

Pi Complex NO2BF4 PCM ONIOM 2.816_94015

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.268139522516

Zero-point correction= 0.157983 (Hartree/Particle)
Thermal correction to Energy= 0.175170
Thermal correction to Enthalpy= 0.176115
Thermal correction to Gibbs Free Energy= 0.106327
Sum of electronic and ZPE= -476.888503
Sum of electronic and thermal Energies= -476.871315
Sum of electronic and thermal Enthalpies= -476.870371
Sum of electronic and thermal Free Energies= -476.940158

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.921	55.714	146.881

C,0,-1.9113442413,0.7193858841,-1.2652827676
C,0,-2.387462751,0.8551293487,0.0433273605
C,0,-3.2057672665,-0.1271989007,0.5963030201
C,0,-3.5703749947,-1.2536675291,-0.1441671134
C,0,-3.0819798056,-1.3792326774,-1.452059962
C,0,-2.2562946223,-0.4095784881,-2.0080230852
C,0,-4.4823434911,-2.3010727046,0.4328603215
H,0,-1.2589117699,1.4748398347,-1.6885735584
H,0,-2.1067565789,1.7204111074,0.6343599493
H,0,-3.5654756015,-0.0160534951,1.6141082538
H,0,-3.3516448721,-2.253420592,-2.0359019315
H,0,-1.8811163507,-0.5302863101,-3.0174954483
H,0,-4.5047624383,-2.2508993776,1.521472229
H,0,-4.1648461935,-3.3023659721,0.1383401373
H,0,-5.504563602,-2.161478653,0.0698329916
N,0,-4.4417737197,1.9044315182,-1.6225648834
O,0,-4.9860692469,0.9394621893,-1.6518528857
O,0,-4.0183126028,2.9319026125,-1.6445336521
F,0,-7.8610013363,4.1099437352,2.8593632491
B,0,-7.9741436719,2.9242578959,2.1641267002
F,0,-6.9267811376,2.091754511,2.5022211565
F,0,-9.1687830447,2.3127265904,2.4802085977
F,0,-7.9325678607,3.1811224723,0.8087195209

Pi Complex NO2BF4 PCM ONIOM 2.817_94021

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.268203592412

Zero-point correction= 0.157942 (Hartree/Particle)
Thermal correction to Energy= 0.175161
Thermal correction to Enthalpy= 0.176105
Thermal correction to Gibbs Free Energy= 0.106148
Sum of electronic and ZPE= -476.888420
Sum of electronic and thermal Energies= -476.871201
Sum of electronic and thermal Enthalpies= -476.870257
Sum of electronic and thermal Free Energies= -476.940213

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.915	55.724	147.237

C,0,3.2760491936,-0.8879710033,-0.9252048117
C,0,2.2043268697,-0.2496363597,-1.5589370835
C,0,1.7511707641,0.9837208904,-1.0965064086
C,0,2.3489571109,1.5969145511,0.0065970155
C,0,3.4250239589,0.948652996,0.6285154259
C,0,3.8908708202,-0.2766252934,0.1672399515
C,0,1.8422554258,2.9108564716,0.5342851741
H,0,3.640677493,-1.8388434413,-1.2972745977
H,0,1.734382432,-0.7091003609,-2.4220091395
H,0,0.9231223906,1.4740137018,-1.5981261439
H,0,3.9034977892,1.4177565709,1.4822166846
H,0,4.7306482066,-0.7565926347,0.6558645007
H,0,1.2008927357,2.7521931326,1.4058887336
H,0,1.2582283221,3.4412695038,-0.2178376725
H,0,2.667502227,3.5516654629,0.8480104685
N,0,1.0499339812,-1.7008949836,0.5977178075
O,0,1.0871192956,-0.8268462671,1.2781476219
O,0,0.9208428743,-2.6371133689,0.0125466021
F,0,-5.0005164593,0.4792774735,-0.2873208908
B,0,-3.7464930501,-0.036602871,-0.038798268
F,0,-2.8241960234,0.9891513917,-0.0021562341
F,0,-3.7456951429,-0.696090603,1.173258157
F,0,-3.4020792148,-0.9231829596,-1.038596893

Pi Complex NO2BF4 PCM ONIOM 2.819_94022

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267271057213

Zero-point correction= 0.157573 (Hartree/Particle)
Thermal correction to Energy= 0.174757
Thermal correction to Enthalpy= 0.175702
Thermal correction to Gibbs Free Energy= 0.106144
Sum of electronic and ZPE= -476.888792
Sum of electronic and thermal Energies= -476.871608
Sum of electronic and thermal Enthalpies= -476.870664
Sum of electronic and thermal Free Energies= -476.940221

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.662	55.771	146.396

C,0,-1.7669860373,0.4379928849,1.6813675992
C,0,-3.0153314954,0.0062482909,1.2245687699
C,0,-3.1001829349,-1.0275335024,0.2949122615
C,0,-1.9479003126,-1.6401644101,-0.2015521695
C,0,-0.7023213921,-1.1991180727,0.2672328894
C,0,-0.6088157943,-0.1786269339,1.2045144449
C,0,-2.0234437407,-2.7452911915,-1.2188090827
H,0,-1.7003728637,1.23199539,2.4168393272
H,0,-3.9201419983,0.467702076,1.6043163848
H,0,-4.0731878369,-1.3599304664,-0.0502209435
H,0,0.205788699,-1.661635886,-0.1107780456
H,0,0.3652847634,0.1440708097,1.558072643
H,0,-1.5320065784,-2.4499082547,-2.1490320281
H,0,-3.0560947605,-3.0076994047,-1.447258038
H,0,-1.5145039131,-3.6397941972,-0.8538188721
N,0,-1.9969710108,1.9227085129,-0.7046033113
O,0,-2.2815234095,2.8371142972,-0.1404157681
O,0,-1.7114470382,1.091239348,-1.3786611424
F,0,2.6861565892,-0.7453013892,-0.6569787702
B,0,3.4730834042,0.1745371517,0.0045722384
F,0,4.1018117035,0.9855656127,-0.9180640671
F,0,2.688280302,0.9531850241,0.8305171315
F,0,4.4190016557,-0.4873166893,0.7588895488

Pi Complex NO2BF4 PCM ONIOM 2.820_94089

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.275441117371

Zero-point correction= 0.158223 (Hartree/Particle)
Thermal correction to Energy= 0.175036
Thermal correction to Enthalpy= 0.175980
Thermal correction to Gibbs Free Energy= 0.110581
Sum of electronic and ZPE= -476.893256
Sum of electronic and thermal Energies= -476.876444
Sum of electronic and thermal Enthalpies= -476.875499
Sum of electronic and thermal Free Energies= -476.940898

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.837	55.662	137.644

C,0,-1.7803215185,-2.8794586443,-0.9005922701
C,0,-0.5932532638,-2.1544925873,-0.9841913274
C,0,0.4640225373,-2.4553342156,-0.133360647
C,0,0.3696833321,-3.4907065767,0.8070579329
C,0,-0.8177635402,-4.2221032636,0.8720486863
C,0,-1.8868411642,-3.9201280366,0.0306266019
C,0,1.5310657496,-3.8122068412,1.7066259892
H,0,-2.6094680604,-2.6541347282,-1.5614931365
H,0,-0.4969799183,-1.35110102,-1.7044633195
H,0,1.3802879272,-1.8770900598,-0.1926584416
H,0,-0.9234897264,-5.0160419145,1.6063202045
H,0,-2.8041282221,-4.4953191013,0.0990740254
H,0,1.2139336841,-4.3903385982,2.5747448124
H,0,2.0240582743,-2.9035100024,2.0552506985
H,0,2.2753484407,-4.4025662855,1.1660015748
N,0,-2.5781445619,-1.6674288805,1.5185570862
O,0,-1.5404816069,-1.4286397765,1.8307954969
O,0,-3.6690661858,-1.7802372972,1.3253234875
F,0,-2.7362807383,-3.6172676554,3.2601699494
B,0,-3.0061134653,-4.7099738941,4.0703110703
F,0,-2.1123288543,-5.7211666496,3.7960486373
F,0,-2.8894800577,-4.3296578373,5.3894519415
F,0,-4.2900055613,-5.1444231342,3.823409547

Pi Complex NO2BF4 PCM ONIOM 2.822_94104

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.275424085266

Zero-point correction= 0.158171 (Hartree/Particle)
Thermal correction to Energy= 0.175004
Thermal correction to Enthalpy= 0.175949
Thermal correction to Gibbs Free Energy= 0.110430
Sum of electronic and ZPE= -476.893308
Sum of electronic and thermal Energies= -476.876474
Sum of electronic and thermal Enthalpies= -476.875530
Sum of electronic and thermal Free Energies= -476.941048

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.817	55.681	137.895

C,0,-2.6552057332,0.7733503251,-1.3523827499
C,0,-1.7921262722,0.4414896821,-0.3004737562
C,0,-1.070800904,1.4362037102,0.3570584502
C,0,-1.1891729967,2.7737897937,-0.0251425435
C,0,-2.0602100957,3.0918555955,-1.0764650335
C,0,-2.792271528,2.1074738352,-1.7302746907
C,0,-0.4198839836,3.8554175132,0.6817531625
H,0,-3.2241100365,-0.0010986385,-1.8540151861
H,0,-1.6828529828,-0.5934291842,0.0060350486
H,0,-0.3871292606,1.1613374935,1.1557015057
H,0,-2.1595714093,4.1272277223,-1.385604238
H,0,-3.4611509871,2.3771609321,-2.5385852632
H,0,-0.0527163013,4.6035935602,-0.022338615
H,0,0.4298388499,3.4468187824,1.2289592785
H,0,-1.0639735202,4.369073867,1.4001194436
N,0,-0.0941434094,0.5028921097,-2.5081823083
O,0,0.1381957321,1.5850196077,-2.4293601441
O,0,-0.1955546064,-0.587389426,-2.7109386673
F,0,1.5258428282,-0.0670363025,-0.5306228491
B,0,2.2671627789,-0.5845943612,0.5208923693
F,0,3.598505616,-0.294796773,0.3160164344
F,0,1.8445552004,-0.0225861251,1.7049812524
F,0,2.0898942215,-1.9501535195,0.5646359999

Pi Complex NO2BF4 PCM ONIOM 2.822_94188

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267726128048

Zero-point correction= 0.157544 (Hartree/Particle)
Thermal correction to Energy= 0.174996
Thermal correction to Enthalpy= 0.175940
Thermal correction to Gibbs Free Energy= 0.104331
Sum of electronic and ZPE= -476.888670
Sum of electronic and thermal Energies= -476.871218
Sum of electronic and thermal Enthalpies= -476.870274
Sum of electronic and thermal Free Energies= -476.941883

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.812	55.863	150.715

C,0,3.2546528065,-0.8646636491,1.0061630731
C,0,3.926618121,-0.1942293588,-0.0172370727
C,0,3.4198036664,1.0011001989,-0.5107299886
C,0,2.245254521,1.5619974258,0.0109206889
C,0,1.590913342,0.8920957844,1.0461039597
C,0,2.0858029413,-0.3135651476,1.5402195591
C,0,1.7165545894,2.8565435186,-0.5431426377
H,0,3.6480451498,-1.7945381462,1.4017817563
H,0,4.8401816432,-0.6072665678,-0.4283936546
H,0,3.9397792787,1.5146769924,-1.3132721829
H,0,0.6842580923,1.3127974974,1.4681129899
H,0,1.5690912282,-0.8188899774,2.3491580921
H,0,2.4553150509,3.6528623975,-0.4292037527
H,0,0.8022222222,3.1636450852,-0.0361825585
H,0,1.5023563495,2.7628015444,-1.6103429619
N,0,1.285718981,-1.8085070817,-0.7828164861
O,0,1.2995618386,-0.8971554651,-1.4128621731
O,0,1.1986888377,-2.7824849799,-0.2544809637
F,0,-4.1481838419,0.9584212382,1.0746439388
B,0,-3.8456818419,0.0832959238,0.0525796099
F,0,-4.812781048,-0.8979095633,-0.0156454424
F,0,-3.7972362994,0.7684838918,-1.1437891636
F,0,-2.6194316283,-0.5018935616,0.2942723707

Pi Complex NO2BF4 PCM ONIOM 2.823_94179

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267244082575

Zero-point correction= 0.157383 (Hartree/Particle)
Thermal correction to Energy= 0.174822
Thermal correction to Enthalpy= 0.175766
Thermal correction to Gibbs Free Energy= 0.104208
Sum of electronic and ZPE= -476.888618
Sum of electronic and thermal Energies= -476.871179
Sum of electronic and thermal Enthalpies= -476.870235
Sum of electronic and thermal Free Energies= -476.941792

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.702	55.858	150.605

C,0,5.1962954816,-4.9741735147,-0.3333115929
C,0,5.6964274127,-5.0082118601,0.9663022195
C,0,4.9794947648,-5.6535887151,1.9701445209
C,0,3.7616064888,-6.2847424811,1.6976827004
C,0,3.2749848288,-6.2557174392,0.3857246327
C,0,3.9794477751,-5.6051988453,-0.6210607552
C,0,2.9836762095,-6.9818068164,2.7801027777
H,0,5.7535338433,-4.4816073619,-1.1224823926
H,0,6.6416147604,-4.5308582546,1.1972870011
H,0,5.3714606535,-5.6699367689,2.9816481287
H,0,2.3358207151,-6.7482557007,0.1542400177
H,0,3.592701886,-5.5982287897,-1.6344532944
H,0,2.8107101434,-8.0274753402,2.5169120983
H,0,2.0050759491,-6.5155110348,2.9168908484
H,0,3.5116943464,-6.9519649429,3.732939509

N,0,3.3299907571,-2.9653886026,0.3393799282
O,0,3.4320901798,-2.476137967,-0.65290943
O,0,3.1620544064,-3.3498508795,1.3644938649
F,0,-1.203758783,-1.5288416203,2.6860683039
B,0,-0.7345048538,-0.2461215523,2.8810189461
F,0,-1.0002926669,0.1505328977,4.1746525952
F,0,0.6278037004,-0.2191452177,2.6626697212
F,0,-1.3562617984,0.6101134072,1.9963818511

Pi Complex NO2BF4 PCM ONIOM 2.825_94068

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267928869545

Zero-point correction= 0.157468 (Hartree/Particle)
Thermal correction to Energy= 0.174778
Thermal correction to Enthalpy= 0.175722
Thermal correction to Gibbs Free Energy= 0.105604
Sum of electronic and ZPE= -476.888824
Sum of electronic and thermal Energies= -476.871515
Sum of electronic and thermal Enthalpies= -476.870570
Sum of electronic and thermal Free Energies= -476.940688

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.675	55.867	147.576

C,0,1.2129154822,-1.1160866734,-0.5547356792
C,0,1.2127612146,-0.9611828235,-1.9411008125
C,0,2.1377672381,-0.1172907274,-2.5437130774
C,0,3.0873667784,0.5795280065,-1.7840138823
C,0,3.0889957467,0.4046072016,-0.3987514585
C,0,2.1594070629,-0.4324406793,0.2149706438
C,0,4.0649531303,1.5059767289,-2.4536176572
H,0,0.5017530644,-1.7818825872,-0.078046863
H,0,0.4923486348,-1.4978610166,-2.5469866574
H,0,2.1303650658,0.0050341866,-3.6220090228
H,0,3.8229293096,0.926450037,0.2064049253
H,0,2.1806116697,-0.5656885873,1.291413887
H,0,3.5734517366,2.439334642,-2.7415063965
H,0,4.4694587227,1.0571782127,-3.362274087
H,0,4.8947298812,1.7547275656,-1.7922114383
N,0,-0.0130906241,1.3964286037,-0.147145753
O,0,0.4762011433,1.8694609155,-1.0220280423
O,0,-0.5864354731,1.0323298985,0.7322539881
F,0,1.561611813,5.4233090971,4.3895379179
B,0,1.1007633187,4.134316172,4.222939407
F,0,0.617052881,3.6561396875,5.4225444849
F,0,0.0894250277,4.1255966473,3.2839806865
F,0,2.1329203755,3.3280201922,3.788785287

Pi Complex NO2BF4 PCM ONIOM 2.826_94040

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267424826797

Zero-point correction= 0.157669 (Hartree/Particle)
Thermal correction to Energy= 0.174927
Thermal correction to Enthalpy= 0.175871
Thermal correction to Gibbs Free Energy= 0.105825
Sum of electronic and ZPE= -476.888564
Sum of electronic and thermal Energies= -476.871307
Sum of electronic and thermal Enthalpies= -476.870362
Sum of electronic and thermal Free Energies= -476.940409

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.768	55.815	147.425

C,0,2.2790254593,-0.8668958293,1.5339750338
C,0,3.3781850835,-0.9515890772,0.6745066042
C,0,3.7157950079,0.1291613466,-0.1375119767
C,0,2.9640216687,1.3050785526,-0.1120336271
C,0,1.8682189355,1.3787955488,0.7595695677
C,0,1.5297192638,0.3102374359,1.5798090349
C,0,3.309030047,2.4747700563,-0.9923642893
H,0,2.0238416631,-1.7023400453,2.1766338681
H,0,3.9778105666,-1.8547864576,0.6500417823
H,0,4.5716492362,0.0557560208,-0.7997908218
H,0,1.2768909519,2.2886395125,0.7905408393
H,0,0.6829510458,0.3883430893,2.2519207369
H,0,2.4608527827,2.7486455889,-1.6239751922
H,0,4.1591052057,2.2518192141,-1.6366793884
H,0,3.5590928304,3.3496821134,-0.3880762362
N,0,1.0603101478,-1.6471592148,-0.8937365881
O,0,1.0309957966,-0.62685003,-1.3247052358
O,0,1.0150440374,-2.7096291945,-0.5708595044
F,0,-3.1858068998,-0.7624580371,-0.6301259266
B,0,-3.9624193907,0.1889397744,-0.0003532794
F,0,-4.9040190038,-0.4370674067,0.7890945535
F,0,-3.1579192064,0.9858342371,0.7878057675
F,0,-4.5937852292,0.9663218018,-0.948431722

Pi Complex NO2BF4 PCM ONIOM 2.829_94116

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266959365789

Zero-point correction= 0.157261 (Hartree/Particle)
Thermal correction to Energy= 0.174598
Thermal correction to Enthalpy= 0.175542
Thermal correction to Gibbs Free Energy= 0.105096
Sum of electronic and ZPE= -476.888998
Sum of electronic and thermal Energies= -476.871661
Sum of electronic and thermal Enthalpies= -476.870717
Sum of electronic and thermal Free Energies= -476.941163

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.562	55.895	148.266

C,0,-5.145308933,-1.5654408088,2.5439999621
C,0,-4.2805325104,-2.6599197471,2.5475041775
C,0,-4.6147720562,-3.8091520978,1.8409282637
C,0,-5.805971514,-3.8877998927,1.1075798322
C,0,-6.6563168283,-2.7795952987,1.0971926514
C,0,-6.3351536829,-1.6280680397,1.8113188849
C,0,-6.1667007474,-5.149727184,0.3731473693

H,0,-4.8858919032,-0.662414665,3.0855366972
H,0,-3.3502796072,-2.6141335772,3.1018224475
H,0,-3.9426773226,-4.6611864806,1.8518499157
H,0,-7.5771402574,-2.8177744502,0.524699499
H,0,-7.0004507501,-0.7719626754,1.7852089065
H,0,-6.6296546558,-5.8692873433,1.0544073413
H,0,-5.2812623642,-5.6246863795,-0.0511617187
H,0,-6.8741594984,-4.9519603634,-0.4322324813
N,0,-6.8986959108,-2.8202246035,4.3762619749
O,0,-6.7530632123,-3.8350038235,3.9557453642
O,0,-7.1130267834,-1.8616726367,4.8955137106
F,0,-7.045775378,-3.9865511185,8.6891262446
B,0,-6.3351899341,-5.0027627844,9.294789567
F,0,-5.708738386,-4.5167989184,10.4229543077
F,0,-7.1982311306,-6.0203034696,9.6436812726
F,0,-5.3882361339,-5.4847593419,8.4144616098

Pi Complex NO2BF4 PCM ONIOM 2.830_93763

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267872230542

Zero-point correction= 0.158479 (Hartree/Particle)
Thermal correction to Energy= 0.175066
Thermal correction to Enthalpy= 0.176010
Thermal correction to Gibbs Free Energy= 0.110018
Sum of electronic and ZPE= -476.889169
Sum of electronic and thermal Energies= -476.872582
Sum of electronic and thermal Enthalpies= -476.871638
Sum of electronic and thermal Free Energies= -476.937630

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.855	55.295	138.892

C,0,-1.0485546681,-2.9668563538,-2.9448666132
C,0,-0.5877366179,-4.1806214114,-2.4424011519
C,0,-0.2190945412,-4.284478622,-1.1037837665
C,0,-0.3152588617,-3.1891842952,-0.2379616737
C,0,-0.7923466484,-1.9778946867,-0.7506376084
C,0,-1.1530227387,-1.8626912037,-2.0889674824
C,0,0.0748239302,-3.2980099046,1.2081705268
H,0,-1.3461803234,-2.8798586104,-3.9837091886
H,0,-0.510924343,-5.0440841207,-3.0924725072
H,0,0.1478181397,-5.2311274791,-0.7215891115
H,0,-0.8804123239,-1.1188452774,-0.0932641402
H,0,-1.5271251644,-0.917905484,-2.4682786715
H,0,-0.7923429506,-3.1278399841,1.8503324649
H,0,0.8344035642,-2.5378173231,1.4802979493
H,0,0.4761818572,-4.2843189531,1.4394048287
N,0,1.5440533851,-1.8325066096,-2.9870770711
O,0,1.313020159,-1.1522081475,-3.8354385837
O,0,1.9069521947,-2.4824127016,-2.1670503173
F,0,3.782330145,-1.8691106323,0.9073327644
B,0,3.3240727208,-1.2632353682,2.0584376823
F,0,3.7837094735,-1.9530867917,3.1596084828
F,0,3.7789575664,0.0380359198,2.101905533
F,0,1.9417630454,-1.2633207596,2.0571953547

Pi Complex NO2BF4 PCM ONIOM 2.830_94055

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266919255288

Zero-point correction= 0.157858 (Hartree/Particle)
Thermal correction to Energy= 0.175081
Thermal correction to Enthalpy= 0.176025
Thermal correction to Gibbs Free Energy= 0.105506
Sum of electronic and ZPE= -476.888207
Sum of electronic and thermal Energies= -476.870984
Sum of electronic and thermal Enthalpies= -476.870040
Sum of electronic and thermal Free Energies= -476.940558

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.865	55.755	148.419

C,0,1.9625589494,-6.6026972739,0.43725645
C,0,2.1016661087,-6.8254354138,1.8107989662
C,0,1.1693010501,-6.3015804574,2.702038984
C,0,0.0888934273,-5.543489451,2.2435344834
C,0,-0.0434695955,-5.3357360536,0.8641937277
C,0,0.8776555142,-5.8620131128,-0.0334784517
C,0,-0.8972968706,-4.936137235,3.2028394124
H,0,2.6790847432,-7.0260032511,-0.2579933052
H,0,2.9291062482,-7.4208016028,2.1808781227
H,0,1.282774766,-6.4840820432,3.7654993205
H,0,-0.8815770363,-4.7535097391,0.4944337203
H,0,0.7530312695,-5.6959509787,-1.0973595131
H,0,-0.8900873992,-5.4539194788,4.1619824209
H,0,-1.9097141123,-4.9684199695,2.7980401178
H,0,-0.6518329636,-3.8863259914,3.3878396112
N,0,3.287948862,-4.2262786185,1.2164681884
O,0,4.2650678278,-4.6068033018,0.8483923867
O,0,2.3748778829,-3.7334020243,1.6042946049
F,0,2.9656704048,1.6683089076,-1.4133419007
B,0,2.5911787464,0.8779945419,-0.3471748567
F,0,2.0379096285,1.6627078172,0.6428468808
F,0,1.6647807988,-0.0535721326,-0.7694761086
F,0,3.6992370496,0.2234774626,0.1518438382

Pi Complex NO2BF4 PCM ONIOM 2.830_94126

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.275092289408

Zero-point correction= 0.158031 (Hartree/Particle)
Thermal correction to Energy= 0.174786
Thermal correction to Enthalpy= 0.175731
Thermal correction to Gibbs Free Energy= 0.110424
Sum of electronic and ZPE= -476.893653
Sum of electronic and thermal Energies= -476.876898
Sum of electronic and thermal Enthalpies= -476.875954
Sum of electronic and thermal Free Energies= -476.941260

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.680	55.684	137.448

C,0,2.5397801517,-0.8425681992,1.0883839021
C,0,3.2780038538,-0.1255860721,0.1523149913
C,0,2.7583829954,1.0445675693,-0.3954398034
C,0,1.5018730632,1.527414271,-0.014832511
C,0,0.7735316391,0.8077229896,0.9378370805
C,0,1.2812498916,-0.3669877538,1.4838977392
C,0,0.9338904142,2.7877946167,-0.6068194001
H,0,2.9380886304,-1.7524372188,1.5223442898
H,0,4.2538162567,-0.479934812,-0.1569052041
H,0,3.3347008753,1.5910568665,-1.1340047562
H,0,-0.2170580731,1.1518832107,1.2277949784
H,0,0.6999780795,-0.9151354795,2.2174978235
H,0,-0.0605696893,2.6072564547,-1.0234026248
H,0,1.5726484277,3.1820804719,-1.3964242772
H,0,0.8274930131,3.5564989205,0.1619633431
N,0,0.6957243948,-1.8234579492,-0.8216760437
O,0,0.4566801065,-2.7465228046,-0.247362658
O,0,0.8683776741,-0.9880480776,-1.5305958235
F,0,-1.6112283502,-0.7953302085,-0.1012904818
B,0,-2.632217863,0.1310427449,0.0553317452
F,0,-2.7359123932,0.4865007019,1.3819908976
F,0,-2.3556909342,1.2431534867,-0.709035804
F,0,-3.814290164,-0.437105729,-0.3671884029

Pi Complex NO2BF4 PCM ONIOM 2.830_94144

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267183559878

Zero-point correction= 0.157622 (Hartree/Particle)
Thermal correction to Energy= 0.174950
Thermal correction to Enthalpy= 0.175894
Thermal correction to Gibbs Free Energy= 0.104563
Sum of electronic and ZPE= -476.888383
Sum of electronic and thermal Energies= -476.871055
Sum of electronic and thermal Enthalpies= -476.870111
Sum of electronic and thermal Free Energies= -476.941441

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.783	55.798	150.128

C,0,2.7772758554,-0.4400459505,-2.7082318387
C,0,1.6545784094,0.3253845703,-3.0270894074
C,0,1.7892193981,1.4520607064,-3.827994494
C,0,3.0383253733,1.8344338587,-4.3380618705
C,0,4.1517025179,1.0529217758,-4.0253513921
C,0,4.0278458525,-0.073704043,-3.2149989157
C,0,3.1602046799,3.0640070707,-5.1954535322
H,0,2.6777596047,-1.3254832459,-2.0901907488
H,0,0.6791696082,0.0423556805,-2.6485177292
H,0,0.9145830054,2.0489389976,-4.0673105596
H,0,5.1254586339,1.3277040057,-4.4166439292
H,0,4.9017515942,-0.6743886465,-2.9872198526
H,0,2.4775844672,3.0107874697,-6.045961549
H,0,4.173989321,3.1854918518,-5.576150218
H,0,2.8995604788,3.959913796,-4.62627019
N,0,3.6889675434,1.4618718201,-0.8203284001
O,0,3.3316399594,2.3380501911,-1.3963212551
O,0,4.0738885085,0.6685562685,-0.1436605165
F,0,0.2541683816,5.0585469393,0.0025122969
B,0,0.528840803,5.2764775793,1.3369173504
F,0,0.2540192135,6.5896024592,1.6553224691
F,0,-0.2483660494,4.4373656819,2.1084004708
F,0,1.86201474,5.0124354632,1.5774429115

Pi Complex NO2BF4 PCM ONIOM 2.831_93989

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266846348776

Zero-point correction= 0.157887 (Hartree/Particle)
Thermal correction to Energy= 0.175085
Thermal correction to Enthalpy= 0.176029
Thermal correction to Gibbs Free Energy= 0.106185
Sum of electronic and ZPE= -476.888195
Sum of electronic and thermal Energies= -476.870997
Sum of electronic and thermal Enthalpies= -476.870053
Sum of electronic and thermal Free Energies= -476.939897

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.867	55.753	147.000

C,0,-3.1405619678,1.0288261601,1.1435492003
C,0,-3.7311585696,0.8124401527,-0.1054177457
C,0,-3.6419409368,-0.4364156949,-0.7140846683
C,0,-2.9597016632,-1.4868625602,-0.0949593145
C,0,-2.380486753,-1.258900934,1.1603305967
C,0,-2.4718194507,-0.0179769461,1.7792632582
C,0,-2.8200630561,-2.8255142055,-0.7659841723
H,0,-3.2256544678,1.9965750365,1.6254152223
H,0,-4.2732137135,1.6149584036,-0.5934965414
H,0,-4.107808408,-0.5961688348,-1.6808284096
H,0,-1.8527181927,-2.0682716163,1.6548046837
H,0,-2.0231276745,0.1355798626,2.7539598052
H,0,-1.8458865969,-2.9058282114,-1.2570083321
H,0,-3.588632825,-2.9724007094,-1.5248263995
H,0,-2.8882112875,-3.6373770232,-0.0406423486
N,0,-0.9205890996,1.4541374785,-0.561506971
O,0,-0.7100395256,0.3767263083,-0.7093548762
O,0,-1.0213046471,2.5577400482,-0.4785386954
F,0,3.4270288679,0.6630400085,-0.7938730352
B,0,4.4189420158,0.0458500932,-0.0592499654
F,0,5.2358420514,-0.6742416349,-0.9052726385
F,0,5.1622930894,1.0028392207,0.5994499208
F,0,3.8438198109,-0.8049424022,0.8619484266

Pi Complex NO2BF4 PCM ONIOM 2.832_93961

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266460911868

Zero-point correction= 0.158104 (Hartree/Particle)
Thermal correction to Energy= 0.175325
Thermal correction to Enthalpy= 0.176269
Thermal correction to Gibbs Free Energy= 0.106450

Sum of electronic and ZPE= -476.887956
Sum of electronic and thermal Energies= -476.870735
Sum of electronic and thermal Enthalpies= -476.869791
Sum of electronic and thermal Free Energies= -476.939610

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.018	55.653	146.945

C,0,-2.2315135423,1.0212003264,1.4366720426
C,0,-3.4033421611,1.003918177,0.6769501569
C,0,-3.733326121,-0.1254662852,-0.0644425444
C,0,-2.9103790045,-1.2576175291,-0.058530937
C,0,-1.7433256113,-1.2303820933,0.7123325469
C,0,-1.4044813716,-0.1049727669,1.4566223591
C,0,-3.2907454582,-2.4877444846,-0.8362405713
H,0,-1.975082175,1.8953014401,2.0255057675
H,0,-4.0556431365,1.8695380513,0.6671666131
H,0,-4.6419394082,-0.1320354387,-0.6574301694
H,0,-1.0949958244,-2.100441649,0.7286929698
H,0,-0.5001032363,-0.1031114868,2.0550925187
H,0,-3.8527961062,-2.231886571,-1.735139956
H,0,-3.9236154919,-3.1370295536,-0.2252034963
H,0,-2.4111380822,-3.0632489126,-1.1265903076
N,0,-0.8811012393,1.6363201987,-0.9761390869
O,0,-1.2446694857,0.7571932077,-1.5434523336
O,0,-0.4634450885,2.5547215958,-0.5118057056
F,0,3.7540246217,0.8671086944,-0.719199305
B,0,3.7679308497,-0.2849554515,0.0404648156
F,0,3.4966850426,-1.3674019983,-0.7706190213
F,0,5.0067604598,-0.4407445522,0.6249150976
F,0,2.8030435707,-0.1960909188,1.0228615466

Pi Complex NO2BF4 PCM ONIOM 2.832_94166

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267253721599

Zero-point correction= 0.157324 (Hartree/Particle)
Thermal correction to Energy= 0.174716
Thermal correction to Enthalpy= 0.175660
Thermal correction to Gibbs Free Energy= 0.104439
Sum of electronic and ZPE= -476.888779
Sum of electronic and thermal Energies= -476.871387
Sum of electronic and thermal Enthalpies= -476.870443
Sum of electronic and thermal Free Energies= -476.941664

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.636	55.920	149.897

C,0,-1.4033866266,-0.1769968077,2.8513700684
C,0,-1.610779403,1.1480783862,3.2382760571
C,0,-2.8313514204,1.7600190366,2.9838701182
C,0,-3.8739532484,1.0661154674,2.3534227182
C,0,-3.6603673981,-0.2628922128,1.9830271069
C,0,-2.4357925002,-0.8822483314,2.2257875156
C,0,-5.1890284307,1.7499528056,2.0981974402
H,0,-0.4551609116,-0.6636113509,3.0518849692
H,0,-0.819422532,1.6994103833,3.7327721874
H,0,-2.9869054982,2.7931861456,3.2779949919
H,0,-4.4564058357,-0.818212213,1.498445408
H,0,-2.2870016454,-1.9175784372,1.9387407794
H,0,-5.6824715213,1.9933672869,3.0421164011
H,0,-5.8615665533,1.1188408283,1.5177738154
H,0,-5.0429441733,2.6874399782,1.5573765363
N,0,-1.0902886592,0.5523765275,0.1319378807
O,0,-1.8273085594,1.3786486107,0.1788766242
O,0,-0.3165699409,-0.2272943831,-0.0359112787
F,0,1.9149403985,2.4362466413,-4.884660271
B,0,2.3844108375,2.3543978409,-3.5904959877
F,0,1.7493583272,3.2997533438,-2.8111016291
F,0,2.1224865249,1.0968658962,-3.0864398134
F,0,3.7440210698,2.5835375575,-3.5733615385

Pi Complex NO2BF4 PCM ONIOM 2.833_94062

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267888788648

Zero-point correction= 0.157385 (Hartree/Particle)
Thermal correction to Energy= 0.174709
Thermal correction to Enthalpy= 0.175654
Thermal correction to Gibbs Free Energy= 0.105819
Sum of electronic and ZPE= -476.889058
Sum of electronic and thermal Energies= -476.871734
Sum of electronic and thermal Enthalpies= -476.870789
Sum of electronic and thermal Free Energies= -476.940624

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.632	55.871	146.979

C,0,-5.327080771,-2.3143656504,-1.5331194867
C,0,-6.4669353609,-1.5171785636,-1.4319622358
C,0,-6.4281494778,-0.3432775333,-0.6896832204
C,0,-5.2549781002,0.0681856888,-0.0421377291
C,0,-4.1157455839,-0.7298594661,-0.1608346396
C,0,-4.1483162956,-1.9137534392,-0.8955691496
C,0,-5.2402239513,1.3321163819,0.7727770954
H,0,-5.3462343993,-3.2251164011,-2.1211594079
H,0,-7.3817937226,-1.811743522,-1.9322462167
H,0,-7.3187363139,0.2720820819,-0.61139439
H,0,-3.1955333515,-0.4283618848,0.3318348965
H,0,-3.251578469,-2.5181320079,-0.9846593818
H,0,-5.745061583,2.1429037011,0.2451610074
H,0,-4.2218176908,1.6481658606,0.9984533792
H,0,-5.7641526878,1.184011118,1.7209485816
N,0,-5.5713063036,-3.326076681,1.1020529029
O,0,-6.0922492356,-2.4210497546,1.4736228669
O,0,-5.0955856771,-4.2991898802,0.8531562987
F,0,0.0072686073,-0.5942375954,2.3757495283
B,0,-1.0688258119,-1.1757785244,3.0124840044
F,0,-1.22351094,-2.4731670678,2.5682209344
F,0,-0.8538476634,-1.1783770443,4.3751625563
F,0,-2.213687417,-0.4584876162,2.7323169055

Pi Complex NO2BF4 PCM ONIOM 2.834_93928

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.268482102561

Zero-point correction= 0.158131 (Hartree/Particle)
Thermal correction to Energy= 0.174916
Thermal correction to Enthalpy= 0.175860
Thermal correction to Gibbs Free Energy= 0.109913
Sum of electronic and ZPE= -476.891068
Sum of electronic and thermal Energies= -476.874283
Sum of electronic and thermal Enthalpies= -476.873338
Sum of electronic and thermal Free Energies= -476.939285

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.761	55.484	138.796

C,0,0.7726607136,-2.9688934205,-2.1885951502
C,0,1.6143452466,-2.6817947944,-1.1084418926
C,0,1.0862277674,-2.5082362421,0.1695875128
C,0,-0.2884192991,-2.6105370914,0.3881621798
C,0,-1.1205653723,-2.9053240186,-0.7007064762
C,0,-0.5996413363,-3.0889396543,-1.9756976249
C,0,-0.874346561,-2.3942518823,1.7563537112
H,0,1.1891713792,-3.1197914933,-3.1779142355
H,0,2.685227827,-2.6066030189,-1.2632707745
H,0,1.7570349265,-2.2792238209,1.0155475177
H,0,-2.1900962017,-2.9933534247,-0.5399061782
H,0,-1.259350441,-3.3231923723,-2.8024627344
H,0,-1.4295759293,-1.4533020062,1.7933000912
H,0,-0.0944846797,-2.3562053003,2.5174883091
H,0,-1.5708247864,-3.1940254582,2.0138595053
N,0,0.7399610983,-0.1443022503,-1.9492382049
O,0,-0.1568919619,-0.1412905953,-1.2980689483
O,0,1.6123753395,0.0023427051,-2.6229071541
F,0,2.7671297116,-1.9120373437,2.4223244625
B,0,3.2283815575,-0.6557659741,2.7708228563
F,0,4.6062155572,-0.6467211504,2.7259209776
F,0,2.7345025173,0.2756061295,1.8809095153
F,0,2.802922327,-0.3464883223,4.0446896352

Pi Complex NO2BF4 PCM ONIOM 2.835_94109

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267159007656

Zero-point correction= 0.157421 (Hartree/Particle)
Thermal correction to Energy= 0.174714
Thermal correction to Enthalpy= 0.175658
Thermal correction to Gibbs Free Energy= 0.105166
Sum of electronic and ZPE= -476.888841
Sum of electronic and thermal Energies= -476.871547
Sum of electronic and thermal Enthalpies= -476.870603
Sum of electronic and thermal Free Energies= -476.941096

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.635	55.864	148.364

C,0,-2.6962157279,-2.9646590894,1.5143892758
C,0,-2.4958658871,-4.1776110912,0.8579831096
C,0,-3.5725281401,-5.0276116268,0.626648461
C,0,-4.8673388661,-4.6830455391,1.0323165277
C,0,-5.0592265979,-3.4569621733,1.6757349329
C,0,-3.9863450582,-2.604982258,1.9205375527
C,0,-6.0221909665,-5.619705704,0.8054262567
H,0,-1.8635386352,-2.2920546635,1.6880077417
H,0,-1.5030609911,-4.4593800371,0.5274648085
H,0,-3.4095753126,-5.972576747,0.1188241061
H,0,-6.0573400168,-3.1670878341,1.987985907
H,0,-4.1533406695,-1.6532078066,2.4134239336
H,0,-5.8313846619,-6.2875417562,-0.0348464835
H,0,-6.9433088263,-5.0696708012,0.6099079028
H,0,-6.1911350664,-6.2400813607,1.6902751698
N,0,-2.9229472051,-4.2360195779,4.0387073081
O,0,-3.4094910624,-5.1432117272,3.6295131101
O,0,-2.4212642766,-3.3911080112,4.5568008692
F,0,-5.5273049145,-4.2254290893,7.7893267269
B,0,-6.0238794675,-5.4242292627,8.2592909184
F,0,-5.3524612497,-5.7776413161,9.4108782902
F,0,-7.3697716081,-5.2904258548,8.527675438
F,0,-5.8392989927,-6.4005250725,7.3017801366

Pi Complex NO2BF4 PCM ONIOM 2.838_93889

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.268588814697

Zero-point correction= 0.158392 (Hartree/Particle)
Thermal correction to Energy= 0.174993
Thermal correction to Enthalpy= 0.175937
Thermal correction to Gibbs Free Energy= 0.110740
Sum of electronic and ZPE= -476.891238
Sum of electronic and thermal Energies= -476.874638
Sum of electronic and thermal Enthalpies= -476.873693
Sum of electronic and thermal Free Energies= -476.938890

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.809	55.365	137.217

C,0,-2.8438467912,0.0789393223,1.3104803987
C,0,-3.3039740838,-0.886137535,0.4164014797
C,0,-2.3960849124,-1.6628473563,-0.293468839
C,0,-1.0142578918,-1.5049070251,-0.1190038282
C,0,-0.5621179482,-0.5477904537,0.790275103
C,0,-1.4669375882,0.2416503735,1.4978329933
C,0,-0.0443157526,-2.358398702,-0.8888390653
H,0,-3.5451527896,0.6846127597,1.8725665739
H,0,-4.3680610769,-1.0268283057,0.2694739662
H,0,-2.7594095841,-2.4049056343,-0.9969677337
H,0,0.5227993331,-0.4099205306,0.9387510457
H,0,-1.0998323408,0.9786491304,2.2039513925
H,0,-0.0607578959,-3.3854081772,-0.5162480524
H,0,0.9758169642,-1.9807586485,-0.7925659542
H,0,-0.3037247534,-2.3913072655,-1.9485776823
N,0,-1.989908091,1.8410138478,-0.7444773212
O,0,-1.8727745787,1.0224717684,-1.4823806512

O,0,-2.1065201257,2.7593244302,-0.1280666873
F,0,2.2759089434,-0.2410809212,1.1157272779
B,0,3.0747542002,0.0937325423,0.037059882
F,0,2.3724570581,0.9265635039,-0.8096677411
F,0,4.1981561311,0.7500844993,0.4935506305
F,0,3.4483425742,-1.0469696226,-0.6402331874

Pi Complex NO2BF4 PCM ONIOM 2.839_94082

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267551188633

Zero-point correction= 0.157620 (Hartree/Particle)
Thermal correction to Energy= 0.174939
Thermal correction to Enthalpy= 0.175883
Thermal correction to Gibbs Free Energy= 0.105513
Sum of electronic and ZPE= -476.888717
Sum of electronic and thermal Energies= -476.871398
Sum of electronic and thermal Enthalpies= -476.870454
Sum of electronic and thermal Free Energies= -476.940824

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.776	55.867	148.107

C,0,2.4107074304,-6.946925232,1.7047979307
C,0,1.6206924415,-6.7876849785,2.8438549686
C,0,0.473187116,-6.0071102358,2.7866861979
C,0,0.0795205821,-5.3803491319,1.5957001958
C,0,0.8687884029,-5.5586942249,0.4583461598
C,0,2.0276611083,-6.331547807,0.5092549582
C,0,-1.1648364228,-4.5359902881,1.5628526411
H,0,3.3030346855,-7.5619079642,1.7394378668
H,0,1.9035687265,-7.2696171067,3.7722542582
H,0,-0.1346834129,-5.8802337589,3.6769818035
H,0,0.5774548851,-5.0891889609,-0.4753919034
H,0,2.6261090494,-6.4665391323,-0.3853417117
H,0,-1.3840746413,-4.187372311,0.5540041667
H,0,-1.0572906593,-3.6620697456,2.2102070017
H,0,-2.0248227284,-5.1030973911,1.9248307564
N,0,3.4971879015,-4.334089373,1.9364398202
O,0,4.4822724033,-4.6436846724,1.5254815159
O,0,2.5759344571,-3.9114922598,2.3838366166
F,0,1.5326261433,0.8395975616,-1.6095031904
B,0,2.0748898755,0.1880922712,-0.5220436989
F,0,1.062976047,-0.2498294703,0.3071463485
F,0,2.8119503867,-0.8956556521,-0.9543956897
F,0,2.8966058224,1.0502082637,0.1739776876

Pi Complex NO2BF4 PCM ONIOM 2.839_94167

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266843435738

Zero-point correction= 0.157399 (Hartree/Particle)
Thermal correction to Energy= 0.174840
Thermal correction to Enthalpy= 0.175784
Thermal correction to Gibbs Free Energy= 0.104487
Sum of electronic and ZPE= -476.888762
Sum of electronic and thermal Energies= -476.871321
Sum of electronic and thermal Enthalpies= -476.870377
Sum of electronic and thermal Free Energies= -476.941674

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.714	55.888	150.057

C,0,1.2653940907,-2.9220586745,-0.6295156783
C,0,0.9512768129,-1.6524180218,-1.1144488579
C,0,1.010812828,-1.3978150505,-2.4796567
C,0,1.3689318969,-2.4015904811,-3.3893781246
C,0,1.6706025344,-3.672191629,-2.8935597369
C,0,1.6229272268,-3.9337329002,-1.5263907395
C,0,1.3973234923,-2.1153042783,-4.8658515496
H,0,1.2141461031,-3.1297480625,0.4336844385
H,0,0.6653365727,-0.8640577851,-0.4277525608
H,0,0.7759782664,-0.4054709129,-2.8513865481
H,0,1.9478336113,-4.4635539384,-3.5817497446
H,0,1.8516391626,-4.9275351746,-1.157364715
H,0,0.3860343729,-2.1668215188,-5.2778980581
H,0,2.0123845196,-2.8380155435,-5.4022094176
H,0,1.7810308285,-1.1138653995,-5.0666383559
N,0,4.0470007526,-2.4648708598,-0.9683805041
O,0,4.2894650634,-3.0203387201,-0.0372633228
O,0,3.9283551671,-1.8773735303,-1.89983358
F,0,5.1913632338,1.5821504539,0.0768537288
B,0,4.6887276973,2.7933529427,0.5068539721
F,0,4.8903441498,2.9152684354,1.865800117
F,0,5.3356933167,3.8179359594,-0.1513914984
F,0,3.3375082003,2.8502471893,0.2346978359

Pi Complex NO2BF4 PCM ONIOM 2.841_94092

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267438081587

Zero-point correction= 0.157393 (Hartree/Particle)
Thermal correction to Energy= 0.174751
Thermal correction to Enthalpy= 0.175695
Thermal correction to Gibbs Free Energy= 0.105148
Sum of electronic and ZPE= -476.888677
Sum of electronic and thermal Energies= -476.871319
Sum of electronic and thermal Enthalpies= -476.870375
Sum of electronic and thermal Free Energies= -476.940921

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.658	55.877	148.477

C,0,-0.9498268238,0.1488013235,-2.6976659523
C,0,-0.4347986656,1.3638196916,-2.2452686967
C,0,0.7910391214,1.3959336352,-1.5924953569
C,0,1.5356737822,0.2257304843,-1.386677605
C,0,1.017101652,-0.982170917,-1.8541435662
C,0,-0.2170462525,-1.0253803576,-2.501201098
C,0,2.8612288044,0.2903267608,-0.6785581935
H,0,-1.9019962297,0.1166336893,-3.2157319137
H,0,-0.9911868773,2.2810623818,-2.3993534237

H,0,1.1843396834,2.3423337504,-1.2349743727
H,0,1.5800161495,-1.8985245054,-1.7123736923
H,0,-0.6019084463,-1.971291495,-2.8666290838
H,0,3.5443479848,0.9615632483,-1.2034941831
H,0,3.3289327393,-0.6918784308,-0.6160370411
H,0,2.7415516377,0.6780661989,0.3359103207
N,0,-1.6799412351,-0.7025651746,-0.086548439
O,0,-0.8568598035,-0.1439406071,0.4017420935
O,0,-2.5541579252,-1.2824984015,-0.4525946907
F,0,-4.5670159487,2.2662142778,2.3349294419
B,0,-5.6789108853,1.4518692448,2.4068253936
F,0,-5.3010524171,0.2026537112,2.8546752197
F,0,-6.5968874421,2.0000047247,3.2768944567
F,0,-6.2402780023,1.3360100665,1.1517523826

Pi Complex NO2BF4 PCM ONIOM 2.843_94060

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267764243661

Zero-point correction= 0.157651 (Hartree/Particle)
Thermal correction to Energy= 0.174953
Thermal correction to Enthalpy= 0.175897
Thermal correction to Gibbs Free Energy= 0.105649
Sum of electronic and ZPE= -476.888608
Sum of electronic and thermal Energies= -476.871306
Sum of electronic and thermal Enthalpies= -476.870362
Sum of electronic and thermal Free Energies= -476.940609

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.784	55.816	147.849

C,0,-1.0580609666,-2.4559652005,0.3085246283
C,0,-0.4303701989,-1.2825376753,0.7270509791
C,0,0.5779346572,-1.3384021656,1.6813525642
C,0,0.9922963533,-2.560630001,2.2297343954
C,0,0.3682879644,-3.7298856759,1.7928744528
C,0,-0.6516949894,-3.6820882048,0.8434402157
C,0,2.078022794,-2.5941855166,3.2702317919
H,0,-1.8399145276,-2.4213972123,-0.4418438187
H,0,-0.7295887211,-0.3282040912,0.3098219986
H,0,1.058624698,-0.4222173144,2.0094840706
H,0,0.6776961296,-4.6868687936,2.1996076669
H,0,-1.1220946852,-4.6010120591,0.5099932781
H,0,2.3554240099,-3.6172351435,3.5235848299
H,0,1.7508328866,-2.0939090548,4.1852841214
H,0,2.9702069103,-2.0735418791,2.9168190705
N,0,-2.5603095034,-2.7023144108,2.7105037569
O,0,-1.7999592756,-2.1681778849,3.3139114558
O,0,-3.4054948649,-3.220583252,2.2089152162
F,0,-2.6110073988,-5.1480712438,7.1393338301
B,0,-3.803778217,-4.6119735166,7.5797392968
F,0,-3.7085820103,-4.3178934766,8.92343201
F,0,-4.0742112332,-3.4579420663,6.8730102395
F,0,-4.8189207113,-5.5227104614,7.37373565

Pi Complex NO2BF4 PCM ONIOM 2.844_94005

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267806869155

Zero-point correction= 0.157654 (Hartree/Particle)
Thermal correction to Energy= 0.174839
Thermal correction to Enthalpy= 0.175783
Thermal correction to Gibbs Free Energy= 0.106240
Sum of electronic and ZPE= -476.888644
Sum of electronic and thermal Energies= -476.871459
Sum of electronic and thermal Enthalpies= -476.870515
Sum of electronic and thermal Free Energies= -476.940058

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.713	55.800	146.365

C,0,2.1942053115,-1.3852442795,3.3599499118
C,0,1.8115932607,-0.0582743596,3.5849046843
C,0,0.5394087012,0.2307171721,4.0721858316
C,0,-0.3752235484,-0.7921297685,4.3329146815
C,0,0.0235509272,-2.116716027,4.110462996
C,0,1.295757696,-2.4152311252,3.6354076621
C,0,-1.7668284997,-0.4832530235,4.8129976994
H,0,3.1900547077,-1.6105036185,2.9944781321
H,0,2.5135146687,0.7463811038,3.3948651454
H,0,0.255144906,1.262172556,4.2516393897
H,0,-0.6747754365,-2.9217626007,4.315858454
H,0,1.5864864596,-3.4471344259,3.476114114
H,0,-2.1285171458,-1.2529603917,5.4958337964
H,0,-2.4602698467,-0.4411475139,3.9681374146
H,0,-1.8061968046,0.4793688638,5.3231706539
N,0,0.8362775863,-0.6610406278,0.9673801129
O,0,1.7752285854,-0.3577927026,0.4562300208
O,0,-0.1609431122,-0.9496868675,1.354945962
F,0,2.2008012931,-4.5776507571,-0.3737573414
B,0,1.4238833418,-5.578387186,-0.9208088838
F,0,1.9818455754,-6.8055614456,-0.6315477014
F,0,0.1522485678,-5.5108799747,-0.3895948519
F,0,1.3583365056,-5.4088700004,-2.2881537841

Pi Complex NO2BF4 PCM ONIOM 2.847_94076

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267489098952

Zero-point correction= 0.157625 (Hartree/Particle)
Thermal correction to Energy= 0.174845
Thermal correction to Enthalpy= 0.175789
Thermal correction to Gibbs Free Energy= 0.105907
Sum of electronic and ZPE= -476.889051
Sum of electronic and thermal Energies= -476.871831
Sum of electronic and thermal Enthalpies= -476.870887
Sum of electronic and thermal Free Energies= -476.940769

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.717	55.809	147.080

C,0,1.0886119246,-1.3210842646,-0.6043259189
C,0,1.5228465623,-1.1204796523,-1.9137513397
C,0,2.4386365654,-0.1130514852,-2.1943834395
C,0,2.9505286063,0.7063060137,-1.1796387686
C,0,2.5164210838,0.4910235127,0.1300926137
C,0,1.5921036753,-0.5109338309,0.4189121607
C,0,3.9652379758,1.7701190955,-1.4966594256
H,0,0.3816206094,-2.11097955,-0.376574105
H,0,1.1448872857,-1.7462965169,-2.7134747472
H,0,2.767639525,0.0430724202,-3.2166305994
H,0,2.8996455332,1.115416376,0.9326930944
H,0,1.2710515365,-0.6689402427,1.4432357274
H,0,3.7486366434,2.2516944683,-2.4512899509
H,0,4.9626024319,1.3287359731,-1.5705359059
H,0,3.9970639645,2.5347048212,-0.7201977274
N,0,-0.593976574,0.9756869195,-0.6229601076
O,0,0.0247505345,1.4980712341,-1.3792993468
O,0,-1.3138836308,0.5457434294,0.1060929877
F,0,2.7048268145,5.0391601545,3.2193681762
B,0,2.0356664012,3.8375504491,3.1202117205
F,0,2.9339403668,2.8319017557,2.8294346303
F,0,1.4047485443,3.5576695269,4.3145324226
F,0,1.0937516201,3.9170163927,2.1144718489

Pi Complex NO2BF4 PCM ONIOM 2.852_94057

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267430511131

Zero-point correction= 0.157373 (Hartree/Particle)
Thermal correction to Energy= 0.174705
Thermal correction to Enthalpy= 0.175649
Thermal correction to Gibbs Free Energy= 0.106061
Sum of electronic and ZPE= -476.889258
Sum of electronic and thermal Energies= -476.871925
Sum of electronic and thermal Enthalpies= -476.870981
Sum of electronic and thermal Free Energies= -476.940570

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.629	55.872	146.461

C,0,1.1765873625,-1.4681046311,4.3651804359
C,0,1.1374317459,-0.1859148568,4.9215125012
C,0,-0.081018914,0.4699777534,5.086426603
C,0,-1.2761546142,-0.134936249,4.6938391043
C,0,-1.222518143,-1.4216132357,4.1405851112
C,0,-0.0129125006,-2.0871430858,3.9816301277
C,0,-2.5950048962,0.5738352287,4.8393244495
H,0,2.1232101452,-1.9853876458,4.2535360872
H,0,2.056835919,0.2922389209,5.2418607007
H,0,-0.1011479105,1.4609860205,5.5270110771
H,0,-2.1454738337,-1.9047105288,3.835549046
H,0,0.0071136108,-3.0850276491,3.5553011158
H,0,-2.5131241834,1.4358807462,5.5012172028
H,0,-3.3559822223,-0.0979245318,5.2399613234
H,0,-2.9514176677,0.9267286223,3.8677075715
N,0,1.180610284,0.2799944363,2.1110506019
O,0,2.2897414499,0.3275438258,2.0687689064
O,0,0.0752870687,0.2956232251,2.0366619484
F,0,0.8394202973,-4.9590183903,2.0033441071
B,0,1.0171073966,-4.8851970992,0.6374053669
F,0,-0.0105279649,-5.5499914432,0.0019065238
F,0,1.0189925588,-3.5617811043,0.2453458468
F,0,2.2228641115,-5.4627118282,0.2983561412

Pi Complex NO2BF4 PCM ONIOM 2.852_94125

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267003972576

Zero-point correction= 0.157376 (Hartree/Particle)
Thermal correction to Energy= 0.174698
Thermal correction to Enthalpy= 0.175642
Thermal correction to Gibbs Free Energy= 0.104863
Sum of electronic and ZPE= -476.888746
Sum of electronic and thermal Energies= -476.871424
Sum of electronic and thermal Enthalpies= -476.870479
Sum of electronic and thermal Free Energies= -476.941259

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.625	55.860	148.967

C,0,1.0533877984,1.052220148,-3.8255433203
C,0,1.1336209068,2.3737914375,-3.3763584345
C,0,2.1925087513,2.774323573,-2.5641278113
C,0,3.1813481689,1.8665533184,-2.1801598071
C,0,3.0923132082,0.5468670178,-2.6435437559
C,0,2.0448185398,0.1409939918,-3.4615518299
C,0,4.3083074235,2.2787068699,-1.2732054026
H,0,0.23818017,0.7449561186,-4.4712640992
H,0,0.3776935003,3.0929680415,-3.6727436109
H,0,2.2498942787,3.8035791913,-2.2255814088
H,0,3.8581000494,-0.1668894587,-2.3568987869
H,0,1.9974374028,-0.8826792089,-3.8140930403
H,0,4.1489208679,1.8904899369,-0.2633878603
H,0,4.3880836079,3.363680643,-1.2062173407
H,0,5.2611004176,1.8827755775,-1.6280873177
N,0,-0.1611616932,0.9235559751,-1.2477323384
O,0,-1.1835478692,1.0496205904,-1.6635949681
O,0,0.8030178718,0.7648082589,-0.7258186356
F,0,-1.4335826944,3.2350879375,3.3625804084
B,0,-2.3993649085,2.255590851,3.4711000644
F,0,-1.9557698524,1.1062746063,2.8490257742
F,0,-2.6444756826,1.9915503442,4.8019045599
F,0,-3.5589014629,2.687223739,2.8608416613

Pi Complex NO2BF4 PCM ONIOM 2.854_93769

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267971080380

Zero-point correction= 0.157854 (Hartree/Particle)
Thermal correction to Energy= 0.174755
Thermal correction to Enthalpy= 0.175699
Thermal correction to Gibbs Free Energy= 0.109794

Sum of electronic and ZPE= -476.889639
Sum of electronic and thermal Energies= -476.872738
Sum of electronic and thermal Enthalpies= -476.871794
Sum of electronic and thermal Free Energies= -476.937699

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.660	55.737	138.708

C,0,2.7553538367,-0.198961917,1.3372238879
C,0,3.3258572958,0.7801018919,0.5248642283
C,0,2.5105376518,1.6474685433,-0.1919251339
C,0,1.1133521027,1.5673515608,-0.1086845312
C,0,0.5522843723,0.5917904341,0.7162680778
C,0,1.363034637,-0.2872211992,1.4330457024
C,0,0.2494893426,2.5220048501,-0.885842256
H,0,3.3841319584,-0.8725288395,1.9083455919
H,0,4.4036195937,0.8631021455,0.4497772378
H,0,2.9587779522,2.4026502504,-0.8295100685
H,0,-0.5312234496,0.5093867131,0.7902335866
H,0,0.910947589,-1.0337699343,2.0772613487
H,0,0.543556564,2.5500119553,-1.9370726564
H,0,0.3517105845,3.5356377429,-0.4911761859
H,0,-0.8033954777,2.2413741111,-0.8283947835
N,0,1.9273248289,-1.8230235427,-0.8596625642
O,0,1.9542851221,-2.771607445,-0.2811737728
O,0,1.8993772614,-0.958886932,-1.5526305762
F,0,-4.3974545784,-0.5212622008,-0.2611253365
B,0,-3.1033333808,-0.1677035455,0.0612832334
F,0,-2.758674659,-0.7534819971,1.2626910324
F,0,-2.254039682,-0.6183969181,-0.9294044052
F,0,-3.0157134655,1.2043972731,0.1671073431

Pi Complex NO2BF4 PCM ONIOM 2.857_93993

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266420595424

Zero-point correction= 0.157772 (Hartree/Particle)
Thermal correction to Energy= 0.175035
Thermal correction to Enthalpy= 0.175979
Thermal correction to Gibbs Free Energy= 0.105984
Sum of electronic and ZPE= -476.888151
Sum of electronic and thermal Energies= -476.870887
Sum of electronic and thermal Enthalpies= -476.869943
Sum of electronic and thermal Free Energies= -476.939939

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.836	55.752	147.318

C,0,4.3078648248,1.2113217647,-2.9354043091
C,0,3.8376258835,2.0373701879,-1.9108266205
C,0,4.1477208932,1.7508318466,-0.5827940204
C,0,4.9238091917,0.6377031189,-0.2538899533
C,0,5.3953900837,-0.1778202419,-1.2922114132
C,0,5.0982383638,0.1047359123,-2.619304369
C,0,5.2437350394,0.2999913598,1.176478912
H,0,4.0790616431,1.4423398634,-3.9697698938
H,0,3.239518964,2.9100550864,-2.1497125617
H,0,3.7791714022,2.3986315874,0.2057173441
H,0,6.0042761798,-1.0431867161,-1.0500161532
H,0,5.4785503625,-0.5336952638,-3.408248061
H,0,4.9133229966,1.0856523036,1.855499186
H,0,6.3178196619,0.1581238326,1.3109189387
H,0,4.7536263307,-0.6317449569,1.4708479177
N,0,1.9347741374,-0.1488274358,-2.1093999303
O,0,2.4353133454,-0.6665175799,-1.2680408039
O,0,1.3397366423,0.2980943648,-2.9341771269
F,0,-2.6375085414,-3.0409677594,1.616614049
B,0,-1.4030592938,-2.4648761402,1.8318565276
F,0,-0.471532643,-3.4498238347,2.0871838324
F,0,-1.0265013838,-1.7586501341,0.7074253349
F,0,-1.473480684,-1.6067336659,2.9094934739

Pi Complex NO2BF4 PCM ONIOM 2.858_94149

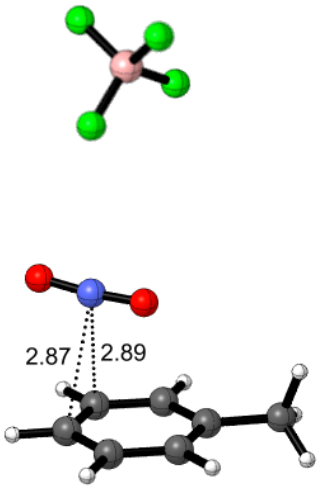
ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267212235626

Zero-point correction= 0.157311 (Hartree/Particle)
Thermal correction to Energy= 0.174683
Thermal correction to Enthalpy= 0.175627
Thermal correction to Gibbs Free Energy= 0.104611
Sum of electronic and ZPE= -476.888790
Sum of electronic and thermal Energies= -476.871418
Sum of electronic and thermal Enthalpies= -476.870474
Sum of electronic and thermal Free Energies= -476.941490

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.615	55.862	149.466

C,0,-4.8384392429,-1.4150876179,0.1284602354
C,0,-4.3742645313,-0.7529209657,1.2686537305
C,0,-4.154922022,0.6237405457,1.2401854542
C,0,-4.3866327247,1.3599692679,0.0778581546
C,0,-4.8560897798,0.6836460963,-1.0570155443
C,0,-5.0860238066,-0.6864568093,-1.034939501
C,0,-4.1402246379,2.8431184245,0.0273716266
H,0,-5.0242988681,-2.4828236825,0.1559669735
H,0,-4.1953515855,-1.3080056309,2.1834173868
H,0,-3.7978301458,1.1276917,2.1320724356
H,0,-5.0455124796,1.2446645769,-1.9667789826
H,0,-5.4559477593,-1.1877974223,-1.9215840552
H,0,-3.8175738502,3.2266734996,0.9949986786
H,0,-5.0470048615,3.375534316,-0.267076848
H,0,-3.3694579689,3.0829410946,-0.7091961955
N,0,-2.001233,-1.3090130104,-0.2025591199
O,0,-2.0465042616,-0.3556777563,-0.7649870836
O,0,-1.8345194515,-2.2756148764,0.3189675604
F,0,3.5258950395,1.0410899965,-1.0660239005
B,0,3.2460632915,0.249376204,0.0282409688
F,0,4.4104378164,-0.3162226392,0.503221206
F,0,2.6691827088,1.0196062087,1.0171572256
F,0,2.368976121,-0.7502735199,-0.3410174059

Pi Complex NO2BF4 PCM ONIOM 2.866_94198



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266440956603

Zero-point correction= 0.157232 (Hartree/Particle)
Thermal correction to Energy= 0.174589
Thermal correction to Enthalpy= 0.175533
Thermal correction to Gibbs Free Energy= 0.104205
Sum of electronic and ZPE= -476.888952
Sum of electronic and thermal Energies= -476.871596
Sum of electronic and thermal Enthalpies= -476.870652
Sum of electronic and thermal Free Energies= -476.941980

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.556	55.911	150.123

C,0,-3.8136900644,0.307942171,0.8369737673
C,0,-3.8952767669,0.2986889649,-0.5589152874
C,0,-3.5093664397,-0.8315794418,-1.2754862269
C,0,-3.0287083219,-1.9659158287,-0.6171628422
C,0,-2.9598605705,-1.9458072019,0.7818427778
C,0,-3.352030945,-0.8253729587,1.5055422655
C,0,-2.5664575853,-3.1728024254,-1.3867261936
H,0,-4.1310678404,1.1818240095,1.3949994825
H,0,-4.2766350615,1.1673114754,-1.0848269785
H,0,-3.5830837718,-0.8318035791,-2.357974237
H,0,-2.5935325812,-2.8220739201,1.3072277131
H,0,-3.2976361227,-0.8331770204,2.5878880654
H,0,-1.4801694695,-3.1513266023,-1.5131119151
H,0,-3.0152457646,-3.206755874,-2.3795203398
H,0,-2.8166825375,-4.0948035021,-0.8604132453
N,0,-1.163284515,1.0380206594,0.0256362307
O,0,-0.8315487524,-0.0146846932,-0.065861352
O,0,-1.3845857401,2.12346682,0.104886118
F,0,3.2052012388,1.8058337968,1.5254638272
B,0,4.1396869612,1.8320325077,0.5104236338
F,0,4.3283475484,3.1339107203,0.0957371993
F,0,5.3320398342,1.3120960376,0.9675911875
F,0,3.683539268,1.0756908851,-0.5497956503

Pi Complex NO2BF4 PCM ONIOM 2.868_93751

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267565186050

Zero-point correction= 0.157873 (Hartree/Particle)
Thermal correction to Energy= 0.174743
Thermal correction to Enthalpy= 0.175687
Thermal correction to Gibbs Free Energy= 0.110136
Sum of electronic and ZPE= -476.889778
Sum of electronic and thermal Energies= -476.872908
Sum of electronic and thermal Enthalpies= -476.871964
Sum of electronic and thermal Free Energies= -476.937515

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.653	55.678	137.965

C,0,-2.6907653831,0.3514104063,1.3517733719
C,0,-3.3717120662,-0.5687835594,0.5569313789
C,0,-2.660318391,-1.5036510775,-0.1865985961
C,0,-1.2606773915,-1.5500480594,-0.1470711834
C,0,-0.5883562619,-0.6308696258,0.6608059143
C,0,-1.2934593279,0.3139711857,1.4036396422
C,0,-0.5063486408,-2.5819949226,-0.9398946995
H,0,-3.2385653023,1.0785355805,1.9403404829
H,0,-4.45419975,-0.5539048432,0.5150878121
H,0,-3.1955397274,-2.2123207442,-0.8100853138
H,0,0.5000418679,-0.6432407211,0.6996164899
H,0,-0.7555448624,1.0168888362,2.0307445533
H,0,-0.9681446161,-2.7479502805,-1.9142263427
H,0,-0.5039878669,-3.5379148988,-0.4097741722
H,0,0.532193011,-2.2841833879,-1.0933318466
N,0,-1.7971772942,1.8959298908,-0.8945078626
O,0,-1.8289155221,1.0259609964,-1.5795917288
O,0,-1.7616881584,2.8455306381,-0.3186119953
F,0,4.4184015092,0.3763205706,-0.0835801347
B,0,3.1060910193,0.0304408181,0.1637522467
F,0,3.0471474345,-0.7910762469,1.2702723725
F,0,2.3710885413,1.1763638974,0.3932505017
F,0,2.5967601792,-0.6327504528,-0.9341348906

Pi Complex NO2BF4 PCM ONIOM 2.870_93870

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267106987355

Zero-point correction= 0.157891 (Hartree/Particle)
Thermal correction to Energy= 0.174886
Thermal correction to Enthalpy= 0.175830
Thermal correction to Gibbs Free Energy= 0.108833
Sum of electronic and ZPE= -476.889649
Sum of electronic and thermal Energies= -476.872655
Sum of electronic and thermal Enthalpies= -476.871711
Sum of electronic and thermal Free Energies= -476.938708

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.742	55.711	141.007

C,0,-3.0726268251,0.2434256471,1.1789611709
C,0,-1.7652802339,-0.1226934507,1.5151368245
C,0,-0.6829099106,0.4773827226,0.8743512526
C,0,-0.8830397662,1.4449163057,-0.112429186
C,0,-2.1977582307,1.8047042247,-0.436763265
C,0,-3.2828851151,1.2176148917,0.2042456635
C,0,0.2836504966,2.1014591146,-0.7974804032
H,0,-3.9136842849,-0.2119900771,1.6890065323
H,0,-1.5924473426,-0.8680828057,2.2841180223
H,0,0.3321396696,0.184649922,1.1337971517
H,0,-2.3674915585,2.5556818484,-1.201534236
H,0,-4.2916171254,1.5139110965,-0.0578442707
H,0,0.4641773879,3.0914648457,-0.3708371695
H,0,0.0940832686,2.2343705525,-1.8637050883
H,0,1.1971800696,1.5130541866,-0.6754910647
N,0,-2.3185280309,-1.7721844905,-0.720501478
O,0,-1.9992722711,-1.0181999883,-1.466256975
O,0,-2.6382088694,-2.6156131476,-0.0718637816
F,0,2.1580477125,-1.0553816274,-0.3537952855
B,0,3.2403365736,-0.2908113164,0.0322473669
F,0,4.2900198185,-1.1291338791,0.349888683
F,0,3.6178509213,0.5365612161,-1.0053430703
F,0,2.9146996462,0.4656452084,1.1387856061

Pi Complex NO2BF4 PCM ONIOM 2.875_94070

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267228760185

Zero-point correction= 0.157816 (Hartree/Particle)
Thermal correction to Energy= 0.175116
Thermal correction to Enthalpy= 0.176060
Thermal correction to Gibbs Free Energy= 0.105422
Sum of electronic and ZPE= -476.888312
Sum of electronic and thermal Energies= -476.871012
Sum of electronic and thermal Enthalpies= -476.870068
Sum of electronic and thermal Free Energies= -476.940706

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.887	55.757	148.671

C,0,3.9063366737,1.8716672295,-2.5472638222
C,0,3.2595686218,2.4558972071,-1.454105135
C,0,3.5565886726,2.0388736206,-0.1570262823
C,0,4.4930763259,1.0299489463,0.0716463762
C,0,5.1374977209,0.4559524866,-1.0335922867
C,0,4.855414587,0.8731890255,-2.3286656114
C,0,4.8043772835,0.550541988,1.4630658512
H,0,3.6869548577,2.2080075743,-3.5543958528
H,0,2.5349644099,3.2475311134,-1.6125003726
H,0,3.0525299813,2.5034799522,0.6840262131
H,0,5.8713605531,-0.3268288617,-0.8695688829
H,0,5.3701530814,0.4205861333,-3.168149197
H,0,4.327408746,1.1774050948,2.21625984
H,0,5.8810277656,0.5541583047,1.6433378055
H,0,4.4543982113,-0.4753260398,1.6043439426
N,0,1.6865084997,0.1400862977,-1.9620599263
O,0,2.3171295349,-0.5089891322,-1.3234808367
O,0,0.9705207846,0.6976293123,-2.6029607252
F,0,-2.4443684265,-2.745850379,1.0760550798
B,0,-1.1388073593,-3.1222488309,1.3139497992
F,0,-1.1178539449,-4.3015006529,2.0280480536
F,0,-0.4878963034,-3.2997910789,0.1101943028
F,0,-0.5021773771,-2.1338570109,2.0362481671

Pi Complex NO2BF4 PCM ONIOM 2.877_93769

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267132492595

Zero-point correction= 0.158214 (Hartree/Particle)
Thermal correction to Energy= 0.175249
Thermal correction to Enthalpy= 0.176193
Thermal correction to Gibbs Free Energy= 0.108904
Sum of electronic and ZPE= -476.888387
Sum of electronic and thermal Energies= -476.871352
Sum of electronic and thermal Enthalpies= -476.870408
Sum of electronic and thermal Free Energies= -476.937697

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.970	55.674	141.622

C,0,3.5600583301,0.2360311215,-0.5485453573
C,0,3.5691628392,-0.5120834574,0.6265622054
C,0,2.5457381593,-1.4202205065,0.8806666167
C,0,1.5019893464,-1.6114760155,-0.0330785499
C,0,1.512955265,-0.8700160923,-1.2174212196
C,0,2.5268121046,0.050208258,-1.473634309
C,0,0.3785717348,-2.5659023481,0.2651553492
H,0,4.3579826109,0.939592477,-0.7571901731
H,0,4.3707498585,-0.3856817745,1.3447122547
H,0,2.5555196279,-1.994145376,1.8016029397
H,0,0.7204284479,-1.0123526832,-1.9451426719
H,0,2.5229300503,0.6128416584,-2.4011259489
H,0,-0.4476460795,-2.0417103124,0.7564401765
H,0,0.7029403337,-3.3672877719,0.929195427
H,0,-0.0141372173,-3.0105266486,-0.6499249687
N,0,1.4204206188,1.9424624293,0.3409278053
O,0,1.063837783,1.1759898313,1.0564163441
O,0,1.7115086485,2.7944247688,-0.309740515
F,0,-2.6783610682,-0.6230737556,0.7853921775
B,0,-3.4901165659,0.1666474056,-0.0020962089
F,0,-2.7109938701,0.8921505164,-0.8805397199
F,0,-4.3634839345,-0.630384603,-0.7114961475
F,0,-4.2022260233,1.0345468786,0.7996964936

Pi Complex NO2BF4 PCM ONIOM 2.879_94110

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267312400944

Zero-point correction= 0.157856 (Hartree/Particle)
Thermal correction to Energy= 0.175140
Thermal correction to Enthalpy= 0.176084
Thermal correction to Gibbs Free Energy= 0.105343

Sum of electronic and ZPE= -476.888595
Sum of electronic and thermal Energies= -476.871311
Sum of electronic and thermal Enthalpies= -476.870367
Sum of electronic and thermal Free Energies= -476.941108

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.902	55.791	148.886

C,0,2.3083781926,-1.5427545649,-3.1785996808
C,0,1.183877978,-2.1108516881,-2.5718267043
C,0,-0.0910376385,-1.6293078715,-2.8656764107
C,0,-0.2664834394,-0.5705761356,-3.7586560596
C,0,0.8689657953,-0.0137720755,-4.3626819607
C,0,2.1430965061,-0.4949249032,-4.0831644294
C,0,-1.6344322979,-0.0182190646,-4.0526132991
H,0,3.2976788305,-1.9308567809,-2.963837944
H,0,1.3013569861,-2.9402412115,-1.8823252601
H,0,-0.9573597347,-2.081967345,-2.3942503078
H,0,0.7473240876,0.8059878752,-5.0635735845
H,0,3.0066997948,-0.0553292023,-4.5682082009
H,0,-2.4168235771,-0.7111022917,-3.743281879
H,0,-1.7548587366,0.1868895865,-5.1173714432
H,0,-1.7896523917,0.9234639211,-3.5187452915
N,0,1.7465624658,0.1019913275,-0.8833036314
O,0,1.1718960956,0.8224032438,-1.4977983368
O,0,2.3287653218,-0.530132726,-0.1795018677
F,0,-1.8525684677,0.998772266,1.6233323397
B,0,-3.0596377601,0.346963077,1.4722792451
F,0,-3.2794976153,-0.4678694556,2.5630659531
F,0,-4.0740054717,1.2759734021,1.3754209878
F,0,-3.0229326237,-0.4199984828,0.3259213659

Pi Complex NO2BF4 PCM ONIOM 2.889_93857

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267215216048

Zero-point correction= 0.157833 (Hartree/Particle)
Thermal correction to Energy= 0.174796
Thermal correction to Enthalpy= 0.175741
Thermal correction to Gibbs Free Energy= 0.108931
Sum of electronic and ZPE= -476.889667
Sum of electronic and thermal Energies= -476.872704
Sum of electronic and thermal Enthalpies= -476.871760
Sum of electronic and thermal Free Energies= -476.938570

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.686	55.699	140.613

C,0,-3.2903349793,-0.0131094848,-0.9143924832
C,0,-2.0445521491,0.1751166832,-1.5247712822
C,0,-0.9390410774,-0.555506486,-1.0992051722
C,0,-1.049288102,-1.4797622204,-0.0557585117
C,0,-2.3012461536,-1.6608100117,0.5423600667
C,0,-3.4143214415,-0.9410538808,0.1158122432
C,0,0.1522729598,-2.2646195103,0.393978568
H,0,-4.1535924382,0.5475133085,-1.2545147832
H,0,-1.9422512217,0.8854968422,-2.3382198156
H,0,0.0260685536,-0.4020207066,-1.5745839405
H,0,-2.4026209791,-2.3734218404,1.354170663
H,0,-4.3754477637,-1.1000664774,0.5900934396
H,0,1.0453851305,-1.6324062597,0.4332995873
H,0,0.3591433605,-3.0762566082,-0.3082826055
H,0,-0.0043090609,-2.706499656,1.3778786659
N,0,-1.8719165659,1.887932334,0.7350351096
O,0,-2.1766785815,2.7665601626,0.127486182
O,0,-1.5403605156,1.0933069489,1.431171867
F,0,2.43397362,0.5524007251,1.1380924878
B,0,3.2284269513,0.0839757902,0.1109978883
F,0,2.5071835654,0.0783765561,-1.0654887149
F,0,4.3189493689,0.9177487086,-0.0317655468
F,0,3.6630895194,-1.191828917,0.4024840875

Pi Complex NO2BF4 PCM ONIOM 2.894_93761

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266705108122

Zero-point correction= 0.157922 (Hartree/Particle)
Thermal correction to Energy= 0.174787
Thermal correction to Enthalpy= 0.175731
Thermal correction to Gibbs Free Energy= 0.109908
Sum of electronic and ZPE= -476.889605
Sum of electronic and thermal Energies= -476.872740
Sum of electronic and thermal Enthalpies= -476.871796
Sum of electronic and thermal Free Energies= -476.937619

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.680	55.655	138.536

C,0,-3.290833929,-0.1041857649,-0.863687202
C,0,-2.0520809325,0.1156419655,-1.4756273807
C,0,-0.9223027046,-0.5696198712,-1.035604206
C,0,-1.0024169476,-1.4760103325,0.0246595678
C,0,-2.2493102616,-1.6890300125,0.6252724544
C,0,-3.3851967966,-1.0178728816,0.1836456544
C,0,0.2187227312,-2.2179006052,0.4943197688
H,0,-4.172659547,0.4187798819,-1.2156936594
H,0,-1.9724021059,0.8143487399,-2.3017106793
H,0,0.0370536913,-0.3948454519,-1.5153436692
H,0,-2.326622883,-2.3898776746,1.450052148
H,0,-4.3411338259,-1.200131896,0.6603162131
H,0,0.1549819724,-2.455536982,1.5567551992
H,0,1.1284573267,-1.6349930875,0.32132807
H,0,0.3219065777,-3.1607622083,-0.0491414693
N,0,-1.9548516622,1.8756369103,0.7710677127
O,0,-1.5819662465,1.1006136618,1.4683284053
O,0,-2.3045345313,2.7340579959,0.1590453969
F,0,2.3785317257,0.7594766002,0.7204649682
B,0,3.2482333738,0.1321744487,-0.1488554229
F,0,4.3055661284,0.978446212,-0.4149572839
F,0,3.7239720269,-1.026710411,0.4281832985
F,0,2.5966488194,-0.1617422372,-1.3289188846

Pi Complex NO2BF4 PCM ONIOM 3.045_94107

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.265798563610

Zero-point correction= 0.157612 (Hartree/Particle)
Thermal correction to Energy= 0.175016
Thermal correction to Enthalpy= 0.175960
Thermal correction to Gibbs Free Energy= 0.104633
Sum of electronic and ZPE= -476.888095
Sum of electronic and thermal Energies= -476.870691
Sum of electronic and thermal Enthalpies= -476.869747
Sum of electronic and thermal Free Energies= -476.941074

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.824	55.769	150.121

C,0,-3.8124303407,1.2448895021,0.5638065754
C,0,-3.6057436488,0.9523810035,-0.7849633239
C,0,-3.2252538928,-0.3331504761,-1.1782828127
C,0,-3.0434906309,-1.3446240607,-0.234431079
C,0,-3.2518128455,-1.0359617659,1.1158485992
C,0,-3.6349833918,0.2408547961,1.5138539533
C,0,-2.6438621259,-2.7365841106,-0.6438832669
H,0,-4.1201254284,2.2389135962,0.8663802518
H,0,-3.7538663513,1.721147417,-1.5361124031
H,0,-3.0760641097,-0.5485902259,-2.2313468515
H,0,-3.1119677011,-1.8109173441,1.8631531543
H,0,-3.7943231966,0.4532091269,2.5645894294
H,0,-3.4519139521,-3.4426259949,-0.4391682278
H,0,-1.7683384602,-3.0732369101,-0.0847523407
H,0,-2.4127089104,-2.7875872174,-1.7078204814
N,0,-0.859323404,1.3930470188,-0.1644168284
O,0,-0.7654082982,0.5347950202,0.527878874
O,0,-0.8607487592,2.2712593388,-0.8427040669
F,0,3.8433007279,-1.115569146,0.8497293954
B,0,4.4440614192,-0.1661377618,0.0491639631
F,0,5.0321274162,0.7972555033,0.8421092815
F,0,5.4022861636,-0.7665532929,-0.7399416859
F,0,3.4902097205,0.4235649837,-0.7552311094

Pi Complex NO2BF4 PCM ONIOM 3.073_94058

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266217593082

Zero-point correction= 0.157860 (Hartree/Particle)
Thermal correction to Energy= 0.175087
Thermal correction to Enthalpy= 0.176031
Thermal correction to Gibbs Free Energy= 0.105441
Sum of electronic and ZPE= -476.888165
Sum of electronic and thermal Energies= -476.870938
Sum of electronic and thermal Enthalpies= -476.869994
Sum of electronic and thermal Free Energies= -476.940584

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.868	55.709	148.569

C,0,-3.8779930585,-0.8256205229,0.2311964376
C,0,-2.9863934712,-0.5728279453,1.2738685826
C,0,-2.1812471735,0.569207822,1.2526518718
C,0,-2.2516199842,1.4738165105,0.1921100692
C,0,-3.1519152464,1.2072009706,-0.8463370907
C,0,-3.9588829341,0.0736233044,-0.8295902075
C,0,-1.375709831,2.6970344569,0.1462481081
H,0,-4.5111468033,-1.7047280696,0.2550449605
H,0,-2.9267369279,-1.2563806121,2.1142799326
H,0,-1.500045915,0.7595630071,2.0759558062
H,0,-3.2218427244,1.9021132701,-1.6772246208
H,0,-4.6520101554,-0.1071553113,-1.6427282638
H,0,-0.5936114026,2.5839637173,-0.6091554565
H,0,-0.892431365,2.876205139,1.1066771938
H,0,-1.9561560417,3.5827748421,-0.1174674472
N,0,-1.0065765552,-1.706691346,-0.422418877
O,0,-1.1200509319,-0.9738079697,-1.2440391855
O,0,-0.8266502047,-2.4871844589,0.3451982827
F,0,4.7662696235,0.8832484057,-0.7830510159
B,0,3.9710785439,0.075313842,0.0019847883
F,0,3.3961429968,-0.9046243254,-0.7814794135
F,0,4.7367085836,-0.5143006655,0.9859338576
F,0,2.9768849781,0.8335809389,0.5856976874

Pi Complex NO2BF4 PCM ONIOM 3.107_93904

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.277412126795

Zero-point correction= 0.158624 (Hartree/Particle)
Thermal correction to Energy= 0.175113
Thermal correction to Enthalpy= 0.176057
Thermal correction to Gibbs Free Energy= 0.112735
Sum of electronic and ZPE= -476.893161
Sum of electronic and thermal Energies= -476.876672
Sum of electronic and thermal Enthalpies= -476.875728
Sum of electronic and thermal Free Energies= -476.939049

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.885	55.496	133.272

C,0,-2.1878616448,-2.4860625768,0.7280848241
C,0,-1.6380220102,-1.2122254535,0.8595436394
C,0,-1.0656934265,-0.570026181,-0.2466768034
C,0,-1.0398828387,-1.1876886753,-1.4966824157
C,0,-1.5887090376,-2.4702393929,-1.6103089767
C,0,-2.1567271651,-3.1147340739,-0.5143616033
C,0,-0.44549168,-0.5027316984,-2.6977636642
H,0,-2.6090073513,-2.9889206877,1.5934803214
H,0,-1.6507072001,-0.7164699497,1.8253719771
H,0,-0.6524646354,0.4267258236,-0.1317161475
H,0,-1.5685692742,-2.9710174016,-2.5728359031
H,0,-2.5697177475,-4.109827569,-0.62895881
H,0,-1.2122671153,-0.3276079841,-3.455368888
H,0,0.3309315583,-1.1182076491,-3.1567094576
H,0,-0.008999042,0.45934876,-2.4302552079
N,0,0.9043357157,-2.3103486059,0.9783492152
O,0,0.7797794677,-3.0251698201,0.1389285601

O,0,1.1902452659,-1.653385303,1.8291297833
F,0,0.0904237504,-4.3129829587,2.5474293155
B,0,-0.6713534408,-3.9445584768,3.6461024982
F,0,-0.0203706968,-4.3103362346,4.8013877793
F,0,-0.8047136215,-2.5706648827,3.5957045133
F,0,-1.9055821304,-4.5486828089,3.5865467506

Pi Complex NO2BF4 PCM ONIOM 3.137_94117

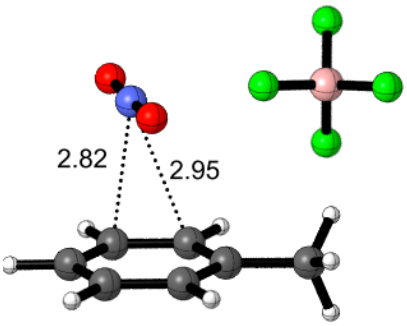
ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.273112150382

Zero-point correction= 0.158058 (Hartree/Particle)
Thermal correction to Energy= 0.174762
Thermal correction to Enthalpy= 0.175706
Thermal correction to Gibbs Free Energy= 0.110625
Sum of electronic and ZPE= -476.893743
Sum of electronic and thermal Energies= -476.877038
Sum of electronic and thermal Enthalpies= -476.876094
Sum of electronic and thermal Free Energies= -476.941175

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.665	55.572	136.975

C,0,5.0182879402,-1.4209373254,-3.5216259863
C,0,5.6357730067,-0.2522877631,-3.0905854836
C,0,5.692859009,0.0512935636,-1.7309230658
C,0,5.1383705619,-0.802736485,-0.7743911138
C,0,4.5167892759,-1.9745908149,-1.2173206336
C,0,4.4562647921,-2.2834310155,-2.5778037159
C,0,5.2081405903,-0.4848616948,0.6945317563
H,0,4.9768201188,-1.6649651231,-4.5761351777
H,0,6.072975203,0.4283443536,-3.8113194422
H,0,6.1734557431,0.9687355348,-1.4081644118
H,0,4.0647667458,-2.6443371292,-0.4886900494
H,0,3.9770120903,-3.2017359596,-2.8999641728
H,0,4.2724087869,-0.7490595009,1.1972634061
H,0,5.4060154915,0.5733368369,0.8650443339
H,0,6.0081857271,-1.0570672599,1.1703438924
N,0,2.1913867355,-0.613867897,-2.4255112214
O,0,2.7283216009,0.3328023135,-2.2192687544
O,0,1.5466508912,-1.4902551112,-2.6490708943
F,0,1.7715185831,-1.111610917,0.1217350758
B,0,1.6196864617,-1.6166818709,1.4045069133
F,0,2.463504437,-2.6914163848,1.5795389225
F,0,1.9091608346,-0.6311695639,2.3226965458
F,0,0.3134498736,-2.0254503863,1.566626177

Pi Complex NO2BF4 PCM ONIOM 3.139_94253



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.273122679758

Zero-point correction= 0.157984 (Hartree/Particle)
Thermal correction to Energy= 0.174740
Thermal correction to Enthalpy= 0.175685
Thermal correction to Gibbs Free Energy= 0.109264
Sum of electronic and ZPE= -476.893819
Sum of electronic and thermal Energies= -476.877063
Sum of electronic and thermal Enthalpies= -476.876118
Sum of electronic and thermal Free Energies= -476.942539

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.651	55.593	139.795

C,0,-3.1804559946,0.4034963697,-0.7960009618
C,0,-1.9577802791,0.3545335062,-1.4690502378
C,0,-0.9840085464,-0.5736427389,-1.0941315133
C,0,-1.2122693228,-1.4686588755,-0.0440316735
C,0,-2.4388288927,-1.4046408946,0.6216876817
C,0,-3.4146989004,-0.4801386035,0.2514593331
C,0,-0.1617316845,-2.4734133604,0.343970515
H,0,-3.937645721,1.1191501966,-1.0922084022
H,0,-1.76442534,1.0340114321,-2.2922612202
H,0,-0.0284035745,-0.59687877,-1.6137977761
H,0,-2.6326245306,-2.0856872258,1.4435422933
H,0,-4.3569157133,-0.4513675739,0.7855571899
H,0,-0.3296845851,-2.8583998627,1.3497442826
H,0,0.8382416036,-2.0300619751,0.303834083
H,0,-0.1720595062,-3.3205905975,-0.3459967995
N,0,-0.7608276865,1.8160468789,0.620523918
O,0,-0.3902113358,2.5527680819,-0.1235337312
O,0,-1.0923919432,1.1656595473,1.4536537791
F,0,3.722527525,0.9550417486,-0.1268884623
B,0,2.7438558186,-0.0070258905,0.0004403664
F,0,1.5629656936,0.608414625,0.388220988
F,0,2.5587510524,-0.6385245965,-1.2097844522
F,0,3.1212078636,-0.9208544215,0.9599658

Pi Complex NO2BF4 PCM ONIOM 3.146_94108

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.273454772103

Zero-point correction= 0.158059 (Hartree/Particle)
Thermal correction to Energy= 0.174823
Thermal correction to Enthalpy= 0.175767
Thermal correction to Gibbs Free Energy= 0.110769
Sum of electronic and ZPE= -476.893790
Sum of electronic and thermal Energies= -476.877026
Sum of electronic and thermal Enthalpies= -476.876082
Sum of electronic and thermal Free Energies= -476.941080

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.703	55.638	136.800

C,0,3.2600129255,0.4714306797,0.6575863815
C,0,2.0723054975,0.4426307223,1.3907724149
C,0,1.0837634238,-0.4995733945,1.0950869655
C,0,1.2649533434,-1.4311893977,0.0675076582
C,0,2.4558998419,-1.3845505066,-0.660961339
C,0,3.4444689892,-0.4446728102,-0.3717468499
C,0,0.2064567731,-2.4581582033,-0.2300118359
H,0,4.0280370767,1.1985603706,0.8912096879
H,0,1.9170514338,1.1493663541,2.1989624156
H,0,0.1549274607,-0.5069955892,1.6616659608
H,0,2.612386753,-2.0929658365,-1.4674467782
H,0,4.3580457592,-0.4305870992,-0.9540279678
H,0,0.3380217755,-2.8901514733,-1.2220114208
H,0,-0.7949938613,-2.0201411615,-0.1722337281
H,0,0.2505077293,-3.2709082653,0.4989332201
N,0,0.7341336936,1.8211017601,-0.6463025512
O,0,0.3424814434,2.538447558,0.1061317846
O,0,1.0806351749,1.1921642608,-1.4900423177
F,0,-3.1397193028,-1.0102696389,-0.8050157135
B,0,-2.7217022125,-0.0361872153,0.0750676387
F,0,-3.7025129285,0.9242550402,0.1978975664
F,0,-2.4635055298,-0.5906646453,1.3096001382
F,0,-1.5708312596,0.5639044909,-0.4136613301

Pi Complex NO2BF4 PCM ONIOM 3.156_94025

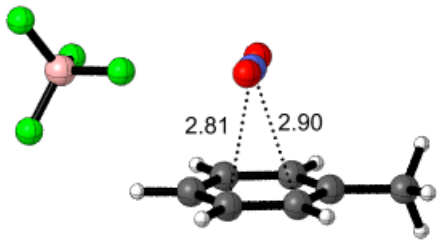
ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266458589435

Zero-point correction= 0.157694 (Hartree/Particle)
Thermal correction to Energy= 0.174970
Thermal correction to Enthalpy= 0.175914
Thermal correction to Gibbs Free Energy= 0.105613
Sum of electronic and ZPE= -476.888179
Sum of electronic and thermal Energies= -476.870902
Sum of electronic and thermal Enthalpies= -476.869958
Sum of electronic and thermal Free Energies= -476.940259

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.795	55.767	147.961

C,0,-3.8286256057,-1.0717485555,0.5317084246
C,0,-2.8063394345,-0.6643613314,1.3862858981
C,0,-2.1779349681,0.5714005994,1.1966401776
C,0,-2.5622370431,1.418446949,0.156100551
C,0,-3.5853643642,0.9917769341,-0.698351804
C,0,-4.2141547574,-0.2365167485,-0.5146869459
C,0,-1.9068942629,2.7583690761,-0.0460774731
H,0,-4.3210132369,-2.0247654287,0.6841026661
H,0,-2.5026784815,-1.2991908607,2.2119215347
H,0,-1.3917652243,0.8823686331,1.8777845898
H,0,-3.8943834114,1.6343968419,-1.5168198559
H,0,-5.0063112085,-0.5418367025,-1.1882911688
H,0,-1.0991685154,2.9171627302,0.668453788
H,0,-2.6344266507,3.562937556,0.081444894
H,0,-1.4968916232,2.8475854189,-1.0543694714
N,0,-0.8924491138,-1.4441912171,-0.5642783356
O,0,-0.3284913612,-1.9875726913,0.2215375758
O,0,-1.3925654215,-0.9470835365,-1.417745049
F,0,3.3900829405,0.8565743383,-0.8210226437
B,0,4.1909037352,0.0561712721,-0.0319336496
F,0,3.4067931902,-0.8801356436,0.6102791324
F,0,5.1176137027,-0.5876239291,-0.8247885631
F,0,4.8393301157,0.8337232959,0.9041357278

Pi Complex NO2BF4 PCM ONIOM 3.158_94252



ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.274019242422

Zero-point correction= 0.157750 (Hartree/Particle)
Thermal correction to Energy= 0.174762
Thermal correction to Enthalpy= 0.175706
Thermal correction to Gibbs Free Energy= 0.108400
Sum of electronic and ZPE= -476.893170
Sum of electronic and thermal Energies= -476.876158
Sum of electronic and thermal Enthalpies= -476.875214
Sum of electronic and thermal Free Energies= -476.942520

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.665	55.749	141.658

C,0,4.1718200974,-2.594843568,-0.5969244901
C,0,4.3367997138,-2.3027378673,-1.9493980158
C,0,4.9162959726,-1.0992039473,-2.3420336363
C,0,5.3435167515,-0.157987826,-1.3992286139
C,0,5.1649240456,-0.4545243179,-0.0472976975
C,0,4.5859173502,-1.6655673053,0.354089587
C,0,5.9893496011,1.1287325058,-1.8387907356
H,0,3.6983468484,-3.5216836419,-0.2872155679
H,0,4.0080629513,-3.0116433557,-2.7001697484
H,0,5.0382617035,-0.8841909453,-3.3986638245
H,0,5.493456896,0.2558151655,0.7046620184
H,0,4.464387305,-1.8794619657,1.4105334537
H,0,6.9789644918,0.9346068905,-2.2585282971

H,0,6.1093292894,1.8189929351,-1.0037013576
H,0,5.3983562272,1.6215119655,-2.6130485362
N,0,2.2899375255,-0.106186477,-0.1038336358
O,0,2.2542580638,-0.2730219572,-1.1986009723
O,0,2.207003002,0.1312987495,0.9784701229
F,0,1.5843783728,-4.6749204894,0.7067101965
B,0,0.7751224777,-3.7358431416,0.1059847184
F,0,0.7787948061,-3.9194130454,-1.2595674781
F,0,-0.5104334053,-3.8535969825,0.5866614189
F,0,1.2464162123,-2.4630433782,0.3931486914

Pi Complex NO2BF4 PCM ONIOM 3.163_93717

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267265488654

Zero-point correction= 0.158040 (Hartree/Particle)
Thermal correction to Energy= 0.174925
Thermal correction to Enthalpy= 0.175869
Thermal correction to Gibbs Free Energy= 0.109640
Sum of electronic and ZPE= -476.888774
Sum of electronic and thermal Energies= -476.871889
Sum of electronic and thermal Enthalpies= -476.870945
Sum of electronic and thermal Free Energies= -476.937174

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.767	55.594	139.390

C,0,5.1918020863,0.2016578552,4.7005408337
C,0,4.7922987579,-0.5202539425,5.8221055054
C,0,4.1441401872,-1.7435408854,5.67353596
C,0,3.880590687,-2.2758302417,4.4070212618
C,0,4.2751056781,-1.5394461871,3.2879470816
C,0,4.9288038206,-0.3109684585,3.4315356011
C,0,3.2092375867,-3.6150611649,4.2644666277
H,0,5.7045645256,1.149381959,4.8113226943
H,0,4.9859324422,-0.1312594792,6.814837323
H,0,3.8384107794,-2.2973703615,6.5554874762
H,0,4.0823284193,-1.933340159,2.2910856008
H,0,5.2423201008,0.235284327,2.5480952508
H,0,3.9068790086,-4.4167305606,4.5183726005
H,0,2.8667755325,-3.7830503071,3.2424968156
H,0,2.3535102544,-3.7021483556,4.9361455988
N,0,2.2363021095,0.5475089329,3.6276885156
O,0,2.0793276831,0.1792273382,4.6602616509
O,0,2.2908012498,0.9733940488,2.6043799776
F,0,3.6316670952,-1.62331694,-0.2358570831
B,0,2.5847909883,-2.5039249684,-0.4135961874
F,0,2.8609765951,-3.3419141225,-1.4733630707
F,0,2.4074008407,-3.252627007,0.7316128159
F,0,1.4297908717,-1.7936835199,-0.6722592502

Pi Complex NO2BF4 PCM ONIOM 3.173_93824

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.277777528472

Zero-point correction= 0.159150 (Hartree/Particle)
Thermal correction to Energy= 0.175184
Thermal correction to Enthalpy= 0.176128
Thermal correction to Gibbs Free Energy= 0.114528
Sum of electronic and ZPE= -476.893626
Sum of electronic and thermal Energies= -476.877592
Sum of electronic and thermal Enthalpies= -476.876648
Sum of electronic and thermal Free Energies= -476.938248

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.930	55.079	129.648

C,0,3.2249727939,0.6106217002,0.4981049261
C,0,2.1432100674,0.5198141093,1.3739561707
C,0,1.1741981404,-0.4733359014,1.1957152533
C,0,1.2672192735,-1.392947329,0.1442048863
C,0,2.3489692521,-1.277910989,-0.7306631169
C,0,3.3188717661,-0.2885337244,-0.5573706205
C,0,0.226950564,-2.4656661738,-0.0204686392
H,0,3.9802632937,1.3734967293,0.6404285115
H,0,2.0567024126,1.2107167536,2.2054377206
H,0,0.3366788402,-0.5368675446,1.8864103441
H,0,2.4382305238,-1.9718817829,-1.5594483119
H,0,4.1480547219,-0.2248753718,-1.2518227443
H,0,0.2464035575,-3.1480030202,0.8319296748
H,0,0.3991947509,-3.0494057994,-0.9239561902
H,0,-0.7952454084,-2.0388325603,-0.0714509433
N,0,0.4100984136,1.7173159396,-0.4615382456
O,0,0.8576782118,1.2427880425,-1.3591437285
O,0,-0.1006393355,2.3089013498,0.3299776321
F,0,-1.9889360723,0.3755662734,1.0966337253
B,0,-2.5618730862,-0.0978933976,-0.0665708647
F,0,-2.4996082611,-1.474810207,-0.0937571456
F,0,-3.8661574113,0.3248137697,-0.1617672891
F,0,-1.8198610086,0.4172551338,-1.1180190049

Pi Complex NO2BF4 PCM ONIOM 3.178_94087

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.273688937032

Zero-point correction= 0.158196 (Hartree/Particle)
Thermal correction to Energy= 0.174943
Thermal correction to Enthalpy= 0.175887
Thermal correction to Gibbs Free Energy= 0.110731
Sum of electronic and ZPE= -476.893405
Sum of electronic and thermal Energies= -476.876658
Sum of electronic and thermal Enthalpies= -476.875714
Sum of electronic and thermal Free Energies= -476.940870

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.778	55.635	137.132

C,0,3.4970237463,-0.408405004,0.1215216464
C,0,3.3011343492,0.5403826174,-0.8758151655
C,0,2.2290987481,1.4301156495,-0.7997993414
C,0,1.3320349676,1.3942504619,0.2694518568
C,0,1.5297496144,0.4269997136,1.2616169383

C,0,2.6032276889,-0.4662854092,1.1908969238
C,0,0.1758359302,2.3541107512,0.3522774846
H,0,4.3347423175,-1.0931569802,0.0726017169
H,0,3.9837146618,0.5936930059,-1.7156720056
H,0,2.091502558,2.1677990119,-1.5831558254
H,0,0.8491631931,0.3818148538,2.1068901459
H,0,2.7477875109,-1.1953187422,1.9808829872
H,0,-0.7762906711,1.8400217257,0.1761328408
H,0,0.2689024687,3.1484241848,-0.3879856944
H,0,0.1186207948,2.8109165055,1.3416494384
N,0,0.6847434024,-1.7998395751,-0.3851206351
O,0,0.8834523865,-1.2220111108,-1.309513621
O,0,0.4199605311,-2.4687137201,0.461953952
F,0,-2.970646463,0.7030262893,1.1526077817
B,0,-2.8535196673,0.0473363501,-0.0531773063
F,0,-3.8666661762,-0.878676202,-0.1757305888
F,0,-2.9243442381,0.9509493848,-1.0907209634
F,0,-1.6360266536,-0.6149067617,-0.104121566

Pi Complex NO2BF4 PCM ONIOM 3.180_94194

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266022363459

Zero-point correction= 0.157283 (Hartree/Particle)
Thermal correction to Energy= 0.174761
Thermal correction to Enthalpy= 0.175705
Thermal correction to Gibbs Free Energy= 0.103846
Sum of electronic and ZPE= -476.888506
Sum of electronic and thermal Energies= -476.871028
Sum of electronic and thermal Enthalpies= -476.870084
Sum of electronic and thermal Free Energies= -476.941943

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.664	55.856	151.241

C,0,3.2793401828,1.843435976,-0.2963201075
C,0,3.2413519392,1.2508368027,0.9636489244
C,0,3.4767911822,-0.1213436599,1.1058495071
C,0,3.7599594409,-0.9189596185,-0.0043123763
C,0,3.7879902268,-0.3098797079,-1.263909985
C,0,3.5514369435,1.0539367256,-1.4117208348
C,0,4.040564773,-2.3909036454,0.1381386949
H,0,3.1026541095,2.9067456844,-0.4063685732
H,0,3.0391257862,1.8544337917,1.8422862044
H,0,3.4555982618,-0.5672309729,2.0954140786
H,0,4.0023254824,-0.9145541396,-2.1396790097
H,0,3.5808396779,1.5005493178,-2.3988026221
H,0,5.0829296902,-2.6062137709,-0.1078915585
H,0,3.418244626,-2.9778649233,-0.5403997362
H,0,3.8577694218,-2.7348536667,1.156256977
N,0,0.629542051,0.2393373097,0.4260075238
O,0,0.8528237814,-0.0748260822,-0.6115937913
O,0,0.3079423207,0.5324042327,1.4467050095
F,0,-5.6842482499,0.5367605657,0.6650256251
B,0,-4.7404756353,-0.098486184,-0.1141805268
F,0,-3.9468492646,-0.8960927845,0.6847809428
F,0,-5.3684379448,-0.8791339917,-1.0618290723
F,0,-3.9532808027,0.8440307414,-0.743776294

Pi Complex NO2BF4 PCM ONIOM 3.191_93775

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267820774694

Zero-point correction= 0.157848 (Hartree/Particle)
Thermal correction to Energy= 0.174765
Thermal correction to Enthalpy= 0.175709
Thermal correction to Gibbs Free Energy= 0.109175
Sum of electronic and ZPE= -476.889080
Sum of electronic and thermal Energies= -476.872163
Sum of electronic and thermal Enthalpies= -476.871219
Sum of electronic and thermal Free Energies= -476.937753

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.666	55.637	140.032

C,0,2.8532320606,0.4448279652,4.0773677583
C,0,2.1013665111,0.4002018353,5.2484884314
C,0,1.1257201115,-0.5787724657,5.4190475367
C,0,0.8777435004,-1.5355002076,4.4294220503
C,0,1.627526897,-1.4748035196,3.2528686516
C,0,2.6110774947,-0.4943821751,3.0774307926
C,0,-0.1580124697,-2.6067055752,4.6412929432
H,0,3.6195045693,1.1989995166,3.9456536626
H,0,2.2742960876,1.1283813264,6.0320377523
H,0,0.5467639172,-0.6035519213,6.3367318381
H,0,1.4508523682,-2.2067296409,2.4655630865
H,0,3.1940319634,-0.4781087305,2.1625988127
H,0,0.1958194278,-3.336607254,5.3731249162
H,0,-0.374039181,-3.14078359,3.7146519582
H,0,-1.0893770955,-2.1856945614,5.0239929131
N,0,0.289534126,0.8876886367,2.2290103188
O,0,-0.0627687741,1.1318896101,3.2502898498
O,0,0.5583110853,0.7253729805,1.1643648547
F,0,1.3461197076,-2.7656092609,-0.0413313397
B,0,0.336572365,-3.6907108575,0.1297403817
F,0,0.8790456899,-4.8974604315,0.5183942171
F,0,-0.5453908892,-3.2455896697,1.0934625038
F,0,-0.338748673,-3.8492043101,-1.0629855898

Pi Complex NO2BF4 PCM ONIOM 3.208_93983

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.274697447668

Zero-point correction= 0.158304 (Hartree/Particle)
Thermal correction to Energy= 0.175013
Thermal correction to Enthalpy= 0.175957
Thermal correction to Gibbs Free Energy= 0.111385
Sum of electronic and ZPE= -476.892915
Sum of electronic and thermal Energies= -476.876205
Sum of electronic and thermal Enthalpies= -476.875261
Sum of electronic and thermal Free Energies= -476.939833

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 109.822 55.625 135.903

C,0,0.4263675733,1.3793791248,0.4081483167
C,0,0.9003036984,0.4351528431,1.313955792
C,0,2.1917812415,-0.0914387456,1.1736898623
C,0,3.0278411385,0.322465029,0.1350311165
C,0,2.5336761747,1.2675675471,-0.7699780058
C,0,1.249370096,1.7896055456,-0.6392355063
C,0,4.4227625054,-0.223929362,-0.0127658127
H,0,-0.5853838986,1.7636952448,0.5010374425
H,0,0.2673293015,0.1025620551,2.1298746591
H,0,2.553096842,-0.8195903319,1.8932422964
H,0,3.1638895989,1.5960224972,-1.5900278933
H,0,0.8878518485,2.5147975481,-1.358784896
H,0,4.6274550043,-0.9946391239,0.730320957
H,0,5.1609350118,0.5709864053,0.1120051792
H,0,4.572528393,-0.6542816204,-1.0051813276
N,0,0.5588023242,-1.693041805,-0.5072027037
O,0,0.7228305098,-1.0704376945,-1.4093790108
O,0,0.355907778,-2.4285438025,0.3012820698
F,0,-2.8933881639,0.704355874,1.3314938947
B,0,-2.9129206203,0.1543225446,0.0688140694
F,0,-2.8399434709,1.1517452755,-0.8788332191
F,0,-1.8302826319,-0.6997389751,-0.0830365153
F,0,-4.0743752545,-0.5658460734,-0.1055587651

Pi Complex NO2BF4 PCM ONIOM 3.215_94153

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266546634745

Zero-point correction= 0.157705 (Hartree/Particle)
Thermal correction to Energy= 0.175147
Thermal correction to Enthalpy= 0.176092
Thermal correction to Gibbs Free Energy= 0.104203
Sum of electronic and ZPE= -476.888028
Sum of electronic and thermal Energies= -476.870585
Sum of electronic and thermal Enthalpies= -476.869641
Sum of electronic and thermal Free Energies= -476.941530

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 109.907 55.760 151.303

C,0,1.7667138673,-1.7776005941,-1.8406867687
C,0,1.454153846,-0.6217503128,-2.5483969888
C,0,2.1720705834,0.5542152192,-2.328300094
C,0,3.2147127536,0.601718855,-1.4011433604
C,0,3.5143104509,-0.5640675564,-0.6864327707
C,0,2.8006740469,-1.7447755978,-0.9043984542
C,0,4.0066164531,1.8617366238,-1.1724610728
H,0,1.2166101894,-2.6943306435,-2.0157858251
H,0,0.6508424821,-0.6319540961,-3.276015235
H,0,1.9178732958,1.4479213856,-2.8887203998
H,0,4.3265665969,-0.5530726306,0.0348583934
H,0,3.0631447832,-2.6409753677,-0.3520688319
H,0,5.0576238554,1.704621843,-1.4242640982
H,0,3.9659838417,2.1692867826,-0.1251461504
H,0,3.6306392233,2.6821563249,-1.7833348315
N,0,1.1286637019,-0.4062653282,0.9971246387
O,0,0.6202862596,0.2157361719,0.2356698865
O,0,1.5648688438,-1.0023460783,1.8251391562
F,0,2.0991684405,4.5455461087,4.7545834585
B,0,1.0431410037,3.7582421559,4.3466079726
F,0,-0.111350009,4.1611736064,4.9841444497
F,0,0.879650548,3.8773591895,2.9815216822
F,0,1.3048763427,2.4400187393,4.6601323439

Pi Complex NO2BF4 PCM ONIOM 3.217_93889

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267250548074

Zero-point correction= 0.158048 (Hartree/Particle)
Thermal correction to Energy= 0.175237
Thermal correction to Enthalpy= 0.176182
Thermal correction to Gibbs Free Energy= 0.107389
Sum of electronic and ZPE= -476.888234
Sum of electronic and thermal Energies= -476.871044
Sum of electronic and thermal Enthalpies= -476.870100
Sum of electronic and thermal Free Energies= -476.938893

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 109.963 55.726 144.787

C,0,3.9573147694,0.3105720139,-0.4117434382
C,0,3.4085395912,0.4008987591,0.8650621716
C,0,2.3442508144,-0.4291810822,1.2351414906
C,0,1.8154566312,-1.3631679025,0.3400639443
C,0,2.3724605846,-1.4348457965,-0.9405427705
C,0,3.4306002318,-0.6096280462,-1.3149010747
C,0,0.666503938,-2.2535774728,0.7310878586
H,0,4.7885636861,0.944626342,-0.6955291545
H,0,3.8159507229,1.1034695508,1.584271759
H,0,1.9363792112,-0.3603213799,2.239372099
H,0,1.9746738124,-2.1511213369,-1.6524764027
H,0,3.8471970088,-0.6900241458,-2.3122294732
H,0,0.5783801293,-2.3338527753,1.8147393928
H,0,0.7921736385,-3.2561800911,0.3205038367
H,0,-0.2803101313,-1.8608481097,0.3474908115
N,0,1.1546015354,1.8540072819,-0.0750040898
O,0,1.1251466132,2.4596741672,0.8546243085
O,0,1.1172749761,1.3260836963,-1.0474004351
F,0,-4.4065313782,0.5784227715,0.9399819586
B,0,-3.6635255909,-0.0932647771,-0.0082741881
F,0,-2.6334133261,-0.769174717,0.6129415869
F,0,-4.4677628313,-0.9908888404,-0.6781200799
F,0,-3.1380936368,0.8147908907,-0.9049321112

Pi Complex NO2BF4 PCM ONIOM 3.221_94009

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266867901234

Zero-point correction= 0.157916 (Hartree/Particle)
Thermal correction to Energy= 0.175144

Thermal correction to Enthalpy= 0.176088
Thermal correction to Gibbs Free Energy= 0.105776
Sum of electronic and ZPE= -476.887953
Sum of electronic and thermal Energies= -476.870726
Sum of electronic and thermal Enthalpies= -476.869781
Sum of electronic and thermal Free Energies= -476.940093

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.904	55.720	147.984

C,0,1.5556200145,1.5754920445,-0.6853394126
C,0,2.2885925767,1.8845290006,0.4584182486
C,0,3.4035202248,1.1246461114,0.8039489733
C,0,3.8137822317,0.0417810676,0.0196504476
C,0,3.0629124392,-0.2696272045,-1.1161963398
C,0,1.9440845708,0.4934085604,-1.4710206975
C,0,5.0443752106,-0.745350419,0.3831464923
H,0,0.6917041497,2.1688271397,-0.960954445
H,0,1.9922460109,2.7194385956,1.082783305
H,0,3.9673818441,1.3773827577,1.6962879107
H,0,3.3629110219,-1.1026773309,-1.744534854
H,0,1.387101458,0.2453206289,-2.3685508735
H,0,5.0759143577,-0.9584561118,1.4529682743
H,0,5.9438860758,-0.1762436186,0.1361840505
H,0,5.0882929006,-1.6896064109,-0.1597713464
N,0,0.8295056288,-1.3782347092,0.3754504086
O,0,1.0977485007,-0.780467718,1.2677298019
O,0,0.504210927,-2.0431241616,-0.4513467486
F,0,-3.6499683631,-1.1474448116,0.1808504607
B,0,-4.1669717354,0.1239860612,0.0367555536
F,0,-3.2997069352,0.8853074252,-0.7200148348
F,0,-5.390903833,0.0569049809,-0.5944631797
F,0,-4.3159212767,0.7016051225,1.2805278047

Pi Complex NO2BF4 PCM ONIOM 3.228_94053

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266407337192

Zero-point correction= 0.157742 (Hartree/Particle)
Thermal correction to Energy= 0.175043
Thermal correction to Enthalpy= 0.175987
Thermal correction to Gibbs Free Energy= 0.105306
Sum of electronic and ZPE= -476.888101
Sum of electronic and thermal Energies= -476.870800
Sum of electronic and thermal Enthalpies= -476.869856
Sum of electronic and thermal Free Energies= -476.940537

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.841	55.741	148.762

C,0,-3.8554348654,-1.319479151,0.7528593789
C,0,-3.683802956,-0.2533884912,1.6314693819
C,0,-3.2942383309,0.9964082371,1.1532643784
C,0,-3.0698843008,1.2122783263,-0.2094069071
C,0,-3.2330580933,0.1323809303,-1.0817481623
C,0,-3.6261023494,-1.1235309806,-0.607615228
C,0,-2.693732763,2.5755033174,-0.7252762244
H,0,-4.1647478832,-2.2901854963,1.1211624208
H,0,-3.8518754441,-0.3934754841,2.6929986154
H,0,-3.1633546307,1.817883813,1.8502107839
H,0,-3.0693128072,0.2759034287,-2.1457400671
H,0,-3.7624407884,-1.9416077464,-1.3067614789
H,0,-2.1310959935,3.1400262077,0.0191199557
H,0,-3.592844516,3.1491030661,-0.9645051604
H,0,-2.0956986387,2.5082577595,-1.6349710016
N,0,-0.7855192093,-1.1939381069,-0.239702394
O,0,-0.821527899,-0.6796788283,0.7397170216
O,0,-0.6501427327,-1.7334561813,-1.2000041987
F,0,3.8093518314,-0.7375386913,0.8116876664
B,0,4.4024370157,0.20542164,-0.002731959
F,0,5.1999724022,1.0339428208,0.7580759804
F,0,5.1697952821,-0.4298154497,-0.9564827276
F,0,3.4232256702,0.9526860601,-0.6247460743

Pi Complex NO2BF4 PCM ONIOM 3.229_94135

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266475122039

Zero-point correction= 0.157610 (Hartree/Particle)
Thermal correction to Energy= 0.174953
Thermal correction to Enthalpy= 0.175897
Thermal correction to Gibbs Free Energy= 0.104442
Sum of electronic and ZPE= -476.888188
Sum of electronic and thermal Energies= -476.870845
Sum of electronic and thermal Enthalpies= -476.869900
Sum of electronic and thermal Free Energies= -476.941356

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.785	55.760	150.391

C,0,3.8290616878,1.2862642092,0.7403010871
C,0,3.6556969672,0.2112530925,1.6090959098
C,0,3.2542456857,-1.0294460271,1.1202124837
C,0,3.0188763256,-1.2290394202,-0.2441269889
C,0,3.1845080737,-0.1419944302,-1.1053711716
C,0,3.5897476368,1.1068080015,-0.6197986869
C,0,2.6207125214,-2.5851163054,-0.7624478612
H,0,4.1483199766,2.250468532,1.1171144396
H,0,3.832443132,0.3387929473,2.6707950717
H,0,3.1221890095,-1.8583725486,1.8083153164
H,0,3.0135829458,-0.2720411213,-2.1698119245
H,0,3.7280819475,1.9310292886,-1.3112672362
H,0,2.2187450046,-2.5240881837,-1.7740198852
H,0,1.8716183659,-3.0492686735,-0.1186108146
H,0,3.4875900321,-3.2499236808,-0.7872927507
N,0,0.751337557,1.1893213836,-0.2334896118
O,0,0.6126477764,1.7384936124,-1.1878115516
O,0,0.791163245,0.6655857726,0.7407946193
F,0,-4.6702668486,0.6815154968,-1.0107767842
B,0,-4.3664886314,-0.1733952347,0.0285124107
F,0,-5.5032343577,-0.843181253,0.428558444
F,0,-3.4185751958,-1.0845807995,-0.3904883968
F,0,-3.862040857,0.5554033415,1.0862538819

Pi Complex NO2BF4 PCM ONIOM 3.231_94060

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266441526657

Zero-point correction= 0.157613 (Hartree/Particle)
Thermal correction to Energy= 0.174934
Thermal correction to Enthalpy= 0.175878
Thermal correction to Gibbs Free Energy= 0.105230
Sum of electronic and ZPE= -476.888221
Sum of electronic and thermal Energies= -476.870900
Sum of electronic and thermal Enthalpies= -476.869956
Sum of electronic and thermal Free Energies= -476.940605

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.773	55.769	148.692

C,0,-0.4190673236,-0.1108187938,3.5945498909
C,0,-1.1910501841,0.9931804677,3.2417311196
C,0,-2.0046615008,0.9495465567,2.1034512529
C,0,-2.0644732225,-0.1955043973,1.3058453305
C,0,-1.2754638996,-1.2920181534,1.6687270873
C,0,-0.4629647818,-1.2535851796,2.7991746575
C,0,-2.9656023303,-0.2649712243,0.1019826841
H,0,0.2066346888,-0.0810026813,4.4784182674
H,0,-1.1747355395,1.8883366003,3.8541611474
H,0,-2.6115625871,1.8126064369,1.8465825376
H,0,-1.2994132359,-2.1885771208,1.0574572161
H,0,0.1377325818,-2.1176424905,3.0585704113
H,0,-3.8533350284,-0.8606935626,0.3280341365
H,0,-2.4608511745,-0.7383754753,-0.7419465829
H,0,-3.299227505,0.7264502406,-0.2052220996
N,0,0.6279916602,1.7325435076,1.1557602803
O,0,0.4711624784,2.8107100778,1.3666005118
O,0,0.8660858793,0.6854776627,0.8871317533
F,0,2.1202774106,1.5080041391,-3.4060068236
B,0,2.7954293645,2.6846856784,-3.6584368345
F,0,2.4668849635,3.1433086,-4.9165801119
F,0,2.4367500024,3.6269443783,-2.716116763
F,0,4.1541583838,2.4592218327,-3.5856359692

Pi Complex NO2BF4 PCM ONIOM 3.236_93860

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266421809273

Zero-point correction= 0.157946 (Hartree/Particle)
Thermal correction to Energy= 0.175144
Thermal correction to Enthalpy= 0.176088
Thermal correction to Gibbs Free Energy= 0.107281
Sum of electronic and ZPE= -476.887940
Sum of electronic and thermal Energies= -476.870742
Sum of electronic and thermal Enthalpies= -476.869798
Sum of electronic and thermal Free Energies= -476.938605

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.904	55.721	144.817

C,0,-1.0520848413,4.0552926138,1.3748907602
C,0,-1.6201718748,2.8192832659,1.6705779456
C,0,-0.8678613864,1.6467609733,1.5320526119
C,0,0.4612135406,1.6917948672,1.1040015183
C,0,1.0133745016,2.9409912383,0.8017246326
C,0,0.2689583863,4.110049239,0.9346709543
C,0,1.2835802159,0.4391645219,0.9609807737
H,0,-1.6298736599,4.9644069355,1.4896143906
H,0,-2.6434408831,2.7615216472,2.0263576274
H,0,-1.3170413041,0.6905822987,1.7831951761
H,0,2.0430923986,2.9968954344,0.4625381449
H,0,0.7223812511,5.0653577612,0.6972585031
H,0,0.7693312762,-0.4247775538,1.3817373905
H,0,2.2431601664,0.5470408534,1.469679154
H,0,1.4966597485,0.2274835288,-0.0908620601
N,0,-1.9778566204,2.1866716248,-1.0997378456
O,0,-2.9340730768,1.6650537189,-0.8878720585
O,0,-1.0526526175,2.7077309305,-1.4125059007
F,0,-0.1563406008,-1.9412388022,-4.1168122754
B,0,0.74116532,-2.0827322744,-3.0783366183
F,0,0.7103774606,-0.9489432756,-2.2926850151
F,0,0.3959741312,-3.1799770832,-2.3172504464
F,0,2.010840368,-2.2549157637,-3.5887311632

Pi Complex NO2BF4 PCM ONIOM 3.237_93813

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267722282933

Zero-point correction= 0.157963 (Hartree/Particle)
Thermal correction to Energy= 0.175049
Thermal correction to Enthalpy= 0.175993
Thermal correction to Gibbs Free Energy= 0.108305
Sum of electronic and ZPE= -476.888476
Sum of electronic and thermal Energies= -476.871391
Sum of electronic and thermal Enthalpies= -476.870447
Sum of electronic and thermal Free Energies= -476.938134

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.845	55.627	142.461

C,0,0.6663989496,-1.3513628322,-0.2853246724
C,0,1.8549539536,-1.7321199654,-0.9037473934
C,0,3.0743952811,-1.2359593787,-0.4481391532
C,0,3.138174701,-0.351966005,0.6327837553
C,0,1.9391925505,0.0350633139,1.237397559
C,0,0.7113760922,-0.4635521206,0.7862299477
C,0,4.4644135666,0.1452774289,1.1424084244
H,0,-0.2867139583,-1.7353304325,-0.633748589
H,0,1.8337520494,-2.4167454503,-1.7436452761
H,0,3.9930606829,-1.5425277416,-0.9377770501
H,0,1.9610753753,0.7162920932,2.0826933331
H,0,-0.208412204,-0.1610242721,1.2791811411
H,0,4.9431079174,-0.6191513964,1.7592813552
H,0,4.3464656687,1.039761477,1.7547055536
H,0,5.1438704715,0.3744761654,0.3201189102
N,0,1.1914638367,1.7840228637,-0.8996660064
O,0,1.7262247773,1.1811950007,-1.659367728

O,0,0.6536187486,2.4790755745,-0.2215541965
F,0,-4.330804864,-0.9166815279,0.8657521579
B,0,-3.5359642363,-0.2386710254,-0.0341219849
F,0,-2.6384814015,0.5558792677,0.6493863525
F,0,-2.85104459,-1.1440903116,-0.8181310962
F,0,-4.3239253685,0.5574842749,-0.839726344

Pi Complex NO2BF4 PCM ONIOM 3.238_93914

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267135462019

Zero-point correction= 0.157588 (Hartree/Particle)
Thermal correction to Energy= 0.174781
Thermal correction to Enthalpy= 0.175725
Thermal correction to Gibbs Free Energy= 0.107245
Sum of electronic and ZPE= -476.888804
Sum of electronic and thermal Energies= -476.871611
Sum of electronic and thermal Enthalpies= -476.870667
Sum of electronic and thermal Free Energies= -476.939147

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.677	55.766	144.129

C,0,0.4274386204,-1.1069622223,-0.1144211646
C,0,0.9577926224,-0.3352574582,-1.1443932856
C,0,2.3365310801,-0.1028282145,-1.2128891135
C,0,3.2045754605,-0.6419382662,-0.2593031274
C,0,2.6538535471,-1.4035467714,0.7753252289
C,0,1.2823593516,-1.6360170943,0.8495887154
C,0,4.6927518475,-0.4385900538,-0.356285357
H,0,-0.643832679,-1.2783205509,-0.0598823284
H,0,0.3009444366,0.0798136111,-1.9020399449
H,0,2.7397278156,0.4877070569,-2.0301861094
H,0,3.3098572333,-1.8222843551,1.5315973516
H,0,0.8810376736,-2.2298577825,1.6625786213
H,0,4.9396084406,0.4132247572,-0.9903176111
H,0,5.1659290916,-1.3231860665,-0.7896856204
H,0,5.1360182387,-0.2797218654,0.6279839958
N,0,1.332634257,1.9331701445,0.5382230464
O,0,1.4674108948,1.313139337,1.4456931796
O,0,1.1899401716,2.6517877823,-0.2958661866
F,0,-2.983209786,-0.88747786,0.9444091191
B,0,-3.550858468,-0.1302129195,-0.0595812832
F,0,-4.3575203034,-0.930408263,-0.8409365738
F,0,-4.3057471295,0.8785556281,0.5034433632
F,0,-2.560128417,0.4275164267,-0.8414599153

Pi Complex NO2BF4 PCM ONIOM 3.242_93631

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.276080899456

Zero-point correction= 0.158860 (Hartree/Particle)
Thermal correction to Energy= 0.175272
Thermal correction to Enthalpy= 0.176216
Thermal correction to Gibbs Free Energy= 0.113061
Sum of electronic and ZPE= -476.890517
Sum of electronic and thermal Energies= -476.874105
Sum of electronic and thermal Enthalpies= -476.873161
Sum of electronic and thermal Free Energies= -476.936316

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.985	55.421	132.920

C,0,-0.5245200261,0.0170458747,3.6629926804
C,0,-0.6344555357,1.211088942,2.9540499914
C,0,-1.8619322273,1.6054477412,2.4255641138
C,0,-3.0072673517,0.8225136516,2.59109031
C,0,-2.8828136823,-0.3839696236,3.2861081311
C,0,-1.6515852678,-0.7831316939,3.8246792482
C,0,-4.334940906,1.2835765865,2.0525581942
H,0,0.4296967289,-0.3019616237,4.065202145
H,0,0.2379896218,1.8370362079,2.8088457663
H,0,-1.9324907692,2.5377743775,1.8751148836
H,0,-3.7557124873,-1.014312225,3.4257982241
H,0,-1.5720468917,-1.7309121195,4.3521981111
H,0,-4.7419262857,2.0772850766,2.6835580394
H,0,-5.0615755834,0.4714261142,2.0283165174
H,0,-4.2326002897,1.6884473056,1.0443849349
N,0,-1.6349317234,-1.7218758998,1.1610963777
O,0,-2.1672128407,-2.6723129423,1.3798029591
O,0,-1.062460227,-0.8429176748,0.7931148475
F,0,-1.2557412541,-3.9559135114,2.78663395
B,0,0.0838516166,-3.8351287792,3.1138925087
F,0,0.5373701309,-2.6927502968,2.4732114485
F,0,0.2276440327,-3.7083541248,4.4754533965
F,0,0.7808738183,-4.9301917627,2.6606032213

Pi Complex NO2BF4 PCM ONIOM 3.245_94016

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.272037025824

Zero-point correction= 0.157778 (Hartree/Particle)
Thermal correction to Energy= 0.174707
Thermal correction to Enthalpy= 0.175651
Thermal correction to Gibbs Free Energy= 0.108993
Sum of electronic and ZPE= -476.891383
Sum of electronic and thermal Energies= -476.874454
Sum of electronic and thermal Enthalpies= -476.873510
Sum of electronic and thermal Free Energies= -476.940168

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.630	55.753	140.294

C,0,2.2781453036,3.569273213,-0.4487834135
C,0,1.4978144028,3.3774687387,0.6894590925
C,0,1.8749037338,2.4431162331,1.650800787
C,0,3.0361101845,1.6783666974,1.5014217943
C,0,3.8059670989,1.871176341,0.3518356553
C,0,3.4331830179,2.8112214751,-0.6168205334
C,0,3.4256393111,0.6668908051,2.5462941689
H,0,1.9911515382,4.3012848399,-1.1939093438
H,0,0.5934202372,3.9577952027,0.8306916252

H,0,1.2590852613,2.3040596917,2.5337765819
H,0,4.717397147,1.2966616568,0.215769742
H,0,4.0579743954,2.9567187252,-1.4916189805
H,0,4.435094453,0.2907727615,2.3795772085
H,0,2.7407613352,-0.1851358985,2.5369750748
H,0,3.3835498743,1.1057228171,3.5445518115
N,0,1.9539530669,0.4650841757,-1.3385892038
O,0,2.7537869887,0.115489489,-2.0253908819
O,0,1.0886367047,0.7421071387,-0.7050807568
F,0,0.4407055041,-3.907431084,-2.4398577643
B,0,0.7954792373,-3.3596021189,-1.2267926384
F,0,0.9683053184,-1.9934626807,-1.3793249474
F,0,-0.197083883,-3.5923463717,-0.3001326903
F,0,1.9775047685,-3.9168295479,-0.7893171877

Pi Complex NO2BF4 PCM ONIOM 3.247_94177

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266265816368

Zero-point correction= 0.157332 (Hartree/Particle)
Thermal correction to Energy= 0.174759
Thermal correction to Enthalpy= 0.175704
Thermal correction to Gibbs Free Energy= 0.103994
Sum of electronic and ZPE= -476.888438
Sum of electronic and thermal Energies= -476.871011
Sum of electronic and thermal Enthalpies= -476.870067
Sum of electronic and thermal Free Energies= -476.941777

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.663	55.860	150.926

C,0,-0.3822921097,-1.721830326,-3.2582543068
C,0,-0.6183366755,-0.3854088187,-3.5681832964
C,0,-0.0158341661,0.6297559932,-2.8154552634
C,0,0.834323189,0.3260072465,-1.7498689759
C,0,1.0548029522,-1.0216762297,-1.4468081162
C,0,0.4560611736,-2.0351484761,-2.1901896536
C,0,1.5106711579,1.4090793662,-0.9524333367
H,0,-0.8435681303,-2.5084780767,-3.8430922843
H,0,-1.2622235815,-0.1248757043,-4.4015894479
H,0,-0.1975336652,1.6682750395,-3.0757085567
H,0,1.7076604648,-1.2790260638,-0.6186017814
H,0,0.6452265881,-3.0715486264,-1.9354986007
H,0,1.1205542018,2.3946066676,-1.2070417205
H,0,2.5852809364,1.4112697377,-1.1491142059
H,0,1.3762901079,1.250933559,0.1195337951
N,0,-2.4219556076,-0.0536719241,-1.3599804112
O,0,-1.8667142432,-0.7508207122,-0.703451483
O,0,-3.055609469,0.6408881834,-1.9493333302
F,0,-5.8769339257,1.4560727858,3.8574906321
B,0,-5.9597874586,1.2753780245,2.4930012681
F,0,-7.2136219143,1.6426927191,2.0515087602
F,0,-5.0072044253,2.0530330785,1.8668705074
F,0,-5.7373760999,-0.052165543,2.188942708

Pi Complex NO2BF4 PCM ONIOM 3.248_93896

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.275067786382

Zero-point correction= 0.158745 (Hartree/Particle)
Thermal correction to Energy= 0.175238
Thermal correction to Enthalpy= 0.176182
Thermal correction to Gibbs Free Energy= 0.112467
Sum of electronic and ZPE= -476.892687
Sum of electronic and thermal Energies= -476.876194
Sum of electronic and thermal Enthalpies= -476.875250
Sum of electronic and thermal Free Energies= -476.938965

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.964	55.489	134.101

C,0,3.5249535956,-0.291063291,-0.3771040656
C,0,3.0036475868,0.6705888164,-1.2390925997
C,0,1.928923396,1.4651535649,-0.842961387
C,0,1.3494502361,1.3203605984,0.4204715227
C,0,1.8740310426,0.3445688833,1.2740381407
C,0,2.95465938,-0.4554579821,0.8817237979
C,0,0.1763112019,2.165886544,0.8370132903
H,0,4.36690136,-0.9013633945,-0.679888728
H,0,3.4365282365,0.80706279,-2.223214615
H,0,1.5353419105,2.211547304,-1.5252566836
H,0,1.4471169667,0.2177244852,2.2647490382
H,0,3.3550999553,-1.1906370116,1.5712560955
H,0,0.1042123026,2.2352022605,1.9226117232
H,0,-0.7638403567,1.7380288385,0.4673881845
H,0,0.2565856946,3.1744839512,0.4306899611
N,0,0.6448645055,-1.7695106898,-0.1114779477
O,0,0.4791952207,-2.3559668065,0.8185844365
O,0,0.7278215631,-1.2898037873,-1.1074020655
F,0,-3.8941655918,-0.8027882436,-0.4290584879
B,0,-2.8588254925,0.0512565423,-0.1174553582
F,0,-1.7374973577,-0.7006044168,0.2007285717
F,0,-2.5773058449,0.8485773679,-1.2052922515
F,0,-3.2098125109,0.8328846766,0.9609254272

Pi Complex NO2BF4 PCM ONIOM 3.254_94079

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.265925774039

Zero-point correction= 0.157622 (Hartree/Particle)
Thermal correction to Energy= 0.174936
Thermal correction to Enthalpy= 0.175881
Thermal correction to Gibbs Free Energy= 0.104925
Sum of electronic and ZPE= -476.888102
Sum of electronic and thermal Energies= -476.870787
Sum of electronic and thermal Enthalpies= -476.869843
Sum of electronic and thermal Free Energies= -476.940798

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.774	55.769	149.338

C,0,3.425335309,-1.722943777,0.628501027
C,0,3.4320424318,-1.301367379,-0.6978954169
C,0,3.4971661006,0.0636655271,-1.00352267
C,0,3.561505987,1.0236379051,0.0085249099
C,0,3.5460059187,0.5835382661,1.3362941534
C,0,3.4795385607,-0.771990587,1.6458627619
C,0,3.6503955642,2.4932834664,-0.3051271248
H,0,3.3808797429,-2.7790352325,0.8659213947
H,0,3.3997317836,-2.0299688209,-1.5010045214
H,0,3.5161913015,0.3795509575,-2.0423409929
H,0,3.5898606084,1.3148748894,2.1373560475
H,0,3.4707952957,-1.0871898989,2.6828631083
H,0,2.8375045568,3.0452254719,0.1719963793
H,0,3.6057147055,2.6756491674,-1.3786634052
H,0,4.5882321116,2.9083581802,0.0704779821
N,0,0.6764390983,-0.4607364284,-0.5713768408
O,0,0.5073087809,-0.7640459326,-1.6251506491
O,0,0.7489276069,-0.1491848529,0.4882048653
F,0,-3.9026291587,-0.8725008469,-0.5527363097
B,0,-4.6939316473,0.0801266036,0.0561465217
F,0,-5.3081797088,0.8504277576,-0.9089444282
F,0,-5.6489287313,-0.5422146453,0.832001942
F,0,-3.9066922179,0.885476209,0.853495266

Pi Complex NO2BF4 PCM ONIOM 3.256_93794

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267615559467

Zero-point correction= 0.158233 (Hartree/Particle)
Thermal correction to Energy= 0.175190
Thermal correction to Enthalpy= 0.176134
Thermal correction to Gibbs Free Energy= 0.109174
Sum of electronic and ZPE= -476.888887
Sum of electronic and thermal Energies= -476.871930
Sum of electronic and thermal Enthalpies= -476.870986
Sum of electronic and thermal Free Energies= -476.937945

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.933	55.587	140.929

C,0,-3.708791379,-0.3555545686,0.5158990411
C,0,-3.2939669549,0.0264731199,-0.7559680974
C,0,-2.0662136553,-0.4212478995,-1.2597075
C,0,-1.2410230952,-1.2616253645,-0.5069426738
C,0,-1.6684501771,-1.6259386684,0.7736488876
C,0,-2.8863314306,-1.1800721434,1.2812999611
C,0,0.0729195539,-1.7578270393,-1.0478219027
H,0,-4.661392756,-0.0171504063,0.9050982881
H,0,-3.9272096378,0.6583717945,-1.3693202405
H,0,-1.7615517305,-0.1308223094,-2.2607462243
H,0,-1.0403374095,-2.2727986011,1.378161719
H,0,-3.1956377745,-1.4818600778,2.2751209581
H,0,0.156301709,-1.5731040201,-2.1188705378
H,0,0.1814756898,-2.8299463287,-0.876533873
H,0,0.9184505283,-1.264114552,-0.5541394814
N,0,-1.3969890213,1.9197703666,0.2222704431
O,0,-1.4773767508,2.564008089,-0.678441976
O,0,-1.2681291724,1.373782008,1.176964389
F,0,2.4822248341,-0.1288853649,1.196700436
B,0,3.2795267076,0.0491583139,0.0844172341
F,0,4.4358347281,0.7024439293,0.4583474173
F,0,3.5998474614,-1.1738999126,-0.4660927913
F,0,2.6080857328,0.8168276353,-0.8460874763

Pi Complex NO2BF4 PCM ONIOM 3.261_94154

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.267181450224

Zero-point correction= 0.157401 (Hartree/Particle)
Thermal correction to Energy= 0.174735
Thermal correction to Enthalpy= 0.175679
Thermal correction to Gibbs Free Energy= 0.104682
Sum of electronic and ZPE= -476.888823
Sum of electronic and thermal Energies= -476.871489
Sum of electronic and thermal Enthalpies= -476.870544
Sum of electronic and thermal Free Energies= -476.941542

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.648	55.831	149.426

C,0,1.8632498918,-0.5860276355,4.873613152
C,0,0.484904449,-0.5805771256,5.0622245772
C,0,-0.144762111,-1.6642205899,5.6874849107
C,0,0.5914845912,-2.7623299104,6.1393055769
C,0,1.9747600455,-2.7558647477,5.9318945489
C,0,2.6053377437,-1.6830705119,5.3078583129
C,0,-0.0705433643,-3.9233474666,6.831510365
H,0,2.3542042082,0.2534246816,4.3964281956
H,0,-0.1066311858,0.2696429091,4.7404723569
H,0,-1.2193111478,-1.6400274148,5.8430065994
H,0,2.5647676024,-3.6029931006,6.2674750068
H,0,3.6791724501,-1.7031367012,5.1621840222
H,0,0.3432440021,-4.058591774,7.8328765772
H,0,0.0957045464,-4.855393965,6.2846119845
H,0,-1.145434657,-3.770731623,6.927345992
N,0,0.0172034908,-2.4562767681,2.9420023376
O,0,1.0196766563,-2.9108347448,3.0604039803
O,0,-0.9920195571,-2.0511763435,2.718943705
F,0,0.0098477318,-6.829550885,2.8644119663
B,0,-0.718200767,-7.6106895596,3.7387268088
F,0,-0.0920957164,-8.8286516678,3.8986942441
F,0,-0.8060096819,-6.970795258,4.9576576562
F,0,-1.9860786208,-7.8027310978,3.2300465234

Pi Complex NO2BF4 PCM ONIOM 3.270_93741

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266875078925

Zero-point correction= 0.158228 (Hartree/Particle)
Thermal correction to Energy= 0.175144
Thermal correction to Enthalpy= 0.176088
Thermal correction to Gibbs Free Energy= 0.109002

Sum of electronic and ZPE= -476.888187
Sum of electronic and thermal Energies= -476.871270
Sum of electronic and thermal Enthalpies= -476.870326
Sum of electronic and thermal Free Energies= -476.937412

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.904	55.594	141.194

C,0,1.8330917235,-0.6380460466,-4.5977882386
C,0,1.1600159759,-1.856601104,-4.5820069289
C,0,-0.1949869393,-1.908903089,-4.2588732926
C,0,-0.908126644,-0.7492258692,-3.9455392555
C,0,-0.2181380454,0.4678722053,-3.948354176
C,0,1.1403222368,0.5265284132,-4.2770675779
C,0,-2.3826179088,-0.8003639275,-3.6479843865
H,0,2.8843735903,-0.5949253592,-4.8557354846
H,0,1.6896427225,-2.7709897925,-4.8226373585
H,0,-0.7068893789,-2.8656295485,-4.252920099
H,0,-0.7519653182,1.3836273999,-3.7105582243
H,0,1.6486788215,1.4845640444,-4.2914311427
H,0,-2.6783935664,-0.0132941492,-2.9514261636
H,0,-2.6703943538,-1.7636195609,-3.2257941888
H,0,-2.9565637419,-0.6576427601,-4.5671456037
N,0,1.1111686223,-0.0636534476,-1.4603376231
O,0,1.203021374,-1.1492619782,-1.6575217171
O,0,1.0548056519,1.0027731063,-1.1578734211
F,0,-3.9459674603,1.6370161991,1.4235012149
B,0,-3.6060497899,0.500016731,0.7210415667
F,0,-3.4384563324,0.8154202095,-0.6117258241
F,0,-2.4249017525,-0.0118108924,1.2191424155
F,0,-4.6042395869,-0.4425493836,0.8508280094

Pi Complex NO2BF4 PCM ONIOM 3.276_94050

file
E(RPM3) = 0.273363507590

Zero-point correction= 0.158064 (Hartree/Particle)
Thermal correction to Energy= 0.175049
Thermal correction to Enthalpy= 0.175993
Thermal correction to Gibbs Free Energy= 0.109095
Sum of electronic and ZPE= -476.891538
Sum of electronic and thermal Energies= -476.874553
Sum of electronic and thermal Enthalpies= -476.873609
Sum of electronic and thermal Free Energies= -476.940507

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.845	55.731	140.800

Pi Complex NO2BF4 PCM ONIOM 3.283_94088

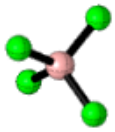
ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.265866408341

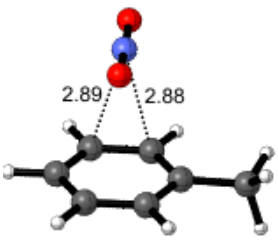
Zero-point correction= 0.157384 (Hartree/Particle)
Thermal correction to Energy= 0.174727
Thermal correction to Enthalpy= 0.175671
Thermal correction to Gibbs Free Energy= 0.104736
Sum of electronic and ZPE= -476.888238
Sum of electronic and thermal Energies= -476.870895
Sum of electronic and thermal Enthalpies= -476.869951
Sum of electronic and thermal Free Energies= -476.940886

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.643	55.832	149.296

C,0,-2.9038078398,-1.9702470564,-0.3773982697
C,0,-3.3169064663,-1.6348291921,0.9097827279
C,0,-3.7810815293,-0.3510004836,1.187637706
C,0,-3.8459789644,0.6258622926,0.1900001665
C,0,-3.4162107602,0.2825981417,-1.0952517632
C,0,-2.9521189735,-1.0059182524,-1.380524605
C,0,-4.391855161,1.9972599219,0.4857064058
H,0,-2.5468185102,-2.9694957416,-0.5961049428
H,0,-3.2749436684,-2.3737181866,1.7017837261
H,0,-4.0992465898,-0.1032588549,2.1952847049
H,0,-3.4625042021,1.0225803709,-1.8889868725
H,0,-2.6398197938,-1.2526060449,-2.3897514817
H,0,-4.1231873763,2.3234778627,1.4913771294
H,0,-5.4829596702,1.9903562278,0.4231203877
H,0,-4.0248490177,2.7354312809,-0.2282083332
N,0,-0.626197699,0.395276516,-0.3722794947
O,0,-0.8203743693,0.0596578695,0.6644734691
O,0,-0.33991566,0.7576099764,-1.3812419393
F,0,4.7689409187,0.6702141974,-1.0391548319
B,0,4.6907398998,0.0432035298,0.1872202617
F,0,3.7441199936,-0.9593397743,0.1293807516
F,0,5.9161021496,-0.4994722148,0.5109560691
F,0,4.3217042898,0.9622656139,1.1480820282

Pi Complex NO2BF4 PCM ONIOM 3.283_94208





ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266064245120

Zero-point correction= 0.157474 (Hartree/Particle)
Thermal correction to Energy= 0.174973

Thermal correction to Enthalpy= 0.175917
Thermal correction to Gibbs Free Energy= 0.103642
Sum of electronic and ZPE= -476.888250
Sum of electronic and thermal Energies= -476.870751
Sum of electronic and thermal Enthalpies= -476.869807
Sum of electronic and thermal Free Energies= -476.942082

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.797	55.812	152.115

C,0,-3.2821416793,-1.9099712114,-0.0495288547
C,0,-3.2511819427,-1.1456738265,1.113328822
C,0,-3.463393069,0.2366361793,1.0522692611
C,0,-3.7154661462,0.8735379249,-0.1657556704
C,0,-3.7316640781,0.0925642537,-1.3257693752
C,0,-3.5191705835,-1.2826958671,-1.2710176684
C,0,-3.9867736581,2.3527708885,-0.2315840729
H,0,-3.1221005292,-2.9804987698,-0.0051957278
H,0,-3.0753153105,-1.6197955256,2.0730680447
H,0,-3.4517871973,0.8207275979,1.9678191384
H,0,-3.913959649,0.5691935336,-2.2837574349
H,0,-3.5371699864,-1.8656187484,-2.1846645116
H,0,-5.0550024649,2.5353661542,-0.3715765618
H,0,-3.4645065417,2.8147748285,-1.0710979256
H,0,-3.6809345593,2.855981414,0.6859481598
N,0,-0.6514952715,-0.0266776263,0.5099307724
O,0,-0.8107934822,-0.1496979432,-0.5785235322
O,0,-0.3909074041,0.1107454837,1.5798409583
F,0,3.7754863154,0.6876935651,-0.8964249574
B,0,4.7198369729,0.0476315636,-0.1200725995
F,0,5.5170377843,-0.7403443378,-0.9233234465
F,0,5.4959376166,0.986580642,0.5262157847
F,0,4.0829828636,-0.744455173,0.8132993976

Pi Complex NO2BF4 PCM ONIOM 3.289_93970

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.265951522336

Zero-point correction= 0.157904 (Hartree/Particle)
Thermal correction to Energy= 0.175175
Thermal correction to Enthalpy= 0.176120
Thermal correction to Gibbs Free Energy= 0.106005
Sum of electronic and ZPE= -476.887805
Sum of electronic and thermal Energies= -476.870534
Sum of electronic and thermal Enthalpies= -476.869590
Sum of electronic and thermal Free Energies= -476.939704

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.924	55.714	147.568

C,0,1.241798972,1.0525571351,-3.4186581415
C,0,1.3243043442,2.431982516,-3.252009379
C,0,2.5487530395,3.028774545,-2.9304489463
C,0,3.7077250032,2.2615856063,-2.7803874794
C,0,3.604460384,0.8765066587,-2.9403640808
C,0,2.3876377154,0.2768248236,-3.2564454015
C,0,5.0353740273,2.9064744945,-2.4843611596
H,0,0.2964240757,0.5875320494,-3.6711027601
H,0,0.4428476062,3.050788378,-3.3820175478
H,0,2.6046741899,4.107452576,-2.8153919031
H,0,4.4894567402,0.2605249827,-2.817175742
H,0,2.3340330942,-0.79914316,-3.375895389
H,0,5.6180862336,3.008706474,-3.4032597631
H,0,5.6224760203,2.3043331428,-1.7892508909
H,0,4.9096620552,3.9028397673,-2.0596741312
N,0,1.4999120489,2.257305761,-0.3680999651
O,0,1.9306332577,1.2384725216,-0.4178547847
O,0,1.0451048506,3.2578294776,-0.2174581243
F,0,3.1265811835,6.3908005569,4.4151143966
B,0,2.2302347926,6.0552387474,3.4223106267
F,0,2.0135320505,4.6923454087,3.4405260046
F,0,1.0362743522,6.7124955372,3.6331550999
F,0,2.7456598628,6.4198019003,2.1954836617

Pi Complex NO2BF4 PCM ONIOM 3.296_93743

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.278823983601

Zero-point correction= 0.158995 (Hartree/Particle)
Thermal correction to Energy= 0.175310
Thermal correction to Enthalpy= 0.176255
Thermal correction to Gibbs Free Energy= 0.113001
Sum of electronic and ZPE= -476.891442
Sum of electronic and thermal Energies= -476.875127
Sum of electronic and thermal Enthalpies= -476.874182
Sum of electronic and thermal Free Energies= -476.937436

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.009	55.298	133.128

C,0,1.8532104707,3.3914186689,-0.7992869791
C,0,1.1813012331,2.9801543081,0.3478140485
C,0,1.7632908503,2.0333559467,1.1986076572
C,0,3.027236593,1.4938907167,0.926738874
C,0,3.6800717101,1.9075692176,-0.2353400674
C,0,3.1011306402,2.8453678981,-1.0900544283
C,0,3.6691852608,0.523830436,1.8818573473
H,0,1.4084507747,4.12353082,-1.4620807223
H,0,0.2099523278,3.3958642396,0.5920857749
H,0,1.2370117252,1.7278808854,2.0985186908
H,0,4.6536261979,1.4932875918,-0.4756780646
H,0,3.6287031264,3.1492305855,-1.9867757001
H,0,4.2179982655,1.0663869859,2.6556834346
H,0,4.3757383086,-0.1302781317,1.3700819734
H,0,2.9233246322,-0.0961927068,2.3818406351
N,0,0.5357478833,0.3719741515,-0.6739207616
O,0,1.3030070977,0.4999792936,-1.4645780635
O,0,-0.3010715895,0.1422072857,0.0228914227
F,0,1.791872477,-3.5104202189,-1.9824985142
B,0,0.8714671522,-2.9030246095,-1.1623467655
F,0,0.0694403782,-2.0437902341,-1.8940398302
F,0,0.0974224306,-3.8470007958,-0.5307336101
F,0,1.5158739541,-2.1127416345,-0.2242362514

Pi Complex NO2BF4 PCM ONIOM 3.302_93903

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266382473702

Zero-point correction= 0.157948 (Hartree/Particle)
Thermal correction to Energy= 0.175123
Thermal correction to Enthalpy= 0.176067
Thermal correction to Gibbs Free Energy= 0.107173
Sum of electronic and ZPE= -476.888265
Sum of electronic and thermal Energies= -476.871090
Sum of electronic and thermal Enthalpies= -476.870146
Sum of electronic and thermal Free Energies= -476.939039

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.891	55.679	144.998

C,0,3.8961618877,-3.9854246303,0.381193286
C,0,4.6652612052,-2.8591674481,0.6620799779
C,0,4.5333371865,-2.2029490087,1.8849112502
C,0,3.6349840108,-2.6553225098,2.8538024541
C,0,2.8557445741,-3.7788624378,2.5549653955
C,0,2.9864848295,-4.4430560411,1.3312229468
C,0,3.5277984705,-1.9746412817,4.1919117626
H,0,4.0021084413,-4.4992752945,-0.5664664813
H,0,5.3704984036,-2.4874155018,-0.0720943186
H,0,5.1391198575,-1.3262829618,2.0904010423
H,0,2.153883547,-4.1525195967,3.2951667719
H,0,2.3841887246,-5.3225069998,1.1302858197
H,0,3.8241908999,-0.9270971653,4.1297536505
H,0,4.1836882514,-2.4622119776,4.9175468039
H,0,2.5105526195,-2.0215495693,4.5855545901
N,0,1.098618489,-2.2935594592,0.8491833191
O,0,1.9065918341,-1.6375205815,0.4721336778
O,0,0.2186566512,-2.8851087153,1.1768891123
F,0,0.6086899595,2.273221099,5.2328650239
B,0,0.0597724779,1.0964116549,4.7689270881
F,0,-1.161371971,0.8840078026,5.3738879535
F,0,-0.11438923,1.1784151343,3.4022244002
F,0,0.9042349802,0.0447507896,5.0588406734

Pi Complex NO2BF4 PCM ONIOM 3.319_94023

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266855800930

Zero-point correction= 0.158045 (Hartree/Particle)
Thermal correction to Energy= 0.175335
Thermal correction to Enthalpy= 0.176279
Thermal correction to Gibbs Free Energy= 0.105622
Sum of electronic and ZPE= -476.887813
Sum of electronic and thermal Energies= -476.870523
Sum of electronic and thermal Enthalpies= -476.869579
Sum of electronic and thermal Free Energies= -476.940236

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	110.024	55.679	148.710

C,0,-1.3817621703,-1.7195658655,-0.3056386346
C,0,-2.3341081933,-1.8821994355,0.6984735157
C,0,-3.4617434,-1.0656099306,0.7371504442
C,0,-3.6674302226,-0.0696101546,-0.222089783
C,0,-2.701298985,0.0915631611,-1.2196151804
C,0,-1.566832466,-0.7274216687,-1.2644352941
C,0,-4.8870316867,0.8116733591,-0.1628693936
H,0,-0.5078220948,-2.3590937164,-0.3420712656
H,0,-2.2009475001,-2.650401368,1.4514565761
H,0,-4.1991706156,-1.2079534281,1.5205850185
H,0,-2.8444270518,0.8476044562,-1.9860135404
H,0,-0.8403123935,-0.5958529921,-2.0592762385
H,0,-5.776470275,0.2291542547,0.0813963174
H,0,-5.0583855486,1.3179054626,-1.1128407326
H,0,-4.7767634371,1.5761564632,0.6108612762
N,0,-0.92077744,1.4516294727,0.5621616085
O,0,-1.2269212131,0.8457186693,1.4366758605
O,0,-0.5687060217,2.1276265574,-0.2443262001
F,0,4.668625193,-1.0729110492,0.7313269688
B,0,4.0676192874,-0.0941090705,-0.0318219594
F,0,3.5223805939,0.8642810948,0.7983080018
F,0,5.0034021024,0.4917069647,-0.8579831594
F,0,3.0656665385,-0.6564562365,-0.7961432058

Pi Complex NO2BF4 PCM ONIOM 3.330_94112

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.266691677891

Zero-point correction= 0.157728 (Hartree/Particle)
Thermal correction to Energy= 0.175120
Thermal correction to Enthalpy= 0.176064
Thermal correction to Gibbs Free Energy= 0.104458
Sum of electronic and ZPE= -476.887859
Sum of electronic and thermal Energies= -476.870467
Sum of electronic and thermal Enthalpies= -476.869523
Sum of electronic and thermal Free Energies= -476.941128

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.889	55.789	150.706

C,0,3.0320197987,-1.3799502638,-0.4393725728
C,0,2.269843893,-0.409517411,0.2077324681
C,0,1.9549205597,-0.5463353919,1.557632715
C,0,2.3944101251,-1.6502041918,2.2937011599
C,0,3.1479031603,-2.6245763297,1.6312581023
C,0,3.4690159057,-2.4911139307,0.2755538355
C,0,2.0823932058,-1.7693891545,3.7615866267
H,0,3.2798110766,-1.2733871318,-1.4887477699
H,0,1.9184100232,0.457042177,-0.3403608441
H,0,1.3611342696,0.2176072203,2.0490393038
H,0,3.5052275118,-3.4896497906,2.1825135602
H,0,4.0675944755,-3.253009243,-0.2122188512
H,0,2.1787541054,-2.798379042,4.1091264001
H,0,1.0717440826,-1.4221064961,3.9810827628
H,0,2.7730339061,-1.1561164563,4.3457725733
N,0,0.8276041006,-3.7257859213,0.4131058798
O,0,0.3434143075,-2.7451099253,0.2404387228

O,0,1.2144791052,-4.755037213,0.5634535341
F,0,1.6731385857,-6.2362816288,-2.9635981571
B,0,2.0522328216,-6.6896217868,-4.2105964289
F,0,1.682300315,-8.0110929338,-4.3479361273
F,0,1.4282319916,-5.932219741,-5.1802073123
F,0,3.4199173737,-6.573008314,-4.3462230808

Pi Complex NO2BF4 PCM ONIOM 3.366_94716

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.312820301687

Zero-point correction= 0.158348 (Hartree/Particle)
Thermal correction to Energy= 0.174303
Thermal correction to Enthalpy= 0.175247
Thermal correction to Gibbs Free Energy= 0.112432
Sum of electronic and ZPE= -476.901252
Sum of electronic and thermal Energies= -476.885297
Sum of electronic and thermal Enthalpies= -476.884353
Sum of electronic and thermal Free Energies= -476.947167

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.377	55.036	132.204

C,0,2.7691748733,-1.6212177632,-0.2947561509
C,0,1.8060982774,-1.3289340468,-1.2740571517
C,0,1.3163172761,-0.0519485052,-1.3795050563
C,0,1.7416609499,0.9579974986,-0.4579750947
C,0,2.8044544722,0.6486610873,0.4584201916
C,0,3.2920102813,-0.631887186,0.5473933723
C,0,1.344054745,2.3788346964,-0.6865888105
H,0,3.1298714946,-2.638771176,-0.1999726501
H,0,1.4519791506,-2.1114683416,-1.9317660663
H,0,0.5653517983,0.2022498349,-2.1205160129
H,0,3.1786871187,1.4374530936,1.1013973496
H,0,4.0591011889,-0.8817600473,1.2677378849
H,0,0.3156014306,2.4496515426,-1.0440244367
H,0,1.9979034433,2.7939939543,-1.4591985704
H,0,1.462750198,2.9811636608,0.2131275944
N,0,0.3814992246,0.3492199553,1.0287569629
O,0,-0.1676389057,1.3200944453,1.348075504
O,0,0.4072108143,-0.7794008259,1.2785478939
F,0,-2.3949306174,-0.4654751541,1.1301606625
B,0,-2.7432950669,-0.3071357142,-0.1972001517
F,0,-3.0331521385,-1.5300290953,-0.7580741592
F,0,-3.830651143,0.5293527983,-0.3034030676
F,0,-1.654039866,0.2550632884,-0.8414070372

Pi Complex NO2BF4 PCM ONIOM 3.372_94096

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.279061853899

Zero-point correction= 0.158195 (Hartree/Particle)
Thermal correction to Energy= 0.174932
Thermal correction to Enthalpy= 0.175876
Thermal correction to Gibbs Free Energy= 0.109974
Sum of electronic and ZPE= -476.892744
Sum of electronic and thermal Energies= -476.876007
Sum of electronic and thermal Enthalpies= -476.875062
Sum of electronic and thermal Free Energies= -476.940965

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.771	55.673	138.704

C,0,2.0012943262,3.6051234769,-0.6916612716
C,0,1.3472562672,3.2657179443,0.4867093558
C,0,1.8509047912,2.2408619644,1.2955702876
C,0,3.02254517,1.5521848426,0.9509779006
C,0,3.6624241208,1.9038027021,-0.2392528697
C,0,3.1585572511,2.9162199861,-1.0528406843
C,0,3.5813693166,0.4789177229,1.8459045569
H,0,1.614621817,4.3944621168,-1.3243088074
H,0,0.4490280045,3.7931681717,0.786674104
H,0,1.3366836434,1.9851825793,2.2176103043
H,0,4.5624063817,1.3756782853,-0.5360477888
H,0,3.671169338,3.1673862872,-1.9741150694
H,0,4.284460338,0.9097450873,2.5628751713
H,0,4.1150141851,-0.2774114156,1.2685250618
H,0,2.7923983288,-0.0182149624,2.4127671381
N,0,0.4595796396,0.6150398607,-0.4533720539
O,0,1.0792538477,0.8012786128,-1.3545957296
O,0,-0.2561111576,0.3306570111,0.3506732764
F,0,2.3522443741,-3.0663726001,-1.4008119397
B,0,1.3768188788,-2.5759548869,-0.565979282
F,0,0.3652833956,-1.9874003944,-1.3059584969
F,0,0.8671077946,-3.5825492718,0.2185541436
F,0,1.8955179476,-1.5681701204,0.2309896931

Pi Complex NO2BF4 PCM ONIOM 3.382_93727

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.277518938346

Zero-point correction= 0.158344 (Hartree/Particle)
Thermal correction to Energy= 0.174923
Thermal correction to Enthalpy= 0.175867
Thermal correction to Gibbs Free Energy= 0.112043
Sum of electronic and ZPE= -476.890975
Sum of electronic and thermal Energies= -476.874395
Sum of electronic and thermal Enthalpies= -476.873451
Sum of electronic and thermal Free Energies= -476.937275

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.766	55.659	134.329

C,0,-0.2639671368,0.1643744557,4.0367281044
C,0,-0.5501259024,1.3975450241,3.4532858604
C,0,-1.7926605863,1.6337005991,2.867780177
C,0,-2.7764878553,0.6450590339,2.8479260839
C,0,-2.4724948299,-0.5969441708,3.4260909304
C,0,-1.230648237,-0.834973727,4.0241571299
C,0,-4.1338321917,0.9065494255,2.2531728333
H,0,0.7047745643,-0.0172739407,4.4852450029
H,0,0.2000426923,2.1795398012,3.4501145739

H,0,-1.9982499821,2.5990242327,2.4181106741
H,0,-3.2183043003,-1.3869376446,3.4166047231
H,0,-1.0174362672,-1.8129016453,4.4479218484
H,0,-4.8123894041,1.2882436715,3.0201460048
H,0,-4.5759291449,-0.0055413079,1.8495440043
H,0,-4.0813071619,1.6501604273,1.4576213456
N,0,-1.1861916478,-1.2707077063,1.115413452
O,0,-1.8542907265,-2.1491138702,0.9754786489
O,0,-0.4414406185,-0.4448930381,1.084088348
F,0,-1.4043597647,-3.7128504674,2.3680745427
B,0,-0.0909041651,-3.9858976105,2.7119132267
F,0,0.6461639126,-2.8826310406,2.3107331415
F,0,0.0209678461,-4.1652921815,4.0704462019
F,0,0.3461964072,-5.1068185201,2.0468857419

Pi Complex NO2BF4 PCM ONIOM 3.406_94020

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.274295003518

Zero-point correction= 0.158065 (Hartree/Particle)
Thermal correction to Energy= 0.174880
Thermal correction to Enthalpy= 0.175825
Thermal correction to Gibbs Free Energy= 0.110851
Sum of electronic and ZPE= -476.892992
Sum of electronic and thermal Energies= -476.876178
Sum of electronic and thermal Enthalpies= -476.875233
Sum of electronic and thermal Free Energies= -476.940207

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.739	55.685	136.748

C,0,-0.0639081568,-0.3717528674,4.1883481227
C,0,-0.3037664744,1.0006098362,4.184852028
C,0,-1.6065449489,1.4896780422,4.1048562205
C,0,-2.6962164036,0.6217102659,4.0271675409
C,0,-2.4416068401,-0.757923892,4.0220238385
C,0,-1.1379186626,-1.2528723946,4.1092167154
C,0,-4.110026867,1.1372262221,3.9811334958
H,0,0.9482545207,-0.7566338113,4.2361953096
H,0,0.5266595824,1.694407915,4.241326558
H,0,-1.7772020693,2.5608249502,4.1025870503
H,0,-3.275488458,-1.451430848,3.9642806314
H,0,-0.9589590942,-2.3252232923,4.0865454615
H,0,-4.1501081792,2.160159743,3.6070669374
H,0,-4.5444894632,1.1316732306,4.9838960841
H,0,-4.7416487192,0.5103692773,3.3491901329
N,0,-1.8805018184,-0.5465102219,1.3116422001
O,0,-2.6961593657,-1.2675079796,1.0835741979
O,0,-1.0549591356,0.1898239824,1.3825598799
F,0,-0.4486284372,-4.4773773182,2.6476138121
B,0,0.4605657683,-3.6421499276,2.0359569371
F,0,-0.2158234828,-2.5692045068,1.4732271243
F,0,1.3702195088,-3.1783061667,2.9601531691
F,0,1.1221608959,-4.3235910385,1.0380945522

Pi Complex NO2BF4 PCM ONIOM 3.408_94164

ONIOM(M062X/6-311G*:PM3)
E(RPM3) = 0.274141138819

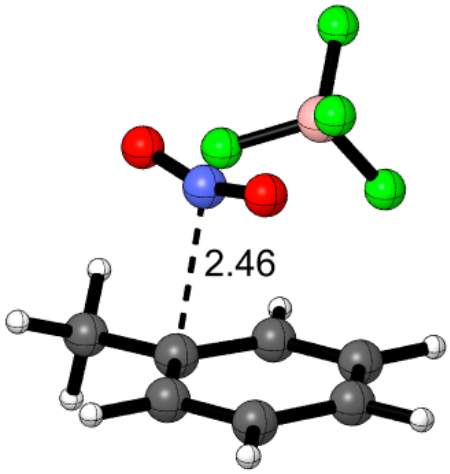
Zero-point correction= 0.158015 (Hartree/Particle)
Thermal correction to Energy= 0.174876
Thermal correction to Enthalpy= 0.175820
Thermal correction to Gibbs Free Energy= 0.109504
Sum of electronic and ZPE= -476.893138
Sum of electronic and thermal Energies= -476.876278
Sum of electronic and thermal Enthalpies= -476.875334
Sum of electronic and thermal Free Energies= -476.941649

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.736	55.710	139.573

C,0,-3.6336609423,-0.5981605817,0.5382173212
C,0,-2.9948052888,0.2803794646,1.4144871802
C,0,-2.0051518573,1.1426989958,0.9528353776
C,0,-1.6257692182,1.1474469828,-0.3929508567
C,0,-2.267218245,0.2542169655,-1.2603047855
C,0,-3.2695297758,-0.6084304646,-0.8022628686
C,0,-0.5554907934,2.0847710775,-0.885340145
H,0,-4.4079169507,-1.2632388852,0.9006527977
H,0,-3.2714849601,0.2947833477,2.4623637999
H,0,-1.5188680623,1.8231693097,1.6443756958
H,0,-1.9967461849,0.2482169451,-2.3121694495
H,0,-3.7631656604,-1.2754601803,-1.4995291138
H,0,-0.7989066481,3.1167644437,-0.6261353718
H,0,-0.4394750467,2.0234160213,-1.9673795207
H,0,0.4131700808,1.8567766628,-0.4252237879
N,0,-0.5306611919,-1.7136202805,-0.3244116655
O,0,-0.8185220633,-1.6613021067,0.7444676556
O,0,-0.1591332508,-1.8738084493,-1.3598672007
F,0,2.9391015672,1.1082499409,-0.9111009083
B,0,2.7148643009,0.5163340587,0.3124469876
F,0,3.8358738271,-0.1842404683,0.701257536
F,0,2.4213203192,1.4763828027,1.2556981268
F,0,1.6502690448,-0.3663676022,0.2068671956

TSs for Toluene + $NO_2^+BF_4^-$ M062X/6-311G*/PCM(CH_2Cl_2)

TS NO2BF4 PCM PURE-M06-2X 3.440_824095 (5a‡)



M062X/6-311G*
E(RM062X) = -900.938230756

Zero-point correction= 0.157181 (Hartree/Particle)
Thermal correction to Energy= 0.172152
Thermal correction to Enthalpy= 0.173096
Thermal correction to Gibbs Free Energy= 0.114136
Sum of electronic and ZPE= -900.781049
Sum of electronic and thermal Energies= -900.766079
Sum of electronic and thermal Enthalpies= -900.765135
Sum of electronic and thermal Free Energies= -900.824095

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.027	53.140	124.092

C,0,-1.0102818907,-0.433536969,1.5651973451
C,0,-0.7782877839,0.8806702567,1.1365812781
C,0,-1.6818068026,1.5052314582,0.2977331748
C,0,-2.8341488766,0.8203091025,-0.1421470076
C,0,-3.0710923804,-0.4890607882,0.3323471484
C,0,-2.1618388761,-1.1104113392,1.1745525989
C,0,-3.8539580601,1.488495173,-1.0129993114
H,0,-0.2872403082,-0.92140422,2.2085329235
H,0,0.1153129439,1.4025694958,1.4574440826
H,0,-1.5064471399,2.5210167525,-0.0405292082
H,0,-3.964883125,-1.0118360067,0.0161749292
H,0,-2.3448882918,-2.1267291697,1.5008345004
H,0,-4.6366898694,1.9247485951,-0.3857815624
H,0,-4.3325036448,0.7620326743,-1.6723652637
H,0,-3.4170700658,2.292561324,-1.6068667788
N,0,-1.4944211238,-0.3484565674,-1.8393753424
O,0,-2.1472515278,-0.0697142997,-2.7167547178
O,0,-0.5794208854,-0.7519383026,-1.3213861869
F,0,-2.3512906532,-2.5956563131,-1.796043987
B,0,-3.7574582321,-2.7949257163,-1.8912966265
F,0,-4.0290752092,-3.748807415,-2.8598446355
F,0,-4.2387787784,-3.1938519143,-0.6408984897
F,0,-4.3371304187,-1.557330811,-2.2454068632

TS NO2BF4 PCM PURE-M06-2X 3.4399_824088

M062X/6-311G*
E(RM062X) = -900.938230779

Zero-point correction= 0.157184 (Hartree/Particle)
Thermal correction to Energy= 0.172153
Thermal correction to Enthalpy= 0.173097
Thermal correction to Gibbs Free Energy= 0.114142
Sum of electronic and ZPE= -900.781047
Sum of electronic and thermal Energies= -900.766078
Sum of electronic and thermal Enthalpies= -900.765133
Sum of electronic and thermal Free Energies= -900.824088

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.028	53.139	124.081

C,0,1.6436415556,2.4802636962,0.1935466235
C,0,2.7282275088,1.7903389991,0.7524260453
C,0,2.9650375674,0.4738760967,0.4046573877
C,0,2.110240449,-0.1863268976,-0.5030579634
C,0,1.0462904869,0.5372725688,-1.0862654784
C,0,0.8139498259,1.858040236,-0.7345132671
C,0,2.3703064536,-1.597518424,-0.9340756463
H,0,1.455283704,3.506796534,0.4858400471
H,0,3.3752681769,2.2888346295,1.4642512718
H,0,3.8006407476,-0.0669250365,0.8362749187
H,0,0.4000948922,0.0428305864,-1.8004635673
H,0,-0.0268533076,2.3856281719,-1.1675987187
H,0,1.4328019345,-2.1125798751,-1.1516054772
H,0,2.9307207363,-2.1552853398,-0.182476137
H,0,2.9608816989,-1.5926658398,-1.8547180814
N,0,0.4825632177,-0.5628494073,1.2999878352
O,0,0.3958489308,-1.6778924841,1.1489206061
O,0,0.338127619,0.4209291673,1.8287933271
F,0,-0.9353662985,-1.7977018116,-1.184405516
B,0,-1.9334756999,-0.8201090709,-0.9816106465
F,0,-1.6415838612,-0.1606178413,0.2455751511
F,0,-1.8836854942,0.1180311927,-2.0168461652
F,0,-3.1829008438,-1.4158478509,-0.9055715491

TS NO2BF4 PCM PURE-M06-2X 3.440_824085

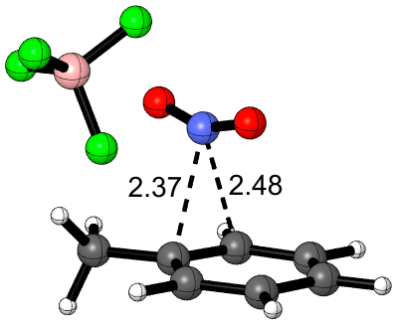
M062X/6-311G*
E(RM062X) = -900.938230783

Zero-point correction= 0.157185 (Hartree/Particle)
Thermal correction to Energy= 0.172154
Thermal correction to Enthalpy= 0.173098
Thermal correction to Gibbs Free Energy= 0.114145
Sum of electronic and ZPE= -900.781046
Sum of electronic and thermal Energies= -900.766077
Sum of electronic and thermal Enthalpies= -900.765133
Sum of electronic and thermal Free Energies= -900.824085

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 108.028 53.138 124.076

C,0,-0.886597005,-0.043161829,1.8571414905
C,0,-2.0661945678,0.6723635012,1.6743680607
C,0,-2.9816788786,0.254823141,0.7205945751
C,0,-2.7232839065,-0.8833805633,-0.0752940723
C,0,-1.5413154489,-1.6191159952,0.1530230016
C,0,-0.6317341918,-1.1978169148,1.1044802585
C,0,-3.7488055818,-1.342457657,-1.0664661522
H,0,-0.1591634294,0.2894978848,2.5884837855
H,0,-2.2671288229,1.5664788112,2.2514757435
H,0,-3.8975348793,0.8109551735,0.5655383636
H,0,-1.3484450811,-2.5099370653,-0.4353904184
H,0,0.2840287906,-1.754315771,1.2642985691
H,0,-4.2644392056,-0.4888149647,-1.5102528017
H,0,-4.5020931214,-1.9483949402,-0.5548194153
H,0,-3.3074530635,-1.9554938287,-1.8535253822
N,0,-1.4629604534,0.720258505,-1.4470491092
O,0,-2.1324296737,0.6514571719,-2.3530016349
O,0,-0.5448487153,1.0091167131,-0.8622748771
F,0,-4.24711686,3.0781891108,0.4898908148
B,0,-3.7905836801,3.0246898613,-0.8303473068
F,0,-4.1143386269,4.1832464573,-1.5193174679
F,0,-2.3775193478,2.8539210349,-0.8173633395
F,0,-4.3469492497,1.8987521634,-1.4751466854

TS NO2BF4 PCM PURE-M06-2X 3.426_824053 (5b‡)



M062X/6-311G*
E(RM062X) = -900.937046606

Zero-point correction= 0.156855 (Hartree/Particle)
Thermal correction to Energy= 0.171835
Thermal correction to Enthalpy= 0.172779
Thermal correction to Gibbs Free Energy= 0.112994
Sum of electronic and ZPE= -900.780191
Sum of electronic and thermal Energies= -900.765212
Sum of electronic and thermal Enthalpies= -900.764268
Sum of electronic and thermal Free Energies= -900.824053

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 107.828 53.127 125.828

C,0,-1.9062710451,-0.7144224971,1.1120366187
C,0,-1.4232682291,0.5169540071,1.52227902
C,0,-1.8554215488,1.6676117661,0.8685863008
C,0,-2.798263357,1.5985031769,-0.1906301725
C,0,-3.317117116,0.3361666821,-0.5466853148
C,0,-2.8624852669,-0.8008384879,0.0817617901
C,0,-3.3068079677,2.8420646507,-0.8521038305
H,0,-1.5533116659,-1.6211596146,1.5891379605
H,0,-0.6982577476,0.5878573657,2.3232499033
H,0,-1.4789733169,2.6402157078,1.1699074626
H,0,-4.0413927923,0.2744634209,-1.3492436796
H,0,-3.2367479526,-1.77233015,-0.2176784293
H,0,-4.3447250949,3.0146198741,-0.5556321238
H,0,-3.2827787038,2.7305108338,-1.9381742914
H,0,-2.7260589476,3.7191998347,-0.5660376328
N,0,-0.7227522512,1.3877473445,-1.3202750352
O,0,-0.4130523872,0.2990091677,-1.2985397925
O,0,-0.5988316137,2.457359757,-1.6826715848
F,0,-2.3724434449,0.931995471,-3.1737352246
B,0,-1.5607825096,1.4226308112,-4.2383060676
F,0,-1.9485753162,0.8423676245,-5.4343836271
F,0,-1.6919252436,2.8122899356,-4.2786498517
F,0,-0.2290434814,1.0833933185,-3.9229043976

TS NO2BF4 PCM PURE-M06-2X 3.393_822143utf00006

M062X/6-311G*
E(RM062X) = -900.935093295

Zero-point correction= 0.156998 (Hartree/Particle)
Thermal correction to Energy= 0.172023
Thermal correction to Enthalpy= 0.172967
Thermal correction to Gibbs Free Energy= 0.112950
Sum of electronic and ZPE= -900.778096
Sum of electronic and thermal Energies= -900.763070
Sum of electronic and thermal Enthalpies= -900.762126
Sum of electronic and thermal Free Energies= -900.822143

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 107.946 53.120 126.317

C,0,2.8575343716,-1.7485595972,0.7241916858
C,0,3.3218246122,-1.4760057777,-0.5447468765
C,0,3.2791891546,-0.1608185115,-1.0179554817
C,0,2.8388846154,0.904336765,-0.1877248236
C,0,2.3963782401,0.6014844355,1.1129351149
C,0,2.3897215431,-0.7047494886,1.5519409344
C,0,2.924309588,2.318423966,-0.6684298844
H,0,2.8432657198,-2.7668533343,1.0931284991
H,0,3.6585592541,-2.2675310726,-1.2003055877
H,0,3.6186307716,0.0603026368,-2.0237488332
H,0,2.0521632158,1.4017793158,1.7577645676
H,0,2.0253796567,-0.9379581822,2.545300314
H,0,2.8539392305,2.3814190427,-1.755452451
H,0,3.8995668021,2.7279821365,-0.3885490993
H,0,2.1561006551,2.946140537,-0.2167430951
N,0,0.9597482053,0.0425795253,-1.4443803582
O,0,0.4842564297,-0.7823151688,-0.8284193645
O,0,0.8894143082,0.8334285422,-2.2605548549
F,0,0.9136057951,-1.6903983293,-5.1846056559
B,0,0.748706945,-2.0006141771,-3.8398436712

F,0,0.588355936,-3.3693316097,-3.6558914209
F,0,1.8924113816,-1.5601281408,-3.1103304159
F,0,-0.3632544316,-1.3074895128,-3.3151692419

TS NO2BF4 PCM PURE-M06-2X 3.3794_822005

M062X/6-311G*
E(RM062X) = -900.935104619

Zero-point correction= 0.156812 (Hartree/Particle)
Thermal correction to Energy= 0.171848
Thermal correction to Enthalpy= 0.172792
Thermal correction to Gibbs Free Energy= 0.113099
Sum of electronic and ZPE= -900.778293
Sum of electronic and thermal Energies= -900.763257
Sum of electronic and thermal Enthalpies= -900.762312
Sum of electronic and thermal Free Energies= -900.822005

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	107.836	53.122	125.634

C,0,-2.3422577904,-2.1331702237,-0.1259724234
C,0,-1.85809662,-1.3353608632,0.888277449
C,0,-2.1088896475,0.0400310022,0.851378149
C,0,-2.9172063585,0.6126353896,-0.1669693145
C,0,-3.4227312073,-0.2296256623,-1.1733217192
C,0,-3.1235111395,-1.5748063816,-1.1606880185
C,0,-3.2784628107,2.0630660985,-0.1144563867
H,0,-2.121672389,-3.1937510893,-0.1388779352
H,0,-1.2357084737,-1.7420662726,1.6737577399
H,0,-1.7118147907,0.6806951533,1.631075373
H,0,-4.0375609866,0.1908728298,-1.9607298583
H,0,-3.4938133356,-2.2170531483,-1.9509822224
H,0,-4.2045976947,2.1752248897,0.4574726187
H,0,-3.4482216398,2.4740130645,-1.1097301083
H,0,-2.5162362047,2.6519480737,0.3982266704
N,0,-0.5976887707,0.6715984436,-0.8403477347
O,0,-0.3784371872,-0.287918325,-1.4043402596
O,0,-0.3491699985,1.758825415,-0.6080311467
F,0,2.0351003561,0.5521943624,-0.6490158623
B,0,2.0994676049,0.1950184418,0.7154208292
F,0,2.8369120484,-0.9729072702,0.8697855832
F,0,2.6484122608,1.2379014613,1.45332161
F,0,0.7599647747,-0.0322723892,1.1487359673

TS NO2BF4 PCM PURE-M06-2X 3.332_821966

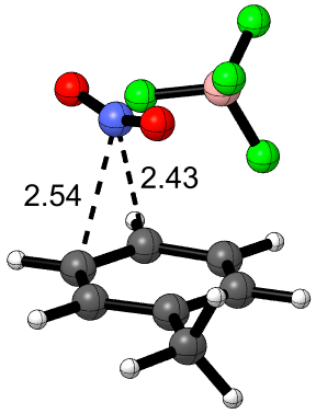
M062X/6-311G*
E(RM062X) = -900.937163256

Zero-point correction= 0.157453 (Hartree/Particle)
Thermal correction to Energy= 0.171946
Thermal correction to Enthalpy= 0.172890
Thermal correction to Gibbs Free Energy= 0.115197
Sum of electronic and ZPE= -900.779710
Sum of electronic and thermal Energies= -900.765217
Sum of electronic and thermal Enthalpies= -900.764273
Sum of electronic and thermal Free Energies= -900.821966

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	107.898	52.379	121.425

C,0,-1.4950406867,-0.727259127,1.1248757157
C,0,-0.9671302018,0.572752383,1.2172511866
C,0,-1.6081955331,1.6039176077,0.5822989224
C,0,-2.7853721567,1.3541190998,-0.2040636468
C,0,-3.3504873719,0.0359741035,-0.1846857477
C,0,-2.6928247006,-0.9892434794,0.4511634979
C,0,-3.5941568161,2.5060104787,-0.7089073374
H,0,-0.968658486,-1.5442018371,1.6058266547
H,0,-0.0603532241,0.7493855787,1.781031956
H,0,-1.2256091862,2.6174646978,0.6324533296
H,0,-4.2839448157,-0.1387012772,-0.7038065206
H,0,-3.0955572352,-1.9934791686,0.425148213
H,0,-3.4530840773,3.3778242165,-0.0698479093
H,0,-4.6489843513,2.2442033471,-0.7550642797
H,0,-3.2953609895,2.7796189468,-1.7250269671
N,0,-1.5366741338,0.7915860311,-1.8403917451
O,0,-1.7922201354,1.5338145416,-2.6901490183
O,0,-0.8198723911,-0.0861743042,-1.614779772
F,0,-2.928099566,-1.0263220374,-2.9557254888
B,0,-4.2775585221,-0.6714927457,-3.1809131284
F,0,-4.6196233506,-0.8937230798,-4.5071914482
F,0,-5.092056258,-1.427411151,-2.3230674715
F,0,-4.4249788109,0.6955911751,-2.8580999948

TS NO2BF4 PCM PURE-M06-2X 2.434_821714



M062X/6-311G*
E(RM062X) = -900.935240397

Zero-point correction= 0.156994 (Hartree/Particle)
Thermal correction to Energy= 0.172169
Thermal correction to Enthalpy= 0.173113
Thermal correction to Gibbs Free Energy= 0.113527
Sum of electronic and ZPE= -900.778246
Sum of electronic and thermal Energies= -900.763071
Sum of electronic and thermal Enthalpies= -900.762127
Sum of electronic and thermal Free Energies= -900.821714

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 108.038 53.282 125.411

C,0,-1.8408225491,-0.9887977627,-1.3499579918
C,0,-3.0567204418,-0.6751782168,-0.7096182153
C,0,-3.2081443809,0.5356870502,-0.0378295163
C,0,-2.152792657,1.4399326882,0.0191445533
C,0,-0.9493675976,1.1275601981,-0.6534280104
C,0,-0.7970677526,-0.0540800742,-1.3470986958
C,0,-2.2648920073,2.7285068827,0.7795339174
H,0,-1.7236515385,-1.9277804049,-1.8781925737
H,0,-3.8771246502,-1.3840148148,-0.7444895564
H,0,-4.1449464914,0.7647631418,0.4574654164
H,0,-0.1321712115,1.8408556728,-0.6161112637
H,0,0.1291968336,-0.2986238572,-1.8492746053
H,0,-1.9719893802,3.5731511913,0.1523016122
H,0,-1.5930478527,2.7189293163,1.6420596407
H,0,-3.2799337084,2.8961788443,1.1378896804
N,0,-1.5033646493,-1.9118188212,0.8773709664
O,0,-1.0194529417,-1.0559878985,1.4292821061
O,0,-1.883371738,-2.966370601,0.7470355636
F,0,0.5913352275,-2.4809993953,-0.1505599389
B,0,0.5916921653,-3.2745218553,-1.3350244455
F,0,-0.6602844372,-3.9088289109,-1.4266415561
F,0,0.7621312013,-2.429029113,-2.4370186522
F,0,1.6111775577,-4.2113582596,-1.2634144351

TS NO2BF4 PCM PURE-M06-2X 2.429_821508

M062X/6-311G*
E(RM062X) = -900.935305625

Zero-point correction= 0.157249 (Hartree/Particle)
Thermal correction to Energy= 0.172359
Thermal correction to Enthalpy= 0.173303
Thermal correction to Gibbs Free Energy= 0.113798
Sum of electronic and ZPE= -900.778057
Sum of electronic and thermal Energies= -900.762947
Sum of electronic and thermal Enthalpies= -900.762003
Sum of electronic and thermal Free Energies= -900.821508

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 108.157 53.083 125.238

C,0,-0.8873318714,0.2541988098,1.4844612488
C,0,-2.1530203705,0.8564791654,1.365946353
C,0,-3.1303394847,0.2617036118,0.5836453864
C,0,-2.8743127181,-0.9468594736,-0.0738040271
C,0,-1.6246308826,-1.56893604,0.1013743991
C,0,-0.6428739491,-0.9901715261,0.880035979
C,0,-3.9066624156,-1.583250754,-0.9572950203
H,0,-0.1136717436,0.7110006717,2.088710938
H,0,-2.3522665534,1.7935483055,1.8736984626
H,0,-4.0983339284,0.7369757723,0.4708170955
H,0,-1.4318380602,-2.5135298397,-0.3964210153
H,0,0.3232189603,-1.4640983507,0.9976789371
H,0,-3.5704577513,-1.5747936865,-1.9976570743
H,0,-4.8616969003,-1.0620820213,-0.9014544158
H,0,-4.0610634357,-2.6276443174,-0.6778283815
N,0,-0.3203710188,1.4620740833,-0.5448390208
O,0,-0.9246565988,0.9620998225,-1.3506008588
O,0,0.3826384836,2.2150595526,-0.0887592391
F,0,2.0522095282,0.433221183,1.0967544864
B,0,2.4528895355,-0.2825675004,-0.0484706186
F,0,3.7052147943,0.1402358728,-0.4687324671
F,0,2.4509760441,-1.6513067589,0.2279047263
F,0,1.4938413368,-0.0199225823,-1.0700888734

TS NO2BF4 PCM PURE-M06-2X 2.4410_821447

M062X/6-311G*
E(RM062X) = -900.935135332

Zero-point correction= 0.157115 (Hartree/Particle)
Thermal correction to Energy= 0.172245
Thermal correction to Enthalpy= 0.173190
Thermal correction to Gibbs Free Energy= 0.113688
Sum of electronic and ZPE= -900.778020
Sum of electronic and thermal Energies= -900.762890
Sum of electronic and thermal Enthalpies= -900.761946
Sum of electronic and thermal Free Energies= -900.821447

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 108.086 53.174 125.231

C,0,-1.7762903842,-0.9983838729,-1.3188325103
C,0,-2.9843544479,-0.7333762897,-0.6604744483
C,0,-3.137258466,0.4627602415,0.00895485
C,0,-2.1189005656,1.4445969125,0.0050206814
C,0,-0.9459894557,1.1970632204,-0.6972636303
C,0,-0.7629131335,-0.018775074,-1.3500185638
C,0,-2.3172715464,2.7185586937,0.772199702
H,0,-1.6364277729,-1.933209418,-1.8500746449
H,0,-3.7753191734,-1.4733293986,-0.6563174208
H,0,-4.0560593785,0.6657181391,0.5498785937
H,0,-0.1437396469,1.9242913123,-0.7096618127
H,0,0.1664966491,-0.217905124,-1.8695800682
H,0,-1.5726544537,3.4665100615,0.5028267823
H,0,-2.2334941323,2.5273185467,1.8458123514
H,0,-3.3122201995,3.1307904893,0.5932077418
N,0,-0.4128900122,-1.5244689998,0.6363324694
O,0,-0.8711369301,-0.8967509837,1.4531185155
O,0,0.2201466732,-2.3605623113,0.2165849809
F,0,1.5051509282,-0.0378859489,0.7193339903
B,0,2.3889852687,0.0387357624,-0.3945759835
F,0,2.1804452874,-1.1068443857,-1.1835599416
F,0,2.0699890293,1.1798857906,-1.1415751985
F,0,3.6998758631,0.0929296367,0.0548295641

TS NO2BF4 PCM PURE-M06-2X 2.419_821322utf00003

M062X/6-311G*
E(RM062X) = -900.935062628

Zero-point correction= 0.157106 (Hartree/Particle)
Thermal correction to Energy= 0.172184

Thermal correction to Enthalpy= 0.173129
Thermal correction to Gibbs Free Energy= 0.113741
Sum of electronic and ZPE= -900.777956
Sum of electronic and thermal Energies= -900.762878
Sum of electronic and thermal Enthalpies= -900.761934
Sum of electronic and thermal Free Energies= -900.821322

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.047	53.192	124.992

C,0,-3.2703514393,-1.043692062,-0.6890301725
C,0,-3.7744870497,-0.0953723686,0.2170112521
C,0,-3.0294739291,1.0329354822,0.50438874
C,0,-1.7961856488,1.2597091742,-0.1315669504
C,0,-1.3485554388,0.3549041005,-1.1025628414
C,0,-2.0698285975,-0.7886997483,-1.3831414592
C,0,-0.9377160985,2.4342214352,0.2282116027
H,0,-3.8462216353,-1.9335468756,-0.9163860085
H,0,-4.7238368527,-0.2694888268,0.7092163049
H,0,-3.388365271,1.7469785659,1.2374283651
H,0,-0.3987128096,0.520685945,-1.5932793261
H,0,-1.6880959314,-1.5070122317,-2.097857078
H,0,0.0174675708,2.0762430912,0.6217991818
H,0,-1.4086401218,3.0725831335,0.9746209194
H,0,-0.7151774509,3.0339754055,-0.6572048653
N,0,-1.8565960702,-2.0343158678,1.0052375321
O,0,-1.3001461621,-1.1743510303,1.4676271687
O,0,-2.1991260017,-3.1067197303,0.8968146061
F,0,0.9638204634,-1.3430042337,-1.9571330906
B,0,1.1313498872,-1.7400263707,-0.6249948872
F,0,2.3499781708,-2.3856165868,-0.4558202221
F,0,1.0450175464,-0.6252891133,0.2242659698
F,0,0.0752068698,-2.6359922872,-0.2854377414

TS NO2BF4 PCM PURE-M06-2X 2.4198_821288

M062X/6-311G*
E(RM062X) = -900.935162090

Zero-point correction= 0.157359 (Hartree/Particle)
Thermal correction to Energy= 0.172449
Thermal correction to Enthalpy= 0.173393
Thermal correction to Gibbs Free Energy= 0.113874
Sum of electronic and ZPE= -900.777803
Sum of electronic and thermal Energies= -900.762713
Sum of electronic and thermal Enthalpies= -900.761769
Sum of electronic and thermal Free Energies= -900.821288

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.213	53.101	125.269

C,0,1.958519396,-1.1145535613,1.2372194673
C,0,2.9921891799,-0.6647537294,0.4016029895
C,0,2.8946141314,0.5825503364,-0.1856624473
C,0,1.7987172951,1.4230672573,0.0833960692
C,0,0.824386326,1.0058223841,0.9963938127
C,0,0.8898892691,-0.2524525927,1.5639623904
C,0,1.6395379029,2.7402345363,-0.6124038477
H,0,2.0201555375,-2.0946302162,1.6966360233
H,0,3.8386604885,-1.30801219,0.1929755168
H,0,3.6638694311,0.9194970828,-0.8721185679
H,0,-0.0235497833,1.6442606884,1.2068744202
H,0,0.1054252939,-0.5896311565,2.2312269769
H,0,1.4928520284,3.544545296,0.1117369549
H,0,0.7446248618,2.7055204344,-1.2394704405
H,0,2.4998131209,2.9803944518,-1.236033176
N,0,0.5253886261,-1.7255958592,-0.6143746453
O,0,0.6004230604,-0.8647132023,-1.3328494699
O,0,0.229541878,-2.7601741867,-0.2657868239
F,0,-2.1823492115,0.9269081215,1.1523506517
B,0,-2.1730384262,0.3227602284,-0.1097543069
F,0,-1.3141148409,1.0231871414,-0.9738314387
F,0,-1.6725968696,-1.0047150415,0.0293992539
F,0,-3.4563056955,0.2743207769,-0.6401113627

TS NO2BF4 PCM PURE-M06-2X 2.435_821006

M062X/6-311G*
E(RM062X) = -900.935138423

Zero-point correction= 0.157267 (Hartree/Particle)
Thermal correction to Energy= 0.172246
Thermal correction to Enthalpy= 0.173191
Thermal correction to Gibbs Free Energy= 0.114132
Sum of electronic and ZPE= -900.777872
Sum of electronic and thermal Energies= -900.762892
Sum of electronic and thermal Enthalpies= -900.761948
Sum of electronic and thermal Free Energies= -900.821006

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.086	53.055	124.299

C,0,-2.7315304569,-1.0596366729,-0.8525009019
C,0,-3.458684925,-0.3572834215,0.1162700198
C,0,-3.016662594,0.8866925373,0.5197973687
C,0,-1.8754072091,1.4854905471,-0.0605531748
C,0,-1.212115834,0.8204648143,-1.0868576522
C,0,-1.6196849842,-0.449126754,-1.4725050947
C,0,-1.3645565641,2.7934783096,0.4598825832
H,0,-3.0542441951,-2.0437336525,-1.1735439675
H,0,-4.3359196318,-0.8047193023,0.5672673939
H,0,-3.5457698826,1.4182167488,1.3041652072
H,0,-0.332214603,1.2624223012,-1.5373011525
H,0,-1.0714897918,-0.9844238398,-2.2391170118
H,0,-0.7973120468,2.6153313112,1.37731235
H,0,-2.1824266924,3.4780109491,0.690906031
H,0,-0.6881246206,3.2641241999,-0.2528650322
N,0,-0.8679100538,-1.7183252024,0.5697389992
O,0,-0.804362628,-0.8864405169,1.3251418752
O,0,-0.6467529113,-2.7508054224,0.1582715094
F,0,1.9225738371,1.04422706,-1.2954986763
B,0,1.8389976723,0.2686769285,-0.1355620336
F,0,3.1053135788,-0.005367248,0.3672307874
F,0,1.0648088569,0.9356669404,0.8290947868
F,0,1.1880076794,-0.9607566147,-0.4516142143

TS NO2BF4 PCM PURE-M06-2X 2.424_820983

M062X/6-311G*
E(RM062X) = -900.933886364

Zero-point correction= 0.157049 (Hartree/Particle)
Thermal correction to Energy= 0.172252
Thermal correction to Enthalpy= 0.173196
Thermal correction to Gibbs Free Energy= 0.112903
Sum of electronic and ZPE= -900.776837
Sum of electronic and thermal Energies= -900.761635
Sum of electronic and thermal Enthalpies= -900.760690
Sum of electronic and thermal Free Energies= -900.820983

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.090	53.155	126.897

C,0,-0.9802296939,0.283338448,1.464761148
C,0,-2.2960323043,0.7185035574,1.2200391317
C,0,-3.1550753693,-0.0696781611,0.4715792865
C,0,-2.7306701865,-1.3074341556,-0.0255699919
C,0,-1.4341839381,-1.7604565433,0.2807218202
C,0,-0.5691757213,-0.9866099429,1.0270880331
C,0,-3.6313016069,-2.144954244,-0.8845116379
H,0,-0.295921351,0.8902559124,2.0442825747
H,0,-2.625182796,1.67795811,1.603002526
H,0,-4.1613537639,0.2740173228,0.2592304292
H,0,-1.1129605238,-2.728525157,-0.0892021388
H,0,0.4352336558,-1.3226643962,1.2465676715
H,0,-3.2920906247,-2.1134875857,-1.9239516183
H,0,-4.6610620194,-1.7904802912,-0.8534619006
H,0,-3.6086380745,-3.1896906027,-0.5694427316
N,0,-0.4260726418,1.3001655673,-0.6651370444
O,0,0.1723767563,2.1715534037,-0.2737807017
O,0,-0.9300651005,0.6505688427,-1.4324375966
F,0,1.9678413544,0.6538921797,1.2726276169
B,0,2.551506657,0.4819647048,0.0020953954
F,0,3.617367127,-0.4007625802,0.0713442553
F,0,1.5455853972,-0.0498487123,-0.8600311503
F,0,2.944163768,1.7222123232,-0.5005053766

TS NO2BF4 PCM PURE-M06-2X 2.398_820850

M062X/6-311G*
E(RM062X) = -900.934626828

Zero-point correction= 0.157042 (Hartree/Particle)
Thermal correction to Energy= 0.172053
Thermal correction to Enthalpy= 0.172997
Thermal correction to Gibbs Free Energy= 0.113776
Sum of electronic and ZPE= -900.777585
Sum of electronic and thermal Energies= -900.762574
Sum of electronic and thermal Enthalpies= -900.761630
Sum of electronic and thermal Free Energies= -900.820850

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	107.965	53.086	124.640

C,0,2.7322567431,-0.995166805,0.5470515269
C,0,3.3246728059,-0.2463328388,-0.4748262467
C,0,2.8728232647,1.035411264,-0.7151261625
C,0,1.8673502689,1.6307872137,0.0852865023
C,0,1.3544681647,0.9175576488,1.1600228443
C,0,1.7565040416,-0.3950853933,1.3790516704
C,0,1.3229771237,2.9820487878,-0.2611283514
H,0,3.0515651958,-2.0124467692,0.7425850269
H,0,4.0959848289,-0.6853217957,-1.095102714
H,0,3.286309782,1.6048277954,-1.5410656738
H,0,0.5787595617,1.3495294955,1.7785759491
H,0,1.3108680826,-0.9699337048,2.1818459873
H,0,1.0285693412,3.5288502907,0.63508463
H,0,0.4237138336,2.851373768,-0.8701578345
H,0,2.0407817988,3.577152935,-0.8256419285
N,0,0.6166164435,-1.442813505,-0.4906263261
O,0,0.3321046087,-2.4669794956,-0.0858249485
O,0,0.5029250915,-0.5982940286,-1.2339380916
F,0,-3.214225774,0.2506481526,0.8071195832
B,0,-1.9607343543,-0.0179918501,0.2809089625
F,0,-1.3445086496,1.1599111643,-0.1739740845
F,0,-1.1262567317,-0.6043831853,1.2665123673
F,0,-2.0486554713,-0.9366111444,-0.7839706881

TS NO2BF4 PCM PURE-M06-2X 2.3272_820767

M062X/6-311G*
E(RM062X) = -900.933402046

Zero-point correction= 0.156838 (Hartree/Particle)
Thermal correction to Energy= 0.171943
Thermal correction to Enthalpy= 0.172887
Thermal correction to Gibbs Free Energy= 0.112635
Sum of electronic and ZPE= -900.776564
Sum of electronic and thermal Energies= -900.761459
Sum of electronic and thermal Enthalpies= -900.760515
Sum of electronic and thermal Free Energies= -900.820767

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	107.896	53.099	126.810

C,0,-1.9044643822,-0.8008658046,1.0364187237
C,0,-1.5095961465,0.446443589,1.5483565094
C,0,-1.9486116838,1.5951673177,0.9325818988
C,0,-2.8345559557,1.5465989707,-0.1698518198
C,0,-3.2872890492,0.3093951323,-0.6229231652
C,0,-2.8323890824,-0.8600775711,-0.0278694826
C,0,-3.2627299954,2.8223426716,-0.8285344634
H,0,-1.565829174,-1.7119757115,1.514449605
H,0,-0.8153748302,0.4883867059,2.3763922977
H,0,-1.6138416625,2.5631904553,1.2899902025
H,0,-3.9841504324,0.2590173476,-1.451340238
H,0,-3.171528379,-1.8253559204,-0.3870753218
H,0,-3.6056852313,3.5433347803,-0.0837237499
H,0,-4.0600982118,2.6543486735,-1.551059017
H,0,-2.4154810325,3.2766632441,-1.3498611488
N,0,-0.4154645765,-0.944789574,-0.7462610577
O,0,-0.2358303599,0.12033448,-1.082011807

O,0,-0.217078547,-2.0607628911,-0.7994152047
F,0,1.0593032055,-0.8269012494,1.2541220009
B,0,2.3660435935,-0.8703170527,0.6842469008
F,0,3.0701450835,0.2665390369,1.0609567935
F,0,3.0117757851,-2.026399935,1.1046100726
F,0,2.1963250647,-0.8939136949,-0.718086529

TS NO2BF4 PCM PURE-M06-2X 2.387_820745

M062X/6-311G*
E(RM062X) = -900.934045808

Zero-point correction= 0.156934 (Hartree/Particle)
Thermal correction to Energy= 0.172037
Thermal correction to Enthalpy= 0.172981
Thermal correction to Gibbs Free Energy= 0.113301
Sum of electronic and ZPE= -900.777112
Sum of electronic and thermal Energies= -900.762009
Sum of electronic and thermal Enthalpies= -900.761065
Sum of electronic and thermal Free Energies= -900.820745

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	107.955	53.135	125.608

C,0,2.7854997738,-1.6997822256,-0.1352851467
C,0,3.6327324203,-0.934404998,-0.9638122363
C,0,3.6264970078,0.4510642606,-0.874427149
C,0,2.782682526,1.0928751939,0.03236097
C,0,1.9737418757,0.313316817,0.8871402397
C,0,1.9906327817,-1.0626815197,0.8288734372
C,0,2.709256927,2.589082452,0.0991166239
H,0,2.7969792092,-2.7814849561,-0.1949708573
H,0,4.2773876252,-1.4340333957,-1.6786039409
H,0,4.2673684387,1.0374756317,-1.5229974933
H,0,1.3214540623,0.8151220052,1.5938619767
H,0,1.3473358477,-1.6514945915,1.4675756804
H,0,1.7790567223,2.9373177459,-0.3593305154
H,0,3.5416002592,3.0560965023,-0.4261817123
H,0,2.7066791615,2.9324656129,1.1351594216
N,0,1.2873072433,-1.3849390543,-1.9663601126
O,0,0.8176882163,-0.3808985556,-1.7633134591
O,0,1.4275730824,-2.3546684929,-2.5309779864
F,0,-2.1934216837,-3.0920386893,-0.0767720342
B,0,-1.139992836,-2.30024487,-0.5000674106
F,0,-1.1179519131,-1.0756682849,0.1757401179
F,0,0.0970796497,-2.9582562277,-0.2731062855
F,0,-1.2205923974,-2.0550223601,-1.8899281277

TS NO2BF4 PCM PURE-M06-2X 3.444_820739

M062X/6-311G*
E(RM062X) = -900.936956537

Zero-point correction= 0.158150 (Hartree/Particle)
Thermal correction to Energy= 0.172803
Thermal correction to Enthalpy= 0.173747
Thermal correction to Gibbs Free Energy= 0.116217
Sum of electronic and ZPE= -900.778806
Sum of electronic and thermal Energies= -900.764154
Sum of electronic and thermal Enthalpies= -900.763209
Sum of electronic and thermal Free Energies= -900.820739

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.435	52.859	121.082

C,0,1.9905369329,-1.1432194098,-1.5561769366
C,0,0.9666255978,-0.2206057925,-1.7792644059
C,0,0.9014608713,0.9318159186,-1.0134760743
C,0,1.8661502208,1.1795673944,-0.0105218727
C,0,2.9186631808,0.2590325096,0.1637478471
C,0,2.9696732974,-0.8988914623,-0.5896044317
C,0,1.8387923501,2.4462947042,0.790749962
H,0,2.0244269843,-2.0581069529,-2.1364420785
H,0,0.2153056877,-0.4143029946,-2.5353083541
H,0,0.1046251245,1.6516859031,-1.1710230325
H,0,3.6642358518,0.4382176767,0.9279691695
H,0,3.7520090635,-1.6225102611,-0.4024158884
H,0,2.2065105446,2.2778323409,1.8050371716
H,0,0.837205576,2.8758378134,0.8391058308
H,0,2.4947051944,3.1871576015,0.3251168359
N,0,0.456004816,-0.253505081,1.3960066797
O,0,0.4671085875,-1.2816219202,0.9436720245
O,0,0.1554955208,0.5588842435,2.1228819069
F,0,2.3099682351,-0.7311536745,2.8439888811
B,0,3.144568775,-1.8789674451,2.6668406142
F,0,2.5118003532,-2.7357572048,1.7566440802
F,0,4.3763107823,-1.4608964641,2.1501766838
F,0,3.3144774523,-2.506459443,3.8944983875

TS NO2BF4 PCM PURE-M06-2X 3.1392_820578

M062X/6-311G*
E(RM062X) = -900.934524532

Zero-point correction= 0.157181 (Hartree/Particle)
Thermal correction to Energy= 0.172131
Thermal correction to Enthalpy= 0.173075
Thermal correction to Gibbs Free Energy= 0.113946
Sum of electronic and ZPE= -900.777344
Sum of electronic and thermal Energies= -900.762393
Sum of electronic and thermal Enthalpies= -900.761449
Sum of electronic and thermal Free Energies= -900.820578

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.014	53.050	124.447

C,0,-3.3366780558,-0.5973561632,0.3432648468
C,0,-2.3068260426,-0.6046035527,1.2700590993
C,0,-1.2300609676,0.3054771788,1.1407197579
C,0,-1.2261902987,1.2932092012,0.1364216559
C,0,-2.2508839072,1.2547562218,-0.7999001496
C,0,-3.2855783638,0.3173939401,-0.7064204223
C,0,-0.1593576434,2.3462318706,0.0798818428
H,0,-4.1562933978,-1.3000911755,0.4228229214
H,0,-2.3055203064,-1.3133155634,2.0912539312

H,0,-0.4280340972,0.2978430153,1.8701514213
H,0,-2.2550298037,1.9708706678,-1.6150482286
H,0,-4.0665752461,0.3155215732,-1.458319046
H,0,0.6261815927,2.1550996524,0.8070711108
H,0,-0.6005003142,3.3250137148,0.2854147476
H,0,0.2982384829,2.381637487,-0.9091515159
N,0,-0.3646482818,-1.4829901688,-0.143768429
O,0,-0.8367787793,-1.3888505208,-1.1644368329
O,0,0.3167583471,-1.9624439405,0.6215347725
F,0,1.8580171704,0.1860735087,1.3541306564
B,0,2.4211552283,0.242083143,0.0623050622
F,0,2.9482045276,1.505918924,-0.1752703885
F,0,3.3916345371,-0.7448228896,-0.0727987487
F,0,1.3710746195,-0.013565124,-0.8701420646

TS NO2BF4 PCM PURE-M06-2X 3.1409_820572

M062X/6-311G*
E(RM062X) = -900.934547624

Zero-point correction= 0.157206 (Hartree/Particle)
Thermal correction to Energy= 0.172155
Thermal correction to Enthalpy= 0.173099
Thermal correction to Gibbs Free Energy= 0.113975
Sum of electronic and ZPE= -900.777342
Sum of electronic and thermal Energies= -900.762393
Sum of electronic and thermal Enthalpies= -900.761449
Sum of electronic and thermal Free Energies= -900.820572

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.029	53.041	124.436

C,0,-3.370588333,-0.6556373104,0.3493715391
C,0,-2.3402104542,-0.6523679232,1.2752980435
C,0,-1.2760115029,0.2729408624,1.1485858232
C,0,-1.2866058276,1.2645103442,0.1481667046
C,0,-2.3124206824,1.216496074,-0.7867533527
C,0,-3.3335535757,0.2644422927,-0.6965083825
C,0,-0.2296417337,2.3271932311,0.0871854573
H,0,-4.1805512367,-1.3697218423,0.4268518764
H,0,-2.329187756,-1.36375597,2.0940346471
H,0,-0.4734330371,0.2738391386,1.8773937984
H,0,-2.3274756862,1.9365768895,-1.5982894792
H,0,-4.1155406103,0.255003632,-1.4473089787
H,0,-0.6895737302,3.3110891632,0.2076256444
H,0,0.2823150152,2.3059220993,-0.8752450568
H,0,0.519713663,2.187719083,0.863039899
N,0,-0.3846453778,-1.4952874088,-0.1447001198
O,0,-0.8619257188,-1.4067051973,-1.1634881764
O,0,0.3071445431,-1.9651282199,0.6171940542
F,0,2.8396580493,1.5808750045,-0.1888375845
B,0,2.3717775299,0.2932108455,0.046393209
F,0,1.332858502,-0.0075522139,-0.8853975514
F,0,3.3875012839,-0.6462969628,-0.0937590685
F,0,1.8135076762,0.2071433886,1.3383310543

TS NO2BF4 PCM PURE-M06-2X 3.055_820543

M062X/6-311G*
E(RM062X) = -900.933591759

Zero-point correction= 0.156954 (Hartree/Particle)
Thermal correction to Energy= 0.172137
Thermal correction to Enthalpy= 0.173081
Thermal correction to Gibbs Free Energy= 0.113049
Sum of electronic and ZPE= -900.776638
Sum of electronic and thermal Energies= -900.761454
Sum of electronic and thermal Enthalpies= -900.760510
Sum of electronic and thermal Free Energies= -900.820543

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.018	53.205	126.350

C,0,-1.8128709796,-0.9661759901,-1.4369061229
C,0,-2.9716093019,-0.7342582824,-0.6976106016
C,0,-3.1084477198,0.458750475,0.0446547894
C,0,-2.1104917238,1.4515209066,0.030192558
C,0,-0.9552590167,1.179838566,-0.6830300585
C,0,-0.8065939897,-0.0174242535,-1.408402822
C,0,-2.3057108206,2.7329623886,0.7911291474
H,0,-1.7052446189,-1.8958700626,-1.978191037
H,0,-3.7642857501,-1.4729947482,-0.6790223216
H,0,-4.0272813908,0.6355776095,0.5961083721
H,0,-0.1471702636,1.9036054963,-0.6897686764
H,0,0.1151405358,-0.191274677,-1.9516274984
H,0,-1.4270414423,3.3729112689,0.7194682186
H,0,-2.5012696874,2.5353262109,1.8476709067
H,0,-3.1634564936,3.2839001123,0.3992857729
N,0,-2.1362866097,-1.0869245663,1.5986018721
O,0,-1.0219982302,-0.9494581471,1.4749079369
O,0,-3.0603406697,-1.4357017304,2.1513541041
F,0,-1.8626753327,-3.2792955561,0.5699564192
B,0,-2.9893657646,-3.9527694726,0.0199673959
F,0,-4.1459835957,-3.3712411126,0.5685977912
F,0,-2.9905017965,-3.7623176152,-1.368296156
F,0,-2.924428338,-5.3025178201,0.3331470099

TS NO2BF4 PCM PURE-M06-2X 2.4184_820386

M062X/6-311G*
E(RM062X) = -900.935155388

Zero-point correction= 0.157396 (Hartree/Particle)
Thermal correction to Energy= 0.172289
Thermal correction to Enthalpy= 0.173233
Thermal correction to Gibbs Free Energy= 0.114769
Sum of electronic and ZPE= -900.777760
Sum of electronic and thermal Energies= -900.762867
Sum of electronic and thermal Enthalpies= -900.761923
Sum of electronic and thermal Free Energies= -900.820386

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.113	53.039	123.047

C,0,2.1902840767,-1.1657337018,-1.2140467939
C,0,1.1209839805,-0.3506208562,-1.6496642157
C,0,0.9459745463,0.9141892759,-1.1130782896
C,0,1.8122109411,1.3837463369,-0.1252783809
C,0,2.9045728667,0.5824030149,0.2667067824
C,0,3.1122019831,-0.6668460286,-0.2858831803
C,0,1.5549816224,2.7098952933,0.5224937977
H,0,2.3324585923,-2.1471724139,-1.652224348
H,0,0.4211432193,-0.7305452373,-2.3847773091
H,0,0.0956563138,1.5141709978,-1.4139484635
H,0,3.5865427599,0.9573307642,1.022310663
H,0,3.956436043,-1.2721154724,0.0208077812
H,0,2.3449459763,2.9813320583,1.2220066779
H,0,0.6027639631,2.6626838771,1.0563978101
H,0,1.4672003704,3.4961121554,-0.2305165776
N,0,0.467960043,-1.7431239342,0.3824408597
O,0,0.5668432277,-0.9643060168,1.1886657608
O,0,0.09477977,-2.7134260593,-0.0683134486
F,0,-1.5914240465,-0.7153143228,-0.3620240376
B,0,-2.0713566007,0.5468568941,0.0959992142
F,0,-1.1431786339,1.0533775506,1.0235788935
F,0,-2.1713396261,1.4134522872,-0.9954392994
F,0,-3.3089423884,0.3696455377,0.7024301037

TS NO2BF4 PCM PURE-M06-2X 2.306_820365

M062X/6-311G*
E(RM062X) = -900.933212549

Zero-point correction= 0.157184 (Hartree/Particle)
Thermal correction to Energy= 0.172295
Thermal correction to Enthalpy= 0.173239
Thermal correction to Gibbs Free Energy= 0.112847
Sum of electronic and ZPE= -900.776028
Sum of electronic and thermal Energies= -900.760918
Sum of electronic and thermal Enthalpies= -900.759973
Sum of electronic and thermal Free Energies= -900.820365

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.117	52.951	127.105

C,0,2.4348138537,-1.3145868312,0.7680728002
C,0,3.344440292,-0.9116576603,-0.2304283759
C,0,3.4188546733,0.4173099464,-0.5709974871
C,0,2.64099661,1.3898634668,0.1041151612
C,0,1.8117776578,0.9942661486,1.1524028843
C,0,1.7080301412,-0.3443001032,1.4939266243
C,0,2.715543961,2.8214194195,-0.3290181604
H,0,2.3731253861,-2.3573071761,1.0566676806
H,0,3.9442603428,-1.6516443078,-0.7456912397
H,0,4.0818317143,0.7381899315,-1.3673700807
H,0,1.2164904472,1.7302964689,1.6787983537
H,0,1.0346067867,-0.6570480575,2.2819587168
H,0,2.2223613955,3.4827971397,0.3816318032
H,0,2.2283256918,2.9397473803,-1.3012899489
H,0,3.7543120223,3.1363122785,-0.4483228357
N,0,0.5403344931,-1.2950610276,-0.5465764378
O,0,0.6098104285,-0.3890126427,-1.2223829897
O,0,0.0489529136,-2.2736739147,-0.2401924816
F,0,-1.0658270744,-0.0364504315,0.9175156755
B,0,-2.281551791,-0.0589040797,0.1738787442
F,0,-2.6503196421,1.2440583607,-0.1422014467
F,0,-2.028268266,-0.7883245756,-1.0079394655
F,0,-3.2669360375,-0.692598733,0.9225165055

TS NO2BF4 PCM PURE-M06-2X 2.2457_820277

M062X/6-311G*
E(RM062X) = -900.934436028

Zero-point correction= 0.157405 (Hartree/Particle)
Thermal correction to Energy= 0.172196
Thermal correction to Enthalpy= 0.173141
Thermal correction to Gibbs Free Energy= 0.114159
Sum of electronic and ZPE= -900.777031
Sum of electronic and thermal Energies= -900.762240
Sum of electronic and thermal Enthalpies= -900.761295
Sum of electronic and thermal Free Energies= -900.820277

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.055	52.527	124.137

C,0,2.1492601033,-0.995536205,1.1494984088
C,0,3.2064409239,-0.411843097,0.4446004345
C,0,2.9935350129,0.7935807323,-0.184211926
C,0,1.7577416558,1.4999035549,-0.0802715647
C,0,0.7389442499,0.9592765523,0.6746676526
C,0,0.9029314715,-0.3069746095,1.2525832274
C,0,1.6031564407,2.8056192441,-0.7959165693
H,0,2.2703147103,-1.9511706324,1.646327824
H,0,4.1582519819,-0.9206156061,0.3662909268
H,0,3.7885526082,1.2360443687,-0.7762579577
H,0,-0.2133938634,1.4652438982,0.77253443
H,0,0.0884773841,-0.735919998,1.8226234546
H,0,0.6087818191,3.2235885092,-0.6484719507
H,0,1.7695882194,2.6700880278,-1.8673194202
H,0,2.3464494045,3.5241040257,-0.4413491174
N,0,0.7232194993,-1.6578364031,-0.4538690311
O,0,0.9951841648,-1.1104999954,-1.4272010844
O,0,0.1965787766,-2.6024581844,-0.0490196378
F,0,-3.7024847419,-0.3303972301,0.0536387594
B,0,-2.4110433849,0.1348622126,0.2638671733
F,0,-2.0083713333,-0.1256626805,1.5900021393
F,0,-1.5136543045,-0.5279093582,-0.6085925905
F,0,-2.3347727981,1.5156048739,0.0275614194

TS NO2BF4 PCM PURE-M06-2X 2.386_820166

M062X/6-311G*
E(RM062X) = -900.934054552

Zero-point correction= 0.157094 (Hartree/Particle)
Thermal correction to Energy= 0.172074
Thermal correction to Enthalpy= 0.173018
Thermal correction to Gibbs Free Energy= 0.113888

Sum of electronic and ZPE= -900.776961
Sum of electronic and thermal Energies= -900.761980
Sum of electronic and thermal Enthalpies= -900.761036
Sum of electronic and thermal Free Energies= -900.820166

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	107.978	53.080	124.449

C,0,2.662863955,-0.9538173389,0.5475773011
C,0,3.3029282193,-0.2085289197,-0.4644461782
C,0,2.9226250564,1.1050014067,-0.7080942142
C,0,1.9069793458,1.6929160432,0.0449535254
C,0,1.3044535926,0.9495578447,1.0837074962
C,0,1.6907066111,-0.3440657983,1.3544920805
C,0,1.4421679335,3.0920416289,-0.228583706
H,0,2.9655347348,-1.9748305725,0.7466419942
H,0,4.0831575053,-0.6713924534,-1.058721438
H,0,3.4059277924,1.6695326624,-1.4973040885
H,0,0.5156744311,1.4106338442,1.6687405269
H,0,1.2046108719,-0.9153445275,2.1328600637
H,0,1.4826084035,3.6928756309,0.6827024038
H,0,0.4016546884,3.0865211929,-0.5638367845
H,0,2.0473338095,3.5765611835,-0.9936278578
N,0,1.2116731408,-1.498052747,-1.2667639288
O,0,1.6323443187,-2.4963794572,-1.591615061
O,0,0.4771571154,-0.6436750417,-1.292070642
F,0,-1.7388376982,-3.6044856516,1.0699230283
B,0,-0.9276647509,-2.6751683606,0.44201542
F,0,-1.2685948854,-1.3690775348,0.808926283
F,0,0.4328088645,-2.8943887564,0.7826354555
F,0,-1.0188460553,-2.7947932776,-0.9635556795

TS NO2BF4 PCM PURE-M06-2X 3.298_819960

M062X/6-311G*
E(RM062X) = -900.933597392

Zero-point correction= 0.157112 (Hartree/Particle)
Thermal correction to Energy= 0.172226
Thermal correction to Enthalpy= 0.173170
Thermal correction to Gibbs Free Energy= 0.113637
Sum of electronic and ZPE= -900.776485
Sum of electronic and thermal Energies= -900.761372
Sum of electronic and thermal Enthalpies= -900.760427
Sum of electronic and thermal Free Energies= -900.819960

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.073	53.194	125.297

C,0,1.8369650052,-1.0828215726,1.50959523
C,0,2.7631935911,-0.8856336433,0.5036692179
C,0,2.7097591776,0.2908534168,-0.2598534037
C,0,1.8022326727,1.3340556048,0.0452037579
C,0,0.8929678583,1.1200321001,1.0756957904
C,0,0.9008663086,-0.0793553906,1.7866185227
C,0,1.8535788962,2.6267445638,-0.7168847224
H,0,1.8234947552,-2.0164969138,2.055947248
H,0,3.4758863137,-1.6603161735,0.2584298039
H,0,3.434609487,0.4424241676,-1.0539498016
H,0,0.1679559223,1.8880603468,1.3209829957
H,0,0.1674532995,-0.2360417389,2.5694560859
H,0,0.9071812932,3.1635814041,-0.6589633827
H,0,2.103611911,2.4635434957,-1.7671940194
H,0,2.632635914,3.2704658426,-0.2994443946
N,0,0.9770984273,-0.6439937116,-1.6440093248
O,0,0.1686128471,-0.9889791838,-0.9447207988
O,0,1.4638342751,-0.4583234501,-2.6487851267
F,0,2.7158560403,-3.8672508421,0.345153912
B,0,1.6924695085,-3.8094075711,-0.6086132158
F,0,0.4897746883,-3.4375407419,0.0051336961
F,0,2.0225867103,-2.8083745081,-1.5737267781
F,0,1.5561700977,-5.0321855006,-1.2548212919

TS NO2BF4 PCM PURE-M06-2X 3.271_819957

M062X/6-311G*
E(RM062X) = -900.933728827

Zero-point correction= 0.157401 (Hartree/Particle)
Thermal correction to Energy= 0.172492
Thermal correction to Enthalpy= 0.173437
Thermal correction to Gibbs Free Energy= 0.113771
Sum of electronic and ZPE= -900.776328
Sum of electronic and thermal Energies= -900.761236
Sum of electronic and thermal Enthalpies= -900.760292
Sum of electronic and thermal Free Energies= -900.819957

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.241	53.059	125.576

C,0,2.0147245719,-1.1252880247,-1.4900910494
C,0,1.059779281,-0.1605400593,-1.8277095093
C,0,0.9893292932,1.0583437247,-1.1519250528
C,0,1.8532627368,1.3305304039,-0.097717552
C,0,2.7767373362,0.3237029595,0.2721494996
C,0,2.8935110742,-0.8725584308,-0.4539638696
C,0,1.840384541,2.6460753052,0.6262318171
H,0,2.0490223134,-2.0756740742,-2.0056122586
H,0,0.3595667283,-0.3626213342,-2.6304979758
H,0,0.249504584,1.7949143758,-1.4453690535
H,0,3.4666407682,0.520425166,1.0873298555
H,0,3.6187333885,-1.6189302322,-0.1603976655
H,0,2.6072867645,3.3046835627,0.2092934368
H,0,2.0670004808,2.5228279179,1.6872041928
H,0,0.8782103481,3.1480084427,0.5279407867
N,0,1.0402862801,-0.6716892205,1.5994317243
O,0,0.2515015489,-1.0137475662,0.8764064625
O,0,1.5002584382,-0.4953444328,2.6184699349
F,0,2.0695001341,-2.8482054502,1.5675773602
B,0,1.7915647562,-3.8281023948,0.5661532857
F,0,0.6136287469,-3.4509722039,-0.0915142729
F,0,2.8572608806,-3.8541359272,-0.3421109865
F,0,1.637840005,-5.0680345077,1.17433589

TS NO2BF4 PCM PURE-M06-2X 2.6887_819594

M062X/6-311G*
E(RM062X) = -900.934845641

Zero-point correction= 0.157950 (Hartree/Particle)
Thermal correction to Energy= 0.172816
Thermal correction to Enthalpy= 0.173760
Thermal correction to Gibbs Free Energy= 0.115252
Sum of electronic and ZPE= -900.776895
Sum of electronic and thermal Energies= -900.762030
Sum of electronic and thermal Enthalpies= -900.761086
Sum of electronic and thermal Free Energies= -900.819594

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.444	52.746	123.141

C,0,-2.3725152963,-1.1840582138,1.1802241997
C,0,-1.1890446447,-0.4904891317,1.5129147256
C,0,-0.9206141857,0.775918181,0.9630481065
C,0,-1.7459657119,1.3018590992,-0.017590935
C,0,-2.8839706831,0.5662604278,-0.3866438966
C,0,-3.2128158336,-0.648680789,0.2211127556
C,0,-1.4179471479,2.6124736492,-0.6756482
H,0,-2.5962376045,-2.1325144265,1.6538465104
H,0,-0.5154102947,-0.8892222495,2.2624521902
H,0,-0.0335371949,1.3120545525,1.2727010583
H,0,-3.5314833868,0.9582404204,-1.165223398
H,0,-4.1115976862,-1.174317721,-0.0768798545
H,0,-2.0526399542,3.410877638,-0.282837663
H,0,-1.5829970548,2.5599411855,-1.7531185418
H,0,-0.3763671507,2.8772813765,-0.4948817359
N,0,-0.1633184527,-1.5387271379,-0.3106456323
O,0,-0.7038767832,-1.203440821,-1.2445621902
O,0,0.6153827433,-2.148982988,0.2413958331
F,0,1.4332237942,0.2326235577,-0.8146430045
B,0,2.2379187357,0.6944580781,0.2628490652
F,0,3.5793278775,0.5381533754,-0.0526262894
F,0,1.9337089097,2.0411034207,0.5017613738
F,0,1.9053370053,-0.0710614835,1.3982605229

TS NO2BF4 PCM PURE-M06-2X 2.586_819521utf00004

M062X/6-311G*
E(RM062X) = -900.932715643

Zero-point correction= 0.157029 (Hartree/Particle)
Thermal correction to Energy= 0.172176
Thermal correction to Enthalpy= 0.173120
Thermal correction to Gibbs Free Energy= 0.113195
Sum of electronic and ZPE= -900.775687
Sum of electronic and thermal Energies= -900.760540
Sum of electronic and thermal Enthalpies= -900.759596
Sum of electronic and thermal Free Energies= -900.819521

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.042	53.172	126.123

C,0,1.7424109949,-1.0657520108,1.2509626052
C,0,2.7843586054,-0.7104945076,0.3685934925
C,0,2.8489304486,0.5801054748,-0.1893436899
C,0,1.8358337633,1.4898172295,0.0507061562
C,0,0.7800296286,1.1021905693,0.9061395654
C,0,0.7391630437,-0.1427605415,1.5163320956
C,0,1.8283761124,2.8573327324,-0.5706790585
H,0,1.7050388707,-2.0546453143,1.689503834
H,0,3.5890493295,-1.4126608398,0.1828232818
H,0,3.681964984,0.8426522415,-0.8317495963
H,0,-0.0224875481,1.8095872037,1.090998154
H,0,-0.0864780378,-0.4181791643,2.1563103693
H,0,1.7478096206,3.6284206805,0.1982193754
H,0,0.9688011846,2.9702436188,-1.2356923683
H,0,2.7346272197,3.0383929924,-1.1474486497
N,0,1.3267839627,-1.5862240304,-1.247554152
O,0,0.4824019787,-0.8475838501,-1.3756090543
O,0,1.9246383344,-2.5007733155,-1.5557900154
F,0,-0.740151014,-2.6698818339,2.1132128465
B,0,-1.1559887508,-2.7578376243,0.7765484202
F,0,-1.577844528,-1.5005471787,0.3233727767
F,0,-0.0409928985,-3.1571200324,-0.0141813447
F,0,-2.1740973046,-3.6940224994,0.6434629565

TS NO2BF4 PCM PURE-M06-2X 2.8006_818867

M062X/6-311G*
E(RM062X) = -900.933304698

Zero-point correction= 0.157588 (Hartree/Particle)
Thermal correction to Energy= 0.172608
Thermal correction to Enthalpy= 0.173552
Thermal correction to Gibbs Free Energy= 0.114438
Sum of electronic and ZPE= -900.775717
Sum of electronic and thermal Energies= -900.760697
Sum of electronic and thermal Enthalpies= -900.759753
Sum of electronic and thermal Free Energies= -900.818867

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.313	52.989	124.415

C,0,-0.3368855723,-1.3350395877,0.4407082457
C,0,-0.6992460203,-0.2460071839,1.2512930834
C,0,-2.0252881806,0.2424587292,1.2539477875
C,0,-2.9735819897,-0.283042188,0.3878985258
C,0,-2.570846589,-1.322223632,-0.4628590138
C,0,-1.278479545,-1.8552288926,-0.4277501787
C,0,-4.3823453643,0.2412282261,0.3359469083
H,0,0.6731575474,-1.7222661924,0.4745503158
H,0,0.0333747258,0.167640295,1.9326837633
H,0,-2.2892859595,1.0523365611,1.9264931589
H,0,-3.2924152948,-1.7328204269,-1.16282063
H,0,-1.0178970767,-2.6708455468,-1.0912182302
H,0,-5.1007313367,-0.5659165994,0.4913084722
H,0,-4.5938581327,0.685383102,-0.6394482506
H,0,-4.5500744977,0.9999129807,1.0999107802
N,0,-0.2978100994,1.3201865102,-0.4490243388
O,0,-0.8309265641,0.9471586756,-1.372092065

O,0,0.3246022042,2.0658022223,0.1313859366
F,0,2.2005819251,0.2936250398,1.0016212795
B,0,2.6736879842,-0.1637901783,-0.2447614792
F,0,2.8133823605,-1.5538729782,-0.2078804074
F,0,1.6950244288,0.1733700799,-1.2220176065
F,0,3.8772160471,0.4496569845,-0.5610520571

TS NO2BF4 PCM PURE-M06-2X 2.801_818858

M062X/6-311G*
E(RM062X) = -900.933304728

Zero-point correction= 0.157591 (Hartree/Particle)
Thermal correction to Energy= 0.172609
Thermal correction to Enthalpy= 0.173553
Thermal correction to Gibbs Free Energy= 0.114446
Sum of electronic and ZPE= -900.775714
Sum of electronic and thermal Energies= -900.760696
Sum of electronic and thermal Enthalpies= -900.759751
Sum of electronic and thermal Free Energies= -900.818858

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.314	52.988	124.401

C,0,-1.3716701134,-0.6558325213,1.2418092285
C,0,-0.9355301892,0.6527453759,1.1479833968
C,0,-1.7042533507,1.6014619389,0.4663799415
C,0,-2.9430290054,1.2851887776,-0.1091750597
C,0,-3.375857617,-0.0301816176,-0.0201096267
C,0,-2.5759558681,-1.0098265211,0.6103670697
C,0,-3.750401349,2.3438372078,-0.8088823159
H,0,-0.7861552695,-1.4097000798,1.7518622925
H,0,0.0069603981,0.9475677583,1.5930847547
H,0,-1.3379677968,2.6207947171,0.3889874731
H,0,-4.3252949637,-0.3233657068,-0.4566037779
H,0,-2.9230196865,-2.0330932838,0.6782408852
H,0,-3.939152002,3.188368415,-0.1434103562
H,0,-4.7101655353,1.9516498371,-1.144157937
H,0,-3.2139527562,2.7263834854,-1.6802526053
N,0,-1.5497085221,-1.2843507278,-1.4815939459
O,0,-1.9819360787,-2.2901398807,-1.7676263971
O,0,-0.926219418,-0.3608712124,-1.6656679411
F,0,0.4172319424,-2.3368186567,-0.5292130986
B,0,0.2064885118,-3.4218460944,0.3678913745
F,0,0.8221677143,-4.5617763407,-0.1284223347
F,0,0.7223587909,-3.0776909855,1.6203375822
F,0,-1.185151836,-3.6194638846,0.4716783974

TS NO2BF4 PCM PURE-M06-2X 2.8758_818627

M062X/6-311G*
E(RM062X) = -900.932099320

Zero-point correction= 0.157024 (Hartree/Particle)
Thermal correction to Energy= 0.171983
Thermal correction to Enthalpy= 0.172927
Thermal correction to Gibbs Free Energy= 0.113472
Sum of electronic and ZPE= -900.775075
Sum of electronic and thermal Energies= -900.760116
Sum of electronic and thermal Enthalpies= -900.759172
Sum of electronic and thermal Free Energies= -900.818627

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	107.921	52.799	125.133

C,0,-0.1779094973,-1.4172019709,0.0343672086
C,0,-1.1399073529,-1.829042212,0.9266388414
C,0,-2.4966567711,-1.4548179549,0.7690119393
C,0,-2.9239379546,-0.6716222814,-0.2867654006
C,0,-1.9349245152,-0.1983408315,-1.1662605582
C,0,-0.5648532458,-0.5608860166,-1.0053518642
C,0,-4.3626490769,-0.2873855503,-0.4821975585
H,0,0.8631472008,-1.6875211945,0.1500799224
H,0,-0.8657456119,-2.4520557157,1.7698008167
H,0,-3.219863819,-1.8029226249,1.498841255
H,0,-2.214635207,0.4274827183,-2.0083514531
H,0,0.177425689,-0.2086557021,-1.710800007
H,0,-5.0048006707,-0.7941554235,0.2367949814
H,0,-4.6981571394,-0.5470015085,-1.4877130002
H,0,-4.4938546384,0.7901111381,-0.3590558006
N,0,-0.8531518506,1.3782220293,0.0226746633
O,0,-1.0573828151,1.1955912709,1.1359391979
O,0,-0.5449167965,2.1773565081,-0.7466933479
F,0,2.3363407419,-0.18952417,-1.303202978
B,0,2.6639364592,0.2522221151,-0.0055172231
F,0,3.7983986387,1.052982433,-0.0421154099
F,0,1.5670819061,0.9971850076,0.4974497674
F,0,2.8681903266,-0.8625200636,0.8185130077

TS NO2BF4 PCM PURE-M06-2X 2.778_818581

M062X/6-311G*
E(RM062X) = -900.931834829

Zero-point correction= 0.157319 (Hartree/Particle)
Thermal correction to Energy= 0.172491
Thermal correction to Enthalpy= 0.173435
Thermal correction to Gibbs Free Energy= 0.113253
Sum of electronic and ZPE= -900.774516
Sum of electronic and thermal Energies= -900.759344
Sum of electronic and thermal Enthalpies= -900.758400
Sum of electronic and thermal Free Energies= -900.818581

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.239	53.065	126.662

C,0,-1.0050072795,0.2799496525,1.5231762953
C,0,-2.2897475524,0.7333179202,1.1771116556
C,0,-3.1695133393,-0.0892267958,0.4405294196
C,0,-2.7467474128,-1.3194120369,-0.0418073752
C,0,-1.4359205739,-1.7217263745,0.2577673947
C,0,-0.5809174981,-0.9458217731,1.0447147868
C,0,-3.6405703038,-2.1891523225,-0.8822337129
H,0,-0.3611461264,0.9133578001,2.1166386597
H,0,-2.6256875557,1.6923191544,1.5516583796

H,0,-4.175294961,0.2617522412,0.2331031748
H,0,-1.0818278089,-2.674571494,-0.1241124013
H,0,0.4168883995,-1.3037606353,1.2671843352
H,0,-3.3492484756,-2.1349772639,-1.9343029912
H,0,-4.6820066867,-1.877475593,-0.8041494876
H,0,-3.5689584979,-3.2334874884,-0.5750855697
N,0,-1.5274760886,1.5818464959,-0.8744236835
O,0,-1.9524229224,2.6278902878,-0.8015344589
O,0,-0.9830037912,0.7424961846,-1.3972316359
F,0,-0.7656106117,3.2347801648,1.6750460703
B,0,0.3290610529,3.5221718034,0.8324563293
F,0,1.4557873991,3.8135856994,1.586682589
F,0,0.5728665241,2.3615691053,0.0401942687
F,0,-0.0051618898,4.5757002677,-0.0169100423

TS NO2BF4 PCM PURE-M06-2X 2.840_818475

M062X/6-311G*
E(RM062X) = -900.931718302

Zero-point correction= 0.157209 (Hartree/Particle)
Thermal correction to Energy= 0.172398
Thermal correction to Enthalpy= 0.173342
Thermal correction to Gibbs Free Energy= 0.113243
Sum of electronic and ZPE= -900.774509
Sum of electronic and thermal Energies= -900.759320
Sum of electronic and thermal Enthalpies= -900.758376
Sum of electronic and thermal Free Energies= -900.818475

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.182	53.116	126.490

C,0,2.6536422561,-0.9929999484,0.5636206246
C,0,3.1583163724,-0.2790537774,-0.533788446
C,0,2.7903488062,1.0732308853,-0.7446874421
C,0,1.8550094252,1.6920344141,0.0771222616
C,0,1.3053652233,0.9305289509,1.1129049969
C,0,1.7044411042,-0.3904685592,1.3623224748
C,0,1.4165626468,3.111746618,-0.1561965167
H,0,2.9526312603,-2.0188128985,0.7208572409
H,0,3.9002928048,-0.739472615,-1.17522762
H,0,3.2355370637,1.6186079521,-1.5712101139
H,0,0.5496719722,1.3799921178,1.74993015
H,0,1.2539937529,-0.9395083454,2.1801515236
H,0,1.3587877725,3.6602110128,0.7849044082
H,0,0.4248420086,3.1379091423,-0.6144528317
H,0,2.1078484278,3.6346071064,-0.816907556
N,0,1.3882615201,-0.6759381156,-1.9586822029
O,0,1.9299163371,-0.8602473875,-2.9394180418
O,0,0.4466342083,-0.6283231276,-1.3335249735
F,0,1.263001083,-4.9893491456,-1.3935587524
B,0,1.2192602327,-3.6070750478,-1.318762625
F,0,0.6827193165,-3.1837656301,-0.0950177196
F,0,2.5219453601,-3.0612089381,-1.4488797693
F,0,0.4384110453,-3.0726466635,-2.3669220696

TS NO2BF4 PCM PURE-M06-2X 3.1393_818379

M062X/6-311G*
E(RM062X) = -900.933595319

Zero-point correction= 0.157755 (Hartree/Particle)
Thermal correction to Energy= 0.172498
Thermal correction to Enthalpy= 0.173442
Thermal correction to Gibbs Free Energy= 0.115216
Sum of electronic and ZPE= -900.775840
Sum of electronic and thermal Energies= -900.761097
Sum of electronic and thermal Enthalpies= -900.760153
Sum of electronic and thermal Free Energies= -900.818379

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.244	52.837	122.548

C,0,-3.3235559084,-0.2403805492,-0.5207739974
C,0,-2.878131179,-0.4202213903,0.777873035
C,0,-1.7576465175,0.3080580222,1.2444675247
C,0,-1.1334059884,1.287473413,0.4484256038
C,0,-1.573265173,1.4174164635,-0.8613523907
C,0,-2.6473680248,0.6606097657,-1.3421372351
C,0,-0.0416549077,2.1461792475,1.0102486085
H,0,-4.1670544932,-0.8043595493,-0.8979606492
H,0,-3.3651893758,-1.1276139754,1.4399434876
H,0,-1.4287666039,0.1753199425,2.2704588066
H,0,-1.070397552,2.1115445318,-1.5244485535
H,0,-2.961715063,0.785062015,-2.3722086451
H,0,0.5920240481,1.5777330943,1.6899725585
H,0,-0.4801871847,2.9804424712,1.5652664955
H,0,0.5886359467,2.5434875651,0.2172970347
N,0,-0.6207997364,-1.5678297531,0.3671568999
O,0,-0.4427956481,-2.1519703977,1.3221083221
O,0,-0.5414729989,-1.392640788,-0.7429983798
F,0,3.1075735489,-0.7572368735,-0.8288008972
B,0,2.2075641028,0.1523688672,-0.2802387995
F,0,1.2794575901,0.5613759927,-1.251374923
F,0,1.4808769465,-0.4958653794,0.7667519857
F,0,2.8742831716,1.2539842641,0.248560108

TS NO2BF4 PCM PURE-M06-2X 3.052_818171

M062X/6-311G*
E(RM062X) = -900.934049352

Zero-point correction= 0.157910 (Hartree/Particle)
Thermal correction to Energy= 0.172527
Thermal correction to Enthalpy= 0.173471
Thermal correction to Gibbs Free Energy= 0.115879
Sum of electronic and ZPE= -900.776140
Sum of electronic and thermal Energies= -900.761522
Sum of electronic and thermal Enthalpies= -900.760578
Sum of electronic and thermal Free Energies= -900.818171

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.262	52.647	121.214

C,0,-2.0181286716,-0.8468271888,0.9555131106
C,0,-1.6402772598,0.3403913135,1.560641443
C,0,-1.9393753415,1.5838888026,0.9377283154
C,0,-2.7216159469,1.6446499021,-0.2349822198
C,0,-3.031913573,0.4407471178,-0.8467852106
C,0,-2.6785896645,-0.786957826,-0.267866971
C,0,-3.1923868878,2.9447625539,-0.8136126851
H,0,-1.7791202651,-1.7993055535,1.410227589
H,0,-1.095400059,0.3375228295,2.4981566861
H,0,-1.6585097821,2.5061636442,1.4346387603
H,0,-3.5724940355,0.4465373266,-1.7871405767
H,0,-2.9410668403,-1.7056743798,-0.7800439302
H,0,-2.8035105569,3.7946793524,-0.2580998679
H,0,-4.2845249974,2.9773338918,-0.7976009777
H,0,-2.8593735506,3.0307424419,-1.8480032587
N,0,0.108966335,1.1443588073,0.0483651966
O,0,-0.0578730115,0.5087311552,-0.8768731349
O,0,0.8188603814,1.7278017798,0.7232453318
F,0,-0.3925887379,3.4520015409,-0.8820192319
B,0,0.1188944672,3.1751291378,-2.1789862943
F,0,-0.8057059113,2.3583064451,-2.8462615761
F,0,0.3327833907,4.3556798092,-2.8715444557
F,0,1.3233685183,2.4675180963,-2.0050560421

TS NO2BF4 PCM PURE-M06-2X 2.8774_817851

M062X/6-311G*
E(RM062X) = -900.932123346

Zero-point correction= 0.157359 (Hartree/Particle)
Thermal correction to Energy= 0.172184
Thermal correction to Enthalpy= 0.173128
Thermal correction to Gibbs Free Energy= 0.114273
Sum of electronic and ZPE= -900.774764
Sum of electronic and thermal Energies= -900.759940
Sum of electronic and thermal Enthalpies= -900.758995
Sum of electronic and thermal Free Energies= -900.817851

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.047	52.687	123.871

C,0,-0.3055309097,-1.4444425884,0.1370791381
C,0,-0.6115834833,-0.4254350119,1.0486605156
C,0,-1.9272315792,0.1241594451,1.0977238567
C,0,-2.939842152,-0.3258666099,0.2333320532
C,0,-2.5845063842,-1.2828833579,-0.6988622072
C,0,-1.2835875774,-1.8401003712,-0.745432729
C,0,-4.3181523552,0.2673574912,0.2988033963
H,0,0.6945296209,-1.8557263555,0.1049316704
H,0,0.1461144674,-0.0859021541,1.7438543201
H,0,-2.1508991025,0.877995239,1.8462648629
H,0,-3.3234743013,-1.6273199814,-1.4146660261
H,0,-1.065533034,-2.5926918708,-1.4939810742
H,0,-4.6509520787,0.3671814151,1.3328006572
H,0,-5.0363326954,-0.3506460587,-0.2385355459
H,0,-4.3258020872,1.264163608,-0.1496116754
N,0,-0.6136173513,1.3953869915,-0.2095120296
O,0,-0.7977603067,1.1047936613,-1.3034263137
O,0,-0.2337305848,2.2392742779,0.4755843079
F,0,2.2998382808,-0.3985605098,1.458161478
B,0,2.7274466814,-0.1521117369,0.137985622
F,0,2.8124761883,-1.3702837741,-0.5492515457
F,0,1.7558268031,0.6631999027,-0.4963372508
F,0,3.954967941,0.4980163488,0.1435545189

TS NO2BF4 PCM PURE-M06-2X 2.776_817301utf00003

M062X/6-311G*
E(RM062X) = -900.930633255

Zero-point correction= 0.157417 (Hartree/Particle)
Thermal correction to Energy= 0.172413
Thermal correction to Enthalpy= 0.173357
Thermal correction to Gibbs Free Energy= 0.113332
Sum of electronic and ZPE= -900.773216
Sum of electronic and thermal Energies= -900.758220
Sum of electronic and thermal Enthalpies= -900.757276
Sum of electronic and thermal Free Energies= -900.817301

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.191	52.726	126.334

C,0,-1.8289284203,-0.7657565707,0.8939667526
C,0,-1.4292142008,0.4485207917,1.3975171205
C,0,-1.9517626803,1.6414831128,0.8645165234
C,0,-2.9136562163,1.6572448101,-0.1499626209
C,0,-3.3041000821,0.431850542,-0.6711649732
C,0,-2.7127591118,-0.7792905041,-0.2066267225
C,0,-3.4703526618,2.9556427973,-0.6640412538
H,0,-1.4275799058,-1.6971950941,1.2662599702
H,0,-0.7085015585,0.4999820375,2.2038956141
H,0,-1.6042883109,2.5879927841,1.2670138431
H,0,-4.0342218903,0.3834111453,-1.4726784629
H,0,-3.0673643874,-1.7274021091,-0.5905436444
H,0,-3.8157326455,3.5810648612,0.1603405897
H,0,-4.3068703483,2.7860989398,-1.3409505379
H,0,-2.7022737068,3.5139037561,-1.2037152014
N,0,-1.3137299306,-0.4556674069,-1.8166460622
O,0,-0.4747100387,0.2393009622,-1.4720308649
O,0,-1.7207921734,-1.0954022849,-2.6756956276
F,0,-0.4826909172,-2.6022484646,-0.7816522722
B,0,0.7056052131,-2.8983295438,-1.5121423529
F,0,1.7881076479,-2.9054288473,-0.6376427995
F,0,0.5621302065,-4.1318240879,-2.139139272
F,0,0.8669431193,-1.8811706269,-2.4736527452

Pi Complexes for Toluene + $NO_2^+BF_4^-$ M062X/6-311G*/PCM(CH_2Cl_2)

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.896_825610

M062X/6-311G*
E(RM062X) = -900.938583160

Zero-point correction= 0.157970 (Hartree/Particle)

Thermal correction to Energy= 0.173870
Thermal correction to Enthalpy= 0.174814
Thermal correction to Gibbs Free Energy= 0.112973
Sum of electronic and ZPE= -900.780613
Sum of electronic and thermal Energies= -900.764713
Sum of electronic and thermal Enthalpies= -900.763769
Sum of electronic and thermal Free Energies= -900.825610

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.105	54.829	130.156

C,0,-3.2836712936,-3.3582062958,-0.449190649
C,0,-3.9330774419,-2.9881248327,-1.6263685303
C,0,-3.2454164433,-3.010560022,-2.8383459772
C,0,-1.9063866986,-3.4040773131,-2.8933543143
C,0,-1.2704718,-3.783830116,-1.7073939679
C,0,-1.9455065851,-3.7574682186,-0.4940817299
C,0,-1.1302674297,-3.3984087368,-4.1820879906
H,0,-3.8165708741,-3.3412325678,0.4954529982
H,0,-4.9735623575,-2.6837983356,-1.5998906655
H,0,-3.7537271621,-2.7102135931,-3.7492115684
H,0,-0.2235867247,-4.0609200392,-1.7263104317
H,0,-1.4211641046,-4.0310882905,0.4138746319
H,0,-1.7245397998,-3.0149967227,-5.0117764418
H,0,-0.7973010016,-4.406915915,-4.4384815515
H,0,-0.2364965291,-2.7785092305,-4.0773093117
N,0,-2.0461247957,-0.7397862508,-0.4447840209
O,0,-2.4720632102,-0.5726430738,0.5663572785
O,0,-1.6601406985,-0.8129227261,-1.4775979773
F,0,2.1723628474,-1.2237550177,0.2454487076
B,0,1.0572297089,-1.9136897121,-0.2057501149
F,0,0.8232240511,-1.6443513963,-1.5630868136
F,0,1.1951586826,-3.2839813721,0.0055679402
F,0,-0.0934391401,-1.4547164216,0.5224070001

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.910_824610

M062X/6-311G*
E(RM062X) = -900.938478053

Zero-point correction= 0.158515 (Hartree/Particle)
Thermal correction to Energy= 0.174305
Thermal correction to Enthalpy= 0.175249
Thermal correction to Gibbs Free Energy= 0.113868
Sum of electronic and ZPE= -900.779963
Sum of electronic and thermal Energies= -900.764173
Sum of electronic and thermal Enthalpies= -900.763229
Sum of electronic and thermal Free Energies= -900.824610

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.378	54.646	129.186

C,0,-0.8391229782,-0.0056112486,1.3390893934
C,0,-1.9779336709,0.7705402966,1.1263326469
C,0,-3.0518627151,0.2605016238,0.3945930617
C,0,-3.0091224776,-1.0324639307,-0.1267477319
C,0,-1.8603499394,-1.8030910042,0.0979668378
C,0,-0.7855957315,-1.2992883781,0.8189471044
C,0,-4.1615256433,-1.6031429336,-0.9100092195
H,0,0.0050781194,0.3878624286,1.8912817371
H,0,-2.0314610951,1.7754681313,1.5328262084
H,0,-3.9331785141,0.8737111352,0.2354607317
H,0,-1.8125411077,-2.8097330069,-0.3067214644
H,0,0.1086437177,-1.8919615648,0.9667248976
H,0,-3.8381611092,-1.9272620932,-1.901857151
H,0,-4.9614024723,-0.8727218581,-1.0329364628
H,0,-4.5758804664,-2.4777702365,-0.4030295529
N,0,-0.3126887202,1.2360925935,-1.239618166
O,0,-0.7108438784,0.3456085483,-1.7638660636
O,0,0.0492179327,2.1858788309,-0.8004106088
F,0,1.6329973486,0.0983181963,-0.7495039287
B,0,2.3814002505,0.3962346161,0.4397277516
F,0,1.8644994432,1.5944154415,0.9585034396
F,0,2.1953962769,-0.6394493273,1.352713726
F,0,3.7181454307,0.5408087403,0.1065718133

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.924_825224

M062X/6-311G*
E(RM062X) = -900.938771871

Zero-point correction= 0.158242 (Hartree/Particle)
Thermal correction to Energy= 0.174070
Thermal correction to Enthalpy= 0.175015
Thermal correction to Gibbs Free Energy= 0.113548
Sum of electronic and ZPE= -900.780530
Sum of electronic and thermal Energies= -900.764702
Sum of electronic and thermal Enthalpies= -900.763757
Sum of electronic and thermal Free Energies= -900.825224

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.231	54.755	129.368

C,0,2.7352194338,-0.1304843549,-2.2094330029
C,0,1.6567446806,0.7596443271,-2.1996293365
C,0,1.678766639,1.889025515,-3.0078280212
C,0,2.7769403513,2.1622083204,-3.829446413
C,0,3.8461826708,1.2639876354,-3.8361367146
C,0,3.8278444161,0.122655279,-3.0358033727
C,0,2.7914487912,3.4180722661,-4.6569011295
H,0,2.7171969376,-1.0167171743,-1.5841048285
H,0,0.8046815371,0.5798449339,-1.5534609641
H,0,0.8522867608,2.5884853141,-2.9707743531
H,0,4.7063335911,1.4617755623,-4.4678929841
H,0,4.6650093005,-0.5661021577,-3.0556649425
H,0,1.9913162175,3.4008875805,-5.4008697131
H,0,3.7392595641,3.5454252812,-5.1804538588
H,0,2.6230378113,4.2853037056,-4.0149323935
N,0,3.668908819,1.9091119825,-0.3340100997
O,0,3.9301177526,2.6328194672,-1.1271794105
O,0,3.4990440812,1.1890789443,0.4929116681
F,0,2.0485467083,4.4409382564,-1.4852247969
B,0,1.1187309046,4.0494620953,-0.5084303862
F,0,0.8885411818,5.0828140162,0.3870480537
F,0,-0.0666188763,3.6230519909,-1.1009185959
F,0,1.6946426259,2.9419955133,0.2039746953

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.926_823642

M062X/6-311G*
E(RM062X) = -900.935838798

Zero-point correction= 0.158157 (Hartree/Particle)
Thermal correction to Energy= 0.174117
Thermal correction to Enthalpy= 0.175062
Thermal correction to Gibbs Free Energy= 0.112197
Sum of electronic and ZPE= -900.777682
Sum of electronic and thermal Energies= -900.761721
Sum of electronic and thermal Enthalpies= -900.760777
Sum of electronic and thermal Free Energies= -900.823642

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.260	54.776	132.310

C,0,1.21426707,-0.726423966,-0.0955206888
C,0,1.26064487,-0.702760051,-1.4892784935
C,0,2.2092316667,0.0797004851,-2.1391323275
C,0,3.1286393195,0.8480643269,-1.4157736072
C,0,3.071275743,0.8148563594,-0.0214792553
C,0,2.1231639982,0.0372475425,0.6388866032
C,0,4.1317225748,1.7172272004,-2.1263517625
H,0,0.4818346577,-1.3418124536,0.4157687981
H,0,0.5606723583,-1.2964194506,-2.0662700882
H,0,2.2416311426,0.0952615186,-3.2241409068
H,0,3.7649524372,1.4153522498,0.5572917973
H,0,2.0822399455,0.0431659828,1.7216118158
H,0,3.7142670727,2.7102133533,-2.3159088638
H,0,4.4151829309,1.2897311829,-3.0891246983
H,0,5.0336850175,1.8492571683,-1.5276222973
N,0,-0.0305975671,1.90986738,0.1553777345
O,0,0.4827824027,2.3029373936,-0.7431713327
O,0,-0.6352804286,1.536435739,1.004965505
F,0,1.8812408299,3.6705911835,3.6966840241
B,0,1.0356213523,2.9255694616,2.899053691
F,0,1.0646933237,1.5685836914,3.243322115
F,0,-0.2802332674,3.393399272,2.9572951358
F,0,1.4566257501,3.0259591303,1.5282075021

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.926_826511

M062X/6-311G*
E(RM062X) = -900.938742887

Zero-point correction= 0.158036 (Hartree/Particle)
Thermal correction to Energy= 0.173959
Thermal correction to Enthalpy= 0.174903
Thermal correction to Gibbs Free Energy= 0.112232
Sum of electronic and ZPE= -900.780707
Sum of electronic and thermal Energies= -900.764784
Sum of electronic and thermal Enthalpies= -900.763840
Sum of electronic and thermal Free Energies= -900.826511

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.161	54.792	131.902

C,0,2.3465828886,-0.8227353157,1.1049569725
C,0,3.1080333345,-0.1788507984,0.1319045298
C,0,2.6714292673,1.0304251606,-0.4065786587
C,0,1.4759099615,1.6150869326,0.0176164275
C,0,0.727538684,0.9664709639,1.0048439972
C,0,1.1524246995,-0.2420025806,1.5421990156
C,0,0.9681914362,2.9003775937,-0.5758847503
H,0,2.6816833013,-1.7644696721,1.5263894756
H,0,4.0397778114,-0.6175826233,-0.2071728968
H,0,3.2641448862,1.5213316601,-1.1719327818
H,0,-0.2154625391,1.3922127201,1.3265798823
H,0,0.5465260592,-0.7376684062,2.2925143588
H,0,-0.0418832789,2.7558799036,-0.9653817083
H,0,1.609702886,3.2527915386,-1.3839633636
H,0,0.9169425699,3.6838553292,0.1840863153
N,0,0.4565728896,-1.7175072605,-0.9417182232
O,0,0.4878473059,-2.7328757618,-0.4951584937
O,0,0.4528326774,-0.7472223097,-1.4702841906
F,0,-1.5275539577,-1.3348756233,0.1433700296
B,0,-2.2936234414,-0.1235466319,0.0457149657
F,0,-2.3587358654,0.4601479337,1.3072964616
F,0,-1.6230819213,0.7194117908,-0.8555555084
F,0,-3.5585476546,-0.4347965433,-0.4294628561

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.957_824442

M062X/6-311G*
E(RM062X) = -900.938601018

Zero-point correction= 0.158570 (Hartree/Particle)
Thermal correction to Energy= 0.174297
Thermal correction to Enthalpy= 0.175241
Thermal correction to Gibbs Free Energy= 0.114159
Sum of electronic and ZPE= -900.780031
Sum of electronic and thermal Energies= -900.764304
Sum of electronic and thermal Enthalpies= -900.763360
Sum of electronic and thermal Free Energies= -900.824442

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.373	54.649	128.558

C,0,-1.7332104415,2.2215669955,1.7371988918
C,0,-1.9456793581,2.7401531656,0.459893556
C,0,-2.6815965404,2.0140648168,-0.4706782204
C,0,-3.2214442682,0.7636644264,-0.1468238104
C,0,-2.999571735,0.2542956791,1.1331988998
C,0,-2.2619935202,0.9735679987,2.071184177
C,0,-4.0332531681,-0.0050096355,-1.1554114374
H,0,-1.1659757363,2.7868866532,2.4688614635
H,0,-1.5369436933,3.707703247,0.1909027504
H,0,-2.8376005375,2.4187969571,-1.4658914748
H,0,-3.3768886441,-0.7250101414,1.4038058866
H,0,-2.0915186865,0.5473753518,3.0529193376
H,0,-3.6702508092,0.1644768565,-2.1704269213
H,0,-5.0798020807,0.3102703726,-1.1238346407
H,0,-4.0049011742,-1.0760535288,-0.9518372656
N,0,0.2703393513,0.2515579558,0.8142582657
O,0,-0.2322195726,0.1449373469,-0.1665347023

O,0,0.8572848817,0.3908894159,1.74282759
F,0,-0.6471226207,-1.745894831,1.5003428805
B,0,-0.8903074543,-2.0193304843,2.8892827157
F,0,-0.2561243056,-1.0025762238,3.6216624029
F,0,-2.2639616279,-1.9871127871,3.1161835187
F,0,-0.3575426587,-3.2590656069,3.2032373369

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.962_827214

M062X/6-311G*
E(RM062X) = -900.939496146

Zero-point correction= 0.158066 (Hartree/Particle)
Thermal correction to Energy= 0.173974
Thermal correction to Enthalpy= 0.174918
Thermal correction to Gibbs Free Energy= 0.112282
Sum of electronic and ZPE= -900.781430
Sum of electronic and thermal Energies= -900.765522
Sum of electronic and thermal Enthalpies= -900.764578
Sum of electronic and thermal Free Energies= -900.827214

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.170	54.792	131.830

C,0,-1.8926823304,0.7570944744,1.1929573165
C,0,-2.7680908276,0.8457076028,0.1119390401
C,0,-3.1916857089,-0.3101938274,-0.5441960334
C,0,-2.7562222099,-1.569017919,-0.128495171
C,0,-1.882753833,-1.6432517733,0.9633093712
C,0,-1.4511279966,-0.4957349726,1.6166809138
C,0,-3.1935898385,-2.8206258651,-0.8418134216
H,0,-1.554361627,1.6527109381,1.7014886451
H,0,-3.1275105592,1.8147681804,-0.2177435851
H,0,-3.8753788184,-0.2298902965,-1.3833087446
H,0,-1.5337892348,-2.6153808458,1.2975909819
H,0,-0.7580324296,-0.5719035915,2.4457155098
H,0,-2.3810434608,-3.222118406,-1.4533892842
H,0,-4.0429218754,-2.6273299602,-1.497625948
H,0,-3.4787434854,-3.5978480837,-0.1304217338
N,0,-0.0433470306,0.7682775097,-1.121074141
O,0,-0.0567797256,-0.3364495691,-1.1295905147
O,0,-0.068100253,1.8728341562,-1.1891064911
F,0,2.3539587381,0.7913606372,-1.0729514301
B,0,2.5436592718,0.8679907241,0.3381662503
F,0,3.248337448,-0.2352041298,0.7803639014
F,0,3.1713056378,2.0550775648,0.6651416024
F,0,1.2239071489,0.8529394522,0.8900399662

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.967_827913

M062X/6-311G*
E(RM062X) = -900.939513201

Zero-point correction= 0.157785 (Hartree/Particle)
Thermal correction to Energy= 0.173822
Thermal correction to Enthalpy= 0.174766
Thermal correction to Gibbs Free Energy= 0.111600
Sum of electronic and ZPE= -900.781729
Sum of electronic and thermal Energies= -900.765692
Sum of electronic and thermal Enthalpies= -900.764747
Sum of electronic and thermal Free Energies= -900.827913

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.075	54.880	132.943

C,0,-0.8792678267,0.2885987742,2.1943375495
C,0,-1.1468714583,1.6567404249,2.2347131334
C,0,-2.4487010063,2.1155662079,2.0802236835
C,0,-3.5105355496,1.2254640016,1.8759978243
C,0,-3.2314433401,-0.140713614,1.8363109025
C,0,-1.9269387274,-0.6091886836,1.9984628894
C,0,-4.9122976405,1.7458905372,1.6995286597
H,0,0.1370560625,-0.0701426295,2.3106718577
H,0,-0.335669918,2.3619572484,2.3693692215
H,0,-2.6497120115,3.1821174072,2.1088829722
H,0,-4.0397213372,-0.8487920488,1.6844512864
H,0,-1.7311956866,-1.6760006585,1.9760346202
H,0,-5.2101669849,2.353750908,2.556714131
H,0,-5.6300853384,0.9323657418,1.5935532372
H,0,-4.9828455927,2.3801410941,0.8124915892
N,0,-1.1234190832,0.2156866337,-0.7620187453
O,0,-1.7940314777,1.0930294935,-0.7229100073
O,0,-0.5177779708,-0.7083369839,-0.8315125563
F,0,1.2217926894,3.2516081533,-1.6071426508
B,0,1.2349072458,1.876076445,-1.4784637652
F,0,0.7822014866,1.507864282,-0.1720175957
F,0,0.2902261793,1.2941732018,-2.3739870894
F,0,2.4890095864,1.3415470636,-1.7037910481

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.967_828376

M062X/6-311G*
E(RM062X) = -900.939491139

Zero-point correction= 0.157703 (Hartree/Particle)
Thermal correction to Energy= 0.173810
Thermal correction to Enthalpy= 0.174754
Thermal correction to Gibbs Free Energy= 0.111115
Sum of electronic and ZPE= -900.781788
Sum of electronic and thermal Energies= -900.765681
Sum of electronic and thermal Enthalpies= -900.764737
Sum of electronic and thermal Free Energies= -900.828376

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.067	54.912	133.941

C,0,-1.4241206998,0.1096301571,-2.2712020279
C,0,-1.0048165116,1.3721750192,-1.8526333958
C,0,0.2526737636,1.5348210442,-1.2860170243
C,0,1.1175776022,0.4459655007,-1.1183688845
C,0,0.6880090287,-0.8122427259,-1.5403482096
C,0,-0.5713312395,-0.9816160605,-2.1171659408
C,0,2.4720536506,0.6432817799,-0.4911955469
H,0,-2.4069928887,-0.018464522,-2.7101740615
H,0,-1.6681642037,2.2226280071,-1.9533922653

H,0,0.5714111504,2.5195580755,-0.9582650008
H,0,1.3436141591,-1.6693811673,-1.4252870755
H,0,-0.8835735614,-1.966107039,-2.4491185101
H,0,3.0512661303,1.3845414275,-1.0461908295
H,0,3.0412306337,-0.2861096914,-0.4691277531
H,0,2.3763447295,1.0084563928,0.5342379816
N,0,-1.9833159585,-0.7659445061,0.5076497662
O,0,-1.2284795385,-0.0472299568,0.8745820575
O,0,-2.6899673085,-1.5481543459,0.1695174788
F,0,-3.6342052871,0.1170242244,2.009215534
B,0,-4.2386726053,1.0670471527,1.1340082195
F,0,-5.5599867215,0.7289830285,0.9124581186
F,0,-4.1045256447,2.3398498973,1.654570079
F,0,-3.503664079,0.964061608,-0.0887707093

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.976_825066

M062X/6-311G*
E(RM062X) = -900.938818196

Zero-point correction= 0.158520 (Hartree/Particle)
Thermal correction to Energy= 0.174296
Thermal correction to Enthalpy= 0.175240
Thermal correction to Gibbs Free Energy= 0.113752
Sum of electronic and ZPE= -900.780299
Sum of electronic and thermal Energies= -900.764522
Sum of electronic and thermal Enthalpies= -900.763578
Sum of electronic and thermal Free Energies= -900.825066

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.372	54.648	129.412

C,0,2.5238069617,-6.4141808544,1.3577215451
C,0,1.6962834247,-6.4848772171,2.4787747398
C,0,0.520225852,-5.7433421622,2.5216030949
C,0,0.1458827331,-4.9191323061,1.4535879027
C,0,0.9756847229,-4.8644649354,0.3334056863
C,0,2.1553870472,-5.6029995549,0.2834140508
C,0,-1.0999876073,-4.0804744334,1.5324506919
H,0,3.4394014152,-6.9942024093,1.3162924931
H,0,1.9685614341,-7.1178836232,3.3157137712
H,0,-0.1167933331,-5.7979843899,3.3993969584
H,0,0.7155770226,-4.2129480716,-0.4926320423
H,0,2.7909962453,-5.5383002277,-0.5932196762
H,0,-1.3610209399,-3.6737698366,0.5554054914
H,0,-0.944761205,-3.2346281125,2.2060548368
H,0,-1.944150112,-4.6620087253,1.9085498917
N,0,3.4373351044,-3.6693987223,2.0550260238
O,0,4.4523873489,-3.8874744305,1.6625897454
O,0,2.4708179009,-3.4301088694,2.5340087553
F,0,1.1415242903,-2.0271274013,-1.1857713399
B,0,1.8283374655,-1.6596435684,-0.0331384829
F,0,1.0228633406,-1.8454272948,1.1002815907
F,0,2.9716246311,-2.5182264207,0.1175217433
F,0,2.2694758566,-0.3465780329,-0.1076227713

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.984_825092

M062X/6-311G*
E(RM062X) = -900.939279115

Zero-point correction= 0.158620 (Hartree/Particle)
Thermal correction to Energy= 0.174375
Thermal correction to Enthalpy= 0.175319
Thermal correction to Gibbs Free Energy= 0.114187
Sum of electronic and ZPE= -900.780659
Sum of electronic and thermal Energies= -900.764904
Sum of electronic and thermal Enthalpies= -900.763960
Sum of electronic and thermal Free Energies= -900.825092

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.422	54.686	128.664

C,0,-2.8901881826,-3.0169865693,1.8699326549
C,0,-2.7571169167,-4.254218692,1.2405703078
C,0,-3.80237106,-5.1719597794,1.2811462844
C,0,-4.9993939706,-4.8789900628,1.9462353939
C,0,-5.1242104146,-3.6342251845,2.5651496127
C,0,-4.0809062162,-2.7112674118,2.5308420598
C,0,-6.1112403308,-5.8899349732,2.0158014315
H,0,-2.0836822001,-2.2929379454,1.8315914097
H,0,-1.8402237484,-4.5008492522,0.7170364045
H,0,-3.689445407,-6.1340393037,0.7902897787
H,0,-6.0346195812,-3.3989533078,3.1027172341
H,0,-4.2006255383,-1.7493524816,3.0186050979
H,0,-6.2542698578,-6.3858810736,1.0538394879
H,0,-7.0468727572,-5.4200434775,2.3174249237
H,0,-5.8763815435,-6.6482841608,2.7650900151
N,0,-2.7102223369,-4.1825991501,4.6105905198
O,0,-2.9380811335,-5.172162047,4.1757434619
O,0,-2.391925215,-3.2270987534,5.0769560989
F,0,-4.8008740545,-3.9268387966,5.5601490713
B,0,-5.76129263,-4.9927088939,5.6134630403
F,0,-6.0550257803,-5.2600736611,6.9426989179
F,0,-6.9018108293,-4.6059509529,4.9161662542
F,0,-5.1680344957,-6.1094124692,5.0060125388

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.984_829231

M062X/6-311G*
E(RM062X) = -900.939542391

Zero-point correction= 0.157751 (Hartree/Particle)
Thermal correction to Energy= 0.173888
Thermal correction to Enthalpy= 0.174832
Thermal correction to Gibbs Free Energy= 0.110311
Sum of electronic and ZPE= -900.781792
Sum of electronic and thermal Energies= -900.765654
Sum of electronic and thermal Enthalpies= -900.764710
Sum of electronic and thermal Free Energies= -900.829231

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.117	54.866	135.796

C,0,0.626289451,1.1962856375,-3.3156390777
C,0,0.5934255513,2.39876298,-2.6096558874
C,0,1.6669726207,2.7652576813,-1.8016182993
C,0,2.7880884421,1.9425416678,-1.6824691954
C,0,2.809659495,0.7393438006,-2.3964331737
C,0,1.741343352,0.3656348343,-3.204834599
C,0,3.9305217623,2.3184795469,-0.777028883
H,0,-0.2042231634,0.9137837242,-3.9535866522
H,0,-0.2685358345,3.0526771638,-2.6848161973
H,0,1.6218712632,3.6940519806,-1.2436216481
H,0,3.6740275739,0.0876189583,-2.3146105908
H,0,1.778890838,-0.5689085696,-3.7530102919
H,0,3.8104288042,1.8508066652,0.2042999258
H,0,3.9760126032,3.3971850657,-0.6244875506
H,0,4.8858804402,1.9858879487,-1.1856481693
N,0,-0.4096416833,0.4528442336,-0.6183067978
O,0,-1.4404396754,0.5172019828,-1.0165762822
O,0,0.6198330307,0.3096332338,-0.2428274961
F,0,-0.5699255403,2.6346010746,0.3203308658
B,0,-1.05020931,2.2946081313,1.6243483478
F,0,-1.2032912586,0.8774763194,1.6038120265
F,0,-0.1118119884,2.6524666935,2.5736289484
F,0,-2.273237974,2.8978087457,1.8442933771

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.991_828973

M062X/6-311G*
E(RM062X) = -900.939538161

Zero-point correction= 0.157822 (Hartree/Particle)
Thermal correction to Energy= 0.173955
Thermal correction to Enthalpy= 0.174899
Thermal correction to Gibbs Free Energy= 0.110565
Sum of electronic and ZPE= -900.781716
Sum of electronic and thermal Energies= -900.765583
Sum of electronic and thermal Enthalpies= -900.764639
Sum of electronic and thermal Free Energies= -900.828973

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.158	54.844	135.402

C,0,-2.2846922853,1.1676504653,1.4597929793
C,0,-3.2071065298,1.0801158566,0.4178057222
C,0,-3.3315187322,-0.1026557348,-0.304438115
C,0,-2.542085334,-1.2175740526,-0.0041628226
C,0,-1.6178945588,-1.115603827,1.0375597966
C,0,-1.4886051467,0.0635711221,1.7663635225
C,0,-2.695497793,-2.5021755474,-0.7739446432
H,0,-2.1902510708,2.0853062674,2.0303269711
H,0,-3.8283964112,1.933169079,0.1695889733
H,0,-4.0483741795,-0.1613116511,-1.1175009384
H,0,-0.9765774777,-1.9589170769,1.2693700754
H,0,-0.7604142065,0.1210112679,2.568044096
H,0,-3.0464581501,-2.3175729813,-1.7900783893
H,0,-3.4247876224,-3.1548547945,-0.2863085816
H,0,-1.7514842576,-3.0458046151,-0.8282431255
N,0,0.0551530432,1.3787157475,-0.3918199672
O,0,-0.4555257844,0.7470539884,-1.1409894742
O,0,0.5309927992,2.0763896264,0.3238003972
F,0,3.6144279388,-0.1603845663,0.2884250529
B,0,2.4583943733,-0.3696154309,-0.4386920086
F,0,2.1960225106,0.7584846628,-1.2704136915
F,0,2.5245952173,-1.515980863,-1.2077244366
F,0,1.3368856578,-0.4468449426,0.4457216071

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.998_824734

M062X/6-311G*
E(RM062X) = -900.939646282

Zero-point correction= 0.158749 (Hartree/Particle)
Thermal correction to Energy= 0.174358
Thermal correction to Enthalpy= 0.175302
Thermal correction to Gibbs Free Energy= 0.114912
Sum of electronic and ZPE= -900.780897
Sum of electronic and thermal Energies= -900.765289
Sum of electronic and thermal Enthalpies= -900.764345
Sum of electronic and thermal Free Energies= -900.824734

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.411	54.607	127.100

C,0,-2.7949119261,0.1536749717,1.0268241998
C,0,-3.103787683,-0.6860289978,-0.0424756691
C,0,-2.1609325537,-1.5989240826,-0.5054846256
C,0,-0.8952631183,-1.6957306278,0.0849841299
C,0,-0.5979525781,-0.851783003,1.1561396532
C,0,-1.5370355233,0.0645596641,1.6254050006
C,0,0.1162133575,-2.6922976633,-0.4117102396
H,0,-3.5274286652,0.8629408147,1.3963824259
H,0,-4.0778697471,-0.6268238228,-0.515017582
H,0,-2.4067125156,-2.2445784846,-1.3433871982
H,0,0.3890964878,-0.8902796174,1.6013671663
H,0,-1.2840763898,0.7117779578,2.4588903124
H,0,-0.1580638181,-3.703142278,-0.09742468
H,0,1.1071623841,-2.4599771321,-0.0243534884
H,0,0.1691580598,-2.6825642427,-1.5013170065
N,0,-0.875738979,1.8239753323,-0.5586945233
O,0,-0.8306816105,1.016334854,-1.311003952
O,0,-0.9612110625,2.6928317951,0.1262817594
F,0,2.4800958657,-0.4871251044,0.6479258368
B,0,2.1349783676,0.4525129325,-0.3220206157
F,0,1.2406037281,1.4129713577,0.2625103519
F,0,3.2579339311,1.1189257885,-0.7913214368
F,0,1.4469829884,-0.1614684118,-1.3769258186

Pi Complex NO_2BF_4 PCM PURE-M06-2X 2.998_827902

M062X/6-311G*
E(RM062X) = -900.939593532

Zero-point correction= 0.157986 (Hartree/Particle)
Thermal correction to Energy= 0.173954
Thermal correction to Enthalpy= 0.174898
Thermal correction to Gibbs Free Energy= 0.111692

Sum of electronic and ZPE= -900.781607
Sum of electronic and thermal Energies= -900.765640
Sum of electronic and thermal Enthalpies= -900.764696
Sum of electronic and thermal Free Energies= -900.827902

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.158	54.795	133.029

C,0,2.3261664919,-0.9977053086,1.595017216
C,0,3.2444286429,-0.9812171634,0.5477972822
C,0,3.3383611639,0.1354955373,-0.2797369141
C,0,2.5215274204,1.2511216323,-0.0797911474
C,0,1.6020708209,1.2214150805,0.972339393
C,0,1.5028101612,0.1109205167,1.8038890261
C,0,2.6178076033,2.4625112585,-0.9686721955
H,0,2.2553526054,-1.8615532617,2.2471142446
H,0,3.8890580107,-1.8357819975,0.3762228813
H,0,4.054360979,0.1378907195,-1.0954277856
H,0,0.9421699659,2.067758007,1.129851912
H,0,0.7790137125,0.1090790979,2.6117751989
H,0,1.6339528491,2.7478549236,-1.3470613564
H,0,3.2734997056,2.2813034779,-1.8205549311
H,0,3.0133681192,3.3163913301,-0.4131905752
N,0,-0.0083644577,-1.408784007,-0.2398906701
O,0,0.5101320735,-0.8596762658,-1.0466101566
O,0,-0.4901324663,-2.0275108325,0.5413585726
F,0,-2.1396536164,-0.9131001387,-1.2177617466
B,0,-2.4221162664,0.3007403282,-0.5251559888
F,0,-3.5907160766,0.1692976578,0.1996976503
F,0,-1.3173041004,0.4849316226,0.3648222102
F,0,-2.4772033416,1.3518667853,-1.4207781197

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.031_827650

M062X/6-311G*
E(RM062X) = -900.940071851

Zero-point correction= 0.157810 (Hartree/Particle)
Thermal correction to Energy= 0.173753
Thermal correction to Enthalpy= 0.174697
Thermal correction to Gibbs Free Energy= 0.112422
Sum of electronic and ZPE= -900.782262
Sum of electronic and thermal Energies= -900.766319
Sum of electronic and thermal Enthalpies= -900.765374
Sum of electronic and thermal Free Energies= -900.827650

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.032	54.908	131.070

C,0,-1.2602447427,-4.2644566936,4.3445311373
C,0,0.1191807165,-4.1870584545,4.523436848
C,0,0.7612771242,-5.074495212,5.383866743
C,0,0.0430272411,-6.0505538488,6.0803148381
C,0,-1.3382901057,-6.1247289793,5.8853550899
C,0,-1.9870172963,-5.2419207269,5.0284396252
C,0,0.7167432509,-6.9818674506,7.0510727303
H,0,-1.7642891456,-3.5781452984,3.6729599356
H,0,0.6943315449,-3.4346729332,3.9956351038
H,0,1.8348305328,-5.0017532459,5.5259619178
H,0,-1.9152261683,-6.8602989991,6.4348765878
H,0,-3.062275814,-5.3067486749,4.9041828578
H,0,0.2928102195,-6.846765433,8.0485511612
H,0,1.7906700585,-6.7997248067,7.1006309119
H,0,0.5598646137,-8.0244813516,6.7654837687
N,0,-1.8015710136,-3.1174914837,7.0974977846
O,0,-0.8473563916,-3.5745655043,7.415856094
O,0,-2.7268973815,-2.5973530413,6.7801903458
F,0,-1.582820535,-5.5932034539,9.169302588
B,0,-2.7989487169,-4.9082323384,9.1356944755
F,0,-3.7140421043,-5.4280556553,10.0233173648
F,0,-2.5535970884,-3.5325372344,9.4018910111
F,0,-3.2969258983,-4.9523805803,7.80480338

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.038_828111

M062X/6-311G*
E(RM062X) = -900.940076145

Zero-point correction= 0.157750 (Hartree/Particle)
Thermal correction to Energy= 0.173744
Thermal correction to Enthalpy= 0.174688
Thermal correction to Gibbs Free Energy= 0.111965
Sum of electronic and ZPE= -900.782326
Sum of electronic and thermal Energies= -900.766333
Sum of electronic and thermal Enthalpies= -900.765388
Sum of electronic and thermal Free Energies= -900.828111

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.026	54.928	132.011

C,0,0.9372398306,-1.03456312,-0.5894022203
C,0,1.2386193959,-0.5680595086,-1.8671814269
C,0,2.3263766526,0.2798268293,-2.0610878496
C,0,3.1292015332,0.6791036651,-0.9887213449
C,0,2.821910539,0.1984052392,0.2863835501
C,0,1.7373716814,-0.6488841243,0.4884776871
C,0,4.2785626724,1.6315206933,-1.1771217036
H,0,0.0934189002,-1.6977808305,-0.4339637168
H,0,0.6260702873,-0.8630472931,-2.7117152237
H,0,2.549648742,0.6467208431,-3.0578513949
H,0,3.419012409,0.5165154876,1.133776086
H,0,1.5090606607,-0.9993225469,1.4890217622
H,0,4.3823494028,1.9320494463,-2.2201014568
H,0,5.2188042381,1.1758575639,-0.8582020999
H,0,4.1237955058,2.5255886979,-0.5692686741
N,0,-0.0953387157,1.6852248563,0.2871516647
O,0,0.6178703987,2.1245665953,-0.4333924838
O,0,-0.8610735707,1.2593413502,0.9650968432
F,0,0.2796806817,3.7088333327,1.6248722465
B,0,1.5207210005,3.2240783036,2.1237034977
F,0,2.5005542576,3.4202607564,1.1479973726
F,0,1.8450227578,3.8307627176,3.3159977647
F,0,1.3384787389,1.8251080455,2.2948551205

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.045_827735

M062X/6-311G*
E(RM062X) = -900.940077246

Zero-point correction= 0.157833 (Hartree/Particle)
Thermal correction to Energy= 0.173791
Thermal correction to Enthalpy= 0.174736
Thermal correction to Gibbs Free Energy= 0.112342
Sum of electronic and ZPE= -900.782244
Sum of electronic and thermal Energies= -900.766286
Sum of electronic and thermal Enthalpies= -900.765342
Sum of electronic and thermal Free Energies= -900.827735

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.056	54.909	131.318

C,0,2.9128898391,0.48379664,-0.5840324522
C,0,3.2071640834,-0.2621321151,0.5554947614
C,0,2.4593050375,-1.3974112637,0.8575998013
C,0,1.4071365515,-1.8078687061,0.0338873318
C,0,1.1267354132,-1.0563591505,-1.109703145
C,0,1.8686414884,0.0792132746,-1.4183339631
C,0,0.5633347991,-3.0064141792,0.3730157476
H,0,3.4955910893,1.3659459221,-0.8256164973
H,0,4.0173584262,0.0413043151,1.2089204388
H,0,2.6880378552,-1.9685095168,1.7517430709
H,0,0.2975911774,-1.3442809923,-1.7464203674
H,0,1.6259649551,0.6544530341,-2.3050354586
H,0,-0.4805097987,-2.7068034287,0.4884465879
H,0,0.8947819039,-3.4808562736,1.2971254829
H,0,0.604886307,-3.7501548982,-0.4260829307
N,0,0.3636959215,1.5944459669,0.6560394545
O,0,0.3102315514,0.6530444936,1.2319263813
O,0,0.4408169271,2.5691131708,0.1349877371
F,0,-1.9421347651,-0.6496399056,0.2378920759
B,0,-2.172463991,0.6113776041,-0.3144720273
F,0,-1.1022100971,0.9097232923,-1.2009200654
F,0,-3.3851389809,0.6837206155,-0.9612487511
F,0,-2.0870646935,1.5843261004,0.7216187863

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.082_828846

M062X/6-311G*
E(RM062X) = -900.938785019

Zero-point correction= 0.157858 (Hartree/Particle)
Thermal correction to Energy= 0.174061
Thermal correction to Enthalpy= 0.175005
Thermal correction to Gibbs Free Energy= 0.109939
Sum of electronic and ZPE= -900.780927
Sum of electronic and thermal Energies= -900.764724
Sum of electronic and thermal Enthalpies= -900.763780
Sum of electronic and thermal Free Energies= -900.828846

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.225	54.856	136.942

C,0,1.3409027005,1.552797146,-1.0520858244
C,0,1.8091977332,1.8374741283,0.2295760222
C,0,2.8357901158,1.0803245579,0.7819690563
C,0,3.412892438,0.0192900195,0.0754096601
C,0,2.9332802289,-0.2600284394,-1.2060279567
C,0,1.9100167637,0.5036472433,-1.7696123857
C,0,4.5364265117,-0.7787426359,0.6816968552
H,0,0.5312544001,2.13161121,-1.4781459947
H,0,1.3666046753,2.6460735721,0.7998590625
H,0,3.1934108277,1.3078709992,1.7813684323
H,0,3.3662127218,-1.0781001374,-1.7733688517
H,0,1.5560081803,0.2753658958,-2.7696536449
H,0,4.3370093971,-1.0079116499,1.7300353251
H,0,5.4707146091,-0.2124937846,0.6440528147
H,0,4.6936130858,-1.7163336121,0.1479092798
N,0,-0.0321601093,-1.0903428283,-0.2612124699
O,0,0.4278772044,-0.8565045538,0.7158620969
O,0,-0.4350034912,-1.383175228,-1.2490525605
F,0,-2.1671837211,-1.2972614172,0.7470229202
B,0,-2.6391990552,0.0413360766,0.586338501
F,0,-1.5900287795,0.7329468481,-0.0972198282
F,0,-3.7839862318,0.0421990504,-0.1884343734
F,0,-2.8433322049,0.6173545392,1.8262228637

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.181_825313

M062X/6-311G*
E(RM062X) = -900.939838216

Zero-point correction= 0.158489 (Hartree/Particle)
Thermal correction to Energy= 0.174100
Thermal correction to Enthalpy= 0.175044
Thermal correction to Gibbs Free Energy= 0.114525
Sum of electronic and ZPE= -900.781349
Sum of electronic and thermal Energies= -900.765738
Sum of electronic and thermal Enthalpies= -900.764794
Sum of electronic and thermal Free Energies= -900.825313

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.249	54.580	127.373

C,0,0.4280663924,-1.7326195446,-0.5014703286
C,0,-0.8768651758,-1.4904098778,-0.9386734265
C,0,-1.1829461102,-0.315576944,-1.6198432413
C,0,-0.1986183173,0.6452802881,-1.8712634458
C,0,1.1024849863,0.3906863156,-1.4339126823
C,0,1.4169129862,-0.7881233592,-0.7567074546
C,0,-0.5723088549,1.9248464361,-2.5682857944
H,0,0.6668482746,-2.6491723107,0.0256992781
H,0,-1.6610252878,-2.2163578079,-0.7496778096
H,0,-2.1991929879,-0.1309933478,-1.947410824
H,0,1.8802270878,1.1256013759,-1.6174440685
H,0,2.4344116711,-0.9641845782,-0.4259745228
H,0,-1.373606563,2.4228435778,-2.0193229524
H,0,-0.9507381629,1.7221328071,-3.5730983238
H,0,0.278383947,2.6016264599,-2.6528410799
N,0,-1.2248234453,0.2343076169,1.3737717494
O,0,-0.340178919,0.8650553916,1.1622240997

O,0,-2.0712799838,-0.4107536811,1.6788385917
F,0,-2.543628696,1.7438204997,0.2304453368
B,0,-3.7932030496,1.3180654787,-0.3385998047
F,0,-4.8269080586,1.978211481,0.3060972398
F,0,-3.778657898,1.6026297152,-1.7002811201
F,0,-3.8836951352,-0.0684010923,-0.129921616

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.187_824934

M062X/6-311G*
E(RM062X) = -900.939888477

Zero-point correction= 0.158650 (Hartree/Particle)
Thermal correction to Energy= 0.174211
Thermal correction to Enthalpy= 0.175155
Thermal correction to Gibbs Free Energy= 0.114954
Sum of electronic and ZPE= -900.781239
Sum of electronic and thermal Energies= -900.765678
Sum of electronic and thermal Enthalpies= -900.764734
Sum of electronic and thermal Free Energies= -900.824934

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.319	54.545	126.703

C,0,2.7045212267,-0.1849626679,1.3212967143
C,0,3.2452063549,0.6317890523,0.3322788173
C,0,2.4370823851,1.551051905,-0.3349009785
C,0,1.0804629258,1.6773795667,-0.025004564
C,0,0.5501062507,0.8621069867,0.9779499425
C,0,1.3509756663,-0.0644010797,1.6427658722
C,0,0.1916809936,2.6552706487,-0.7448846336
H,0,3.3277888973,-0.904431011,1.839938336
H,0,4.294870174,0.5487346277,0.0734719138
H,0,2.8649497372,2.1727243806,-1.1155409891
H,0,-0.5025969604,0.9401679062,1.2229437791
H,0,0.9134970938,-0.6938475181,2.4108958226
H,0,0.562643117,2.8669841738,-1.7488461973
H,0,0.1428212655,3.6032470084,-0.2018296658
H,0,-0.8212801653,2.258325724,-0.8173257953
N,0,0.7294055613,-1.6788101951,-0.685250406
O,0,0.2201213226,-2.4027040557,-0.0203042457
O,0,1.2915579471,-1.0344423303,-1.3882901476
F,0,-3.3642110674,-1.1348018418,-0.775157018
B,0,-2.2770046382,-0.4758894384,-0.2245416541
F,0,-1.8250565007,-1.1400175776,0.9276679577
F,0,-1.1939042721,-0.4944690216,-1.167793754
F,0,-2.5838313147,0.8494277575,0.0719598935

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.188_825412

M062X/6-311G*
E(RM062X) = -900.939815265

Zero-point correction= 0.158459 (Hartree/Particle)
Thermal correction to Energy= 0.174067
Thermal correction to Enthalpy= 0.175011
Thermal correction to Gibbs Free Energy= 0.114403
Sum of electronic and ZPE= -900.781356
Sum of electronic and thermal Energies= -900.765748
Sum of electronic and thermal Enthalpies= -900.764804
Sum of electronic and thermal Free Energies= -900.825412

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.229	54.568	127.561

C,0,-1.7898816071,-2.8902163023,-1.0844161286
C,0,-0.5995805204,-2.175573497,-1.0008772486
C,0,0.3456603445,-2.4998846375,-0.0269771826
C,0,0.1239174738,-3.5427106509,0.8740693341
C,0,-1.0707997664,-4.2629554471,0.7743780492
C,0,-2.0209992221,-3.9390190393,-0.1903220578
C,0,1.1117366064,-3.8850741552,1.9553850373
H,0,-2.5270012112,-2.6427349893,-1.839626743
H,0,-0.4048927542,-1.3612716155,-1.6898852617
H,0,1.2662635954,-1.9278653365,0.035549755
H,0,-1.2601737197,-5.0738742757,1.4679582795
H,0,-2.9427673681,-4.5091755559,-0.2439585396
H,0,0.6284618307,-3.8150230492,2.931443982
H,0,1.9764373761,-3.2210565072,1.9355367197
H,0,1.4654362899,-4.9131143963,1.8466786042
N,0,-2.7682530898,-1.947087017,1.7995704401
O,0,-1.8369482361,-1.3573833986,1.6975253889
O,0,-3.7504543013,-2.4507005432,1.885226629
F,0,-1.8118020739,-3.1130210107,3.5460317168
B,0,-2.2880495354,-4.4264073837,3.8834456185
F,0,-1.2183800543,-5.3137667293,3.8246162866
F,0,-2.8468509034,-4.3887171258,5.1501803492
F,0,-3.2568256535,-4.7666943367,2.9235255716

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.189_824858

M062X/6-311G*
E(RM062X) = -900.939899573

Zero-point correction= 0.158697 (Hartree/Particle)
Thermal correction to Energy= 0.174251
Thermal correction to Enthalpy= 0.175195
Thermal correction to Gibbs Free Energy= 0.115042
Sum of electronic and ZPE= -900.781203
Sum of electronic and thermal Energies= -900.765649
Sum of electronic and thermal Enthalpies= -900.764704
Sum of electronic and thermal Free Energies= -900.824858

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.344	54.522	126.603

C,0,2.906949854,0.6761250119,0.6403598081
C,0,1.7026454713,0.4796855419,1.3194966808
C,0,0.8962586933,-0.6158625268,1.0185719656
C,0,1.2700919418,-1.5306947325,0.0306329341
C,0,2.4786470157,-1.3259171773,-0.6397507529
C,0,3.2930522267,-0.2351602865,-0.3384158064
C,0,0.374100766,-2.6965291438,-0.2894638802
H,0,3.5358723271,1.526749423,0.876832242
H,0,1.3869269029,1.1801544495,2.0858086727
H,0,-0.0428142126,-0.7536492233,1.5412832925

H,0,2.782727701,-2.0230945521,-1.4146394746
H,0,4.2256047884,-0.0946966779,-0.8735443063
H,0,0.5759408892,-3.5329238694,0.385620335
H,0,0.5281163425,-3.0494938184,-1.3101824577
H,0,-0.6712632255,-2.4122765814,-0.165273172
N,0,0.3280920719,1.6097963877,-0.9859398642
O,0,0.7785837929,0.9095046679,-1.715248253
O,0,-0.0897374992,2.3854794416,-0.3156547103
F,0,-1.6643419159,1.1209860658,1.2996211953
B,0,-2.2873367769,0.2286169927,0.4119907963
F,0,-2.3231970044,-1.0514091359,0.9600225204
F,0,-3.557585808,0.6720884578,0.0817930856
F,0,-1.4819583423,0.1928472853,-0.7770988508

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.189_825651

M062X/6-311G*
E(RM062X) = -900.939827037

Zero-point correction= 0.158396 (Hartree/Particle)
Thermal correction to Energy= 0.174055
Thermal correction to Enthalpy= 0.175000
Thermal correction to Gibbs Free Energy= 0.114176
Sum of electronic and ZPE= -900.781431
Sum of electronic and thermal Energies= -900.765772
Sum of electronic and thermal Enthalpies= -900.764827
Sum of electronic and thermal Free Energies= -900.825651

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.221	54.598	128.015

C,0,-2.8322277737,-4.3493292628,-0.5116668038
C,0,-3.667235587,-4.1647892802,-1.608547912
C,0,-3.1498717338,-3.6768793048,-2.8091685598
C,0,-1.7942871648,-3.3700547127,-2.9379935606
C,0,-0.9608515209,-3.5695585454,-1.8326524329
C,0,-1.4725605128,-4.0494064043,-0.6301492958
C,0,-1.2200944782,-2.808793641,-4.2100228555
H,0,-3.2293098322,-4.7282120382,0.4230635203
H,0,-4.7238371009,-4.3958827201,-1.5320010745
H,0,-3.813341374,-3.5266122589,-3.6552643303
H,0,0.0932326566,-3.3321167277,-1.9143343704
H,0,-0.8065905302,-4.1902796844,0.2149749152
H,0,-0.468522359,-3.483813184,-4.6266906285
H,0,-0.7193007142,-1.8618319623,-4.0017449387
H,0,-1.9913164518,-2.648443811,-4.9639829312
N,0,-2.1493765293,-1.2432430388,-0.2697897675
O,0,-1.4674550503,-1.2249394669,0.6020611972
O,0,-2.9023659254,-1.2237631015,-1.0809568547
F,0,1.360184381,-1.4565717658,-2.6151181554
B,0,0.8405232884,-0.7731135942,-1.5200359247
F,0,0.9062529773,-1.5740107098,-0.3681894755
F,0,1.4951244501,0.4310238132,-1.3178006871
F,0,-0.5516799148,-0.5098549984,-1.7650949737

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.234_824226

M062X/6-311G*
E(RM062X) = -900.936710619

Zero-point correction= 0.158182 (Hartree/Particle)
Thermal correction to Energy= 0.174185
Thermal correction to Enthalpy= 0.175130
Thermal correction to Gibbs Free Energy= 0.112484
Sum of electronic and ZPE= -900.778528
Sum of electronic and thermal Energies= -900.762525
Sum of electronic and thermal Enthalpies= -900.761581
Sum of electronic and thermal Free Energies= -900.824226

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.303	54.812	131.849

C,0,4.2454573101,-2.7180703235,-0.4866097869
C,0,4.350940463,-2.4569922,-1.8510129158
C,0,4.8477056999,-1.2364458466,-2.2970307528
C,0,5.2473744787,-0.2457346836,-1.3931916373
C,0,5.1336632167,-0.5153280291,-0.0280829248
C,0,4.6401325675,-1.7435286787,0.4235388461
C,0,5.7986406315,1.0660014965,-1.8883174114
H,0,3.8283549103,-3.6550953067,-0.1402010726
H,0,4.0258104032,-3.2024701189,-2.5672687481
H,0,4.9203473608,-1.0423806986,-3.3629625656
H,0,5.4423623343,0.2368249608,0.6920520287
H,0,4.5573182908,-1.9326088384,1.4886130777
H,0,6.7802341379,0.9214172881,-2.3461284374
H,0,5.9120200447,1.7826212543,-1.0741052179
H,0,5.1487012093,1.5073752087,-2.6467328101
N,0,2.1751754636,-0.2799855106,-0.0061144746
O,0,2.1156760675,-0.5746967332,-1.069072002
O,0,2.1949311974,0.105385034,1.0340969724
F,0,1.6935304338,-4.5235858425,0.2539199869
B,0,0.9802209843,-3.3697625154,-0.0572402315
F,0,1.2304063877,-2.9757363945,-1.3790082068
F,0,-0.3801442817,-3.5504583581,0.150160195
F,0,1.4344069886,-2.3036571639,0.7939556888

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.278_828463

M062X/6-311G*
E(RM062X) = -900.941417319

Zero-point correction= 0.158272 (Hartree/Particle)
Thermal correction to Energy= 0.174123
Thermal correction to Enthalpy= 0.175068
Thermal correction to Gibbs Free Energy= 0.112955
Sum of electronic and ZPE= -900.783145
Sum of electronic and thermal Energies= -900.767294
Sum of electronic and thermal Enthalpies= -900.766350
Sum of electronic and thermal Free Energies= -900.828463

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.264	54.696	130.727

C,0,-1.1872823781,3.6315802963,0.8289433573
C,0,-1.6006933305,2.3358517309,1.1447693826
C,0,-0.6646129431,1.3129218045,1.2739732178
C,0,0.7008511922,1.5597493949,1.0922390447
C,0,1.1000279451,2.8617355832,0.7864226113
C,0,0.1676172991,3.8904714185,0.6532380911
C,0,1.6961892241,0.4364596811,1.1998545557
H,0,-1.9152522665,4.4286399419,0.7317288147
H,0,-2.6539625483,2.1249669462,1.2980413875
H,0,-0.9939258097,0.3057988156,1.5076985684
H,0,2.1545415802,3.0743897777,0.6423730293
H,0,0.5018077912,4.8929753016,0.4108045462
H,0,1.6058574083,-0.0723972405,2.1622800976
H,0,2.7190600725,0.8007326873,1.1015654659
H,0,1.5115000003,-0.3033614011,0.4180668548
N,0,-1.2826613721,1.5472679034,-1.6995791587
O,0,-2.3131839366,1.1443925852,-1.6707217138
O,0,-0.2846470534,2.017251015,-1.7596166233
F,0,-0.5543961358,-0.1634651169,-3.2286461017
B,0,-0.0534207317,-1.095951756,-2.2750697654
F,0,-0.4290811778,-0.5590085834,-1.0028610684
F,0,-0.6423373646,-2.3303996711,-2.4584461281
F,0,1.3267164353,-1.1571044144,-2.3525722657

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.281_828248

M062X/6-311G*
E(RM062X) = -900.941709578

Zero-point correction= 0.158256 (Hartree/Particle)
Thermal correction to Energy= 0.173992
Thermal correction to Enthalpy= 0.174936
Thermal correction to Gibbs Free Energy= 0.113462
Sum of electronic and ZPE= -900.783454
Sum of electronic and thermal Energies= -900.767718
Sum of electronic and thermal Enthalpies= -900.766774
Sum of electronic and thermal Free Energies= -900.828248

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.182	54.666	129.384

C,0,-0.3566508889,0.2877816534,3.2797219507
C,0,-1.017303971,1.3231369554,2.6172649763
C,0,-1.5667873415,1.1106021483,1.3547470394
C,0,-1.4664735306,-0.1346730182,0.7269279174
C,0,-0.8169817951,-1.1663138205,1.4086650706
C,0,-0.2639025471,-0.9602889129,2.671484038
C,0,-1.9934855423,-0.3343767733,-0.6679978928
H,0,0.0676522092,0.4517344852,4.2634818719
H,0,-1.1110486499,2.2961182632,3.0884265651
H,0,-2.0681344428,1.9238314407,0.8412216525
H,0,-0.7356536326,-2.1429671768,0.9418357425
H,0,0.2396478452,-1.7752132232,3.1792195977
H,0,-2.2342050084,-1.381459989,-0.8561158875
H,0,-1.2436935346,-0.0164637601,-1.397314509
H,0,-2.8890166106,0.2645419352,-0.8403278015
N,0,1.3752701838,1.7409685849,0.9023599153
O,0,1.3491740029,2.8121030462,1.1811729391
O,0,1.4561031021,0.6611383587,0.6832932984
F,0,-0.0757077989,2.1633850917,-0.9387803872
B,0,0.8923215701,2.1969346228,-1.9919230208
F,0,0.723382196,3.3343317993,-2.7551557187
F,0,2.153984686,2.2248122687,-1.3293813725
F,0,0.7822085992,1.0381631201,-2.744592885

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.293_826543

M062X/6-311G*
E(RM062X) = -900.938018478

Zero-point correction= 0.157623 (Hartree/Particle)
Thermal correction to Energy= 0.173649
Thermal correction to Enthalpy= 0.174593
Thermal correction to Gibbs Free Energy= 0.111476
Sum of electronic and ZPE= -900.780396
Sum of electronic and thermal Energies= -900.764369
Sum of electronic and thermal Enthalpies= -900.763425
Sum of electronic and thermal Free Energies= -900.826543

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	108.966	54.877	132.842

C,0,-0.1282562982,-0.4948018958,4.1134327163
C,0,-0.2961572025,0.8846727328,4.0708531952
C,0,-1.5759675064,1.4382677229,4.0439683119
C,0,-2.7113003767,0.6272981097,4.0656482516
C,0,-2.5301524166,-0.7601887345,4.1125490878
C,0,-1.2519434244,-1.319208929,4.1364489789
C,0,-4.0946098501,1.2233621543,4.0696873062
H,0,0.8577187468,-0.9408960104,4.1012599901
H,0,0.5701917111,1.5362262784,4.0468962433
H,0,-1.6938814737,2.5165620313,4.0024138837
H,0,-3.4008906631,-1.4100955893,4.1377410211
H,0,-1.1280662067,-2.3955884728,4.1602352611
H,0,-4.0814796559,2.257268563,3.7228448625
H,0,-4.5113524577,1.2169647623,5.0801886737
H,0,-4.7760296997,0.6554060978,3.4335586669
N,0,-1.7525657384,-1.0170713715,1.2969635208
O,0,-2.2974158455,-1.9783353499,1.2297385898
O,0,-1.2726551872,-0.0195145598,1.287124108
F,0,-0.7875700467,-3.8557367788,2.1938555591
B,0,0.4944007611,-3.3134807342,2.0098285304
F,0,0.316800947,-2.0152952771,1.4195050296
F,0,1.1311253983,-3.1615932612,3.2383985913
F,0,1.243960185,-4.0982222882,1.1483676204

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.351_828876

M062X/6-311G*
E(RM062X) = -900.941679148

Zero-point correction= 0.158260 (Hartree/Particle)
Thermal correction to Energy= 0.174035
Thermal correction to Enthalpy= 0.174979
Thermal correction to Gibbs Free Energy= 0.112803
Sum of electronic and ZPE= -900.783419

Sum of electronic and thermal Energies= -900.767644
Sum of electronic and thermal Enthalpies= -900.766700
Sum of electronic and thermal Free Energies= -900.828876

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.208	54.679	130.861

C,0,-4.6720445495,-1.3561255034,0.0203870703
C,0,-4.0514805331,-0.9090785365,1.1856874949
C,0,-3.4466628142,0.348286831,1.2226614287
C,0,-3.4514351224,1.181294076,0.100604797
C,0,-4.0859034092,0.7224786301,-1.0574047248
C,0,-4.6893521908,-0.531051507,-1.1019237694
C,0,-2.762728993,2.5184614793,0.1098115952
H,0,-5.1454877372,-2.330613761,-0.0082514475
H,0,-4.0455125429,-1.5353432653,2.0717808001
H,0,-2.9605912596,0.6852607227,2.1325295772
H,0,-4.0987138151,1.3560014876,-1.9391606113
H,0,-5.1720449687,-0.864744547,-2.0135509607
H,0,-2.4899957302,2.8162328407,1.1220968222
H,0,-3.4029990503,3.2900238791,-0.3225837646
H,0,-1.8436234147,2.4677286801,-0.4779655286
N,0,-1.3218533119,-1.4187658636,0.069717911
O,0,-1.6459235674,-1.0374954521,-0.9156162625
O,0,-1.011872907,-1.8714129426,1.0309213704
F,0,0.2298573296,1.3796541435,-1.262637894
B,0,0.6373850368,0.7304334351,-0.1027873223
F,0,1.7248675624,1.3379779894,0.4833770313
F,0,-0.4649056507,0.6897131985,0.8035124478
F,0,0.9197456392,-0.6307580148,-0.4058130602

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.378_823817

M062X/6-311G*
E(RM062X) = -900.938779720

Zero-point correction= 0.158695 (Hartree/Particle)
Thermal correction to Energy= 0.174204
Thermal correction to Enthalpy= 0.175148
Thermal correction to Gibbs Free Energy= 0.114963
Sum of electronic and ZPE= -900.780085
Sum of electronic and thermal Energies= -900.764576
Sum of electronic and thermal Enthalpies= -900.763632
Sum of electronic and thermal Free Energies= -900.823817

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.315	54.548	126.670

C,0,-3.1766916697,0.405147725,-0.789498797
C,0,-2.037032545,0.3016477909,-1.5828908326
C,0,-1.0334735513,-0.6134374831,-1.2559575198
C,0,-1.1526020698,-1.4438623184,-0.1380408884
C,0,-2.2995758103,-1.3239059835,0.651823331
C,0,-3.3013630857,-0.4106118491,0.3331253321
C,0,-0.0873868727,-2.4541416438,0.1907296624
H,0,-3.9580387174,1.1122639684,-1.0427481569
H,0,-1.9279694011,0.9270131031,-2.4627620672
H,0,-0.1396293818,-0.6785748587,-1.8660883709
H,0,-2.4075644588,-1.9533989559,1.529878419
H,0,-4.1809483348,-0.3349826503,0.9627124025
H,0,0.1617213647,-2.4267892054,1.2521329649
H,0,0.8229710252,-2.2558962635,-0.3736149469
H,0,-0.4338908879,-3.4628099088,-0.049882836
N,0,-0.268253384,1.6874279109,0.3533189997
O,0,0.4268644823,2.023661483,-0.440905313
O,0,-0.9902187976,1.4521221152,1.1580293576
F,0,2.9879599237,1.2656209989,0.4947580692
B,0,2.3759347562,0.0179948248,0.3726966965
F,0,1.1556426582,0.0680538817,1.1316819179
F,0,2.0235910136,-0.2008502546,-0.967384807
F,0,3.172539744,-1.0024554269,0.853802383

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.379_825489

M062X/6-311G*
E(RM062X) = -900.938705281

Zero-point correction= 0.158235 (Hartree/Particle)
Thermal correction to Energy= 0.174004
Thermal correction to Enthalpy= 0.174948
Thermal correction to Gibbs Free Energy= 0.113216
Sum of electronic and ZPE= -900.780471
Sum of electronic and thermal Energies= -900.764702
Sum of electronic and thermal Enthalpies= -900.763758
Sum of electronic and thermal Free Energies= -900.825489

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.189	54.728	129.925

C,0,5.0359678023,-1.4192549029,-3.5178172376
C,0,5.5163269546,-0.2064617963,-3.0278772333
C,0,5.5411052512,0.0361996888,-1.6568274354
C,0,5.0883048008,-0.9212340681,-0.7444408747
C,0,4.6012885266,-2.1307734932,-1.2476470599
C,0,4.577052603,-2.3811579742,-2.6218724752
C,0,5.1434704099,-0.6668656478,0.7372949252
H,0,5.0207182965,-1.6123130039,-4.5841944042
H,0,5.8715229629,0.5530858533,-3.7154297582
H,0,5.9158313423,0.9858671958,-1.28717423
H,0,4.2296909006,-2.8775160651,-0.5551966665
H,0,4.2061641078,-3.332748548,-2.9879000488
H,0,4.5538543304,-1.4036484643,1.2814570403
H,0,4.7472508438,0.3201254518,0.9779599772
H,0,6.1763110135,-0.714116059,1.0925764109
N,0,2.0563904881,-0.9317489485,-1.9997373851
O,0,2.5276604311,0.0016387013,-2.3613136262
O,0,1.5191447449,-1.8599274986,-1.7219372119
F,0,2.2716177534,-0.2303421659,0.1656389745
B,0,1.7570064829,-1.168919609,1.1268052571
F,0,2.3420830975,-2.4135627568,0.8448695467
F,0,2.0835065409,-0.7409487248,2.3995503658
F,0,0.379534815,-1.2473267648,0.9347260495

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.423_822985

M062X/6-311G*

E(RM062X) = -900.937556839

Zero-point correction= 0.158613 (Hartree/Particle)
Thermal correction to Energy= 0.174294
Thermal correction to Enthalpy= 0.175238
Thermal correction to Gibbs Free Energy= 0.114572
Sum of electronic and ZPE= -900.778944
Sum of electronic and thermal Energies= -900.763263
Sum of electronic and thermal Enthalpies= -900.762319
Sum of electronic and thermal Free Energies= -900.822985

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.371	54.626	127.683

C,0,0.4017946698,1.7110812507,0.3101736678
C,0,0.7281748427,0.7384032063,1.2502803114
C,0,1.9392528611,0.0551391118,1.15327642
C,0,2.844298533,0.3261514132,0.1184166259
C,0,2.502551002,1.3056606558,-0.8157280724
C,0,1.2949781459,1.9958026259,-0.7185245211
C,0,4.1617192961,-0.4007610354,0.0489542608
H,0,-0.557111968,2.2076028088,0.3666955866
H,0,0.0232963472,0.4946436756,2.0353369808
H,0,2.1897457521,-0.7022884386,1.8911795012
H,0,3.1877327573,1.5313803101,-1.6268665492
H,0,1.0458934397,2.7478851161,-1.4587308992
H,0,4.0552763778,-1.4458651468,0.3467256759
H,0,4.8868955108,0.0568906014,0.7269327344
H,0,4.582582051,-0.3702735109,-0.9567134437
N,0,0.4197669688,-1.5536495995,-0.7186796746
O,0,0.2071828859,-0.7291272943,-1.4222657297
O,0,0.6627458674,-2.4365707849,-0.0920823649
F,0,-2.3722881807,0.7533954637,1.286801276
B,0,-2.4414282147,-0.1864708741,0.2612929516
F,0,-2.0892801726,0.3946523026,-0.9643214095
F,0,-1.483566439,-1.2262722208,0.5270401398
F,0,-3.7037773337,-0.7562396369,0.1897185318

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.534_823904

M062X/6-311G*
E(RM062X) = -900.937909738

Zero-point correction= 0.158688 (Hartree/Particle)
Thermal correction to Energy= 0.174418
Thermal correction to Enthalpy= 0.175362
Thermal correction to Gibbs Free Energy= 0.114005
Sum of electronic and ZPE= -900.779222
Sum of electronic and thermal Energies= -900.763492
Sum of electronic and thermal Enthalpies= -900.762548
Sum of electronic and thermal Free Energies= -900.823904

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.449	54.572	129.136

C,0,-0.1827941978,0.2710149976,4.1029893471
C,0,-0.5586636205,1.4778532671,3.5152248257
C,0,-1.7991906838,1.601067815,2.895548805
C,0,-2.6890395883,0.5243948776,2.8554795715
C,0,-2.2942166155,-0.6851518431,3.4422925836
C,0,-1.0528442145,-0.8143756347,4.0630405722
C,0,-4.0532673079,0.6682286928,2.2327242557
H,0,0.7870320144,0.174580425,4.5768642047
H,0,0.1177476268,2.325082974,3.5359859398
H,0,-2.0835087382,2.5448127762,2.4408573187
H,0,-2.9583561717,-1.5426129381,3.4066769306
H,0,-0.7653888027,-1.7675403734,4.4903206773
H,0,-4.7902878347,0.93437274,2.9949556785
H,0,-4.3861171335,-0.2648821686,1.7741758964
H,0,-4.0657504871,1.451787923,1.4739016776
N,0,-0.9710671392,-1.1700906807,0.9739511364
O,0,-1.7980523853,-1.8489011527,0.6863754483
O,0,-0.1434470013,-0.456901479,1.1533270096
F,0,-1.8354157599,-3.6100469986,2.6341818651
B,0,-0.4611318306,-3.8927924241,2.7176449467
F,0,0.2237135286,-2.8168810341,2.0593462666
F,0,-0.0561607853,-3.9328434937,4.0482510546
F,0,-0.1666673721,-5.0787564677,2.0633665884

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.645_825367

M062X/6-311G*
E(RM062X) = -900.939301383

Zero-point correction= 0.158242 (Hartree/Particle)
Thermal correction to Energy= 0.174002
Thermal correction to Enthalpy= 0.174946
Thermal correction to Gibbs Free Energy= 0.113935
Sum of electronic and ZPE= -900.781059
Sum of electronic and thermal Energies= -900.765299
Sum of electronic and thermal Enthalpies= -900.764355
Sum of electronic and thermal Free Energies= -900.825367

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.188	54.800	128.409

C,0,-3.3774283996,-0.5490399188,0.7441193801
C,0,-2.4252231216,0.1666412721,1.4692105575
C,0,-1.5037190101,0.9743913772,0.8131193981
C,0,-1.5207855639,1.0880298281,-0.5825299331
C,0,-2.4796030763,0.361043599,-1.3001722189
C,0,-3.4026111038,-0.4504206569,-0.6440070119
C,0,-0.5421555025,1.9921391313,-1.2852106194
H,0,-4.0906115952,-1.1828845432,1.2583036371
H,0,-2.394347408,0.0853075844,2.549742893
H,0,-0.7437674509,1.5047551527,1.3751760737
H,0,-2.506176698,0.4410404415,-2.3829315661
H,0,-4.1376131209,-1.0036604171,-1.2174029247
H,0,-0.8661500535,3.0325949134,-1.1962779136
H,0,-0.4749433335,1.7601298805,-2.3497924395
H,0,0.4530968102,1.9228107284,-0.843724195
N,0,-0.1593801647,-1.4104047382,-0.7358147305
O,0,-0.7885982834,-1.9690477065,-0.0154037438
O,0,0.4839737901,-0.9527153849,-1.5140411295
F,0,2.3709172822,0.5031175326,-0.5214230599
B,0,2.1019300588,0.4198355529,0.8535514224
F,0,3.2363193042,0.0578088338,1.5598633814

F,0,1.5856287256,1.6316580191,1.3112346512
F,0,1.0993409148,-0.5941524813,1.0214040911

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.689_828697

M062X/6-311G*
E(RM062X) = -900.940818005

Zero-point correction= 0.157931 (Hartree/Particle)
Thermal correction to Energy= 0.173884
Thermal correction to Enthalpy= 0.174828
Thermal correction to Gibbs Free Energy= 0.112121
Sum of electronic and ZPE= -900.782887
Sum of electronic and thermal Energies= -900.766934
Sum of electronic and thermal Enthalpies= -900.765990
Sum of electronic and thermal Free Energies= -900.828697

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.114	54.838	131.980

C,0,3.5239603318,-3.107381134,0.3385598937
C,0,3.9653116205,-1.9103904588,0.9035781095
C,0,3.9904230906,-1.7551489644,2.2834862183
C,0,3.5762385835,-2.7907196001,3.1301626937
C,0,3.1382031206,-3.9866461465,2.551613153
C,0,3.1114029379,-4.1461733514,1.1657555847
C,0,3.6135523984,-2.6070914127,4.6245992043
H,0,3.4990691624,-3.2247822722,-0.7385062341
H,0,4.2803130404,-1.0939786016,0.2637427592
H,0,4.3123727018,-0.8146983167,2.7171257173
H,0,2.8202134519,-4.8031985046,3.193394659
H,0,2.7677821861,-5.081041323,0.7377470512
H,0,4.6455987948,-2.5988104861,4.9834653318
H,0,3.089221161,-3.4122316009,5.1418438574
H,0,3.1596681271,-1.6553553988,4.9068638133
N,0,0.7704594187,-2.1939564854,2.617102198
O,0,0.9766599879,-1.8876404998,1.5750730053
O,0,0.507085039,-2.5530689592,3.6311810888
F,0,1.0617540931,1.2201335107,1.918341358
B,0,0.6847463688,0.6790951457,3.1373414844
F,0,0.4429634538,1.6421793567,4.0918148578
F,0,-0.4617262884,-0.1438631009,2.9505512321
F,0,1.7135333182,-0.2128960959,3.580349163

Pi Complex NO_2BF_4 PCM PURE-M06-2X 3.732_828669

M062X/6-311G*
E(RM062X) = -900.941337422

Zero-point correction= 0.158135 (Hartree/Particle)
Thermal correction to Energy= 0.174048
Thermal correction to Enthalpy= 0.174992
Thermal correction to Gibbs Free Energy= 0.112668
Sum of electronic and ZPE= -900.783203
Sum of electronic and thermal Energies= -900.767290
Sum of electronic and thermal Enthalpies= -900.766345
Sum of electronic and thermal Free Energies= -900.828669

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	109.217	54.811	131.171

C,0,2.0296250026,3.3580986294,-0.9172365859
C,0,1.3634673117,3.2950016454,0.3020153471
C,0,1.6977269818,2.307794741,1.2291035816
C,0,2.6985276153,1.369627402,0.9523369127
C,0,3.3596808587,1.4471545694,-0.2789321807
C,0,3.03208978,2.4313120286,-1.2032250613
C,0,3.0705337203,0.3008328745,1.9467914117
H,0,1.7696024559,4.1211825851,-1.6416558061
H,0,0.5836269764,4.0113305191,0.5344648761
H,0,1.1774949453,2.2662640506,2.1817766363
H,0,4.1234821196,0.7141887153,-0.5149429536
H,0,3.5525170884,2.4724178105,-2.1533602293
H,0,4.0384913656,0.5233074247,2.4024788138
H,0,3.1532588356,-0.6705014774,1.4549682237
H,0,2.3361761969,0.2268594835,2.7506609317
N,0,0.3880880379,0.0730773907,-0.2550159791
O,0,0.4846511392,0.623010531,-1.2088380795
O,0,0.2145863121,-0.442721144,0.7094671887
F,0,2.0532083379,-2.5834674987,-2.6548032634
B,0,1.5610253326,-2.4204242908,-1.3754787311
F,0,0.1959900283,-2.0142984308,-1.4243862297
F,0,1.6852881721,-3.5672675835,-0.614976118
F,0,2.2448532861,-1.3402992757,-0.7266626054

Nitrations of Toluene Including a Sulfuric Acid Molecule

The transition structures in this section were located in M06-2X/6-311G*/PCM calculations with ε=109.

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.45_370364

m062x/6-311G*
E(RM062X) = -1176.50893228

Zero-point correction= 0.182468 (Hartree/Particle)
Thermal correction to Energy= 0.198253
Thermal correction to Enthalpy= 0.199197
Thermal correction to Gibbs Free Energy= 0.138569
Sum of electronic and ZPE= -1176.326464
Sum of electronic and thermal Energies= -1176.310679
Sum of electronic and thermal Enthalpies= -1176.309735
Sum of electronic and thermal Free Energies= -1176.370364

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.406	56.282	127.604

C,0,1.3698326556,0.0182068278,1.4911963992
C,0,2.5899498691,-1.3255273713,-0.6470028025
C,0,2.5940893992,0.4706352542,0.9465071895
C,0,0.7850171121,-1.1386896379,0.9525362602
C,0,3.2089348477,-0.2115676862,-0.1023284159
C,0,1.3770795171,-1.7899398491,-0.1128843569
C,0,0.7390432258,0.7231195096,2.6549407415

H,0,3.0407593302,-1.8429758482,-1.4853334544
H,0,3.0653574329,1.3518361486,1.3710279924
H,0,-0.1445732827,-1.5073785323,1.3724876921
H,0,4.1478659522,0.148454098,-0.5043464175
H,0,0.8992693438,-2.6610971288,-0.5449385977
N,0,0.7211368096,1.566735618,-0.3987408832
O,0,0.7166108908,0.906855788,-1.3075953998
O,0,0.5326120611,2.4831485281,0.2294796734
S,0,-2.4736213367,-0.2006640567,-0.2076509075
O,0,-1.6137190458,-1.004965783,-1.2627611712
O,0,-2.6152763146,-1.2079812018,1.0015424144
O,0,-3.7639241745,0.1036251227,-0.7479302073
O,0,-1.5879778941,0.8219883888,0.2705558856
H,0,-3.3619253283,-1.823071045,0.9167004716
H,0,-2.1352756725,-1.5760798946,-1.8497466355
H,0,0.9970519161,0.2022755461,3.5811898657
H,0,1.0977454939,1.749088853,2.7505217536
H,0,-0.348702808,0.7294223517,2.5667709102

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.42_370300

m062x/6-311G*
E(RM062X) = -1176.50889413

Zero-point correction= 0.182381 (Hartree/Particle)
Thermal correction to Energy= 0.198114
Thermal correction to Enthalpy= 0.199058
Thermal correction to Gibbs Free Energy= 0.138594
Sum of electronic and ZPE= -1176.326513
Sum of electronic and thermal Energies= -1176.310780
Sum of electronic and thermal Enthalpies= -1176.309836
Sum of electronic and thermal Free Energies= -1176.370300

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.318	56.277	127.257

C,0,1.2896093973,-0.0464573232,1.45272334
C,0,2.6550744219,-1.3535333857,-0.625937531
C,0,2.499232734,0.4696367623,0.9287105508
C,0,0.786408799,-1.2356836003,0.9118388947
C,0,3.1923251081,-0.1989456589,-0.0817417674
C,0,1.4483104282,-1.8679490353,-0.1267989498
C,0,0.6069055638,0.6403404102,2.5973056112
H,0,3.1628907709,-1.8620530078,-1.4364668036
H,0,2.9076929475,1.3826906203,1.3516899088
H,0,-0.1348646109,-1.6511579069,1.3043400249
H,0,4.1246637266,0.2063122471,-0.4550082315
H,0,1.0313890275,-2.769715771,-0.5598021815
N,0,0.7331289131,1.47343085,-0.5546129554
O,0,0.6922168606,0.7363151395,-1.40072942
O,0,0.5760197374,2.4443930554,-0.0046960422
S,0,-2.5146102658,-0.1972536271,-0.027546193
O,0,-1.7738866623,-1.1599251811,-1.0394291764
O,0,-2.5734654388,-1.0379761449,1.3098029412
O,0,-3.8403722439,0.0830171506,-0.4894992455
O,0,-1.5650632966,0.8439824497,0.2392611957
H,0,-3.3429942107,-1.6269909727,1.3724551751
H,0,-2.3599207049,-1.7843090339,-1.4971480685
H,0,1.1304754874,0.40677344,3.5284774831
H,0,0.6310003855,1.7276022352,2.4871356241
H,0,-0.429244875,0.3183642884,2.6921748161

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.41_370239

m062x/6-311G*
E(RM062X) = -1176.50813056

Zero-point correction= 0.182483 (Hartree/Particle)
Thermal correction to Energy= 0.198280
Thermal correction to Enthalpy= 0.199224
Thermal correction to Gibbs Free Energy= 0.137891
Sum of electronic and ZPE= -1176.325648
Sum of electronic and thermal Energies= -1176.309851
Sum of electronic and thermal Enthalpies= -1176.308907
Sum of electronic and thermal Free Energies= -1176.370239

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.422	56.198	129.085

C,0,1.3192603856,-0.0574419201,1.464644467
C,0,2.665139579,-1.3432928232,-0.6425476287
C,0,2.5160913703,0.4714784346,0.923054857
C,0,0.8191013379,-1.2488871114,0.9256319627
C,0,3.2023984729,-0.1898217369,-0.0986145123
C,0,1.4699306077,-1.8698081535,-0.126912706
C,0,0.647189778,0.6170336186,2.6221405683
H,0,3.1632125906,-1.8437464535,-1.4639492006
H,0,2.9258615469,1.3837004103,1.3463805772
H,0,-0.0856939709,-1.681977874,1.3384540709
H,0,4.1260767193,0.2248704597,-0.4826999663
H,0,1.0560534081,-2.7753207518,-0.5551313111
N,0,0.7784556459,1.4961839707,-0.5281052404
O,0,0.7100447106,0.7669805789,-1.3807276458
O,0,0.6330934374,2.4686636714,0.0243601844
S,0,-2.4126198876,-0.2152591959,0.1449491901
O,0,-1.8475892434,-1.0417161677,-1.0795586929
O,0,-2.6408870744,-1.0854888126,1.2616294104
O,0,-3.7822862796,0.3613850718,-0.38278063
O,0,-1.5376748886,0.9165451346,0.2455844139
H,0,-4.5407127391,-0.2251157614,-0.2295320171
H,0,-2.2165559644,-1.9364763584,-1.1621386398
H,0,1.181977764,0.3769430016,3.5452161407
H,0,0.6651695171,1.7050640689,2.5208113836
H,0,-0.3864828231,0.2896156993,2.7274249649

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.44_370143

m062x/6-311G*
E(RM062X) = -1176.50824968

Zero-point correction= 0.182460 (Hartree/Particle)
Thermal correction to Energy= 0.198238
Thermal correction to Enthalpy= 0.199182
Thermal correction to Gibbs Free Energy= 0.138107
Sum of electronic and ZPE= -1176.325789
Sum of electronic and thermal Energies= -1176.310012

Sum of electronic and thermal Enthalpies= -1176.309067
Sum of electronic and thermal Free Energies= -1176.370143

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.396	56.166	128.544

C,0,1.3772607127,0.0120189635,1.5014506462
C,0,2.5807194907,-1.340933762,-0.6419454989
C,0,2.5600179472,0.5003584927,0.8986639033
C,0,0.8268428595,-1.1860931251,1.0180598905
C,0,3.1690577184,-0.187264205,-0.1512847688
C,0,1.4087854916,-1.841583617,-0.0499525105
C,0,0.7587134538,0.7222472444,2.6679510624
H,0,3.0235529982,-1.8640071945,-1.4809596429
H,0,3.0070587524,1.4128854535,1.281033254
H,0,-0.0664511689,-1.5859199104,1.4867762148
H,0,4.077588265,0.1999454197,-0.5955925424
H,0,0.9589062347,-2.7482927333,-0.4368036722
N,0,0.6320262879,1.487948704,-0.4076070606
O,0,0.6085050705,0.8007559305,-1.2967766779
O,0,0.4345264432,2.4217196343,0.1932109351
S,0,-2.4386267361,-0.449940583,0.0520734533
O,0,-1.7555697949,-1.0919547737,-1.2217763486
O,0,-2.6772330264,-1.4590667182,1.0419713208
O,0,-3.8080510151,0.111798337,-0.4922057014
O,0,-1.64107296,0.7079999921,0.3376562814
H,0,-4.5362867182,-0.5295685407,-0.4601985373
H,0,-2.0587895924,-1.9917470298,-1.4259070134
H,0,1.0605134407,0.2291791595,3.5961748331
H,0,1.0873236107,1.7605823447,2.7305800184
H,0,-0.3307677655,0.6929085168,2.6131811616

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.46_370093

m062x/6-311G*
E(RM062X) = -1176.50757660

Zero-point correction= 0.182598 (Hartree/Particle)
Thermal correction to Energy= 0.198434
Thermal correction to Enthalpy= 0.199379
Thermal correction to Gibbs Free Energy= 0.137484
Sum of electronic and ZPE= -1176.324979
Sum of electronic and thermal Energies= -1176.309142
Sum of electronic and thermal Enthalpies= -1176.308198
Sum of electronic and thermal Free Energies= -1176.370093

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.520	56.117	130.268

C,0,1.3848620334,0.0290383966,1.5069950078
C,0,2.5867102601,-1.3253173034,-0.6351977056
C,0,2.6188747783,0.4609716968,0.9704829222
C,0,0.7837427465,-1.1178298372,0.962173494
C,0,3.2240994008,-0.2265681915,-0.0810832119
C,0,1.3656815084,-1.7739399677,-0.1055320323
C,0,0.7533351081,0.7422114696,2.6654340651
H,0,3.0312379998,-1.8456719895,-1.4750707434
H,0,3.105087154,1.3311453047,1.4004590576
H,0,-0.1487209234,-1.4762935517,1.3857014382
H,0,4.1709409849,0.11811688,-0.4780310821
H,0,0.87608982,-2.6369851287,-0.5405432009
N,0,0.7646321665,1.6035632932,-0.3757379748
O,0,0.7797579269,0.9560178475,-1.2931681569
O,0,0.5655177477,2.506643153,0.2666164004
S,0,-2.3306739583,-0.2437026587,-0.3217590812
O,0,-1.7845358479,-1.1048442768,-1.3301453991
O,0,-2.7641249993,-1.0915664957,0.9392309991
O,0,-3.6780388901,0.4041512115,-0.8223708262
O,0,-1.567567074,0.8453653336,0.2190395463
H,0,-3.1334527834,-1.9631635245,0.7224083616
H,0,-4.1858688527,-0.1565359382,-1.4309680176
H,0,0.9346150909,0.1796474853,3.5852836517
H,0,1.1718980744,1.7398650899,2.8040936088
H,0,-0.3278114714,0.820673702,2.533065879

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.43_369922

m062x/6-311G*
E(RM062X) = -1176.50753881

Zero-point correction= 0.182345 (Hartree/Particle)
Thermal correction to Energy= 0.198187
Thermal correction to Enthalpy= 0.199131
Thermal correction to Gibbs Free Energy= 0.137617
Sum of electronic and ZPE= -1176.325193
Sum of electronic and thermal Energies= -1176.309352
Sum of electronic and thermal Enthalpies= -1176.308408
Sum of electronic and thermal Free Energies= -1176.369922

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.364	56.256	129.468

C,0,1.2356313461,-2.0638017922,1.0980799472
C,0,3.28809509,-0.8672120359,-0.3361021218
C,0,1.4209414079,-0.6963756079,1.1910857181
C,0,2.0906581285,-2.847513665,0.3064154189
C,0,2.4366496239,-0.0643935603,0.4604456658
C,0,3.1324573218,-2.2532553507,-0.3860338494
H,0,0.4262129361,-2.5355760427,1.6425301782
H,0,4.0939216986,-0.3925389455,-0.8878343759
H,0,0.7788552522,-0.100995869,1.8302420737
H,0,1.9341221421,-3.9175099001,0.2431636589
C,0,2.6612747547,1.4135432414,0.5684120398
H,0,3.8030696639,-2.8496606407,-0.9920507362
N,0,1.3674431689,-0.283383964,-1.8523078481
O,0,0.7192059899,-1.1962028107,-1.7527515249
O,0,1.7627546045,0.6692987718,-2.3073577681
S,0,-1.4387591055,0.9826602834,0.1832064153
O,0,-1.8812427779,-0.3223801846,0.5789578596
O,0,-0.9502828136,1.7933386948,1.450922699
O,0,-2.6504183125,1.8303333467,-0.3644387819
O,0,-0.3875159307,1.1592020706,-0.7767175808
H,0,-3.5019860867,1.6121687968,0.0486700994
H,0,-1.4708944577,1.6278268674,2.2538183258
H,0,3.4335710916,1.6107289721,1.3173436136
H,0,3.0175585126,1.8379129998,-0.3730433382
H,0,1.7513867512,1.9312283244,0.871590212

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.46_369483

m062x/6-311G*
E(RM062X) = -1176.50823352

Zero-point correction= 0.182931 (Hartree/Particle)
Thermal correction to Energy= 0.198567
Thermal correction to Enthalpy= 0.199511
Thermal correction to Gibbs Free Energy= 0.138751
Sum of electronic and ZPE= -1176.325303
Sum of electronic and thermal Energies= -1176.309666
Sum of electronic and thermal Enthalpies= -1176.308722
Sum of electronic and thermal Free Energies= -1176.369483

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.603	56.035	127.881

C,0,-0.2180113637,-0.1126305268,0.1802629739
C,0,0.3424060906,0.3065852992,2.8883152504
C,0,1.1164260489,-0.0452716501,0.6383155167
C,0,-1.2637689474,0.0857346119,1.1068190417
C,0,1.3911183545,0.1622877867,1.981841526
C,0,-0.9860071472,0.2816401352,2.4467414479
C,0,-0.523012904,-0.2797282672,-1.2776102735
H,0,0.5559327187,0.4479907321,3.9412499018
H,0,1.9259258497,-0.1668930112,-0.0739010462
H,0,-2.2902194855,0.0719895234,0.7565812467
H,0,2.4170451447,0.1949099367,2.3272358604
H,0,-1.7960646639,0.4140849958,3.1542404267
N,0,-0.0508388814,-2.4795270392,0.8678731912
O,0,0.0939673567,-2.4907770615,1.9830529681
O,0,-0.1789248807,-2.9045203753,-0.1693899789
S,0,-3.3627752532,-2.4236822665,2.3141267481
O,0,-2.4169375421,-2.612282905,3.5682324851
O,0,-4.0247686248,-1.1535562514,2.3886856836
O,0,-4.414012081,-3.5911866857,2.450365735
O,0,-2.5415107099,-2.7810905869,1.1930591711
H,0,-5.190925217,-3.3591328703,2.9846338586
H,0,-2.7657760184,-2.2331677475,4.3914090888
H,0,-0.6658188957,0.704403524,-1.7326805234
H,0,0.2927110129,-0.7725277751,-1.8079532678
H,0,-1.4446129607,-0.8448025253,-1.430524032

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.46_369466

m062x/6-311G*
E(RM062X) = -1176.50823358

Zero-point correction= 0.182934 (Hartree/Particle)
Thermal correction to Energy= 0.198569
Thermal correction to Enthalpy= 0.199513
Thermal correction to Gibbs Free Energy= 0.138768
Sum of electronic and ZPE= -1176.325300
Sum of electronic and thermal Energies= -1176.309665
Sum of electronic and thermal Enthalpies= -1176.308721
Sum of electronic and thermal Free Energies= -1176.369466

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.604	56.034	127.849

C,0,1.1223484806,-1.4486463115,1.1981616853
C,0,3.3522312733,-1.0312245389,-0.4300078128
C,0,1.6854665978,-0.1883762866,1.1235312701
C,0,1.6664662364,-2.502005332,0.4534159251
C,0,2.793472644,0.0522640414,0.2833623755
C,0,2.7908594794,-2.2965513705,-0.3439892793
H,0,0.2597581439,-1.6200186513,1.8313047162
H,0,4.2227688108,-0.8594496239,-1.0545007027
H,0,1.2733930678,0.6307732153,1.7028799772
H,0,1.2148361598,-3.485694278,0.5048555919
C,0,3.4274977546,1.4096648036,0.2406655957
H,0,3.2150460949,-3.1179067984,-0.9081951792
N,0,1.2861131834,0.2102248444,-1.6674738973
O,0,0.678113685,-0.7354951924,-1.693394278
O,0,1.6380124012,1.2306737396,-1.9957905964
S,0,-1.587938157,0.8027673121,0.4426646838
O,0,-1.8850446015,-0.6147955595,-0.1938826122
O,0,-1.4003494101,0.6723935427,1.8585899124
O,0,-2.8928848116,1.6360961444,0.1436636017
O,0,-0.5752077512,1.3665879583,-0.403201941
H,0,-3.5782235284,1.5500657725,0.8261545267
H,0,-2.4164259186,-1.2012505984,0.3689124387
H,0,2.6813353016,2.2018387017,0.3286367614
H,0,4.1145477064,1.5150093666,1.0849764295
H,0,4.0036611574,1.5587610989,-0.6732961922

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.41_369431

m062x/6-311G*
E(RM062X) = -1176.50796125

Zero-point correction= 0.182600 (Hartree/Particle)
Thermal correction to Energy= 0.198286
Thermal correction to Enthalpy= 0.199230
Thermal correction to Gibbs Free Energy= 0.138530
Sum of electronic and ZPE= -1176.325362
Sum of electronic and thermal Energies= -1176.309676
Sum of electronic and thermal Enthalpies= -1176.308731
Sum of electronic and thermal Free Energies= -1176.369431

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.426	56.076	127.753

C,0,1.6935849268,-0.0488377843,1.3751181221
C,0,2.3071921671,-1.3308718179,-1.0494263994
C,0,3.0325735634,-0.3260155166,1.0077240719
C,0,0.6723333934,-0.4283545046,0.4960903578
C,0,3.3325300127,-0.9922094361,-0.1823472755
C,0,0.9770263366,-1.0447141656,-0.7063265994
C,0,1.3887835579,0.5887865398,2.6981685075
H,0,2.5270620281,-1.8199232042,-1.9906857426
H,0,3.8330557271,-0.0551175613,1.6900546743
H,0,-0.3589216442,-0.2249526291,0.7605862834
H,0,4.3629481289,-1.2129973849,-0.4318441065

H,0,0.1790369257,-1.3144784519,-1.388109288
N,0,2.6299180279,1.9145798219,-0.03810725
O,0,2.2972111521,1.6371619076,-1.073687291
O,0,3.0180334575,2.5652739116,0.7963834255
S,0,-0.9785961719,2.8782676368,1.0805579929
O,0,-1.7571749663,1.7309211821,1.4311784093
O,0,-0.89843469,3.7446742479,2.3987109964
O,0,-1.7620540179,3.8008368484,0.0674283074
O,0,0.3313182402,2.7453395257,0.5071568683
H,0,-2.7087394423,3.8836992547,0.2679892228
H,0,-0.3063524559,4.5112020053,2.3274826336
H,0,1.8606438514,1.5721744021,2.7918164698
H,0,0.3150281117,0.708149629,2.8402293785
H,0,1.7803067802,-0.0251214561,3.512126231

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.46_368778

m062x/6-311G*
E(RM062X) = -1176.50700707

Zero-point correction= 0.182525 (Hartree/Particle)
Thermal correction to Energy= 0.198277
Thermal correction to Enthalpy= 0.199221
Thermal correction to Gibbs Free Energy= 0.138229
Sum of electronic and ZPE= -1176.324482
Sum of electronic and thermal Energies= -1176.308730
Sum of electronic and thermal Enthalpies= -1176.307786
Sum of electronic and thermal Free Energies= -1176.368778

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.421	56.105	128.370

C,0,1.3946979783,-0.0557317179,1.4106703258
C,0,2.5965104742,-1.3471213873,-0.7668013543
C,0,2.7012776845,0.2622481542,1.0434316612
C,0,0.7174835086,-1.073308511,0.7045850326
C,0,3.2983369615,-0.360627795,-0.0446633928
C,0,1.3151493467,-1.7319461181,-0.3520101919
C,0,0.7040874993,0.6785930168,2.5193367303
H,0,3.0756464489,-1.8490913124,-1.5997397348
H,0,3.2475641528,1.0144773191,1.6019276877
H,0,-0.2917084246,-1.3369431089,1.0031503886
H,0,4.3042575434,-0.0887561973,-0.3445837785
H,0,0.7874051077,-2.5155296604,-0.8815680512
N,0,1.8749467474,0.6908139326,-1.9502585436
O,0,0.9915638252,1.0290934874,-1.3422776891
O,0,2.5873814247,0.6680569707,-2.8243024294
S,0,2.7605797852,3.5474474246,0.042068451
O,0,1.5746869327,3.2612473783,0.7894117996
O,0,3.930781786,3.5640422298,1.1046720636
O,0,2.7409294207,5.0240329851,-0.51329426
O,0,3.1385779666,2.7368793158,-1.0842639486
H,0,2.3892413696,5.6729105098,0.11798914
H,0,4.815303293,3.6462366356,0.7115308755
H,0,1.4169547004,1.216941569,3.1432532544
H,0,0.0127237386,1.4128390861,2.0962990254
H,0,0.1253637288,-0.0046472067,3.1429129384

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.46_368547

m062x/6-311G*
E(RM062X) = -1176.50468519

Zero-point correction= 0.181786 (Hartree/Particle)
Thermal correction to Energy= 0.197922
Thermal correction to Enthalpy= 0.198867
Thermal correction to Gibbs Free Energy= 0.136138
Sum of electronic and ZPE= -1176.322899
Sum of electronic and thermal Energies= -1176.306763
Sum of electronic and thermal Enthalpies= -1176.305819
Sum of electronic and thermal Free Energies= -1176.368547

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.198	56.454	132.023

C,0,1.2677255647,-0.2738113823,1.1842970915
C,0,3.3604761659,-1.1187237732,-0.4852835656
C,0,2.4883613582,0.433587296,1.1438574021
C,0,1.117005835,-1.4337782834,0.4174886517
C,0,3.5283672382,-0.0015637461,0.3237503146
C,0,2.1397461266,-1.8300640224,-0.4200544269
H,0,0.4717936477,0.048598038,1.846312348
C,0,4.4389908761,-1.588171053,-1.4157146455
H,0,2.6190970015,1.3113739766,1.767095726
H,0,0.1954082149,-1.9998656946,0.4680226282
H,0,4.4617046005,0.54891241,0.3022518279
H,0,2.0156950593,-2.7096314183,-1.0433804186
N,0,0.9721990184,1.4067789076,-0.5897857242
O,0,1.2662112358,0.8318816188,-1.5125912917
O,0,0.5323986874,2.2765095201,-0.0168767976
S,0,-2.3363193718,-0.187245601,0.1195295487
O,0,-3.1224700733,-1.2060879069,-0.7948549798
O,0,-1.9855159743,-0.8142940557,1.3620710599
O,0,-3.3764328134,0.9731326461,0.3758106407
O,0,-1.3382781929,0.3848391195,-0.7348653401
H,0,-3.9922167858,0.7945459141,1.1050597592
H,0,-3.6628099414,-1.8419513464,-0.2989843191
H,0,4.704205127,-2.6254043464,-1.1984645768
H,0,4.0895756932,-1.554575751,-2.4505349132
H,0,5.3352407023,-0.975150066,-1.3330769994

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.45_368434

m062x/6-311G*
E(RM062X) = -1176.50729410

Zero-point correction= 0.182563 (Hartree/Particle)
Thermal correction to Energy= 0.198250
Thermal correction to Enthalpy= 0.199194
Thermal correction to Gibbs Free Energy= 0.138860
Sum of electronic and ZPE= -1176.324731
Sum of electronic and thermal Energies= -1176.309044
Sum of electronic and thermal Enthalpies= -1176.308100
Sum of electronic and thermal Free Energies= -1176.368434

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 124.404 56.087 126.985

C,0,1.3100653065,-0.0525074452,1.4020342769
C,0,2.750095371,-1.2779419147,-0.6710712871
C,0,2.5649921709,0.4509845922,0.9856086631
C,0,0.8106838299,-1.2042044967,0.7724871446
C,0,3.2892139805,-0.1750267281,-0.0283800861
C,0,1.5096854864,-1.7953101939,-0.2628001386
C,0,0.565635967,0.584895985,2.536424248
H,0,3.2867425216,-1.7495844079,-1.4853465359
H,0,2.9735896278,1.3242889725,1.4846598671
H,0,-0.1291553263,-1.6282787846,1.1095092169
H,0,4.2508217575,0.2218291509,-0.3294233621
H,0,1.101241392,-2.6665396163,-0.7613046679
N,0,0.8228566282,1.5748990957,-0.4767126438
O,0,0.9268161118,0.9635723329,-1.4140399804
O,0,0.5442398906,2.4578814559,0.1666575797
S,0,-2.467121347,-0.3016936189,0.0147883296
O,0,-2.0677696494,-1.503190713,-0.9323465655
O,0,-2.6289233234,-0.8767920607,1.3104927842
O,0,-3.9097884639,0.1075937761,-0.4722429497
O,0,-1.5620863099,0.7983580926,-0.2069334373
H,0,-3.9155642702,0.7284046269,-1.2190875323
H,0,-1.7419664325,-1.2361028878,-1.8073600897
H,0,0.8600079755,0.1098692429,3.4766020966
H,0,0.7987612757,1.6472455136,2.6283190562
H,0,-0.5122121704,0.4610820309,2.4231120137

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.45_368346

m062x/6-311G*
E(RM062X) = -1176.50607699

Zero-point correction= 0.182224 (Hartree/Particle)
Thermal correction to Energy= 0.198085
Thermal correction to Enthalpy= 0.199029
Thermal correction to Gibbs Free Energy= 0.137731
Sum of electronic and ZPE= -1176.323853
Sum of electronic and thermal Energies= -1176.307992
Sum of electronic and thermal Enthalpies= -1176.307048
Sum of electronic and thermal Free Energies= -1176.368346

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 124.300 56.231 129.012

C,0,1.2951943995,-0.4934208794,1.3829299282
C,0,3.1982355277,-1.2049080253,-0.5411415225
C,0,2.6099500371,0.0061859866,1.4654221616
C,0,0.9585112498,-1.410473959,0.3765303891
C,0,3.5484368367,-0.3521059492,0.5093468865
C,0,1.8955192641,-1.7406820081,-0.5820501736
H,0,0.5633492242,-0.2226839373,2.1345611248
C,0,4.1788235132,-1.5400680491,-1.6249973408
H,0,2.8775470183,0.677800256,2.273178504
H,0,-0.0356893642,-1.8397851307,0.3445010875
H,0,4.5554579218,0.045490518,0.5644607902
H,0,1.6319179568,-2.4213739795,-1.3844616387
N,0,0.9888057256,1.4647454521,-0.0574557741
O,0,1.4882848939,1.1818888097,-1.0230037291
O,0,0.4007470691,2.1030531493,0.6634276309
S,0,-2.2983802868,0.0875322091,-0.3112001854
O,0,-2.4071564182,-1.4614062512,-0.6003856389
O,0,-1.8009167758,0.1441111727,1.1925477233
O,0,-3.5843261383,0.7041431221,-0.4297248773
O,0,-1.1630333909,0.5268684789,-1.0693149528
H,0,-2.5119310556,0.1239172018,1.8531946275
H,0,-3.2504928699,-1.8544101805,-0.3222362388
H,0,3.9678276614,-0.9383741554,-2.5141856442
H,0,5.2032440839,-1.3351756744,-1.3158345241
H,0,4.0985689166,-2.5884161774,-1.9162286134

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.44_368221

m062x/6-311G*
E(RM062X) = -1176.50532400

Zero-point correction= 0.182100 (Hartree/Particle)
Thermal correction to Energy= 0.198138
Thermal correction to Enthalpy= 0.199083
Thermal correction to Gibbs Free Energy= 0.137103
Sum of electronic and ZPE= -1176.323224
Sum of electronic and thermal Energies= -1176.307186
Sum of electronic and thermal Enthalpies= -1176.306241
Sum of electronic and thermal Free Energies= -1176.368221

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 124.334 56.382 130.447

C,0,1.2042125192,-0.1373309213,1.4380541965
C,0,2.7287361883,-1.0708580895,-0.7161641512
C,0,2.4202322414,0.4722254201,1.1258366128
C,0,0.7891810188,-1.2589440339,0.6901726644
C,0,3.1744399643,0.0263039244,0.0492876823
C,0,1.5524052058,-1.7426040163,-0.3536017168
C,0,0.3355392341,0.3944457811,2.538067218
H,0,3.3353887364,-1.4371144579,-1.5363768167
H,0,2.7704354133,1.3059993972,1.7231395369
H,0,-0.14610799,-1.7448121896,0.9468186123
H,0,4.1070835091,0.5182036409,-0.2050004504
H,0,1.2290966048,-2.6097319546,-0.9162493125
N,0,1.593874083,0.7054541483,-1.9449699837
O,0,0.6607965344,0.8875092435,-1.3441673016
O,0,2.2947685133,0.7931075924,-2.8247902306
S,0,2.8695312951,3.6943825003,-0.0377849025
O,0,1.7513820532,3.6801233498,1.0812707905
O,0,4.0696991897,3.2889757421,0.6183467704
O,0,3.0487633572,5.2241942852,-0.3779655467
O,0,2.3771971457,3.0068427027,-1.2049979325
H,0,2.4129314165,5.5620379462,-1.0294884127
H,0,0.8437700641,3.7439112097,0.7423338876
H,0,-0.5215210551,0.9226790057,2.1095955364
H,0,-0.0582282917,-0.4158976999,3.1538932737
H,0,0.8792520491,1.0924794735,3.1736119761

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.42_368199

m062x/6-311G*
E(RM062X) = -1176.50519050

Zero-point correction= 0.182050 (Hartree/Particle)
Thermal correction to Energy= 0.198019
Thermal correction to Enthalpy= 0.198963
Thermal correction to Gibbs Free Energy= 0.136991
Sum of electronic and ZPE= -1176.323141
Sum of electronic and thermal Energies= -1176.307172
Sum of electronic and thermal Enthalpies= -1176.306228
Sum of electronic and thermal Free Energies= -1176.368199

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.259	56.397	130.430

C,0,1.1922289591,-0.6843599428,1.4325987854
C,0,3.2683159534,-1.215575417,-0.373339391
C,0,2.1282355489,0.3036827796,1.1181572445
C,0,1.2647407505,-1.9140191107,0.8025061283
C,0,3.1936467409,0.0491930522,0.2247052759
C,0,2.3060141876,-2.1749843787,-0.1036672
H,0,0.401122122,-0.468774656,2.1397801341
H,0,4.0750544431,-1.4328258682,-1.0643051275
H,0,2.0617369677,1.276648808,1.5955903046
H,0,0.5225380192,-2.6765968944,1.0067336745
C,0,4.2409875695,1.0969708745,-0.0172981801
H,0,2.3585684744,-3.140612582,-0.5924572876
N,0,1.1582276499,0.9092461963,-1.1253243353
O,0,0.751211123,-0.0665269275,-1.5019250919
O,0,1.339245627,2.0200285593,-1.0758366194
S,0,-2.0448105084,0.1474984983,0.1858626066
O,0,-1.9792681624,-0.9616770381,-0.7218497451
O,0,-2.1273652885,-0.3803154106,1.6733427557
O,0,-3.3978062496,0.9350589946,-0.0086351873
O,0,-1.0209514659,1.1527428217,0.2035444459
H,0,-4.1435285451,0.3754802117,-0.2796086387
H,0,-2.6339664001,-1.2034289961,1.7716118579
H,0,5.0199448872,1.0150896562,0.7458144794
H,0,4.7117652646,0.9769012527,-0.9927123072
H,0,3.8277363322,2.1050575171,0.0576774181

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.43_368154

m062x/6-311G*
E(RM062X) = -1176.50633068

Zero-point correction= 0.182762 (Hartree/Particle)
Thermal correction to Energy= 0.198529
Thermal correction to Enthalpy= 0.199473
Thermal correction to Gibbs Free Energy= 0.138177
Sum of electronic and ZPE= -1176.323569
Sum of electronic and thermal Energies= -1176.307802
Sum of electronic and thermal Enthalpies= -1176.306858
Sum of electronic and thermal Free Energies= -1176.368154

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.579	55.947	129.009

C,0,1.3246840153,-0.1352029004,1.4953650177
C,0,2.7387165081,-1.0877992152,-0.7213613676
C,0,2.5749911437,0.4040532847,1.1742321529
C,0,0.8246241528,-1.2073294265,0.7306843306
C,0,3.2784047467,-0.0565658818,0.0736997951
C,0,1.5303607644,-1.6987837113,-0.3494601539
C,0,0.5142014072,0.4348373339,2.6193409495
H,0,3.3002178138,-1.4644494736,-1.5684310657
H,0,2.9893381254,1.197662279,1.7857120253
H,0,-0.1309079015,-1.6454159618,0.9978578913
H,0,4.2375842458,0.3770324031,-0.186302691
H,0,1.1423531694,-2.5256480754,-0.9318095255
N,0,1.6109814073,0.7242692583,-1.8835224669
O,0,0.7820540325,1.0274151658,-1.1863087195
O,0,2.2144220707,0.720685632,-2.8370980506
S,0,2.8798789688,3.6392533307,-0.0613472209
O,0,1.465497718,3.4261103154,0.6170718576
O,0,3.9205152914,3.4293813308,0.9028126657
O,0,2.8610203596,5.1498406006,-0.5160395003
O,0,2.8120768667,2.8768114962,-1.2735618684
H,0,3.1598447812,5.7698803074,0.1691935635
H,0,1.4128337856,3.7343396761,1.5361553777
H,0,1.1422638731,0.9665545483,3.3340602336
H,0,-0.2136279072,1.1476622161,2.2184250196
H,0,-0.0436724388,-0.3429225323,3.1419597503

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.50_368101

m062x/6-311G*
E(RM062X) = -1176.50660328

Zero-point correction= 0.182466 (Hartree/Particle)
Thermal correction to Energy= 0.198227
Thermal correction to Enthalpy= 0.199172
Thermal correction to Gibbs Free Energy= 0.138502
Sum of electronic and ZPE= -1176.324137
Sum of electronic and thermal Energies= -1176.308376
Sum of electronic and thermal Enthalpies= -1176.307432
Sum of electronic and thermal Free Energies= -1176.368101

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.390	56.181	127.690

C,0,1.4209347188,0.027249842,1.2521282174
C,0,3.0262519673,-1.36915888,-0.5691194524
C,0,2.6038563894,0.6119188228,0.7794803448
C,0,1.0829131423,-1.2839034426,0.8603522568
C,0,3.3761007297,-0.0702123026,-0.1383551524
C,0,1.8927441855,-1.9750320821,-0.032393294
H,0,0.7989240191,0.5530904252,1.9675038121
C,0,3.8634756162,-2.0621224218,-1.6012695572
H,0,2.8853912069,1.6050399858,1.1068862189
H,0,0.1850583869,-1.7473977008,1.2533437037
H,0,4.2699108996,0.3931738169,-0.5426270469
H,0,1.6296267319,-2.9852808747,-0.3268759235
N,0,0.0901106523,0.4669185759,-0.7539128971

O,0,0.8450712369,0.3953138682,-1.585149786
O,0,-0.9054714714,0.7097092376,-0.2794289196
S,0,-0.4892130776,-2.7512885288,-2.4542642478
O,0,0.7972221178,-2.1500227322,-3.1541983162
O,0,-0.2113353839,-4.0710991247,-1.9679701109
O,0,-1.5553383865,-2.8149490439,-3.6158626925
O,0,-0.9374959126,-1.7067351569,-1.5804414722
H,0,-1.5518338991,-3.6512432253,-4.1091053942
H,0,1.2976807333,-2.7869651871,-3.6898807178
H,0,3.6021907941,-3.1164867523,-1.6874335088
H,0,3.7136105982,-1.5907655766,-2.5769216432
H,0,4.9252420049,-1.9793425419,-1.3622174206

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.45_367948

m062x/6-311G*
E(RM062X) = -1176.50450469

Zero-point correction= 0.181829 (Hartree/Particle)
Thermal correction to Energy= 0.197883
Thermal correction to Enthalpy= 0.198827
Thermal correction to Gibbs Free Energy= 0.136557
Sum of electronic and ZPE= -1176.322676
Sum of electronic and thermal Energies= -1176.306622
Sum of electronic and thermal Enthalpies= -1176.305677
Sum of electronic and thermal Free Energies= -1176.367948

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.174	56.404	131.059

C,0,1.3059363286,-0.1845987137,1.2828123849
C,0,3.2403817907,-1.1472512183,-0.5051910293
C,0,2.5830201518,0.4123182838,1.2161040466
C,0,1.0276354223,-1.3108393375,0.4982773232
C,0,3.5420096615,-0.0804244969,0.3365534623
C,0,1.9721283953,-1.7623325136,-0.4000588001
H,0,0.5663730354,0.1856507649,1.9843286106
C,0,4.2268661504,-1.6439763368,-1.5189879854
H,0,2.8138385954,1.2547861082,1.8586412284
H,0,0.0710170548,-1.8115147797,0.5875058612
H,0,4.5187713069,0.3866420195,0.2884584116
H,0,1.746508587,-2.6099756172,-1.0386802733
N,0,1.0441910742,1.5360102161,-0.4363517726
O,0,1.3451001538,1.009261321,-1.3855528605
O,0,0.6161424385,2.3839001207,0.1774183934
S,0,-2.2277599982,-0.1199904913,0.0266513479
O,0,-2.3729455343,-1.5781025794,-0.5661562289
O,0,-2.0098306692,-0.296494823,1.4263063841
O,0,-3.669956717,0.497998984,-0.1203601364
O,0,-1.3025234289,0.625676073,-0.7892432105
H,0,-3.8461096418,0.8897702495,-0.9910061353
H,0,-2.290924138,-1.6240978982,-1.532433674
H,0,4.2864787025,-2.7336684765,-1.5033891241
H,0,3.9076552916,-1.3513951521,-2.5234578006
H,0,5.2207559867,-1.2336097063,-1.3452494228

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.47_367776

m062x/6-311G*
E(RM062X) = -1176.50698426

Zero-point correction= 0.182836 (Hartree/Particle)
Thermal correction to Energy= 0.198424
Thermal correction to Enthalpy= 0.199368
Thermal correction to Gibbs Free Energy= 0.139208
Sum of electronic and ZPE= -1176.324148
Sum of electronic and thermal Energies= -1176.308560
Sum of electronic and thermal Enthalpies= -1176.307616
Sum of electronic and thermal Free Energies= -1176.367776

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.513	56.060	126.617

C,0,-0.182898926,-0.093589264,0.1478782505
C,0,0.3931473862,0.2838510685,2.8589777528
C,0,1.1478579764,0.0823607856,0.5803498537
C,0,-1.2206688668,-0.0319894324,1.1034318987
C,0,1.4311847568,0.2623727671,1.9233062794
C,0,-0.9334493371,0.1517590681,2.4463386853
C,0,-0.503760729,-0.2381763031,-1.3093700668
H,0,0.6209526686,0.4102731504,3.9108282444
H,0,1.9489981806,0.0598309068,-0.1505886161
H,0,-2.2495395575,-0.1348760167,0.7757316867
H,0,2.4574912449,0.3745899585,2.2506634849
H,0,-1.7383809235,0.1824714693,3.1713306469
N,0,0.0222179876,-2.4833145884,0.7946158865
O,0,0.3511905142,-2.4997587352,1.8688177482
O,0,-0.2504508322,-2.8879587663,-0.221365092
S,0,-3.3678951491,-2.5495558824,2.4578000436
O,0,-2.7945882768,-2.7314956473,3.9192193287
O,0,-3.9283543994,-1.2380123837,2.4290685618
O,0,-4.5867089034,-3.5493208857,2.3958316638
O,0,-2.3714612,-2.9656659796,1.5022934272
H,0,-4.3415388109,-4.458593101,2.1588037408
H,0,-2.2317110873,-3.5147562033,4.0307173711
H,0,-0.6830539458,0.7506004181,-1.7408684724
H,0,0.3195290266,-0.6941680564,-1.8610638565
H,0,-1.4094417968,-0.827594347,-1.4638824513

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.45_367760

m062x/6-311G*
E(RM062X) = -1176.50395742

Zero-point correction= 0.182287 (Hartree/Particle)
Thermal correction to Energy= 0.198322
Thermal correction to Enthalpy= 0.199266
Thermal correction to Gibbs Free Energy= 0.136197
Sum of electronic and ZPE= -1176.321671
Sum of electronic and thermal Energies= -1176.305636
Sum of electronic and thermal Enthalpies= -1176.304692
Sum of electronic and thermal Free Energies= -1176.367760

	E	CV	S

KCal/Mol Cal/Mol-K Cal/Mol-K
Total 124.449 56.110 132.739

C,0,1.3018632539,-0.1069590375,1.4253909544
C,0,2.6765326666,-1.2914041261,-0.7101003457
C,0,2.5402480382,0.4082640586,0.9802268409
C,0,0.7899306157,-1.2501139068,0.8170435544
C,0,3.2358003697,-0.1894686532,-0.0502400537
C,0,1.4595871348,-1.8369861869,-0.2516315288
C,0,0.5763580161,0.579145547,2.5439588056
H,0,3.2072569701,-1.7642101539,-1.5288746884
H,0,2.9484290807,1.2876651275,1.4678287269
H,0,-0.1489287218,-1.6695924739,1.1595830508
H,0,4.2004478892,0.1948891451,-0.3590435659
H,0,1.0510268059,-2.7168743658,-0.7361209348
N,0,1.0219510261,-0.0683699724,-2.0417445636
O,0,0.7165186825,0.7836261389,-1.3725861015
O,0,1.0637572662,-0.6655426202,-2.9994356031
S,0,4.148870552,1.99399554,-2.6466277464
O,0,3.9974626988,2.8449404637,-1.3223211578
O,0,5.3228216402,1.2061194323,-2.4576513956
O,0,4.5070294565,3.0636623857,-3.7494194082
O,0,2.8798147884,1.3900457453,-2.9670260484
H,0,3.735332728,3.4952550458,-4.1504675623
H,0,3.1484705242,3.3088035421,-1.2381528913
H,0,1.202554912,0.6115551911,3.4386927359
H,0,0.3494423934,1.6127664785,2.2717516878
H,0,-0.3555827874,0.072132655,2.7892442388

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.47_367357

m062x/6-311G*
E(RM062X) = -1176.50600394

Zero-point correction= 0.182633 (Hartree/Particle)
Thermal correction to Energy= 0.198369
Thermal correction to Enthalpy= 0.199313
Thermal correction to Gibbs Free Energy= 0.138647
Sum of electronic and ZPE= -1176.323371
Sum of electronic and thermal Energies= -1176.307635
Sum of electronic and thermal Enthalpies= -1176.306691
Sum of electronic and thermal Free Energies= -1176.367357

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 124.478 56.086 127.682

C,0,1.3857235316,-0.0896439679,1.4121306041
C,0,2.5741746083,-1.3639937917,-0.7834142686
C,0,2.6947737114,0.2198175953,1.0482161038
C,0,0.697322221,-1.0892383588,0.690776014
C,0,3.2856174939,-0.3944347943,-0.0484970196
C,0,1.2879474076,-1.73930518,-0.3749502189
C,0,0.7037855868,0.6369897831,2.5314591943
H,0,3.0480409627,-1.8598240505,-1.6230042323
H,0,3.2514587279,0.9577706327,1.6151789187
H,0,-0.3146626896,-1.346351207,0.985513736
H,0,4.293798451,-0.1273198392,-0.3449347164
H,0,0.7516617918,-2.5093189952,-0.9156664195
N,0,1.8885641938,0.7058700238,-1.9354796496
O,0,1.0043081385,1.0426100657,-1.327812362
O,0,2.6065300236,0.6901853504,-2.805045064
S,0,2.7671774618,3.5359844499,0.0790515572
O,0,1.5320728637,3.2868712974,0.765419974
O,0,3.9689188911,3.5112216628,1.1060336917
O,0,2.789055606,5.0057215991,-0.4940969171
O,0,3.1937973088,2.7002816633,-1.0057572645
H,0,2.3055558986,5.6483112926,0.0499572861
H,0,3.7530915684,3.8836898151,1.9764431761
H,0,1.4245717382,1.1426673308,3.1737204569
H,0,0.0354421802,1.3982199465,2.1189898056
H,0,0.1025783227,-0.0445903241,3.1350656142

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.47_367350

m062x/6-311G*
E(RM062X) = -1176.50600378

Zero-point correction= 0.182637 (Hartree/Particle)
Thermal correction to Energy= 0.198371
Thermal correction to Enthalpy= 0.199315
Thermal correction to Gibbs Free Energy= 0.138654
Sum of electronic and ZPE= -1176.323367
Sum of electronic and thermal Energies= -1176.307633
Sum of electronic and thermal Enthalpies= -1176.306689
Sum of electronic and thermal Free Energies= -1176.367350

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 124.480 56.083 127.673

C,0,1.4474524532,0.0526059121,1.2664205643
C,0,3.0173548927,-1.3601478601,-0.5765056695
C,0,2.6056289584,0.6425367878,0.7442307153
C,0,1.1156323839,-1.2700918483,0.9105323047
C,0,3.3602682041,-0.0481276944,-0.1835099147
C,0,1.9088146606,-1.9683702355,0.0091701533
H,0,0.8406309888,0.5852658632,1.9898489187
C,0,3.8226672434,-2.068266077,-1.6233964974
H,0,2.88343263,1.6459103686,1.0424988425
H,0,0.2370776088,-1.7385726389,1.339860437
H,0,4.2349821926,0.419699491,-0.6229465824
H,0,1.653263105,-2.989174062,-0.2526825842
N,0,0.0411237165,0.4322830824,-0.7235611342
O,0,0.7841485968,0.3634874091,-1.5648342864
O,0,-0.9453861341,0.6536879006,-0.2239258657
S,0,-0.3687972422,-2.6539249343,-2.4975862442
O,0,0.8953987513,-2.3430040381,-3.1007167549
O,0,-0.2938585462,-4.0630596153,-1.7848343151
O,0,-1.4725296385,-2.8493403921,-3.6078676522
O,0,-0.9604427631,-1.781463843,-1.5249590145
H,0,-1.1348253288,-3.2227904718,-4.4380389815
H,0,0.2525420091,-4.7148305226,-2.2534420646
H,0,3.640456824,-3.1426064321,-1.6050326355
H,0,3.5385905636,-1.7003483446,-2.6134574814
H,0,4.8898188706,-1.8836658045,-1.4913102575

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.27_367301

m062x/6-311G*
E(RM062X) = -1176.50416316

Zero-point correction= 0.182152 (Hartree/Particle)
Thermal correction to Energy= 0.198172
Thermal correction to Enthalpy= 0.199116
Thermal correction to Gibbs Free Energy= 0.136862
Sum of electronic and ZPE= -1176.322011
Sum of electronic and thermal Energies= -1176.305991
Sum of electronic and thermal Enthalpies= -1176.305047
Sum of electronic and thermal Free Energies= -1176.367301

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.355	56.279	131.025

C,0,1.175857137,-0.2923308959,1.2760808552
C,0,3.256935894,-1.2148096919,-0.3444163068
C,0,2.3045277143,0.5106309128,1.0189643123
C,0,1.0744619331,-1.5395044254,0.6854132724
C,0,3.3877698757,0.0356144552,0.2466906507
C,0,2.110318251,-1.9859302586,-0.1392942137
H,0,0.3868651978,0.0818033234,1.9172898212
H,0,4.0529342979,-1.5970580393,-0.9734843541
H,0,2.3860650659,1.4798176433,1.5011293721
H,0,0.2014809117,-2.157980262,0.855528096
C,0,4.6318567427,0.861640535,0.0887708816
H,0,2.0294324334,-2.9531533282,-0.6218482658
N,0,1.1556746024,1.2823394581,-0.9579864112
O,0,1.0959763618,0.3884333165,-1.6381960628
O,0,1.0217712819,2.3620164829,-0.6573072695
S,0,-2.2009761508,-0.089096922,0.130139374
O,0,-2.2647895056,-1.2632359659,-0.9254370796
O,0,-2.0326673396,-0.7238814542,1.3965676924
O,0,-3.6610400283,0.5079189903,0.1287692369
O,0,-1.2841925675,0.9197806311,-0.3384009061
H,0,-3.8067828379,1.1895883052,-0.5467203775
H,0,-2.1810032413,-0.9727228606,-1.8478667464
H,0,5.2659721767,0.7464305379,0.9719282741
H,0,5.2064790332,0.5490838709,-0.7824426008
H,0,4.3991867606,1.9237026415,-0.0061642448

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.08_366987

m062x/6-311G*
E(RM062X) = -1176.50525318

Zero-point correction= 0.182356 (Hartree/Particle)
Thermal correction to Energy= 0.198117
Thermal correction to Enthalpy= 0.199061
Thermal correction to Gibbs Free Energy= 0.138266
Sum of electronic and ZPE= -1176.322897
Sum of electronic and thermal Energies= -1176.307136
Sum of electronic and thermal Enthalpies= -1176.306192
Sum of electronic and thermal Free Energies= -1176.366987

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.320	56.249	127.954

C,0,1.0642829031,-0.1910019511,0.8572016353
C,0,3.312362018,-1.3397429729,-0.4452653805
C,0,2.3328540429,0.3597195632,0.9946346116
C,0,0.9003634367,-1.288223651,0.0220877017
C,0,3.4413590385,-0.2130372422,0.3564197321
C,0,2.0167178283,-1.8411163596,-0.6523836985
H,0,0.2151280707,0.2396509746,1.3718170285
C,0,4.5180385257,-1.9874264648,-1.0643686397
H,0,2.4753463119,1.2374855904,1.6140559918
H,0,-0.0784372606,-1.7322427133,-0.1209177675
H,0,4.4223640161,0.2269759647,0.501958599
H,0,1.8753577834,-2.710917876,-1.2863424187
N,0,1.2054572961,-0.209110597,-2.2169007761
O,0,1.7056266123,0.7569320164,-1.9226136285
O,0,0.5864126765,-0.8750830344,-2.8915720119
S,0,3.6253354799,-1.79851512,-4.414825598
O,0,3.0852359611,-1.5563792946,-5.8775366202
O,0,4.9767125332,-2.2706116045,-4.4592989501
O,0,2.6717417416,-2.9279296006,-3.8423650219
O,0,3.2546458484,-0.6295941973,-3.6716464133
H,0,2.905026295,-3.8304408853,-4.113720406
H,0,3.4796541128,-2.1409146914,-6.5453541589
H,0,4.2434113916,-2.85559267,-1.6628975712
H,0,5.0602228877,-1.2814407428,-1.6959818175
H,0,5.2032574492,-2.3219254406,-0.2827334214

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.32_366879

m062x/6-311G*
E(RM062X) = -1176.50595018

Zero-point correction= 0.182866 (Hartree/Particle)
Thermal correction to Energy= 0.198662
Thermal correction to Enthalpy= 0.199606
Thermal correction to Gibbs Free Energy= 0.139072
Sum of electronic and ZPE= -1176.323084
Sum of electronic and thermal Energies= -1176.307288
Sum of electronic and thermal Enthalpies= -1176.306344
Sum of electronic and thermal Free Energies= -1176.366879

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.662	56.151	127.406

C,0,1.1085620742,-0.2488348089,1.4023740487
C,0,3.1518427109,-1.2621083817,-0.2211803818
C,0,2.2033713882,0.5522548538,1.035904418
C,0,1.0153069306,-1.5368531384,0.9118139198
C,0,3.2665485885,0.0412639094,0.2570190922
C,0,2.0344528622,-2.0332234456,0.0874544274
H,0,0.3330840962,0.1599431148,2.038057263
H,0,3.9363028428,-1.6759184144,-0.8448183478
H,0,2.2770467127,1.5621893031,1.4274695401
H,0,0.1594390989,-2.1548347827,1.1527430666
C,0,4.481179254,0.8812240417,-0.0142754834
H,0,1.9556904546,-3.038829345,-0.3095784124
N,0,1.1332783534,1.1215136362,-1.0731729833

O,0,0.8970020257,0.139817299,-1.5657765739
O,0,1.1683828642,2.2438212077,-0.9588502661
S,0,-2.2148626553,0.0774294377,-0.0469725995
O,0,-1.6230199757,-1.1007051158,-0.9204570525
O,0,-2.0728862925,-0.4571432735,1.43435924
O,0,-3.5960679673,0.2832914669,-0.362753197
O,0,-1.2440237344,1.1278694997,-0.1538942252
H,0,-2.8142818676,-1.011637322,1.7270369958
H,0,-2.2561011444,-1.8085786006,-1.1218277369
H,0,4.9811131079,0.5747973144,-0.9326455636
H,0,4.2292610817,1.9408705657,-0.0850058499
H,0,5.1925601907,0.7736009782,0.8092736615

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.34_366676

m062x/6-311G*
E(RM062X) = -1176.50534938

Zero-point correction= 0.182861 (Hartree/Particle)
Thermal correction to Energy= 0.198602
Thermal correction to Enthalpy= 0.199546
Thermal correction to Gibbs Free Energy= 0.138674
Sum of electronic and ZPE= -1176.322488
Sum of electronic and thermal Energies= -1176.306747
Sum of electronic and thermal Enthalpies= -1176.305803
Sum of electronic and thermal Free Energies= -1176.366676

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.625	55.982	128.117

C,0,1.2020189926,-0.3673889648,1.4445043513
C,0,3.1585399948,-1.2360862468,-0.3601711874
C,0,2.26455754,0.4742110407,1.0731457544
C,0,1.0951041214,-1.6195117654,0.8717464693
C,0,3.2870068187,0.0328136834,0.2021402096
C,0,2.0703576489,-2.0428199142,-0.0434254925
H,0,0.4631383183,-0.016510661,2.1545421113
H,0,3.910654614,-1.5938269046,-1.0542468703
H,0,2.3511420177,1.454272931,1.5318961228
H,0,0.2676986108,-2.2701471364,1.1274396267
C,0,4.4773181402,0.9041556419,-0.0765072292
H,0,1.9797550588,-3.0201301588,-0.5033758659
N,0,1.1061104328,1.190204373,-0.9362821885
O,0,0.8314569505,0.2454508869,-1.4799422906
O,0,1.1565987743,2.30268679,-0.7519469964
S,0,-2.0732472153,-0.0054145773,0.2829611131
O,0,-1.7304138191,-0.9318312735,-0.9536344531
O,0,-2.0681113214,-0.7837351706,1.4874049614
O,0,-3.529525979,0.5153984,-0.0226902064
O,0,-1.2221185471,1.138059927,0.1195889867
H,0,-4.2330820096,-0.0832787572,0.2763865461
H,0,-2.0638120255,-1.8404782009,-0.8769143972
H,0,5.2432340778,0.729554188,0.6842819888
H,0,4.9140514588,0.6835663236,-1.0501125788
H,0,4.2191583465,1.9637235459,-0.0352834852

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 2.48_366653

m062x/6-311G*
E(RM062X) = -1176.50596937

Zero-point correction= 0.182740 (Hartree/Particle)
Thermal correction to Energy= 0.198294
Thermal correction to Enthalpy= 0.199238
Thermal correction to Gibbs Free Energy= 0.139316
Sum of electronic and ZPE= -1176.323229
Sum of electronic and thermal Energies= -1176.307675
Sum of electronic and thermal Enthalpies= -1176.306731
Sum of electronic and thermal Free Energies= -1176.366653

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	124.431	56.006	126.117

C,0,1.3522633047,-0.0195415153,1.3283820503
C,0,2.4465352315,-1.3946200832,-0.8624728545
C,0,2.6886480109,0.1607868421,0.9927535471
C,0,0.5779885775,-0.9257374524,0.5677011814
C,0,3.2326213324,-0.4995628256,-0.1077459176
C,0,1.1184970249,-1.6270947558,-0.4925057853
C,0,0.7170283771,0.7207420242,2.4669605349
H,0,2.8874005657,-1.9293940893,-1.6958976955
H,0,3.3126272491,0.8287991863,1.5762639826
H,0,-0.4635497268,-1.072192888,0.8344470906
H,0,4.2704265838,-0.3390381104,-0.3784169579
H,0,0.5120370379,-2.3258858961,-1.0550534411
N,0,2.1282205238,0.8182392138,-1.9410543308
O,0,1.172726589,1.1578002875,-1.452108971
O,0,2.9568936909,0.8271231435,-2.7078839766
S,0,2.6765281212,3.5683213891,0.2757722734
O,0,1.3493821715,3.2781854802,0.7367785152
O,0,3.6990798786,3.4652551397,1.4774410502
O,0,2.7784027408,5.0759025011,-0.1790232758
O,0,3.2766438857,2.8091451153,-0.7830626331
H,0,2.2087833678,5.6777477228,0.3272618995
H,0,3.3415503177,3.7648404766,2.3288265743
H,0,0.2213406114,0.0248487074,3.1471720193
H,0,1.450913145,1.3000518674,3.0259121401
H,0,-0.0401606122,1.4105025191,2.0870439805

Toluene / NO2+ / H2SO4 TS M06-2X/6-311G*/PCM 3.33_365619

m062x/6-311G*
E(RM062X) = -1176.50419780

Zero-point correction= 0.182762 (Hartree/Particle)
Thermal correction to Energy= 0.198553
Thermal correction to Enthalpy= 0.199497
Thermal correction to Gibbs Free Energy= 0.138579
Sum of electronic and ZPE= -1176.321436
Sum of electronic and thermal Energies= -1176.305645
Sum of electronic and thermal Enthalpies= -1176.304701
Sum of electronic and thermal Free Energies= -1176.365619

	E	CV	S

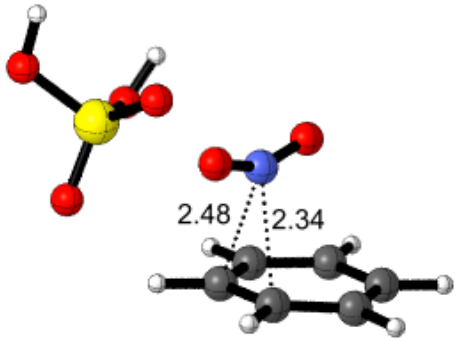
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 124.594 56.096 128.212

C,0,1.207224956,-0.4414402954,1.4662233836
C,0,3.1390746344,-1.2098816994,-0.4068561848
C,0,2.2535196544,0.4273434969,1.1132931721
C,0,1.1008799143,-1.6684487104,0.8412656855
C,0,3.2630487115,0.0365642126,0.2048673644
C,0,2.0645751596,-2.0414336336,-0.1070874676
H,0,0.4816607619,-0.1284310852,2.2066565655
H,0,3.8828303524,-1.5295296314,-1.1280714383
H,0,2.3364385553,1.3890684717,1.6100946494
H,0,0.2788376174,-2.3344208354,1.0735586102
C,0,4.4358107554,0.935824575,-0.0595665661
H,0,1.9755206664,-2.9985959642,-0.607843994
N,0,1.033508995,1.2009461916,-0.8525691503
O,0,0.7716523901,0.2700879486,-1.4253578422
O,0,1.0630472585,2.3043282633,-0.6205457089
S,0,-2.0950696249,-0.1538776196,0.1582897852
O,0,-1.764951982,-1.2195628577,-0.7306416733
O,0,-2.1323776797,-0.805157671,1.598485605
O,0,-3.5998150515,0.2256134325,-0.1242503018
O,0,-1.3031846286,1.052108745,0.2017037211
H,0,-3.8500033037,1.1107615924,0.187772152
H,0,-2.2903920892,-0.1765345613,2.3218731849
H,0,5.217330656,0.7447626661,0.6810955425
H,0,4.8589540773,0.759655083,-1.0481053643
H,0,4.1622962435,1.9888918858,0.0264342703

Nitrations of Benzene Including a Sulfuric Acid Molecule

An exploratory series of calculations was performed to evaluate the system of main text reference 23. This system includes an explicit molecule of sulfuric acid, in addition to benzene and NO_2^+. Some studies used water as the implicit solvent, while others, as marked, used ε=109 following reference 6a's implicit solvent model. These calculations used M06-2X/6-311++G** to match reference 23.

Optimized TS for the nitration of benzene / H_2SO_4 in water



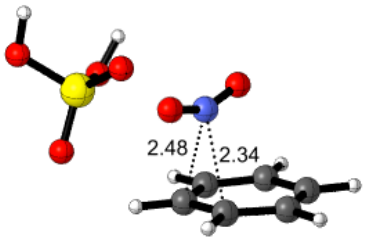
scrf=(solvent=water)
m062x/6-311++G**
E(RM062X) = -1137.22862808

Zero-point correction= 0.153518 (Hartree/Particle)
Thermal correction to Energy= 0.167849
Thermal correction to Enthalpy= 0.168793
Thermal correction to Gibbs Free Energy= 0.109978
Sum of electronic and ZPE= -1137.075110
Sum of electronic and thermal Energies= -1137.060779
Sum of electronic and thermal Enthalpies= -1137.059835
Sum of electronic and thermal Free Energies= -1137.118650

E CV S
KCal/Mol Cal/Mol-K Cal/Mol-K
Total 105.327 50.407 123.788

C,0,1.2433883745,-0.2428223357,1.1741211346
C,0,3.2943184877,-1.1350187881,-0.49811605
C,0,2.4466176734,0.4942952656,1.0452095581
C,0,1.0755898379,-1.4243688504,0.4586013985
C,0,3.4906760392,0.0142088326,0.2390290224
C,0,2.0844538117,-1.8496470019,-0.392629401
H,0,0.4608506769,0.1151282607,1.8337410466
H,0,4.0711679665,-1.499049796,-1.1587907331
H,0,2.5853451564,1.3932714356,1.6345974174
H,0,0.1603458322,-1.9953723859,0.555020991
H,0,4.4197906862,0.5654986479,0.1748355994
H,0,1.9498081449,-2.7498970189,-0.9801122743
N,0,1.1228535636,1.4545719814,-0.6344400695
O,0,1.2655007808,0.8176657575,-1.559305763
O,0,0.75964207,2.3989157682,-0.116817001
S,0,-2.2531235255,-0.1416098159,0.1329334456
O,0,-2.5308283627,-1.5123349896,-0.6079892351
O,0,-1.9476169669,-0.4902553231,1.4849294104
O,0,-3.6671070702,0.5625482192,0.1677795461
O,0,-1.3451991631,0.6484907141,-0.6615341492
H,0,-3.8703163879,1.0342564115,-0.6573255767
H,0,-2.5559936257,-1.4161329885,-1.5745903172

Optimized TS for the nitration of benzene / H_2SO_4 with eps=109



Scrf=(solvent=generic=read)
eps=109
epsinf=2.016
rsolv=2.5
m062x/6-311++G**
E(RM062X) = -1137.22898495

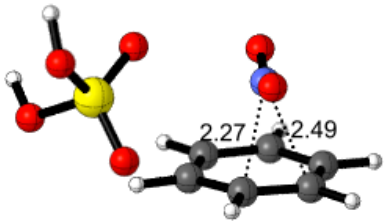
Zero-point correction= 0.153524 (Hartree/Particle)
Thermal correction to Energy= 0.167855
Thermal correction to Enthalpy= 0.168799
Thermal correction to Gibbs Free Energy= 0.109969
Sum of electronic and ZPE= -1137.075461
Sum of electronic and thermal Energies= -1137.061130

Sum of electronic and thermal Enthalpies= -1137.060186
Sum of electronic and thermal Free Energies= -1137.119016

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	105.331	50.401	123.819

C,0,1.242229262,-0.2448802291,1.1737812552
C,0,3.2950184823,-1.1345787946,-0.4977707368
C,0,2.444681072,0.493686734,1.0452197534
C,0,1.0757760891,-1.4260757829,0.4576120736
C,0,3.4899217265,0.0145488139,0.2397514058
C,0,2.0855476353,-1.8500807307,-0.393303153
H,0,0.45915009,0.1123503552,1.8331059991
H,0,4.072528475,-1.4978054547,-1.1580908063
H,0,2.5822941935,1.3925330657,1.6350247473
H,0,0.1609428559,-1.9978938175,0.5530424584
H,0,4.4184997629,0.5668119345,0.1762523485
H,0,1.951860377,-2.7500742962,-0.9813959988
N,0,1.1248023446,1.4540022475,-0.6340665089
O,0,1.2656724531,0.8166855998,-1.5590530862
O,0,0.7623867002,2.3993057846,-0.1173646692
S,0,-2.2535307302,-0.1414817273,0.133387552
O,0,-2.5324499553,-1.5105811573,-0.6099975757
O,0,-1.9493717504,-0.4929767513,1.4850282739
O,0,-3.6667661412,0.5642251148,0.1687845505
O,0,-1.3442351656,0.6489954291,-0.6590153533
H,0,-3.8686273514,1.0383106443,-0.6553063893
H,0,-2.5561664256,-1.4126849816,-1.5764781407

TS for the nitration of benzene / H_2SO_4 in water



scrf=(solvent=water)
m062x/6-311++G**
E(RM062X) = -1137.22726102

Zero-point correction= 0.154049 (Hartree/Particle)
Thermal correction to Energy= 0.166019
Thermal correction to Enthalpy= 0.166963
Thermal correction to Gibbs Free Energy= 0.114796
Sum of electronic and zero-point Energies= -1137.073212
Sum of electronic and thermal Energies= -1137.061242
Sum of electronic and thermal Enthalpies= -1137.060298
Sum of electronic and thermal Free Energies= -1137.112465

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	104.179	44.476	109.795

C,0,1.3808052492,-0.1790984205,1.2150657253
C,0,3.2485195488,-1.1046086776,-0.5984768334
C,0,2.6600428452,0.4238640053,1.1419762024
C,0,1.0813986765,-1.3063225731,0.4319121017
C,0,3.5902400313,-0.0471016994,0.2309442152
C,0,2.0014636881,-1.7434294623,-0.4902389748
H,0,0.6649692357,0.1701832907,1.9463477573
H,0,3.9581589183,-1.4563187812,-1.3349639493
H,0,2.8919539507,1.2578040922,1.7907612374
H,0,0.124883694,-1.7976488336,0.5427540226
H,0,4.562211449,0.4173184686,0.1530787729
H,0,1.7737778722,-2.5807993605,-1.1342095695
N,0,0.921870416,1.4081211505,-0.3438201047
O,0,1.2999043668,1.0488741651,-1.349674275
O,0,0.3454188767,2.1660555624,0.2810778143
S,0,-2.245054708,-0.0880996204,-0.0392357781
O,0,-2.5956427662,-1.5966039417,-0.2591598342
O,0,-1.7988912621,0.0159803287,1.3056628391
O,0,-3.6278408463,0.6344200468,-0.1015994545
O,0,-1.4174556668,0.364476163,-1.1158316087
H,0,-3.8800348189,0.8515530891,-1.0127155056
H,0,-2.6805347504,-1.8162769919,-1.2005068005

TS for the nitration of benzene / H_2SO_4 with eps=109

Scrf=(solvent=generic=read)
eps=109
epsinf=2.016
rsolv=2.5
m062x/6-311++G**
E(RM062X) = -1137.22760470

Zero-point correction= 0.154042 (Hartree/Particle)
Thermal correction to Energy= 0.166015
Thermal correction to Enthalpy= 0.166960
Thermal correction to Gibbs Free Energy= 0.114783
Sum of electronic and zero-point Energies= -1137.073563
Sum of electronic and thermal Energies= -1137.061589
Sum of electronic and thermal Enthalpies= -1137.060645
Sum of electronic and thermal Free Energies= -1137.112821

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	104.176	44.478	109.814

C,0,1.3808052492,-0.1790984205,1.2150657253
C,0,3.2485195488,-1.1046086776,-0.5984768334
C,0,2.6600428452,0.4238640053,1.1419762024
C,0,1.0813986765,-1.3063225731,0.4319121017
C,0,3.5902400313,-0.0471016994,0.2309442152
C,0,2.0014636881,-1.7434294623,-0.4902389748
H,0,0.6649692357,0.1701832907,1.9463477573
H,0,3.9581589183,-1.4563187812,-1.3349639493
H,0,2.8919539507,1.2578040922,1.7907612374
H,0,0.124883694,-1.7976488336,0.5427540226
H,0,4.562211449,0.4173184686,0.1530787729
H,0,1.7737778722,-2.5807993605,-1.1342095695
N,0,0.921870416,1.4081211505,-0.3438201047
O,0,1.2999043668,1.0488741651,-1.349674275
O,0,0.3454188767,2.1660555624,0.2810778143
S,0,-2.245054708,-0.0880996204,-0.0392357781
O,0,-2.5956427662,-1.5966039417,-0.2591598342
O,0,-1.7988912621,0.0159803287,1.3056628391

O,0,-3.6278408463,0.6344200468,-0.1015994545
O,0,-1.4174556668,0.364476163,-1.1158316087
H,0,-3.8800348189,0.8515530891,-1.0127155056
H,0,-2.6805347504,-1.8162769919,-1.2005068005

π-complex for the nitration of benzene / H_2SO_4 in water

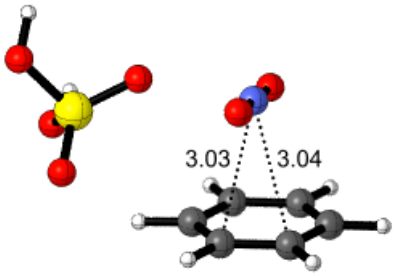
scrf=(solvent=water)
m062x/6-311++G**
E(RM062X) = -1137.23415202

Zero-point correction= 0.155069 (Hartree/Particle)
Thermal correction to Energy= 0.170106
Thermal correction to Enthalpy= 0.171051
Thermal correction to Gibbs Free Energy= 0.110779
Sum of electronic and ZPE= -1137.079083
Sum of electronic and thermal Energies= -1137.064046
Sum of electronic and thermal Enthalpies= -1137.063101
Sum of electronic and thermal Free Energies= -1137.123373

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	106.743	51.966	126.852

C,0,-0.9484656687,-0.0958313958,1.415685958
C,0,-2.4985233005,0.9219691104,-0.6665822876
C,0,-2.1695753588,-0.6947296552,1.0962301636
C,0,-0.5104501523,1.01695238,0.6984043148
C,0,-2.9449086834,-0.182758343,0.0560612586
C,0,-1.281345557,1.5214935754,-0.346147518
H,0,-0.3459424069,-0.4857560768,2.2287996837
H,0,-3.0985052251,1.315955275,-1.4783130989
H,0,-2.5195391988,-1.5492474998,1.6643745114
H,0,0.425828332,1.4952381555,0.9615944067
H,0,-3.8936702599,-0.6448707343,-0.1893621263
H,0,-0.9358962077,2.3820712125,-0.9068075186
N,0,-0.2127135319,-1.9998584634,-0.8229670052
O,0,-0.5938534734,-1.3214462013,-1.6078150001
O,0,0.1556999359,-2.7231636999,-0.0702641559
S,0,2.775474817,-0.0625828872,0.087093629
O,0,2.7911920658,1.4877746247,-0.2261532251
O,0,2.6008747025,-0.1816026979,1.4982360877
O,0,4.2527268263,-0.5261252244,-0.2174217048
O,0,1.8760197432,-0.7113554716,-0.8399859564
H,0,4.4244555654,-0.6450780745,-1.1667535342
H,0,2.6511170367,1.6829520913,-1.1679068827

π-complex for the nitration of benzene / H_2SO_4 with eps=109



Scrf=(solvent=generic=read)
eps=109
epsinf=2.016
rsolv=2.5
m062x/6-311++G**
E(RM062X) = -1137.23458220

Zero-point correction= 0.155119 (Hartree/Particle)
Thermal correction to Energy= 0.170140
Thermal correction to Enthalpy= 0.171085
Thermal correction to Gibbs Free Energy= 0.110960
Sum of electronic and ZPE= -1137.079463
Sum of electronic and thermal Energies= -1137.064442
Sum of electronic and thermal Enthalpies= -1137.063498
Sum of electronic and thermal Free Energies= -1137.123622

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	106.765	51.962	126.543

C,0,-0.9495407485,-0.0982248932,1.4167261157
C,0,-2.496323829,0.9220697864,-0.6670537172
C,0,-2.1717932407,-0.6945188796,1.0969163102
C,0,-0.5084864255,1.0127317903,0.6986735394
C,0,-2.9454397792,-0.1813297013,0.0561186405
C,0,-1.2776613332,1.5186299609,-0.3466770122
H,0,-0.3480548955,-0.4893785751,2.2299728952
H,0,-3.0949533001,1.3168006123,-1.4793926484
H,0,-2.5236470391,-1.5483022815,1.664904813
H,0,0.4294069547,1.4882867817,0.9608188285
H,0,-3.8948843515,-0.6418544685,-0.189601185
H,0,-0.9293205909,2.3775322051,-0.9081277399
N,0,-0.2097875277,-1.9999551707,-0.8195094553
O,0,-0.5969115274,-1.3261797078,-1.6053247294
O,0,0.1650186105,-2.7190308474,-0.0659426744
S,0,2.7725626398,-0.0589612752,0.0854612185
O,0,2.7933954028,1.4926596087,-0.2245519727
O,0,2.5935365545,-0.1820676821,1.4955723955
O,0,4.2496720714,-0.5250306049,-0.2187218175
O,0,1.8744260969,-0.7027825209,-0.8459105766
H,0,4.4173338872,-0.649264124,-1.1683038917
H,0,2.6514523708,1.6881699872,-1.1660473365

π-complex for the nitration of benzene / H_2SO_4 in water

scrf=(solvent=water)
m062x/6-311++G**

E(RM062X) = -1137.23314059

Zero-point correction= 0.154885 (Hartree/Particle)
Thermal correction to Energy= 0.167843
Thermal correction to Enthalpy= 0.168787
Thermal correction to Gibbs Free Energy= 0.113564
Sum of electronic and zero-point Energies= -1137.078256
Sum of electronic and thermal Energies= -1137.065298
Sum of electronic and thermal Enthalpies= -1137.064354
Sum of electronic and thermal Free Energies= -1137.119577

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	105.323	46.356	116.227

C,0,-0.955283465,-0.1057099629,1.4039216634
C,0,-2.5178520175,0.9239144691,-0.6538848587
C,0,-2.1778167772,-0.6984036471,1.0937760304
C,0,-0.5199107666,1.0047153947,0.6879183645
C,0,-2.9590374425,-0.1810349314,0.0652762617
C,0,-1.2988121343,1.5167889802,-0.3428557623
H,0,-0.3457120177,-0.5031311685,2.2053269232
H,0,-3.1228766812,1.3224303173,-1.4569336746
H,0,-2.5224918833,-1.5551757486,1.6577815543
H,0,0.4209498772,1.474138041,0.9417801135
H,0,-3.9088872364,-0.639404964,-0.1740938968
H,0,-0.9561746404,2.376475848,-0.9027405283
N,0,-0.2040249944,-1.982195065,-0.8134908081
O,0,-0.5996272496,-1.3185179382,-1.6012947585
O,0,0.1823263949,-2.6813476205,-0.0495564516
S,0,2.7920359765,-0.0471988992,0.0719566357
O,0,2.8311427958,1.4864442527,-0.2298308349
O,0,2.5720152855,-0.1736158788,1.4667059658
O,0,4.2558148627,-0.5211441686,-0.1903436684
O,0,1.9207494966,-0.6787835571,-0.8767275061
H,0,4.4201903288,-0.692903265,-1.1310814612
H,0,2.6932822885,1.6736595121,-1.1716093031

π-complex for the nitration of benzene / H_2SO_4 with eps=109

Scrf=(solvent=generic=read)

eps=109
epsinf=2.016
rsolv=2.5
m062x/6-311++G**

Zero-point correction= 0.154875 (Hartree/Particle)
Thermal correction to Energy= 0.167837
Thermal correction to Enthalpy= 0.168781
Thermal correction to Gibbs Free Energy= 0.113547
Sum of electronic and zero-point Energies= -1137.078694
Sum of electronic and thermal Energies= -1137.065732
Sum of electronic and thermal Enthalpies= -1137.064788
Sum of electronic and thermal Free Energies= -1137.120022

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	105.319	46.361	116.251

C,0,-0.955283465,-0.1057099629,1.4039216634
C,0,-2.5178520175,0.9239144691,-0.6538848587
C,0,-2.1778167772,-0.6984036471,1.0937760304
C,0,-0.5199107666,1.0047153947,0.6879183645
C,0,-2.9590374425,-0.1810349314,0.0652762617
C,0,-1.2988121343,1.5167889802,-0.3428557623
H,0,-0.3457120177,-0.5031311685,2.2053269232
H,0,-3.1228766812,1.3224303173,-1.4569336746
H,0,-2.5224918833,-1.5551757486,1.6577815543
H,0,0.4209498772,1.474138041,0.9417801135
H,0,-3.9088872364,-0.639404964,-0.1740938968
H,0,-0.9561746404,2.376475848,-0.9027405283
N,0,-0.2040249944,-1.982195065,-0.8134908081
O,0,-0.5996272496,-1.3185179382,-1.6012947585
O,0,0.1823263949,-2.6813476205,-0.0495564516
S,0,2.7920359765,-0.0471988992,0.0719566357
O,0,2.8311427958,1.4864442527,-0.2298308349
O,0,2.5720152855,-0.1736158788,1.4667059658
O,0,4.2558148627,-0.5211441686,-0.1903436684
O,0,1.9207494966,-0.6787835571,-0.8767275061
H,0,4.4201903288,-0.692903265,-1.1310814612
H,0,2.6932822885,1.6736595121,-1.1716093031

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