A New Tool to Guide Halofunctionalization Reactions: the Halenium Affinity (*HalA*) Scale

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Table of Contents:

I. General remarks:

All reactions were carried out in flame-dried glassware under an atmosphere of dry nitrogen or argon. Molecular sieves (4Å) were dried at 160 °C under 0.25 mtorr pressure prior to use. Unless otherwise mentioned, solvents were purified as follows. THF was distilled from sodium benzophenone ketyl. NMR spectra were obtained using a 500 MHz Varian NMR spectrometer and referenced using the residual ^{1}H peak from the deuterated solvent. Infrared spectra were measured on a Nicolet IR/42 spectrometer FT-IR (thin film, NaCl cells). For HRMS (ESI) analysis, a Waters 2795 (Alliance HT) instrument was used and referenced against Polyethylene Glycol (PEG-400-600).

Column chromatography was performed using Silicycle 60Å, 35-75 μm silica gel. Pre-coated 0.25 mm thick silica gel 60 F254 plates were used for analytical TLC and visualized using UV light, iodine, potassium permanganate stain, *p*-anisaldehyde stain or phosphomolybdic acid in EtOH stain.

Halenium sources used in this study: *N*-chlorosuccinimide (NCS), *N*-bromosuccinimide (NBS), *N*-iodosuccinimide (NIS), 1,3-dichloro-5,5-dimethylhydantoin (DCDMH), 1,3-dibromo-5,5-dimethylhydantoin (DBDMH) and *N*-chlorophthalimide (NCP) were re-crystallized prior to use. Chlorodiethylsulfonium hexachloroantimonate (CDSC), bromodiethylsulfonium bromopentachloroantimonate (BDSB), iododiethylsulfonium iodopentachloroantimonate (IDSI) were synthesized as reported previously.[1] Substituted pyridines were distilled and stored over KOH prior to use (except 4-bromopyridine which was distilled immediately after basification of its commercially available HCl salt and used right away). All other commercially available reagents and solvents were used as received unless otherwise mentioned.

II. Guide to halenium affinity (*HalA*) calculations:

Since we have derived parallels between protonation and halogenation chemistry, the evaluation of gas phase Halenium Affinity (*HalA*) is essentially similar to the reported methods used for derivation of Proton Affinity (*PA*).[2] We define the computationally evaluated *HalA* as the molar enthalpy change for a given Lewis base (:LB) upon its attachment to a halenium ion (X^+), as shown below:

$$HalA = -\Delta E(elec) - \Delta ZPE - \Delta E'(vib) + \frac{5}{2}RT \ ;$$

$$E'_{(vib)}\ (T) = \sum_{i=1}^{3n-6} \frac{Nhv_i}{e^{Nhv_i/RT} - 1}$$

where; $\Delta E_{(elec)} = E_{(electronic)}(\text{X-LB adduct}) - [E_{(electronic)}(:LB) + E_{(electronic)}(X^+)]$; zero point energy change $\Delta ZPE = ZPE(\text{X-LB adduct}) - ZPE(:LB)$; $\Delta E'_{(vib)} = E'_{(vib)}(\text{X-LB adduct}) - E'_{(vib)}(:LB)$ i.e. difference in temperature dependence of vibrational energy; N is Avogadro's number, *h* is Planck's constant, and n_i is the i^{th} vibrational frequency. Finally, the 5/2 RT quantity accounts for translational degrees of freedom and the ideal gas value for the change from two particles to one.

The acceptor fragment (Lewis base) may be neutral or anionic (i.e. the X-LB complex is cationic or neutral), leading to two distinct cases:

$$\Delta H_{rxn}(X^+ + :LB \rightarrow X\text{-}LB^+) \text{ or } \Delta H_{rxn}(X^+ + :LB^- \rightarrow X\text{-}LB)$$

The *HalA* values (gas phase) in kcal/mol are derived at T = 298.15 K (unless noted otherwise) assuming ideal gas behavior.

Ab initio assessments may provide accurate *HalA* values, but their computational expense quickly becomes impractical with increasing molecular size. A Density Functional Theory (DFT) approach is affordable and widely available to most organic chemists who wish to evaluate *HalA* values and apply them in the planning of halofunctionalization reactions. Our combined theoretical-experimental optimizations for the best compromise between computational expense and reliability of *HalA* values, have led us to the application of the following basis sets based on the halenium ion under consideration: a.) for fluorenium, chlorenium and bromenium ions - B3LYP/6-31G*. b.) for iodenium ion – B3LYP/6-31G*/LANL2DZ. To calculate *HalA* values from theory for gas phase reactions (appropriate solvent models can be applied if necessary) the following steps were followed:

1. An appropriate basis set must be chosen based on the halenium ion under consideration.
2. The Lewis base is initially subjected to a conformational search at the level of theory decided from step 1. To confirm that each structure was a true minimum, vibrational analyses were performed. If necessary, the lowest energy conformer can be re-subjected to a full geometry optimization to verify convergence.
3. The halenium ion (in its triplet state) is also subjected to the same level of theory for a geometry optimization.

4. The Lewis base-halenium ion adduct is then subjected to step 2 as described above. If there are multiple nucleophilic sites within the same molecule (Lewis base), then separate calculations must be initiated with appropriate attachment of the halenium ion to each nucleophilic site.

5. The following three values are extracted from each of the output files for geometry minimized Lewis base (lowest energy conformer) and the Lewis base-halenium ion adduct/complex: a.) electronic energy (E), b.) zero point energy (ZPE) and, c.) temperature dependence of vibrational energy $E'_{(vib)}$.

The electronic energy of the halenium ion is also obtained from its corresponding output file.

6.) Finally, these values (converted to kcal/mol) are then substituted in the following equation to obtain the *HalA* (X) for the Lewis base.

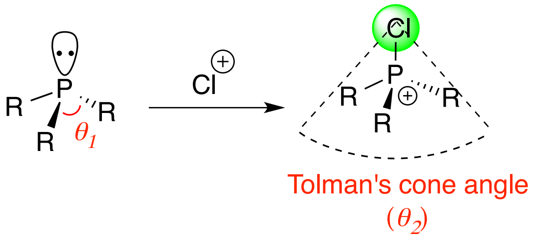
$$HalA = -\Delta E(elec) - \Delta ZPE - \Delta E'(vib) + \frac{5}{2}RT \;;$$

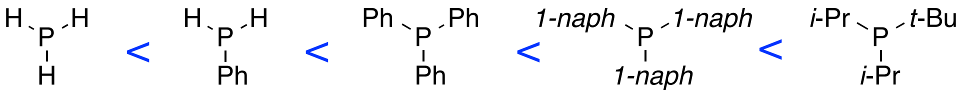
Alternatively, the excel file template provided as a separate section of supporting information can be used to obtain the *HalA* value by simply entering the six values obtained from the output files for geometry minimized Lewis base (lowest energy conformer) and the Lewis base-halenium ion adduct/complex.

III. Interpreting the halenium affinity table:

The Halenium affinity table (attached as a separate section of supporting information) provides over 500 *HalA* (Cl) values for various halenium acceptors that are categorized based on functional groups. Each category includes an organized trend of *HalA* values for acceptors based on their ring size, substitution pattern, nucleophilicity etc. For searching a category of acceptors or even a particular acceptor, the table also provides labels and molecular formulas. The labels are based on the functionalities and/or the acceptor atom. For instance, the *HalA* (Cl) of morpholine can be found by searching the document for molecular formula- C_4H_9NO. Since, morpholine incorporates nitrogen and oxygen atoms serving as halenium ion acceptors, searching the document under the label '**NO**' will lead to a quick recognition of compounds incorporating **N**itrogen and **O**xygen atoms that have been evaluated for halenium affinity (e.g. N-methyl morpholine, 4-hydroxypyridine, methoxypyridines, amides etc.). Apart from simply being a listing of *HalA* (Cl) values, the table also provides the reader with useful and handy trends that can be interpreted based on their ring size, steric strain etc. The following four examples illustrate a few of several trends.

Example 1

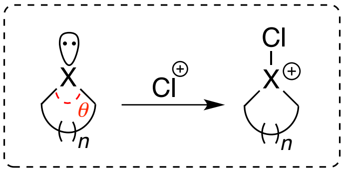


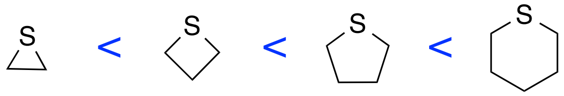


Label	**P1**	**P2**	**P6**	**P8**	**P5**
θ_1	93.4°	93.0°	102.6°	103.0°	107.4°
θ_2	48.0°	51.0°	106.1°	123.5°	146.1°
HalA (Cl)	156.0	184.6	215.0	221.3	220.5

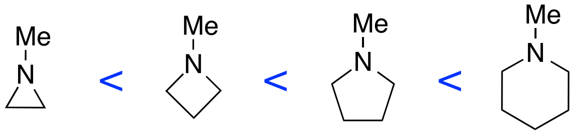
The relationship of sterics incorporated in substituted phosphines to their electron donating ability can be best described by the Tolman's concept of cone angles.[3] To represent the trend of halenium affinity in phosphines, we have employed the cone angle where the metal center is replaced by a chlorine atom. As shown above, the increasing steric demand of the substituents on phosphine leads to an increased internal angle (θ_1) for R-P-R (**P1**-93.4° <**P2**-93.0° < **P6**-102.6° < **P8**-103.0°< **P5**-107.4°) eventually shifting the trigonal pyramidal geometry of the phosphine towards trigonal planar. Thus in sterically bulky phosphines, the R-P bond gains more '*s*' character leading to higher '*p*' character in the lone pair. A lone pair with more '*p*' character is less bound to the nucleus and displays enhanced nucleophilicity for the free phosphine. Meanwhile, as substituent bulk increases, the strain in the larger cone angle (θ_2) cases of the halo-phosphonium ion opposes this effect, leading to a leveling off of the rate of increase in the *HalA* (Cl) values.

Example 2





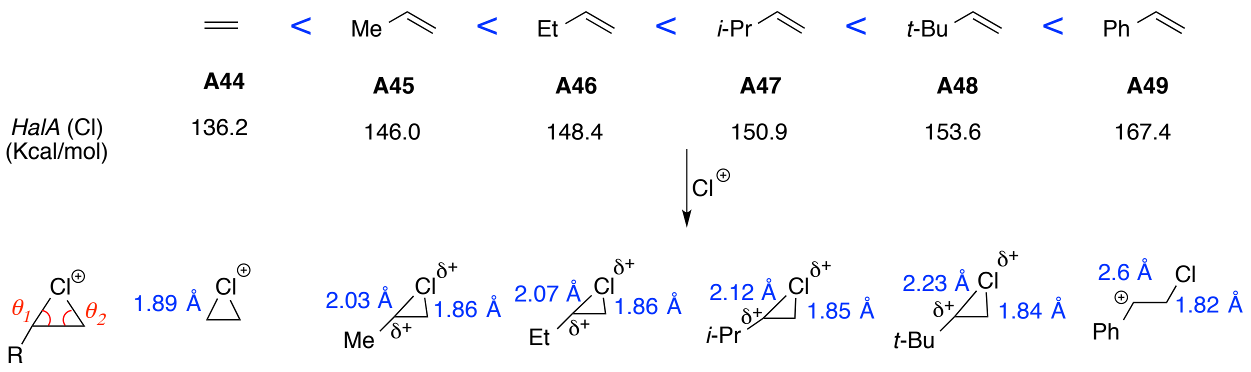
Label	**S13**	**S14**	**S15**	**S16**
∠C-S-C (θ)	47.5°	76.6°	93.7°	97.8°
HalA (Cl) (Kcal/mol)	147.3	155.2	159.1	161.5



Label	**N58**	**N59**	**N60**	**N61**
∠C-N-C (θ)	61.4°	90.5°	104.6°	111.7°
N-Cl (Å)	1.76	1.79	1.80	1.80
HalA (Cl) (Kcal/mol)	157.4	164.3	165.4	165.9

As described for example 1 above, a similar trend of *HalA* (Cl) is observed for compounds **S13** to **S16** and **N58** to **N61**. With increasing ring size, the angle strain for C-N-C or C-S-C (θ) is relieved. The increase in '*p*' character of the lone pair with increasing ring size enhances the nucleophilicity of the heteroatoms and hence their halenium affinity. In contrast, as we go from left to right the increasing '*p*' character of the lone pair results in a longer bond to the chlorine atom (intrinsic effect due to the geometry). This can be seen from increasing N-Cl distance in the chlorinated analogs. Among the compounds shown above, the lone pair electrons in **S13** and **N58** are tightly bound to the nucleus as they have the highest '*s*' character and hence the resulting S-Cl or N-Cl bond is the strongest.

Example 3

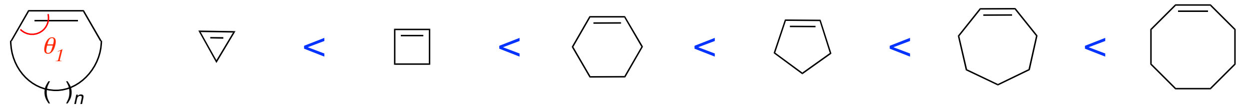


	A44	**A45**	**A46**	**A47**	**A48**	**A49**
HalA (Cl) (Kcal/mol)	136.2	146.0	148.4	150.9	153.6	167.4

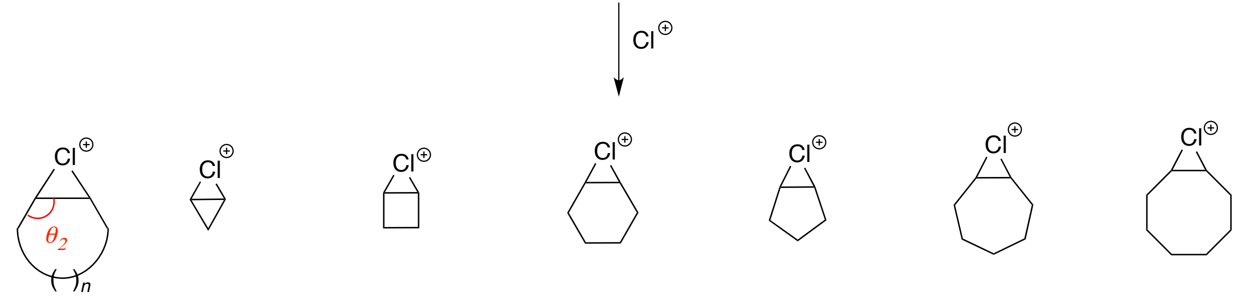
Label	**A44**-Cl	**A45**-Cl	**A46**-Cl	**A47**-Cl	**A48**-Cl	**A49**-Cl
θ_1	67.3°	61.8°	60.5°	58.7°	54.9°	43.6°
θ_2	67.3°	74.4°	76.1°	78.7°	84.2°	102.2°

The ascending trend of *HalA* (Cl) values in this example (as anticipated) displays the increasing reluctance of chlorenium ion to form a three membered cyclic intermediate (chloriranium ion) with the increasing inductive and hyperconjugative donating effects of the substituent on the terminal olefin. Ethylene (**A44**) by itself forms a symmetrically bridged chloriranium ion **A44**-Cl. The increasing donating effect of the substituents (**A45**-**A48**) distorts this symmetry as indicated by the C-Cl distances and the bond angles θ_1 and θ_2. The phenyl ring in styrene (**A49**) stabilizes the chlorenium ion via resonance electron donation. The delocalization of this positive charge results in the corresponding chloromethyl carbenium ion **A49**-Cl.[4]

Example 4



	A86	**A87**	**A89**	**A88**	**A90**	**A91**
θ_1	64.6°	94.4°	123.5°	112.1°	128.0°	131.5°
HOMO (LUMO)	-9.6 eV (4.9 eV)	-9.4 eV (5.1 eV)	-9.1 eV (5.2 eV)	-9.1 eV (5.2 eV)	-9.1 eV (5.1 eV)	-9.1 eV (5.0 eV)
HalA (Cl) (Kcal/mol)	141.1	147.9	154.8	155.5	156.9	159.2



	A86-Cl	**A87**-Cl	**A89**-Cl	**A88**-Cl	**A90**-Cl	**A91**-Cl
θ_2	61.7°	91.9°	120.8°	109.2°	125.2°	130.1°
θ *for parent cycloalkane*	60.0°	89.4°	111.5°	103.3°	~116.0°	~117.0°

Forming a chlorenium ion adduct of the above cycloalkenes leads to re-hybridization of the olefinic carbons from sp^2 (∠C-C=C = 120°) to hybridization between sp^2 and sp^3 (similar to oxirane carbons). The initial strain introduced due to presence of olefinic carbons (in the parent cycloalkene) can be relieved to a certain extent if the concomitant re-hybridization in its chlorenium adduct leads to a bond angle (θ_2) that is close to the corresponding bond angle (θ) in the parent cycloalkane. As shown above, the *HalA* (Cl) value of the cycloalkenes increase with the ring size, except for **A88** and **A89**. Cyclopropene (**A86**) incorporates a higher ring strain and angular strain θ_1 = 64.6° (55.4° deviation from the normal bond angle of 120° for an sp^2 carbon). Formation of the chlorenium ion adduct **A86**-Cl, alleviates this strain to a certain extent as θ_2 (61.7°)

approaches the natural bond angle in cyclopropane (θ = 60.0°) *via* partial hybridization of the sp^2 carbons. Though cyclobutene undergoes similar changes in its bond angles upon formation of **A87**-Cl, it has a relatively higher *HalA* (Cl). A switch in the trend of *HalA* (Cl) values is observed for cyclopentene (**A88**) and cyclohexene (**A89**). Their orbital energies being similar, the only difference arises due to the change in angle strain upon formation of **A88**-Cl and **A89**-Cl. The resulting hybridization in **A88**-Cl brings θ_2 (109.2°) closer to the bond angle in the parent cyclopentane (θ = 103.3°, $\theta_2 - \theta$ = 5.9°) in comparison to formation of **A89**-Cl, which results in elevated angle strain as θ_2 (120.8°) deviates further from cyclohexane (θ = 111.5°, $\theta_2 - \theta$ = 9.3°). Finally, as θ_1 increases with increasing ring size (θ_1-**A91**), the corresponding change in the geometry of the olefin escalates its nucleophilicity.

IV. Equilibrium and titration studies on halopyridinium salts:

a. Screening of chlorenium sources for the formation of chloropyridinium complexes of 1a:

To test the validity of theoretically evaluated halenium affinity values, we studied the possibility for the formation of chloropyridinium complexes *via* ^{1}H NMR. In this respect, 2,4,6-trimethylpyridine **1a** was initially chosen as a model substrate and acetone-d_6 was identified as the optimum solvent of choice. The corresponding halo-pyridinium salts of **1a** displayed low solubility in other commercially available deuterated solvents. Halo-pyridinium salts of **1a** were found to be soluble in tetrahydrofuran-d_8 (THF), but this solvent was prohibitively expensive for the large number of planned experiments. Furthermore, the possibility of chlorination of acetone under reaction conditions was ruled out based on three control experiments (see section **III-h** for further discussion), thus assuring that acetone is not a reactive solvent.

The formation of halo-pyridinium complex (**1a**-X) was monitored by observing the

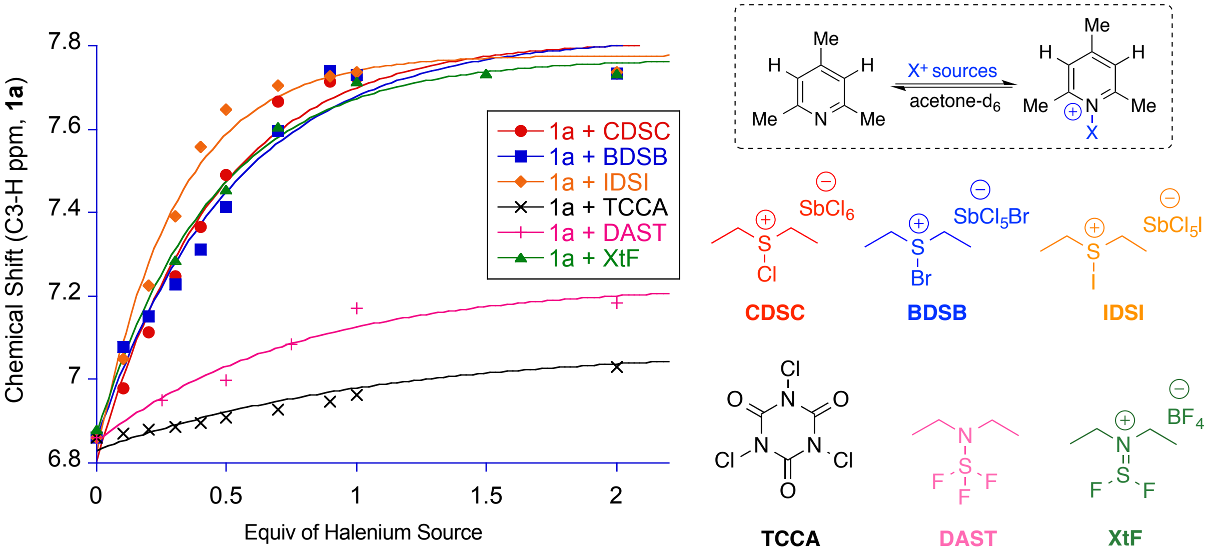


Figure S1. Plot for titration of **1a** with various halenium ion sources representing the chemical shift change of C3-H (ppm, **1a**) as a function of added halenium ion source.

chemical shift (ppm) change of the C3-H aromatic hydrogens of **1a** upon treatment with various amounts of halenium sources (X^+). As seen in Figure S1, halenium ion sources such as NCS, NCP, dichloramine-T and TCCA with *HalA* values lower than **1a** did not fully transfer halenium ion to **1a**, whereas XtalFluor-E®, CDSC, BDSB, and IDSI did form the halo-pyridinium salts. A significant downfield shift of C3-H (approximately 0.9 ppm) is evident when 1.0 equivalent of the latter halenium sources are added to **1a** (since the extent of positive charge localized on the pyridine nucleus is the same in the halo-pyridinium salts **1a**-F, **1a**-Cl, **1a**-Br and **1a**-I, the extent of downfield chemical shift observed for C3-H was also the same upon addition of 1.0 equiv of halenium sources). After addition of 1.0 equivalent of halenium ion source to **1a**, there no further observable change in the chemical shift of C3-H (of **1a**-Cl) as the titration is extended beyond 1.0 equiv of the halenium source (indication for the formation of 1:1 complex). Based on the *HalA* values, TCCA and DAST do not have the ability to completely transfer X^+ ion, resulting only in stronger halogen bonding that leads to a 0.16 and 0.34 ppm downfield shift of C3-H, respectively. No chemical shift changes were observed when NCS, DCDMH, dichloramine-T, and N-chlorophthalimide sources were used. Addition of up to 5.0 equiv of TCCA (i.e. 15.0 equiv of active chlorenium ion) did not shift C3-H further downfield. However, with this excess of halogenating reagent, new peaks appeared in the aromatic region of the ^{1}H-NMR spectrum, suggesting side reactions such as benzylic chlorination. EI-MS studies on the crude mixture displayed masses for mono, di- and tri-chlorinated **1a**). Radical chlorination of the aromatic ring can be ruled out since the same product was obtained when the experiment was repeated in the dark.

Table S1. Absolute and relative *HalA* values (gas phase) of **1a** in comparison to different halenium sources. Since SM8 is not compatible for elements >Kr, the gas phase *HalA* values are depicted for comparison of the halenium (F, Cl, Br and I) sources.

Entry	**Halenium source**	**Halenium Ion (X)**	***HalA* (X) of 1a (kcal/mol)**	***HalA* (X) of halenium ion source (kcal/mol)**	***ΔHalA* (kcal/mol)**
1	DAST	F^+	288.8	432.2	143.4
2	XtF	F^+	288.8	294.7	5.9
3	NCS	Cl^+	168.2	290.1	121.9
4	DCDMH	Cl^+	168.2	275.7	107.5
5	NCP	Cl^+	168.2	286.7	118.5
6	Dichloramine-T	Cl^+	168.2	273.3	105.1
7	TCCA	Cl^+	168.2	253.0	84.8
8	CDSC	Cl^+	168.2	161.3	-6.9
9	BDSB	Br^+	179.4	133.2	-46.2
10	IDSI	I^+	141.1	96.7	-44.4

NCS, DCDMH, NCP and Dichloramine-T, and have 121.9, 107.5, 118.5, and 105.1 (kcal/mol) higher gas phase chlorenium affinities than trimethyl pyridine, respectively (Table S1, entries 3-6). These large differences are corroborated by the experimental data and explain why the corresponding halo-pyridinium complexes are not formed. In organic solvents, conversion of neutral species into charged products is typically uphill in energy, so the conjugate anion of the halenium ion donor will always be more potent acceptor than **1a**. Thus, it is no surprise that chlorenium ion transfer from neutral donors to substituted pyridines to yield halo-pyridiniums is unlikely. Therefore, for all subsequent experiments, CDSC was employed as the chlorenium donor, BDSB as the Br^+ donor and IDSI as the I^+ donor; the corresponding gas phase *Hal*A values (gas phase) are 161.3, 133.2, and 96.7 kcal/mol, respectively (Table S1, entries 8-10).

b. Titration studies of pyridine derivatives with CDSC:

Substituted pyridines 4-phenylpyridine (**1h**), 4-cyanopyridine (**1f**), pyridine 4-carbaldehyde (**1i**), 4-trifluoromethylpyridine (**1e**), and 4-dimethylaminopyridine (**1j**) were titrated with CDSC (0.0-2.0 equiv) in acetone-d_6 at room temperature (Figure S2). The range of *HalA* (Cl) values (gas phase) for these pyridines spans from 145.2 to 176.0 kcal/mol. B3LYP/6-31G*/SM8 is not compatible for the antimony (VI) chloride counterion associated with CDSC, hence we resorted comparing gas phase *HalA* (Cl) values of diethyl sulfide and substituted pyridines. The gas phase *HalA* (Cl) values are 161.3 for diethyl sulfide and 168.2 for **1a**. Figure S2 depicts the downfield shifts of the pyridines' C3-H resonances as they are titrated with CDSC (0.0-2.0 equiv), forming chloro-pyridinium complexes. In all cases the formation of a 1:1 complex of Lewis base:halonium ion was confirmed on the basis of the unchanged chemical shifts of C3-H beyond addition of a stoichiometric equivalent of CDSC.

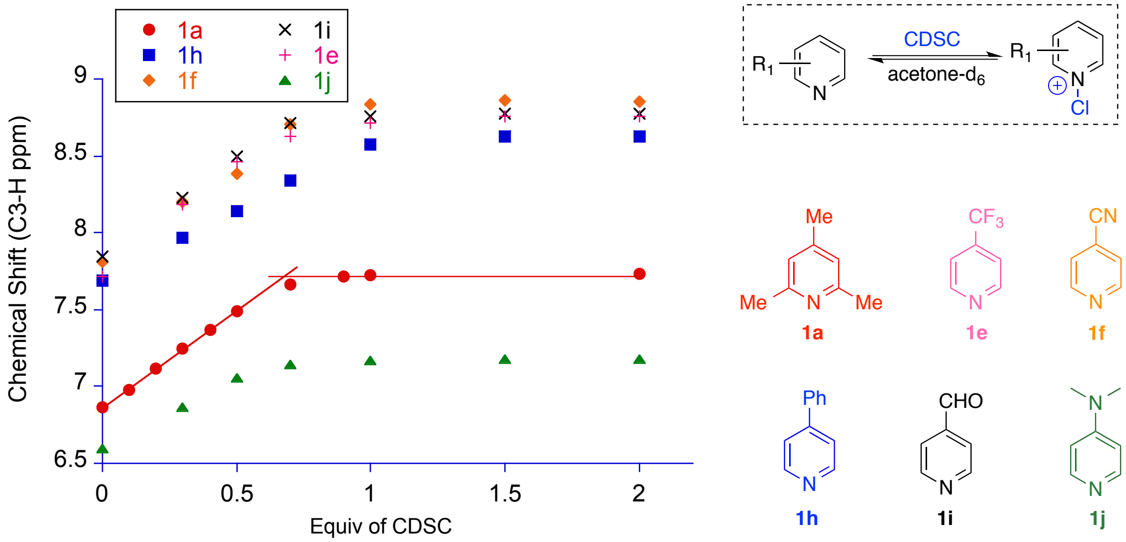


Figure S2. Plot for titration of pyridines **1a-i** with various CDSC representing the chemical shift change of C3-H (ppm) as a function of added CDSC. The biphasic nature of the data for the titration of **1a** is illustrated by two straight lines.

As Table S2 shows, halenium ion transfer to substituted pyridines can be easily monitored from the downfield chemical shift change of the aromatic proton (*meta* proton, C3-H). The most electron rich pyridine **1j** (DMAP) shows an attenuated shift as a result of the electron donating C_4-*N,N*-dimethylamine, which prior to chlorenium transfer alters the chemical shift of the C3-H significantly in comparison to other substituted pyridines. The observed chemical shift change between the free pyridine derivatives and their protonated analogs (~1 ppm downfield), closely matches those observed upon treatment of pyridine derivatives **1a**-**j** with 1.0 equiv of CDSC. This clearly suggests complete chlorenium atom transfer to the nitrogen in all these pyridines to form the corresponding chloropyridinium salts. However, the exact chemistry of Cl^+ delivery by CDSC is not completely understood. The range of *HalA* (Cl) values (SM8-acetone) for the pyridines in Table S2 spans from 137.2 to 154.3 kcal/mol, while that simply calculated for diethyl sulfide is 151.6, yet as noted above, complete chlorenium transfer is clearly indicated by the NMR results. Exploratory studies of possible explanations

Table S2. Absolute and relative *HalA* values in kcal/mol obtained from gas phase and (SM8-acetone) calculation of pyridine derivatives **1a**-**j** in comparison to diethyl sulfide–mimicking CDSC. [a]The Δ*HalA* values displayed below represent the difference in *HalA* (Cl) values between the pyridine derivatives and diethyl sulfide. The *HalA* value of diethyl sulfide is 161.3 kcal/mol (gas phase) and 151.6 kcal/mol (SM8-acetone).

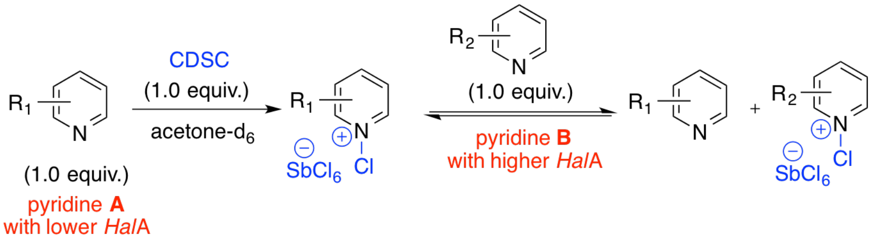
Entry	Pyridine derivatives	*Hal*A gas phase	*HalA*	Δ*Hal*A gas phase	Δ*Hal*A SM8-acetone[a]	Δppm (C3-H)
1	**1j** (4-NMe_2)	176.0	154.3	14.7	2.7	0.576
2	**1a** (2,4,6-trimethyl)	168.2	148.2	6.9	-3.4	0.868
3	**1h** (4-Ph)	165.7	145.7	4.4	-5.9	0.936
4	**1i** (4-CHO)	150.8	140.8	-10.5	-10.8	0.921
5	**1f** (4-CN)	145.2	138.0	-16.1	-13.6	1.048
6	**1e** (4-CF_3)	149.3	137.2	-12.0	-14.4	1.050

involving differential ion pairing of the $SbCl_6^-$ counterion with Et_2SCl^+ vs the chloropyridinium cations are not accessible to the present method as the SM8 solvent model included in the Spartan code does not extend to antimony. Hence, we focus our analysis on comparisons of the *HalA* values within the same class (i.e. the pyridine derivatives in this case) of Lewis bases.

c. Qualitative analysis of competition experiments between pyridine derivatives:

To validate the *Hal*A scale on a more conclusive manner, the equilibrium of various substituted chloropyridiniums were investigated. In a typical experiment, a stock solution of CDSC (1.0 equiv) was added at room temperature to an acetone-*d_6* solution of pyridine **A** (1.0 equiv), which has a lower calculated *HalA* than diethyl sulfide. Complete formation of the chloro-pyridinium complex (**A**-Cl) was then confirmed by ^{1}H NMR analysis. To this complex (**A**-Cl), pyridine **B** (1.0 equiv), chose to have a higher calculated *HalA* value than **A** was added to generate **B**-Cl *via* abstraction of chlorenium

Table S3. Absolute and relative *HalA* values in kcal/mol (SM8-acetone) of pyridine derivatives **1a-j**.



Entry	Pyridine derivatives (A)	*Hal*A (kcal/mol) of pyridines (A)	(A_{Cl}/A)	Pyridine derivatives (B)	*Hal*A (kcal/mol)	(B_{Cl}/B)
1	**1e** (4-CF_3)	137.2	0.35	**1a** (2,4,6-trimethyl)	148.2	0.80
2	**1f** (4-CN)	138.0	0.37	**1a** (2,4,6-trimethyl)	148.2	0.80
3	**1f** (4-CN)	138.0	0.52	**1e** (4-CF_3)	137.2	0.56
4	**1e** (4-CF_3)	137.2	0.04	**1j** (4-NMe_2)	154.3	0.75
5	**1a** (2,4,6-trimethyl)	148.2	0.29	**1j** (4-NMe_2)	154.3	0.79
6	**1i** (4-CHO)	150.8	0.29	**1h** (4-Ph)	165.7	1.0
7	**1h**	165.7	0.28	**1a**	168.2	0.70

ion from **A**-Cl. The established equilibrium was then analyzed *via* ^{1}H-NMR analysis. The amount of each chlorinated pyridine derivative was determined by examining the chemical shift change of C3-H and correlating it with the titration data of each substituted pyridine with CDSC (Figure S2). For example, in the competition between **1e** and **1a**, C3-H for **1e**-Cl under the equilibrium mixture resonates at 8.27 ppm. Using linear interpolation based on the biphasic behavior seen between the limiting shifts observed for unchlorinated and chlorinated pyridines in titrations with CDSC, this shift indicates that 0.35 mol fraction of **1e** is chlorinated. Similarly, C3-H of **1a**, resonating at 7.67 ppm correlates to a 0.80 mol fraction of **1a**. (Note: the sum of the individual mole fractions is over 100% (0.35 + 0.80 = 1.15) and this can be attributed to the fact that the actual chemical shift observed for C3-H under sub-stoichiometric amounts of halenium source is influenced by dimerization). Table S3 shows the fraction of chlorinated pyridine **A** and **B**, extracted from the titration curves in Figure S2 based on the changes in the chemical shifts of C3-H aromatic proton of the substituted pyridines. This shows a correlation between the calculated chlorenium affinities and experimental results. As anticipated, pyridine **B** with higher *HalA* value yields a greater ratio of $\mathbf{B}_{\mathrm{Cl}}$:**B**. This is a fair *qualitative* comparison to display the transfer of chlorenium ion from pyridine **A** (with a relatively lower *HalA*) to pyridine **B** exhibiting a relatively higher *HalA* value. Pyridine derivative **1a** has 18.9 and 23.0 kcal/mol higher *HalA* than **1e** and **1f**, respectively, and thus the chlorenium ion is mostly transferred to **1a** (with 0.80 equivalents chlorinated, Table S3, entry 1 and 2). The smallest difference in the fraction of chlorinated complex is observed between **1f** and **1e** (0.56 versus 0.52, Table S3, entry 3). This is in complete agreement with the *HalA* values of the two pyridines. *HalA* (Cl) of **1f** is 138.0 kcal/mol and *HalA* (Cl) of **1e** is 137.2 kcal/mol.

These experiments qualitatively display the correlation between theoretically calculated *HalA* values and the fraction of chlorinated pyridine observed by ^{1}H NMR. However, these experimental results cannot be used for quantitative analysis. As shown in Figures S1 and S2, the titration curves are nonlinear prior to addition of full stoichiometric equivalent amounts of halenium ion sources (CDSC, BDSB and IDSI), clearly suggesting the possibility of dimerization. This dimerization was confirmed when treatment of **1a** with 0.5 equivalents of BDSB (or IDSI) in $CDCl_3$ displayed a downfield shift of the C3-H to 7.2 ppm. The extent of this shift is in accordance to the reported halogenated dimers of **1a**.[5] The tendency of halo-pyridinium to undergo dimerization with the free base when subjected to sub-stoichiometric amounts of halenium source limits the quantitative analysis.[6] Moreover, the rapid exchange of chlorenium ion between the chlorinated and non-chlorinated acceptors leads to an averaged NMR signal, which does not allow for a direct measure of each species *via* integration.

Seeking reliable means for qualitative and quantitative analysis, we attempted to block pyridine-halogen-pyridine dimerization and the fast exchange of halenium ion in order to observe the chlorinated and non-chlorinated species under NMR timescale. Our rigorous optimizations identified pyridines **1b** and **1c** as model candidates for this study. Chlorinated **1b**-Cl and **1c**-Cl and their non-chlorinated counterparts **1b** and **1c** could be observed by ^{1}H NMR at -90 °C in acetone-d_6. This enables the integration of each individual species (free base and its chlorinated analog) such that the ratios of chlorinated and non-chlorinated counterparts could be obtained.

d. ^{1}H-NMR analysis of chlorination of 4-methyl-2,6-di-tert-butyl pyridine (1c):

To rigorously confirm *HalA* assessments on a quantitative scale, we resorted to equilibrium studies of chloropyridinium salts. Addition of 0.5 equiv of CDSC to **1c** in acetone-*d₆* at room temperature led to the observation of two species (broad peaks) by ^{1}H NMR (Figure S3). Lowering the temperature to -30 °C, resulted in two sharp peaks corresponding to **1c** and chlorinated **1c**-Cl in a 1:1 ratio. This demonstrates that **1c** has a slow exchange with its chlorinated form (**1c**-Cl) under the NMR timescale; thus enabling the observation of the chlorinated pyridine and its free base by ^{1}H-NMR analysis at -30 °C. The bulky *t*-butyl substituents on the *ortho* positions efficiently inhibited the dimerization and the rapid intermolecular transfer of halenium ions. **1c** was

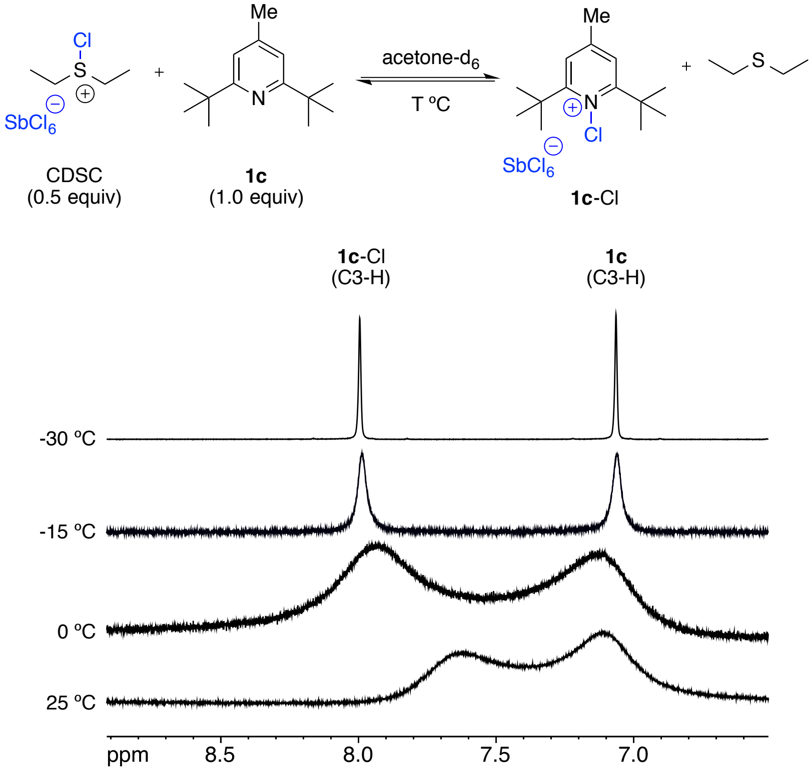
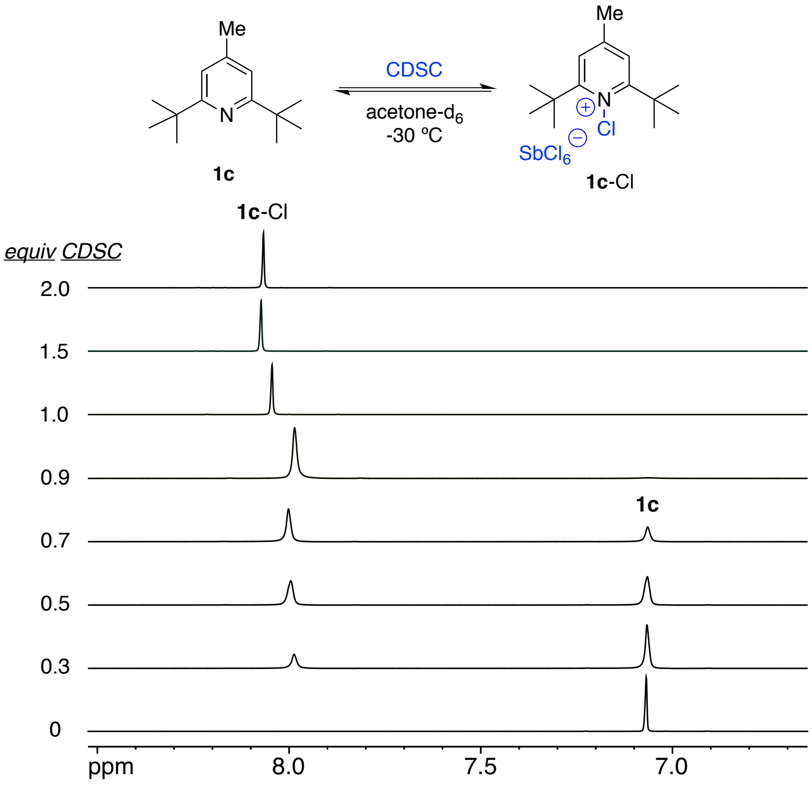


Figure S3. ^{1}H NMR spectra of **1c** at different temperatures under sub-stoichiometric amounts (0.5 equiv) of CDSC.

then titrated with CDSC to observe the ratios of **1c** and **1c**-Cl at -30 °C. Figure S4 shows the overlay of ^{1}H NMR spectra (C3-H) with different amounts of CDSC. The resonance at 7.06 ppm corresponds to the free base, while the downfield peak at 8.06 ppm corresponds to **1c**-Cl. Upon addition of 1.0 equiv of CDSC, the resonance at 7.06 ppm disappears, and only **1c**-Cl is observed (8.06 ppm, Figure S4, entry 6).

e. Formation of halopyridinium salts of 1c with different halenium donors:

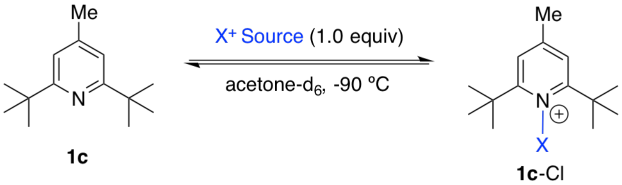


Entry	CDSC (equiv)	1c (%)	1c-Cl (%)
1	0.0	100	0.0
2	0.3	69.0	30.0
3	0.5	53.0	50.0
4	0.7	31.0	70.0
5	0.9	3.0	90.0
6	1.0	0.0	100
7	1.5	0.0	100
8	2.0	0.0	100

Figure S4. Titration data for chlorination of **1c** with CDSC.

Since **1c** and **1c**-Cl can be observed as separate entities under the NMR timescale at -30 °C, we initiated similar studies with different halenium sources to observe the formation of **1c**-X and validate the theoretical *HalA* estimates. The counter anions of DAST and TCCA have a higher *HalA* than **1c** (Table S4, entries 1 and 3) therefore, as anticipated, ^{1}H NMR showed no evidence of their transferring halenium ion. Similarly, as expected from the *HalA* values, only CDSC, BDSCB and IDSI led to a complete transfer of halenium ion to **1c** forming the corresponding halo-pyridinium salts (Table S4, entries 4-6).

Table S4. Absolute *HalA* values and experimentally observed ratios of **1c** and **1c**-X using different halenium ion sources. Since SM8 is not compatible for elements >Kr, the gas phase *HalA* values are depicted for comparison of the halenium (F, Cl, Br and I) sources.



1c **1c**-Cl

Entry	Halenium source	Halenium ion (X)	***Hal*A (X) of 1c gas phase (kcal/mol)**	***Hal*A of Halenium source gas phase (kcal/mol)**	**(1c-Cl)%**
1	DAST	F^+	287.9	432.2	0.0
2	XtF	F^+	287.9	294.7	47.0
3	TCCA	Cl^+	153.1	253.0	0.0
4	CDSC	Cl^+	153.1	161.3	100
5	BDSB	Br^+	160.4	133.2	100
6	IDSI	I^+	118.4	96.7	100

f. Quantitative analysis *via* competition experiments:

The optimized conditions mentioned above were employed to study the competition for chlorenium ion capture between **1a** and **1c**. Since, **1a** has a 15.0 kcal/mol higher chlorenium affinity than **1c**, halenium ions should preferentially bind to **1a** over **1c** with an equilibrium constant > 10^{10}. As shown by the ^{1}H-NMR spectra overlay (Figure S5), titration of the pre-formed **1c**-Cl complex with **1a** leads to a corresponding decrease in the concentration of **1c**-Cl as the chlorenium ion is now transferred onto the stronger Lewis base **1a** (intensity of the peak at 8.06 ppm for **1c**-Cl decreases while the intensity of the peak at 7.06 ppm which corresponds to free **1c**, increases). Moreover, a careful inspection of Figure S5 indicates a downfield shift of the

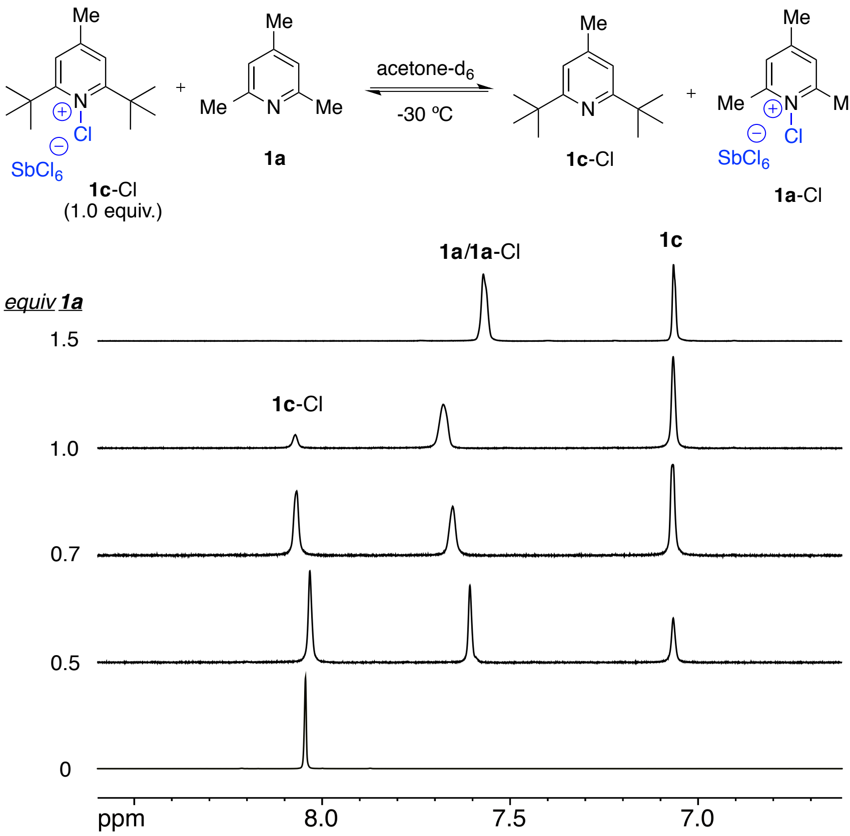


Figure S5. Quantification of *HalA* assessment *via* competitive chlorination between **1c** and **1a**.

chlorinated species **1a**-Cl and **1c**-Cl until the mixture is titrated with 1.0 equiv of **1a**, a Lewis base capable of undergoing dimerization (as discussed earlier). The fraction of **1c**-Cl listed in Table S5 is derived from the integration of these two peaks corresponding to **1c** and **1c**-Cl. Formation of **1a**-Cl is also revealed by the downfield shift of C3-H of **1a**. The fraction of **1a**-Cl (Table S5) is derived by correlating its observed chemical shift to its titration data (Figure S2). Similarly, as shown below (Figure S6), the fraction of **1c**-Cl and **1a** was plotted against the number of equivalents of **1a** added.

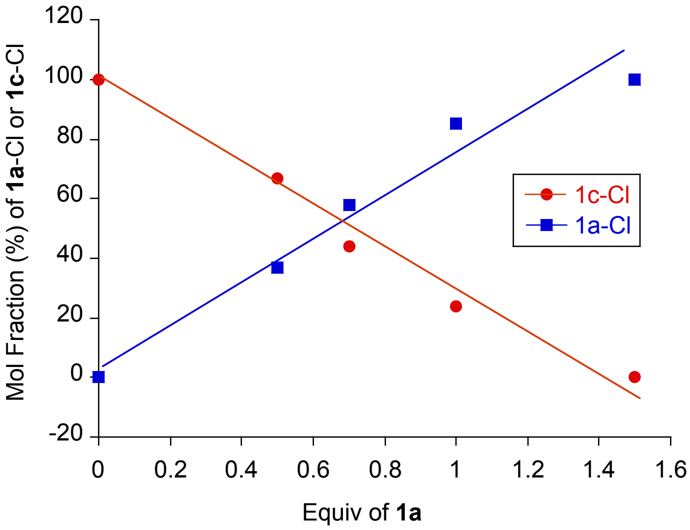


Figure S6. Plot for mol fraction (%) of **1a**-Cl and **1c**-Cl vs equiv of **1a** added.

Table S5. Data for titration of **1c**-Cl with **1a**. *Hal*A $(Cl)_{\mathbf{1c}}$ = 127.2 kcal/mol (SM8-acetone). *Hal*A $(Cl)_{\mathbf{1a}}$ = 148.2 kcal/mol (SM8-acetone).

Entry	1a (equiv)	(1c-Cl)%	(1a-Cl)%
1	0.0	100	0.0
2	0.5	67.0	37.0
3	0.7	44.0	58.0
4	1.0	16.0	85.0
5	1.5	0.0	100

Note: Although our NMR analysis conditions were chosen to minimize exchange and dimerization of **1c** and **1c**-Cl, the formation of hetero-dimers of **1c**-Cl with free **1a** is possible, and dimerization of **1a** with **1a**-Cl certainly occurs even under low temperature

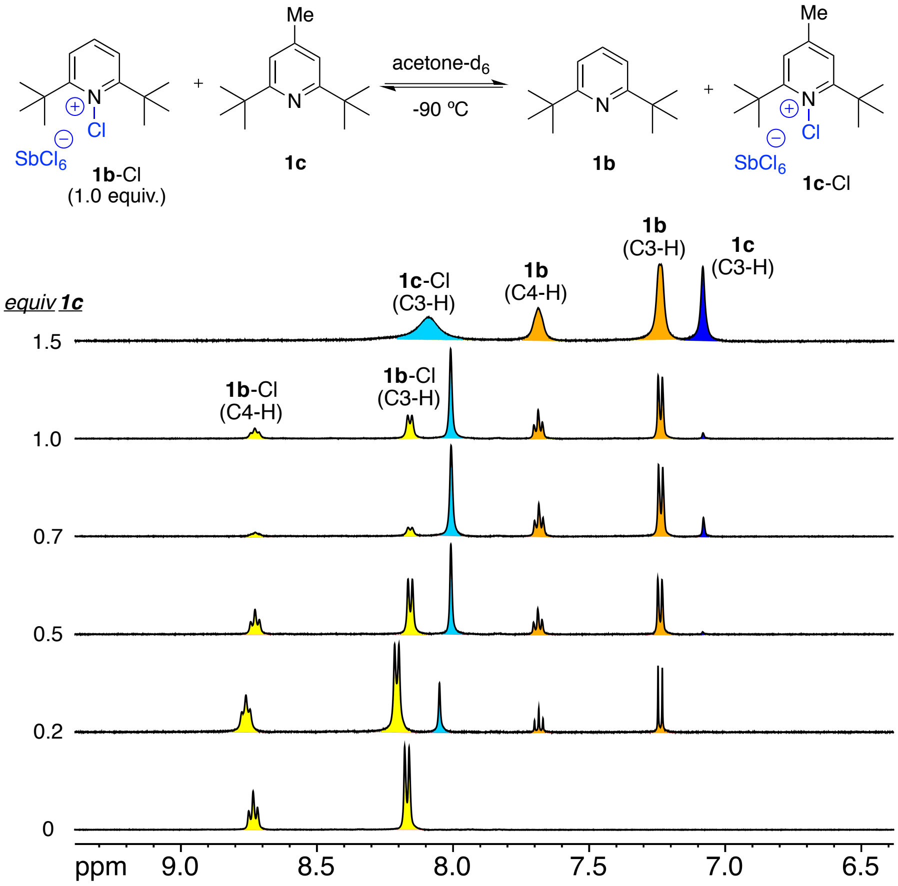


Figure S7. Overlay of ^1H NMR spectra displaying the titration of **1b**-Cl with **1c**.

Table S6. Data for titration of **1c**-Cl with **1b**. *Hal*A $(Cl)_{\mathbf{1c}}$ = 127.2 kcal/mol. *Hal*A $(Cl)_{\mathbf{1b}}$ = 126.1 kcal/mol (B3LYP/6-31G*/SM8-acetone).

Entry	1c (equiv)	(1b-Cl)%	(1c-Cl)%
1	0.0	100	0.0
2	0.2	82.0	100.0
3	0.3	69.0	97.0
4	0.5	58.0	98.0
5	0.6	37.0	93.0
6	0.7	36.7	95.0
7	0.9	19.8	86.2
8	1.0	12.0	88.0
9	1.5	0.0	56.0

condition in the presence of sub-stoichiometric amounts of halenium ion source.

To thwart the competing dimerization, we resorted on competition studies using 2,6-di-*tert*-butylpyridine (**1b**) and **1c**. At -90 °C in acetone-d_6 the free bases **1b** and **1c** were distinctly observed from the corresponding chloropyridiniums **1b**-Cl and **1c**-Cl by ^{1}H-NMR. The fraction of free bases **1b** and **1c** was derived simply by integration of the corresponding peaks at 7.06 (**1c**) and 8.06 (**1c**-Cl) ppm (see Figure S7). Furthermore, the C3-H resonances of **1b** and **1b**-Cl were distinctly observable at 7.24 and 8.16 ppm, respectively, whereas the corresponding C4-H could be observed at 7.69 and 8.73 ppm. The overlay of ^{1}H-NMR spectra at different equivalents of **1c** is shown in Figure S7. As the spectra show, addition of the stronger Lewis base **1c** depletes **1b**-Cl**,** confirming the equilibrium shift anticipated by *HalA* calculations. When an equimolar mixture of **1b** and **1c** was treated with 1.0 equiv of CDSC, an equilibrium mixture of **1b**-Cl and **1c**-Cl (in a 1:7 ratio, Table S6, entry 8) was observed by ^{1}H-NMR. The experimental result is in complete accord with the theoretical *Hal*A predictions at the B3LYP/6-31G*/SM8 (acetone) level of theory (Δ*Hal*A at -90 °C = 1.1 kcal/mol; predicting a 1:7 ratio). The

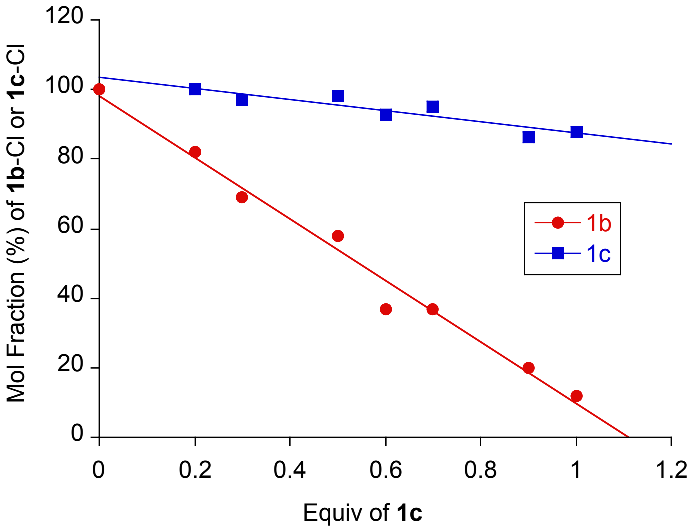
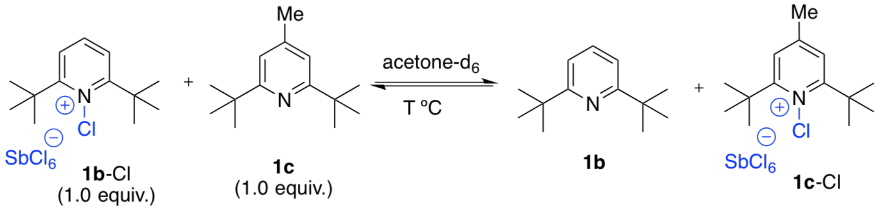


Figure S8. Plot for mol fraction (%) of **1b**-Cl and **1c**-Cl vs equiv of **1c** added.

fraction of chlorinated **1b** and **1c** were plotted against the equivalents of added **1c** (Figure S8). This study not only validates quantification via *HalA* but also highlights its value in predicting the outcome of reactions involving subtle steric and electronic changes.

The competition reaction between **1b** and **1c** was repeated at different temperatures (ranging from -90 °C to -30 °C) to probe the effect on chlorenium ion

Table S7. Effect of temperature on equilibrium ratios of **1b**-Cl and **1c**-Cl in presence of their free bases **1b** and **1c**.



1b-Cl (1.0 equiv.) **1c** (1.0 equiv.) **1b** **1c**-Cl

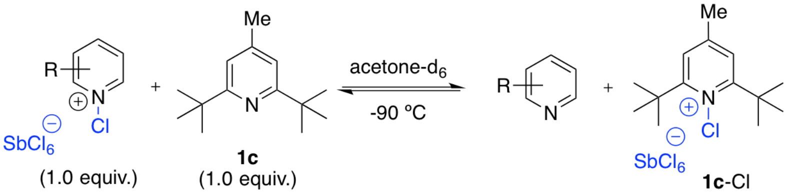
Entry	Temperature (°C)	Δ*Hal*A (kcal/mol) at T °C	(1b-Cl)%	(1c-Cl)%
1	-30	1.104	17.0	88.0
2	-50	1.094	20.0	87.0
3	-70	1.091	22.0	85.0
4	-90	1.081	21.0	83.0

transfer. Table S7 displays the fraction of chlorinated **1b** and **1c** at different temperatures (listed *HalA* values were calculated using the SM8 model to simulate acetone). The calculated Δ*HalA* values decrease upon lowering the temperature, which is in agreement with the experimental results (fraction of **1c** that is chlorinated drops from 88.0 to 83.0 %). Note that a slight excess of chlorenium donor is reflected in the >100% sum of these percentages.

g. Competition study for chlorenium ion transfer from 1c-Cl to pyridines derivatives (a quantitative trend):

Having qualitatively and quantitatively validated the chlorenium ion transfers, **1c** was subjected to similar competition studies with a series of pyridines exhibiting different electronic and steric profiles. Pyridine derivative (**A**) with a lower inherent *HalA* than **1c** was chlorinated by its reaction with CDSC. To this chloropyridinium complex **A**-

Table S8. Data for observed equilibrium ratios when 1.0 equiv of **1c** is added to chloropyridinium derivatives **1(a-j)**-Cl. *HalA* values are estimated at the B3LYP/6-31G*/SM8 (acetone) level of theory.



Entry	Pyridine Derivatives (A)	*HalA* (A) (kcal/mol)	*HalA* (1c) (kcal/mol)	ΔHalA (kcal/mol)	(1c-Cl)%
1	**1f** (4-CN)	138.0	127.2	+10.8	100
2	**1e** (4-CF_3)	137.2	127.2	+10.0	97
3	**1b** (2,6-di-*t*-Bu)	126.1	127.2	-1.1	88
4	**1g** (4-Br)	138.8	127.2	+11.6	53
5	**1d** (4-*t*-Bu)	146.3	127.2	+19.1	4
6	**1a** (2,4,6-trimethyl)	148.2	127.2	+21.0	0
7	**1h** (4-Ph)	145.7	127.2	+18.5	32
8	**1j** (4-NMe_2)	154.3	127.2	+27.1	30

Cl, 1.0 equiv of **1c** was added and the corresponding ratio at equilibrium was evaluated by ^{1}H NMR. As shown in Table S8 (entry 1-3), the difference in *HalA* between **1c** and the corresponding pyridine derivative **1f**, **1e**, and **1b** correlates to the observed equilibrium ratio of **1c**-Cl by ^{1}H NMR. Thus, the fraction of **1c**-Cl calculated from experimental results compliments the theoretical *HalA* estimates. On the other hand, 4-bromopyridine (**1g**), 4-tert-butylpyriidine (**1d**), and 2,4,6-trimethylpyridine (**1a**), which have higher *HalA* values than **1c** also demonstrate experimental results that comply with the theoretical estimations (entry 4-6). The calculated Δ*HalA* values decrease upon

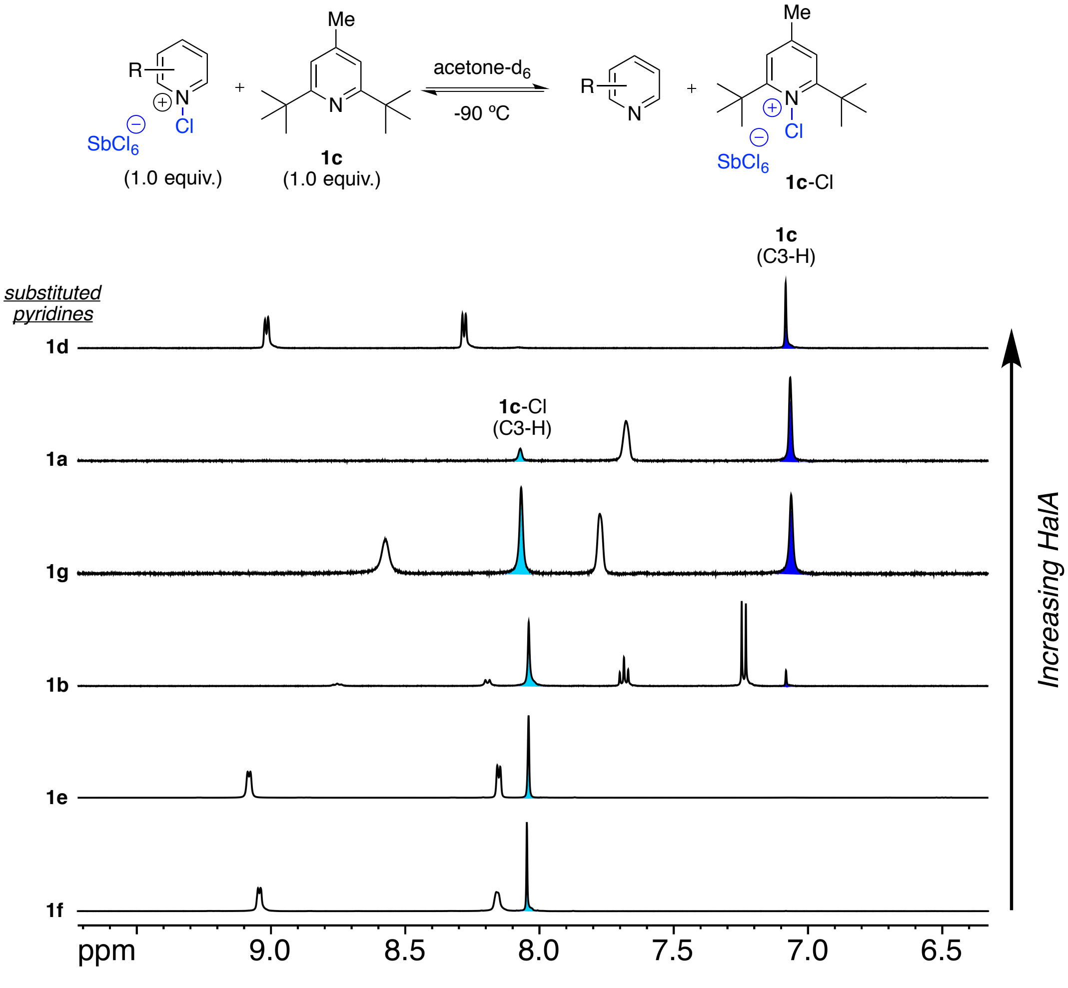


Figure S9. Overlay of ^{1}H NMR spectra displaying equilibrium ratios when chloropyridinium derivatives **1**(**a**-**f**)-Cl were treated with 1.0 equiv of **1c**.

lowering the temperature, which is in agreement with the experimental results (fraction of **1c** that is chlorinated drops from 88.0 to 83.0 %). The identity of this precipitated could not established due to instability of the chlorinated complexes, hence reliable experimental results were not obtained upon chlorination of **1h** and **1j**.

The overlay of ^{1}H-NMR spectra of **1c**-Cl in competition with other pyridines is shown in Figure S9. These examples clearly demonstrate the validity of *HalA* as an efficient tool that allows quantitative ranking of halenium ion affinities for Lewis bases.

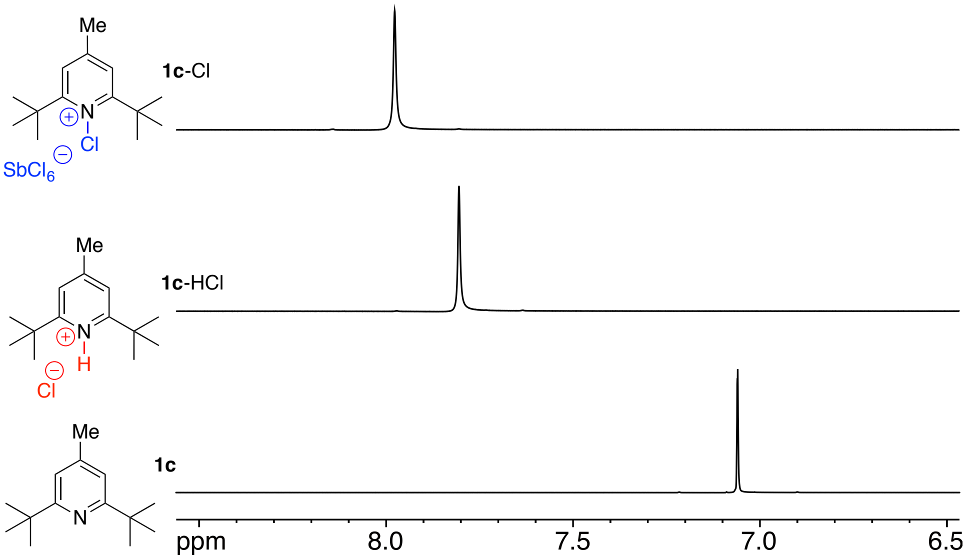


Figure S10. Overlay of ^{1}H NMR spectra of **1c**-Cl, **1c**-HCl and **1c** displaying their relative chemical shifts.

h. Control experiments:

The halo-pyridinium salts with antimony (VI) halide as the counter anion were insoluble in most of the commercially available deuterated solvents. Although THF-*d₆* was efficient in dissolving these salts, it was not economically viable for the entire set of planned experiments. Furthermore, use of acetonitrile-*d₃* led to Ritter-type reactions causing decomposition of the halo-pyridinium salts. Hence, for all the above experiments involving analyses of halo-pyridinium salts, acetone-*d₆* was identified as the optimum solvent. We were aware of the possibility that treatment of pyridines with halenium sources in acetone might lead to protonation (rather than chlorination) of the pyridinium nitrogen atom yielding α-chloroacetone as the end product. The protonated pyridines would exhibit a similar downfield shift of the C3-H and thus lead to an erroneous result. This possibility was ruled out based on our control experiments - 1.) by observing no change in chemical shift of the chloropyridiniums upon addition of K_2CO_3,

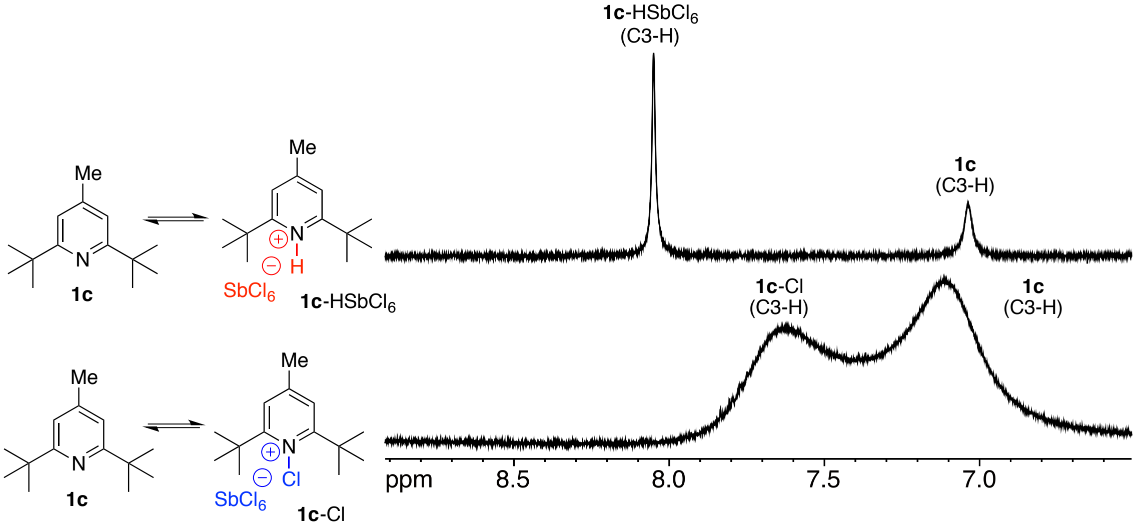


Figure S11. Overlay of ^{1}H NMR spectra displaying the protonated salt (**1c**-$HSbCl_6$) and the analogous chlorinated salt (**1c**-Cl) in presence of the free base (**1c**) in acetone-*d₆* at room temperature.

2.) by employing THF as a solvent and observing identical behavior as seen with acetone-*d*$_6$, and, 3.) by successfully initiating a chlorolactonization of alkenoic acid using the *in situ* generated chloro-pyridinium **1a**-Cl.

1.) To verify whether the species under consideration were chloro-pyridinium salts, we deliberately synthesized their protonated analogs by bubbling HCl gas in the ethereal solution of **1c** at 0 °C followed by filtration of the precipitated salt (**1c**-HCl). The salt was dried and suspended in 1,2-dichloroethane and treated with 1.5 equiv of $SbCl_5$ at -40 °C. This yielded the protonated pyridinium-$SbCl_6$ salt. Having the same counter anion - $SbCl_6^-$, ^{1}H NMR spectra of **1c-H** (protonated salt) and **1c**-Cl (chlorinated salt) were compared in acetone-*d*$_6$ at room temperature (Figure S11). The equilibrium mixture of **1c** and **1c**-Cl at room temperature shows a set of poorly resolved peaks between 7.0-7.6 ppm. In contrast, the equilibrium mixture of **1c** and **1c**-$HSbCl_6$ displays a set of two sharp peaks at 7.06 and 8.06 ppm corresponding to the protonated salt and the free base, respectively. The difference in their chemical shifts (ppm) and broadness of the peak clearly confirms the identity of two different species (protonated and chlorinated) and the relative rate of exchange (compared to NMR timescale) under similar conditions. Furthermore, the protonated and chlorinated species shown above were subjected to 1.0 equiv of K_2CO_3 and the resulting mixtures were analyzed by ^{1}HNMR. Upon addition of K_2CO_3 at room temperature, the peak corresponding to **1c**-$HSbCl_6$ disappeared instantaneously with increased intensity for the peak due to free **1c**. However, addition of K_2CO_3 to the equilibrium mixture of **1c** and **1c**-Cl did not lead to any immediate observable change in the intensity or ratio of the free base and its chlorinated counterpart. When this solution was left at room temperature for over 30 min, some evidence of decomposition of **1c**-Cl was observed by ^{1}H NMR. This clearly shows that under the standard optimized conditions, the addition of halenium source leads to the formation of halo-pyridinium salts rather than simple protonation.

2.) Chlorination of **1c** with CDSC was performed using non-deuterated THF as a solvent (^{1}H NMR spectrum at -90 °C was obtained using suppression of THF resonances). A similar behavior (when acetone-d_6 was employed) of **1c** and **1c**-Cl was observed leading to two distinct peaks in ^{1}H NMR at 7.06 ppm for **1c** and 8.06 ppm for

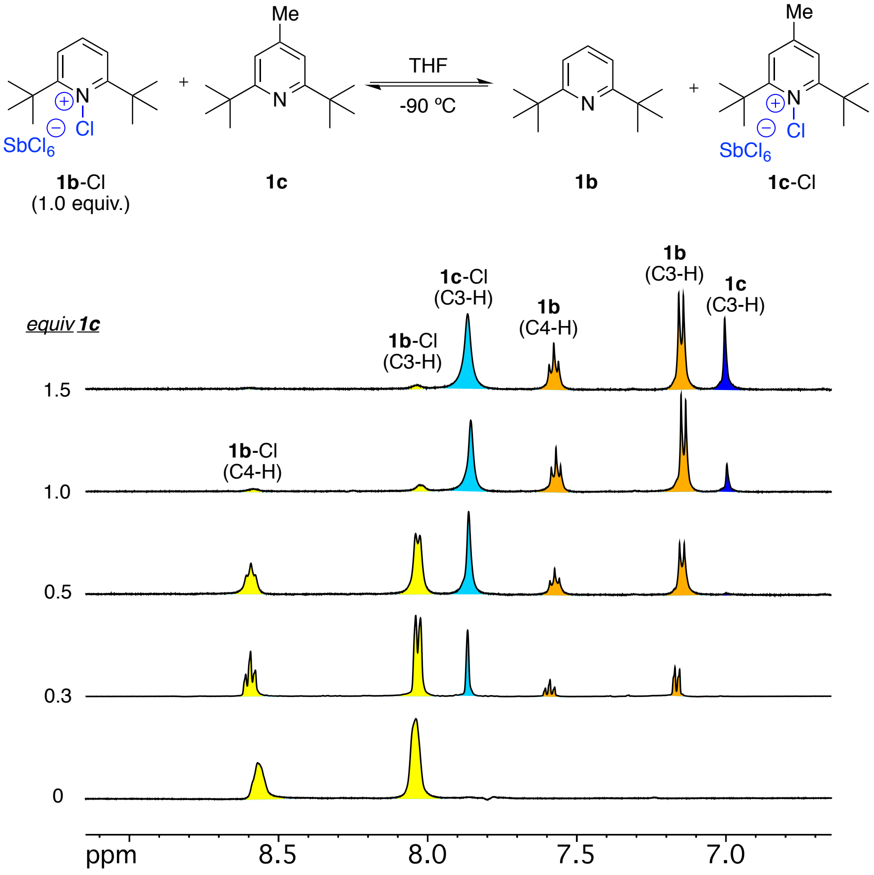


Figure S12. Competition for chlorenum ion capture between **1b** and **1c** at -90 °C in THF as a solvent. The chemical shifts (ppm) for the free bases (**1b** and **1c**) and the corresponding chlorenium salts (**1b**-Cl and **1c**-Cl) are identical to those observed in acetone-d_6 at -90 °C.

1c-Cl (Figure S12). Since there are no enolizable protons available in THF, the appearance of the downfield peak at 8.06 ppm clearly demonstrates formation of **1c**-Cl.

3.) Finally, the *in-situ* generated complex – **1a**-Cl (using 1.0 equiv each, **1a** and CDSC) in $CDCl_3$ was treated with 1.0 equiv of alkenoic acid (**17**) at room temperature (Figure S13). The chlorenium ion from **1a**-Cl was transferred to the alkenoic acid (**17**), successfully initiating a chlorolactonization reaction yielding the chlorolactone (**17a**).

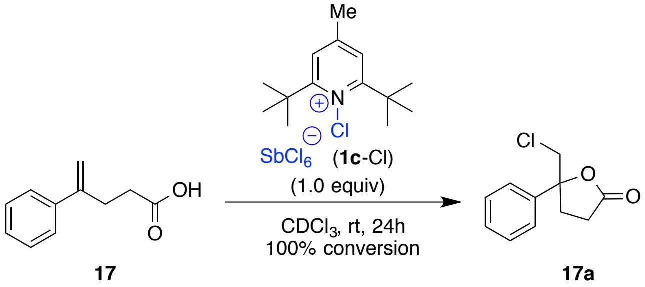
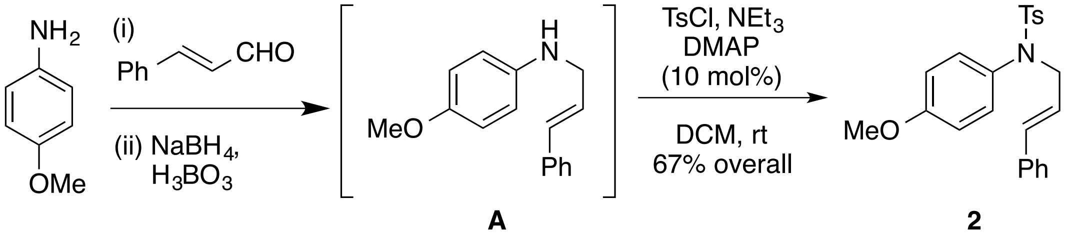


Figure S13. Chlorolactonization of **17** using **1c**-Cl as an active chlorenium source.

V. Synthesis of substrates and intramolecular chlorocyclization of alkenes:

a. Synthesis of substrates **2**, **4** and **9**:



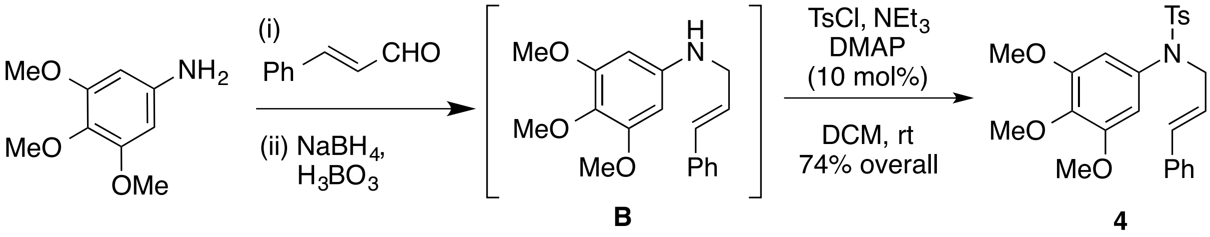
***N*-cinnamyl-*N*-(4-methoxyphenyl)-4-methylbenzenesulfonamide (2)**:

Intermediate (**A**) was synthesized as reported previously.[7] *p*-Anisidine (1.0 g, 8.12 mmol) was placed in a porcelain mortar along with freshly distilled *trans*-cinnamaldehyde (1.02 mL, 1.0 equiv, 8.12 mmol). This mixture was grinded using a pestle for about 10 min until a bright yellow solid was obtained. Part of this mixture was analyzed by ^{1}H NMR to verify completion of the reaction (imine formation is quantitative). To this crude imine, a 1:1 mixture (pre-mixed) of $NaBH_4$ (768 mg, 2.5 equiv, 20.3 mmol) and H_3BO_3 (1.26 g, 2.5 equiv, 20.3 mmol) were added at once. Mixing was continued using mortar and pestle for another 20 min until a dry yellow solid was obtained. The reaction mixture was then transferred to a separatory funnel. The motor was washed with CH_2Cl_2 (15 mL) and the washings were transferred to the same separatory funnel. This solution was then washed with 50% aqueous $NaHCO_3$ solution following by 5 mL of brine. The organics were separated, dried over anhydrous Na_2SO_4, filtered, concentrated and then subjected to the next step without further purification. The crude amine **A** was transferred to a 100 mL round bottom flask and dissolved in dry CH_2Cl_2 (10 mL). To this mixture were added NEt_3 (2.3 mL, 2.0 equiv, 16.24 mmol) and

4-(*N*,*N*-dimethylamino)pyridine (91 mg, 0.1 equiv, 0.81 mmol) followed by tosyl chloride (1.86 g, added in 3 portions). This mixture was allowed to stir for 5 h at room temperature and the progress of the reaction was monitored by thin layer chromatography (TLC). Upon completion of the reaction, the organics were poured in a separatory funnel and washed with satd. aqueous $NaHCO_3$ solution. The organics were separated, dried over anhydrous Na_2SO_4, filtered, concentrated and subjected to purification using silica gel column chromatography employing 20% ethyl acetate in hexanes as eluent. Pure product **2** was obtained as a white solid (2.14 g, 67% overall yield).

Analytical data for **2**: White solid, mp 79 °C; ^1H NMR (500 MHz, $CDCl_3$) δ 7.54-7.51 (2H, m.), 7.26-7.20 (7H, m.), 6.98-6.94 (2H, m.), 6.79-6.76 (2H, m.), 6.35 (1H, dd, *J* = 16.0, 5.0 Hz), 6.13-6.06 (1H, m.), 4.29 (2H, ddd, *J* = 1.5, 5.0, 11.0 Hz), 3.76 (3H, s.), 2.42 (3H, s.) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.0, 143.3, 136.4, 135.7, 133.7, 131.7, 129.4, 129.4, 128.5, 127.8, 126.4, 124.2, 114.1, 55.3, 53.6, 21.6 ppm; IR (film) 3019, 2932, 2837, 1595, 1507 (s), 1447, 1346 (s), 1249, 1162 (s), 684 cm^{-1}. HRMS (ESI) Calculated Mass for $C_{23}H_{24}NO_3S$: ($[M+H]^+$) = 394.1477, Found ($[M+H]^+$) = 394.1478.

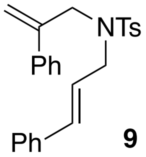
N-cinnamyl-4-methyl-N-(3,4,5-trimethoxyphenyl)benzenesulfonamide (4):



The same procedure used for the synthesis of **2** (as described above) was employed for the synthesis of **4**. Using 1.0 g (5.5 mmol) of 3,4,5-trimethoxyaniline, pure product (**4**) was isolated (2.14 g, 74% overall yield).

Analytical data for **4**: White solid, mp 121 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (2H, dd, J = 8.0 Hz.), 7.27-7.19 (7H, m.), 6.38 (1H, d, J = 16.0 Hz.), 6.23 (2H, s.), 6.10 (1H, ddd, J = 6.5, 13.5, 16.0 Hz), 4.27 (2H, dd, J = 1.0 Hz, 7.0 Hz.), 3.80 (3H, s.), 3.66 (6H, s.), 2.41 (3H, s.) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.0, 143.6, 137.7, 136.3, 135.7, 134.8, 133.9, 129.4, 128.6, 127.9, 127.8, 126.4, 124.1, 106.5, 60.9, 56.1, 53.7, 21.5 ppm; IR (film) 3000, 2938, 2837, 1595 (s), 1503, 1454, 1416, 1347, 1232, 1163 (s), 1128 (s), 661 cm^{-1}. HRMS (ESI) Calculated Mass for $C_{25}H_{28}NO_5S$: ([M+H]$^+$) = 454.1688, Found ([M+H]$^+$) = 454.1685.

N-cinnamyl-4-methyl-N-(2-phenylallyl)benzenesulfonamide (9):

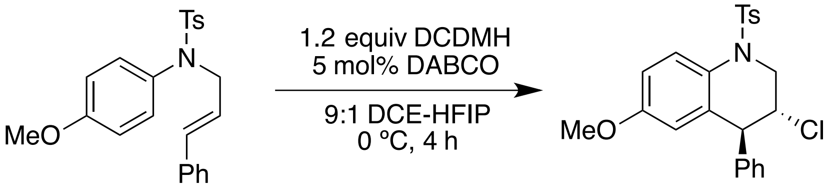


9

Substrate **9** was synthesized as reported previously.[8]

Analytical data for **9**: Crystalline white solid, mp 130 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (2H, d, *J* = 8.0 Hz.), 7.39-7.37 (2H, m.), 7.31-7.19 (8H, m.), 7.13 (2H, d, *J* = 6.5 Hz.), 6.30 (1H, d, *J* = 15.5 Hz.), 5.78 (1H, ddd, *J* = 7.0, 14.0 and 16.0 Hz.), 5.45 (1H, apparent singlet.), 5.24 (1H, d, *J* = 1.0 Hz.), 4.26 (2H, s.), 3.86 (2H, d, *J* = 7.0 Hz.), 2.41 (3H, s.) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.3, 142.8, 138.5, 137.0, 136.2, 134.1, 129.6, 128.5, 128.4, 128.0, 127.8, 127.4, 126.6, 126.3, 123.4, 116.3, 50.6, 48.9, 21.5 ppm; IR (film) 3056, 3031, 2922, 1599, 1495, 1447, 1340 (s), 1159 (s), 1093, 910, 738, 659 cm^{-1}. HRMS (ESI) Calculated Mass for $C_{25}H_{26}NO_2S$: ($[M+H]^+$) = 404.1684, Found ($[M+H]^+$) = 404.1687.

b. Chlorocyclization of alkenes **2**, **4** and **9**:



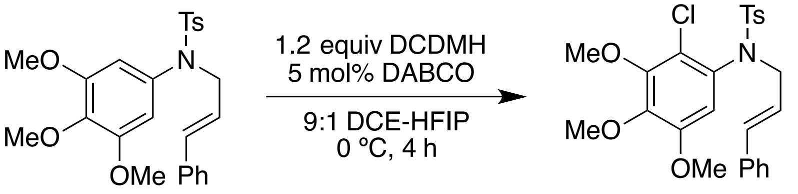
trans-3-chloro-6-methoxy-4-phenyl-1-tosyl-1,2,3,4-tetrahydroquinoline (3):

A 5 mL round bottom flask containing a stir bar was charged with **2** (100 mg, 0.25 mmol) and dissolved in a 9:1 mixture of 1,2-dichloroethane:hexafluoroisopropanol (2.5

mL). To this solution 1,4-diazabicyclo[2.2.2]octane (1.5 mg, 0.05 equiv, ~0.01 mmol) was added and the reaction mixture was placed in an ice bath for about 5 min. Subsequently, 1,3-dichloro-5,5-dimethylhydantoin (DCDMH) (60 mg, 1.2 equiv, 0.31 mmol) was added and stirring was continued for another 3.5 h. The progress of the reaction was monitored by TLC and upon complete consumption of substrate **2**, the reaction was quenched with 10% aqueous sodium sulfite (1 mL). The organics were then separated, dried over anhydrous Na_2SO_4, filtered, concentrated and subjected to purification using silica gel column chromatography employing 10% ethyl acetate in hexanes as eluent. After purification, pure product **3** was obtained as a white solid (101 mg, 93%).

Analytical data for **3**: White solid, mp 118 °C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82 (1H, d, *J* = 9.0 Hz.), 7.55 (2H, d, *J* = 8.5 Hz.), 7.27 (2H, d, *J* = 8.0 Hz.), 7.19 (1H, t, *J* = 8.0 Hz.), 7.11 (2H, t, *J* = 7.0 Hz.), 6.70 (1H, dd, *J* = 3.0 and 9.5 Hz.), 6.47 (2H, d, *J* = 7.5 Hz.), 6.13 (1H, d, *J* = 2.0 Hz.), 4.65 (1H, dd, *J* = 4.0 and 13.5 Hz.), 3.89 (1H, d, *J* = 9.5 Hz.), 3.76-3.70 (1H, m.), 3.60-3.56 (4H, m.), 2.44 (3H, s.) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.4, 144.2, 141.1, 136.3, 133.5, 130.0, 128.8, 128.6, 128.3, 127.5, 127.4, 126.5, 114.9, 113.1, 57.0, 55.2, 54.2, 52.3, 21.5 ppm; IR (film) 3030, 2928, 2838, 1610 (s), 1493 (s), 1356 (s), 1248, 1163 (s), 1037, 910, 801, 736 cm^{-1}. HRMS (ESI) Calculated Mass for $C_{23}H_{23}NO_3ClS$: ($[M+H]^+$) = 428.1087, Found ($[M+H]^+$) = 428.1087.

Attempted chlorocyclization of substrate **4**:



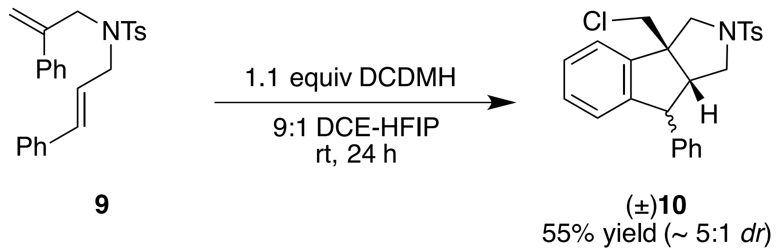
4

5, 73% yield

Compound **4** (100 mg, 0.22 mmol) was subjected to the same chlorocyclization conditions (as described above for substrate **2**) and 79 mg (73% yield) of the ring-chlorinated product **5** was obtained as pale yellow oil.

Analytical data for **5**: Pale yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$) two rotamers (~2.5:1 ratio) along *N*-Ts were observed at room temperature. Heating the sample to 50 °C did not lead to complete convergence of the spectral lines corresponding to the rotamers. Major rotamer: δ 7.68 (1H, d, *J* = 8.0 Hz.), 7.27-7.19 (10H, m.), 6.54 (1H, s.), 6.30 (1H, d, *J* = 16.0 Hz.), 6.18 (1H, ddd, *J* = 7.0, 13.5 and 16.0 Hz.), 4.41-4.38 (1H, m.), 4.20-4.14 (1H, m.), 3.86 (3H, s.), 3.80 (3H, s.), 3.68 (3H, s.), 2.41 (3H, s.) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.5, 150.4, 143.6, 136.3, 134.2, 131.5, 129.6, 129.5, 128.5, 127.9, 127.3, 126.4, 123.9, 111.7, 61.1, 56.1, 53.1, 21.6 ppm; IR (film) 3023, 2940, 1596, 1576, 1485 (s), 1444, 1396, 1351, 1240, 1163 (s), 1112 (s), 1016, 870, 661 cm-1. HRMS (ESI) Calculated Mass for $C_{25}H_{27}NO_5ClS$: ([M+H]$^+$) = 487.1220, Found ([M+H]$^+$) = 487.1221.

Chlorocyclization of substrate **9**:



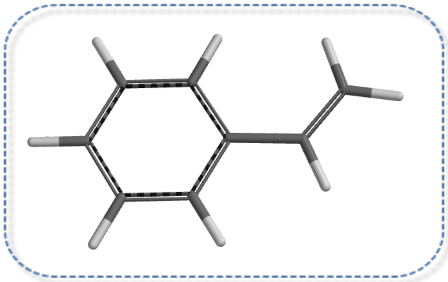
In a 5 mL round bottom flask containing a stir bar, **9** (100 mg, 0.25 mmol) was dissolved in a 9:1 mixture of 1,2-dichloroethane:hexafluoroisopropanol (2.5 mL). Then, 1,3-dichloro-5,5-dimethylhydantoin (DCDMH) (54 mg, 1.1 equiv, 0.27 mmol) was added and the reaction mixture was stirred for 24 h. The progress of the reaction was monitored by TLC and upon complete consumption of substrate **9**, the reaction was quenched with 10% aqueous sodium sulfite (1 mL). The organics were then separated, dried over anhydrous Na_2SO_4, filtered, concentrated and subjected to purification using silica gel column chromatography employing 20% ethyl acetate in hexanes as eluent. After purification, product **10** was obtained as a white solid (60 mg, 55% yield). Crude ^1H NMR analysis indicated a 5:1 *dr* for **10**. Although complete conversion of **9** was attained (as judged by TLC and ^1H NMR), the mass balance was accounted by a complex mixture of products, which were inseparable by chromatography (identity of these products could not be assigned due to overlapping peaks in NMR). An analytically pure sample of **10** was obtained *via* preparative TLC. The relative stereochemistry of the major diastereomer could not be assigned with the aid of NOESY experiments owing to the nature of *cis*-(5,5) fusion in the tricyclic framework of **10**.

Analytical data for **10**: White waxy solid; ^{1}H NMR (500 MHz, $CDCl_3$) 5:1 *dr*, major diastereomer: δ 7.67 (2H, d, *J* = 8.0 Hz.), 7.32-7.20 (8H, m.), 7.07 (2H, d, *J* = 7.5 Hz.), 6.89 (1H, d, *J* = 8.0 Hz.), 4.15 (1H, d, *J* = 5.5 Hz.), 3.67 (2H, s.), 3.47 (2H, dd, *J* = 3.5 and 9.5 Hz.), 3.34 (1H, d, *J* = 9.5 Hz.), 3.28 (1H, dd, *J* = 6.5 and 9.5 Hz.), 2.88 (1H, ddd, *J* = 2.5, 6.5 and 8.5 Hz.), 2.42 (3H, s.) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 145.4, 144.1, 144.0, 143.9, 132.0, 129.7, 128.8, 128.8, 128.1, 127.9, 127.0, 125.7, 123.3, 60.0, 57.5, 56.7, 53.9, 49.9, 21.6 ppm; IR (film) 3928, 2961, 2867, 1598, 1453, 1349 (s), 1260, 1165 (s), 1099, 1026, 911, 807, 702, 665 cm^{-1}. HRMS (ESI) Calculated Mass for $C_{25}H_{25}NO_2ClS$: ($[M+H]^+$) = 438.1295, Found ($[M+H]^+$) = 438.1297.

VI. Quantum mechanical modeling studies:

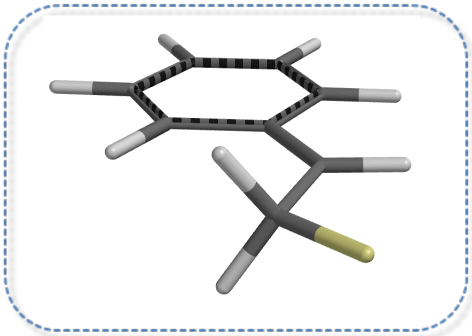
Based on the nature of halenium ion (F, Cl, Br or I), full optimizations for all conformations of the 'halenium ion' acceptors and the corresponding 'Lewis base-halenium ion' complexes were performed using density functional calculations at the B3LYP/6-31G* level (with the LANL2DZ(d) pseudopotential and basis used for iodine) as implemented in the Spartan-10 software running on Macintosh and Linux platforms. To confirm that each structure was a true minimum, vibrational analyses were performed. For structures presented in Figure 2, Figure 5b and Figure 6 in the manuscript, the *HalA* (Cl) values were calculated using the energies obtained from a full geometry optimization of the structures in simulated acetone at B3LYP/6-31G*/SM8 level of theory. Alternatively, when the *gas phase* energies of the same structures were corrected for solvation in simulated acetone using the SM8 model available in the Spartan code to run single point (i.e. B3LYP/6-31G*/SM8) calculations, the resulting data led to the same conclusion. To verify convergence and consistency of the optimizations, a number of examples were re-optimized from multiple starting points; energetic variations of 0.02 kcal/mol or less were found among these calculated structures. Relative enthalpies $\Delta H°_{rel}$ were calculated for the *gas phase* structures by including zero-point and thermal corrections to 298.15 K. Importantly, neither the vibration nor the solvation corrections introduced differences between relative E° and relative H° values that were large enough to reorder the relative energy structures; thus, either set of data led to the same conclusions.

Cartesian coordinates for geometry minimized styrene:



Atom			X	Y	Z
1	H	H1	3.8906963	-0.1039465	0.0006791
2	C	C1	2.8698467	0.2657609	0.0010817
3	C	C2	1.8324097	-0.5808014	-0.0009399
4	H	H2	2.7517904	1.3461327	0.0033224
5	H	H3	2.0454119	-1.6501016	-0.0027489
6	C	C3	0.3985202	-0.2467405	-0.0006402
7	C	C4	-2.3724006	0.2865908	0.0003848
8	C	C5	-0.0834339	1.0750850	-0.0010208
9	C	C6	-0.5422606	-1.2906386	0.0000292
10	C	C7	-1.9121771	-1.0300166	0.0005909
11	C	C8	-1.4498423	1.3375891	-0.0004488
12	H	H6	0.6174931	1.9048299	-0.0018638
13	H	H7	-0.1890770	-2.3197190	0.0002462
14	H	H8	-2.6188624	-1.8558522	0.0012169
15	H	H9	-1.7991778	2.3669659	-0.0007321
16	H	H10	-3.4389364	0.4948622	0.0008431

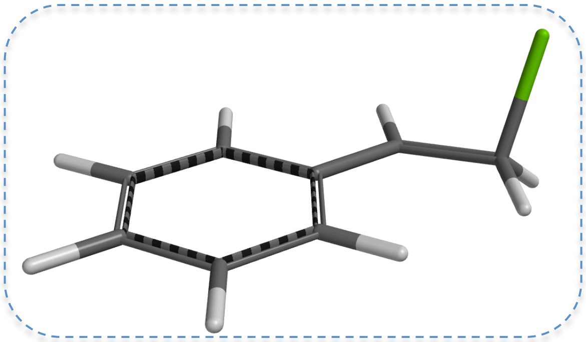
Cartesian coordinates for geometry minimized styrene + F cation:



Atom			X	Y	Z
1	H	H2	2.8006008	0.8488801	0.6519632
2	C	C1	2.7085660	0.2902544	-0.2938554
3	C	C2	1.5334306	-0.6181780	-0.2430910
4	H	H3	2.5850185	1.0299477	-1.1015570
5	H	H4	1.7830570	-1.6715264	-0.3782480
6	C	C3	0.2035457	-0.2816827	-0.0507188

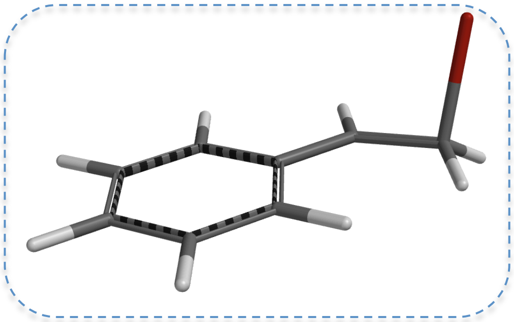
7	C	C4	-2.5045408	0.2809256	0.3249902
8	C	C5	-0.2361024	1.0744593	0.1365294
9	C	C6	-0.7692893	-1.3400906	-0.0410085
10	C	C7	-2.1064585	-1.0547618	0.1451608
11	C	C8	-1.5733418	1.3422209	0.3209874
12	H	H6	0.4856653	1.8855877	0.1324170
13	H	H7	-0.4356001	-2.3641986	-0.1821204
14	H	H8	-2.8453117	-1.8490166	0.1531099
15	H	H9	-1.9168737	2.3614270	0.4627659
16	H	H10	-3.5578961	0.5047057	0.4714904
17	F	F1	3.8455304	-0.4389539	-0.5088152

Cartesian coordinates for geometry minimized styrene + Cl cation:



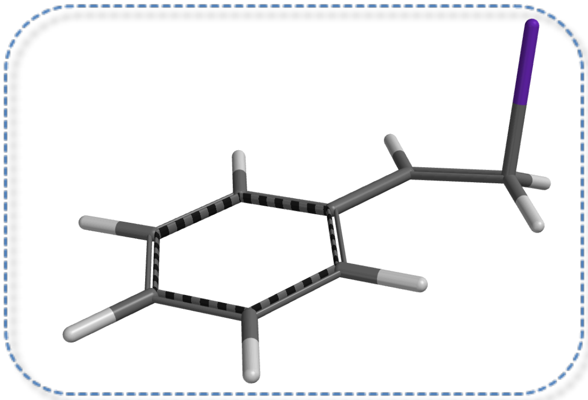
	Atom		X	Y	Z
1	Cl	Cl1	3.2758162	0.0329725	-1.8063251
2	H	H2	3.5289469	-0.0248172	0.5680118
3	C	C1	2.7218866	0.2924718	-0.0971674
4	C	C2	1.5507764	-0.6129596	-0.0072821
5	H	H3	2.5110803	1.3505918	0.0440545
6	H	H4	1.7990723	-1.6737210	-0.0222951
7	C	C3	0.2067354	-0.2710434	0.0403656
8	C	C4	-2.5261721	0.2862665	0.1816959
9	C	C5	-0.2565230	1.0888791	0.0506730
10	C	C6	-0.7568595	-1.3372371	0.0969362
11	C	C7	-2.1046711	-1.0552540	0.1714872
12	C	C8	-1.6064943	1.3533468	0.1197515
13	H	H6	0.4526671	1.9073041	-0.0037532
14	H	H7	-0.4056968	-2.3653040	0.0845860
15	H	H8	-2.8352386	-1.8558000	0.2181726
16	H	H9	-1.9665647	2.3766974	0.1247055
17	H	H10	-3.5887611	0.5076062	0.2363835

Cartesian coordinates for geometry minimized styrene + Br cation:



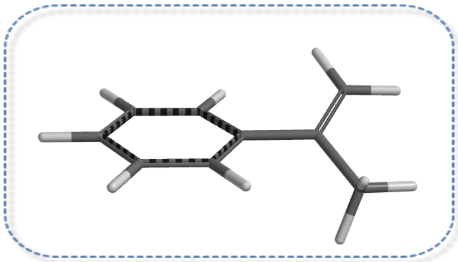
	Atom		X	Y	Z
1	H	H2	3.5697360	-0.0504926	0.5475900
2	C	C1	2.7137838	0.2913182	-0.0319186
3	C	C2	1.5582490	-0.6125257	0.0299976
4	H	H3	2.5259948	1.3517069	0.1031904
5	H	H4	1.8038016	-1.6736580	0.0441067
6	C	C3	0.2050238	-0.2699339	0.0549767
7	C	C4	-2.5422655	0.2870390	0.1691956
8	C	C5	-0.2622947	1.0902243	0.0582713
9	C	C6	-0.7607195	-1.3372320	0.1043399
10	C	C7	-2.1141792	-1.0555682	0.1637094
11	C	C8	-1.6177899	1.3545758	0.1150925
12	H	H6	0.4442188	1.9103845	0.0134268
13	H	H7	-0.4108292	-2.3647834	0.0969540
14	H	H8	-2.8416681	-1.8570948	0.2036541
15	H	H9	-1.9764367	2.3767833	0.1182231
16	H	H10	-3.6039676	0.5069392	0.2149216
17	Br	Br1	3.3093428	0.0523175	-2.0057309

Cartesian coordinates for geometry minimized styrene + I cation at the B3LYP/6-31G*/LANL2DZ level:



Atom			X	Y	Z
1	H	H2	3.5660177	-0.0553705	0.5724722
2	C	C1	2.7079995	0.2982736	0.0078013
3	C	C2	1.5599104	-0.5963249	0.0434782
4	H	H3	2.5287101	1.3580360	0.1445492
5	H	H4	1.8021039	-1.6548963	0.0955743
6	C	C3	0.2014926	-0.2589280	0.0433076
7	C	C4	-2.5325765	0.2831161	0.1677538
8	C	C5	-0.2668403	1.0894980	0.0546987
9	C	C6	-0.7508916	-1.3226186	0.0883419
10	C	C7	-2.1010179	-1.0491769	0.1523919
11	C	C8	-1.6172590	1.3483483	0.1180072
12	H	H6	0.4334051	1.9150566	0.0170130
13	H	H7	-0.3995600	-2.3490830	0.0759140
14	H	H8	-2.8235147	-1.8555499	0.1907949
15	H	H9	-1.9779479	2.3699122	0.1321514
16	H	H10	-3.5945859	0.4984912	0.2199692
17	I	I1	3.2645546	-0.0187839	-2.1242187

Cartesian coordinates for geometry minimized α-methylstyrene:



Atom			X	Y	Z
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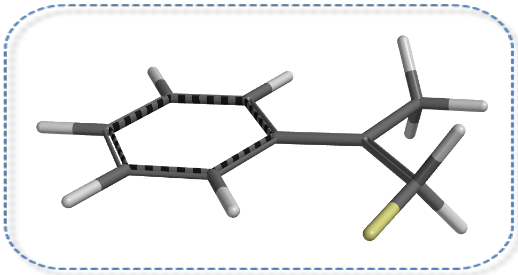
2	C	C1	-0.4286364	1.3767145	0.3754165
3	C	C4	-1.4766033	-0.8504688	1.6715387
4	C	C2	0.0410623	0.1002697	0.0136178
5	C	C6	-1.3892479	1.5375872	1.3704535
6	C	C5	-1.9175001	0.4238483	2.0275127
7	C	C3	-0.5145509	-1.0094413	0.6737549
8	H	H6	-1.7367719	2.5357278	1.6248454
9	H	H5	-2.6712871	0.5487679	2.8002426
10	H	H3	-0.1837947	-2.0110102	0.4172445
11	H	H4	-1.8819748	-1.7273009	2.1701069
12	C	C7	1.0786076	-0.0715433	-1.0405486
13	C	C8	1.9807647	0.8846413	-1.3109147
14	H	H8	2.0297302	1.8131786	-0.7504886
15	C	C9	1.0973657	-1.3792354	-1.8012150
16	H	H2	1.3966913	-2.2169699	-1.1577300
17	H	H10	0.1063311	-1.6244976	-2.2022647
18	H	H14	2.7179693	0.7566693	-2.0985613

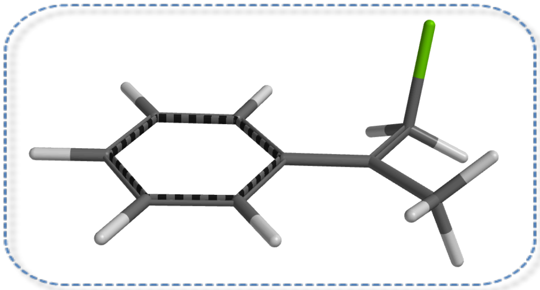
19	H	H7	1.8062168	-1.3373140	-2.6332862

Cartesian coordinates for geometry minimized α-methylstyrene + F cation:



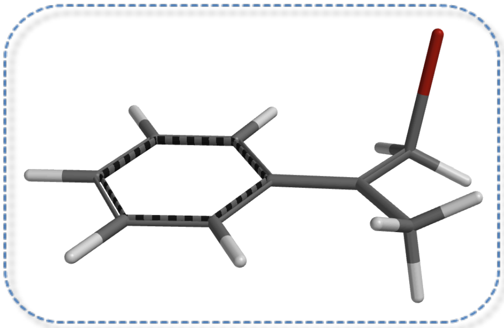
Atom			X	Y	Z
1	H	H1	0.8268993	1.9386516	0.7763814
2	C	C1	-0.0748199	1.3466181	0.7544581
3	C	C4	-2.4366449	-0.1956646	0.6883418
4	C	C2	-0.0841211	0.0831349	0.0673998
5	C	C6	-1.2177010	1.8098166	1.3786756
6	C	C5	-2.3929706	1.0458066	1.3506329
7	C	C3	-1.3092163	-0.6698768	0.0553704
8	H	H6	-1.2039172	2.7654028	1.8921011
9	H	H5	-3.2856129	1.4171075	1.8467243
10	H	H3	-1.3499687	-1.6261442	-0.4517926
11	H	H4	-3.3548840	-0.7733159	0.6769108
12	C	C7	1.0490968	-0.4357215	-0.5833723
13	C	C8	2.4079159	0.1818604	-0.6473422
14	H	H8	2.6411853	0.3464377	-1.7126624
15	C	C9	1.0223894	-1.7419414	-1.3223742
16	H	H2	0.8367010	-2.5681402	-0.6235004
17	H	H10	0.2232622	-1.7632673	-2.0709981
18	H	H14	3.1285884	-0.5680494	-0.2826502
19	H	H7	1.9694056	-1.9432586	-1.8291552
20	F	F1	2.6044127	1.3505437	0.0368513

Cartesian coordinates for geometry minimized α-methylstyrene + Cl cation:



Atom			X	Y	Z
1	H	H1	0.8524194	1.8777405	0.7165050
2	C	C1	-0.0810083	1.3318856	0.6510305
3	C	C4	-2.5061903	-0.0938857	0.5581270
4	C	C2	-0.1230751	0.0425115	0.0205688
5	C	C6	-1.2133218	1.8736161	1.2232405
6	C	C5	-2.4269518	1.1669125	1.1725448
7	C	C3	-1.3752485	-0.6575056	0.0027165
8	H	H6	-1.1682477	2.8411187	1.7119204
9	H	H5	-3.3174398	1.6013467	1.6185220
10	H	H3	-1.4492442	-1.6287982	-0.4703050
11	H	H4	-3.4520204	-0.6242397	0.5260742
12	C	C7	1.0279102	-0.5162342	-0.5687384
13	C	C8	2.3205086	0.2521563	-0.6608431
14	H	H8	2.1970268	1.3308190	-0.7283068
15	C	C9	1.0981013	-1.8830376	-1.1487562
16	H	H2	2.0446183	-2.3540930	-0.8564681
17	H	H10	0.2761186	-2.5452394	-0.8848084
18	H	H14	2.9264954	-0.0974754	-1.4974917
19	H	H7	1.1388190	-1.7911799	-2.2469288
20	Cl	Cl1	3.2307301	-0.1264182	0.8613968

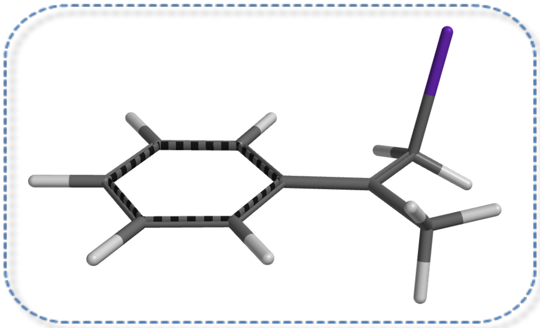
Cartesian coordinates for geometry minimized α-methylstyrene + Br cation:



Atom			X	Y	Z
1	H	H1	0.8327779	1.9119966	0.7084753

2	C	C1	-0.0916941	1.3530424	0.6406643
3	C	C4	-2.5047018	-0.1024158	0.5433834
4	C	C2	-0.1135219	0.0558758	0.0226009
5	C	C6	-1.2404550	1.8914536	1.1944123
6	C	C5	-2.4492275	1.1703719	1.1432342
7	C	C3	-1.3585396	-0.6598175	0.0018075
8	H	H6	-1.2110206	2.8648339	1.6689701
9	H	H5	-3.3475157	1.5991107	1.5750232
10	H	H3	-1.4135317	-1.6384902	-0.4570390
11	H	H4	-3.4415030	-0.6454718	0.5113394
12	C	C7	1.0489179	-0.5024899	-0.5660970
13	C	C8	2.3221833	0.2610903	-0.6707408
14	H	H8	2.2417243	1.3418603	-0.6355645
15	C	C9	1.0847678	-1.8753920	-1.1566583
16	H	H2	2.0994897	-2.2806491	-1.1424513
17	H	H10	0.4182202	-2.5863016	-0.6680319
18	H	H14	2.9416736	-0.0617910	-1.5049186
19	H	H7	0.7861214	-1.8127022	-2.2171424
20	Br	Br1	3.3958347	-0.2841144	1.0087333

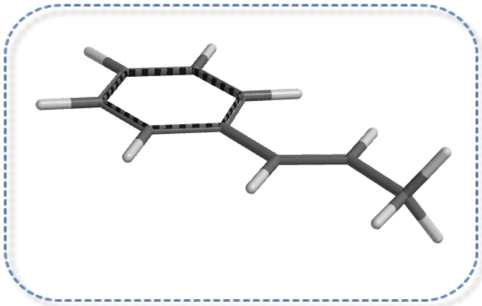
Cartesian coordinates for geometry minimized α-methylstyrene + I cation at the B3LYP/6-31G*/LANL2DZ level:



Atom			X	Y	Z
1	H	H1	0.8216134	1.9349950	0.6952996
2	C	C1	-0.0974624	1.3649121	0.6285659
3	C	C4	-2.4905437	-0.1062810	0.5325283
4	C	C2	-0.1048925	0.0669882	0.0276392
5	C	C6	-1.2518304	1.8998675	1.1662200
6	C	C5	-2.4499482	1.1694591	1.1156606
7	C	C3	-1.3372975	-0.6571308	0.0060733
8	H	H6	-1.2329263	2.8812592	1.6283797
9	H	H5	-3.3559224	1.5960944	1.5368294
10	H	H3	-1.3795844	-1.6426269	-0.4422513
11	H	H4	-3.4228396	-0.6601748	0.4999604
12	C	C7	1.0635820	-0.4921789	-0.5559665
13	C	C8	2.3305740	0.2606205	-0.6583741
14	H	H8	2.2610386	1.3417721	-0.5902834
15	C	C9	1.0721913	-1.8617905	-1.1622284

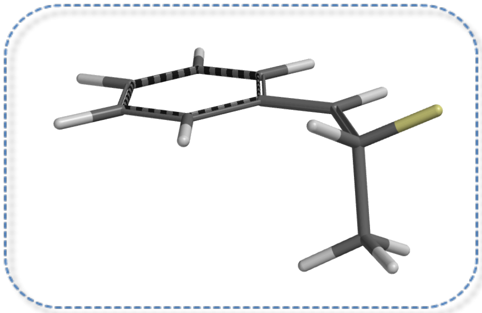
16	H	H2	2.0889431	-2.2095317	-1.3515531
17	H	H10	0.5561395	-2.6042419	-0.5487047
18	H	H14	2.9373174	-0.0429563	-1.5102082
19	H	H7	0.5500666	-1.8147397	-2.1304459
20	I	I1	3.4417814	-0.4243156	1.1128594

Cartesian coordinates for geometry minimized *trans*-β-methylstyrene:



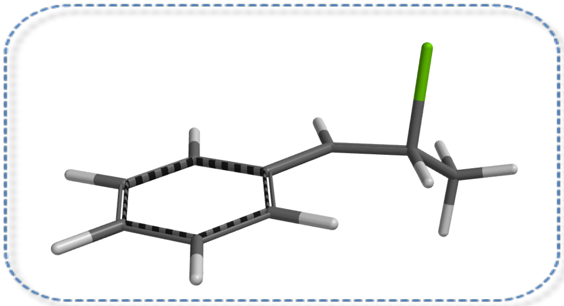
Atom			X	Y	Z
1	H	H1	-0.3032617	1.4434338	-1.2951095
2	C	C1	-0.2150847	1.3742470	-0.2145948
3	C	C4	-0.0084324	1.2430075	2.5620160
4	C	C2	-0.0119607	0.1209177	0.3934372
5	C	C6	-0.3097799	2.5340009	0.5486210
6	C	C5	-0.2062783	2.4766153	1.9417906
7	C	C3	0.0862075	0.0823323	1.7954828
8	H	H6	-0.4670086	3.4895036	0.0544467
9	H	H5	-0.2816820	3.3841314	2.5347258
10	H	H3	0.2416392	-0.8755999	2.2871534
11	H	H4	0.0722434	1.1821635	3.6443459
12	C	C7	0.1021490	-1.1377356	-0.3598294
13	H	H7	0.2068386	-2.0296220	0.2601989
14	C	C8	0.0986798	-1.3016486	-1.6911815
15	H	H8	0.0036050	-0.4336645	-2.3438352
16	C	C9	0.2234347	-2.6262418	-2.3843957
17	H	H2	0.3212531	-3.4486447	-1.6676358
18	H	H10	-0.6515615	-2.82 92254	-3.0174953
19	H	H14	1.0989995	-2.6479705	-3.0481412

Cartesian coordinates for geometry minimized *trans*-β-methylstyrene + F cation:



Atom			X	Y	Z
1	H	H1	1.6950242	0.2018471	-0.6603466
2	C	C1	1.1474801	0.4843242	0.2327420
3	C	C4	-0.2977428	1.2584934	2.5425834
4	C	C2	-0.2884213	0.4247253	0.2449821
5	C	C6	1.8268403	0.9112594	1.3518993
6	C	C5	1.1065941	1.2968524	2.5018730
7	C	C3	-0.9929841	0.8307952	1.4300967
8	H	H6	2.9105386	0.9618797	1.3520224
9	H	H5	1.6532101	1.6384720	3.3768001
10	H	H3	-2.0785636	0.7914027	1.4371534
11	H	H4	-0.8250115	1.5645290	3.4398285
12	C	C7	-1.0321893	-0.0079843	-0.8424875
13	H	H7	-2.1195756	0.0060996	-0.7554595
14	C	C8	-0.5512188	-0.5607180	-2.1364050
15	H	H8	0.3502814	-0.0488542	-2.4946380
16	C	C9	-0.2847499	-2.0741329	-1.9983349
17	H	H2	0.5579302	-2.2719746	-1.3306097
18	H	H10	-1.1722955	-2.5941163	-1.6280814
19	H	H14	-0.0501390	-2.4513359	-2.9980698
20	F	F1	-1.5550074	-0.3615634	-3.0655486

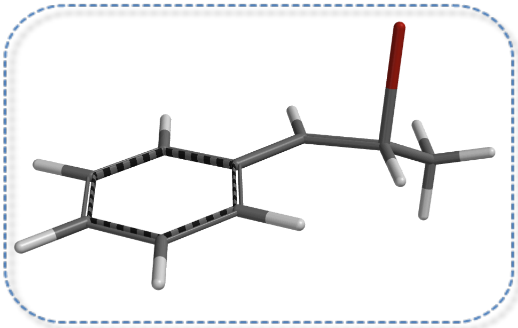
Cartesian coordinates for geometry minimized *trans*-β-methylstyrene + Cl cation:



Atom			X	Y	Z
1	H	H1	1.8415927	0.3792221	-0.5524955
2	C	C1	1.2525920	0.6380542	0.3202823
3	C	C4	-0.2896535	1.3234001	2.5927255
4	C	C2	-0.1422605	0.3073176	0.3750987
5	C	C6	1.8458243	1.2924901	1.3783517
6	C	C5	1.0785012	1.6332895	2.5100144
7	C	C3	-0.8985295	0.6715536	1.5397491
8	H	H6	2.8997233	1.5476129	1.3442432
9	H	H5	1.5573512	2.1495495	3.3377162
10	H	H3	-1.9558636	0.4253881	1.5798343
11	H	H4	-0.8582175	1.5982875	3.4747316
12	C	C7	-0.8070644	-0.3658755	-0.6457541
13	H	H7	-1.8663492	-0.5760463	-0.4981623
14	C	C8	-0.2765590	-0.8240323	-1.9543484

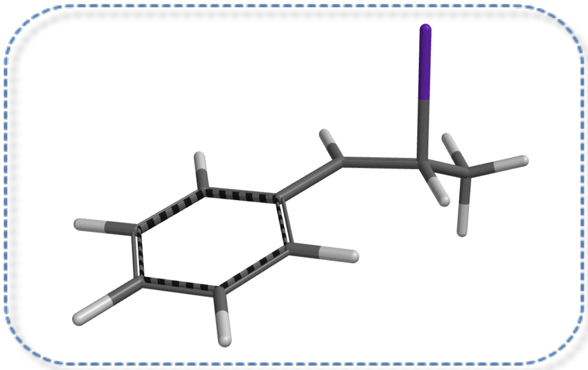
15	H	H8	0.7972271	-0.6813895	-2.0677326
16	C	C9	-0.7048959	-2.2291680	-2.3552876
17	H	H2	-0.2155746	-2.9613526	-1.7026519
18	H	H10	-1.7888340	-2.3546941	-2.2843876
19	Cl	Cl1	-1.0731909	0.4521031	-3.0067585
20	H	H14	-0.3958189	-2.4257099	-3.3851683

Cartesian coordinates for geometry minimized *trans*-β-methylstyrene + Br cation:



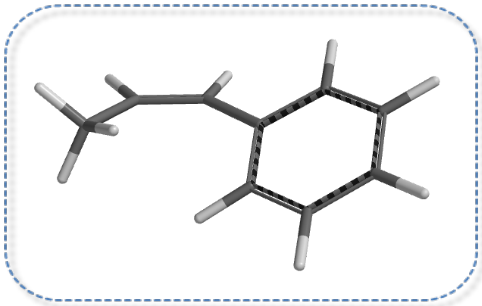
Atom			X	Y	Z
1	H	H1	1.8574729	0.3830576	-0.5330532
2	C	C1	1.2617372	0.6444875	0.3333469
3	C	C4	-0.2904247	1.3409636	2.5990273
4	C	C2	-0.1292304	0.2929226	0.3901490
5	C	C6	1.8468260	1.3248348	1.3859169
6	C	C5	1.0756437	1.6724980	2.5167296
7	C	C3	-0.8910606	0.6634599	1.5511735
8	H	H6	2.8957440	1.5930012	1.3471919
9	H	H5	1.5456894	2.2057584	3.3365620
10	H	H3	-1.9439914	0.4038623	1.5960776
11	H	H4	-0.8644809	1.6179014	3.4748436
12	C	C7	-0.7866125	-0.4129093	-0.6258795
13	H	H7	-1.8380584	-0.6510893	-0.4669806
14	C	C8	-0.2356687	-0.9020513	-1.9008857
15	H	H8	0.8341550	-0.7594681	-2.0334701
16	C	C9	-0.7310299	-2.2520803	-2.3839682
17	H	H2	-0.2724791	-3.0425599	-1.7753894
18	H	H10	-1.8184063	-2.3407703	-2.3106930
19	H	H14	-0.4376409	-2.4160850	-3.4232182
20	Br	Br1	-1.0781843	0.6342663	-3.0774805

Cartesian coordinates for geometry minimized *trans*-β-methylstyrene + I cation:



	Atom		X	Y	Z
1	H	H1	1.8494486	0.4237718	-0.5496064
2	C	C1	1.2515656	0.6678248	0.3201486
3	C	C4	-0.2852244	1.3201876	2.5871639
4	C	C2	-0.1321358	0.3299062	0.3668280
5	C	C6	1.8402660	1.3137967	1.3850405
6	C	C5	1.0759639	1.6379051	2.5175545
7	C	C3	-0.8879579	0.6788587	1.5236835
8	H	H6	2.8924886	1.5702541	1.3530702
9	H	H5	1.5503198	2.1431802	3.3521744
10	H	H3	-1.9428120	0.4287196	1.5638640
11	H	H4	-0.8598802	1.5772193	3.4689331
12	C	C7	-0.7883929	-0.3803678	-0.6546760
13	H	H7	-1.8324835	-0.6314673	-0.4804312
14	C	C8	-0.2316178	-0.9099972	-1.8949633
15	H	H8	0.8369943	-0.7660635	-2.0198083
16	C	C9	-0.7154934	-2.2725801	-2.3491641
17	H	H2	-0.2478077	-3.0362309	-1.7185189
18	H	H10	-1.7985210	-2.3752239	-2.2697020
19	H	H14	-0.4223518	-2.4638129	-3.3810689
20	I	I1	-1.1523684	0.7441194	-3.1205218

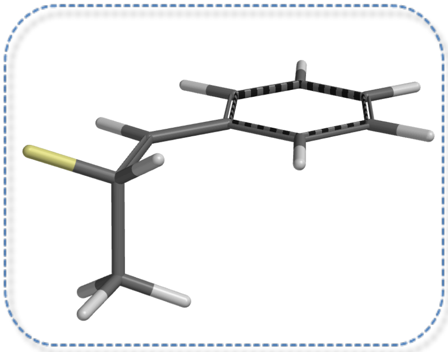
Cartesian coordinates for geometry minimized *cis*-β-methylstyrene:



Atom	X	Y	Z

1	H	H1	-0.9234456	0.9465027	-1.1015877
2	C	C1	-0.5814928	0.8807578	-0.0740923
3	C	C4	0.1704031	0.7208959	2.6057955
4	C	C2	-0.1651186	-0.3597750	0.4426459
5	C	C6	-0.6050526	2.0207735	0.7290371
6	C	C5	-0.2230467	1.9491230	2.0696045
7	C	C3	0.1905473	-0.4172493	1.8033731
8	H	H6	-0.9354075	2.9668141	0.3075209
9	H	H5	-0.2440752	2.8384877	2.6937307
10	H	H3	0.4958038	-1.3709947	2.2281328
11	H	H4	0.4578425	0.6490724	3.6516742
12	C	C7	-0.1259336	-1.6009607	-0.3527417
13	H	H7	-0.3228481	-2.5049577	0.2243823
14	C	C8	0.1518614	-1.7686650	-1.6572552
15	H	H8	0.1111787	-2.7914341	-2.0322993
16	C	C9	0.5563012	-0.7370371	-2.6731029
17	H	H2	0.9129031	0.1874253	-2.2107370
18	H	H10	1.3567311	-1.1305768	-3.3118026
19	H	H14	-0.2771514	-0.4782021	-3.3422782

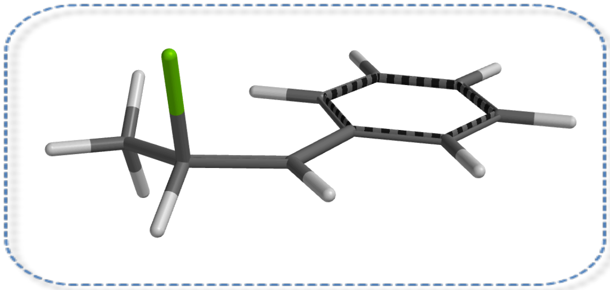
Cartesian coordinates for geometry minimized *cis*-β-methylstyrene + F cation:



	Atom		X	Y	Z
1	H	H1	1.1119258	1.1495487	-0.8902513
2	C	C1	0.6798624	1.0649594	0.1012788
3	C	C4	-0.4077372	0.8127077	2.7050387
4	C	C2	0.1023642	-0.1792678	0.5297595
5	C	C6	0.6954936	2.1448640	0.9555887
6	C	C5	0.1540619	2.0187079	2.2521613
7	C	C3	-0.4347183	-0.2773156	1.8595014
8	H	H6	1.1295815	3.0884175	0.6421690
9	H	H5	0.1787208	2.8758949	2.9197088
10	H	H3	-0.8642102	-1.2203051	2.1858766
11	H	H4	-0.8128270	0.7434694	3.7089588
12	C	C7	0.0403306	-1.2998401	-0.2845878
13	H	H7	-0.3913257	-2.2105820	0.1331818
14	C	C8	0.4378418	-1.4373396	-1.7109923
15	H	H8	1.3519814	-0.8768709	-1.9421268
16	C	C9	-0.7141760	-0.9792857	-2.6296449
17	H	H2	-1.6356511	-1.5198861	-2.3977861

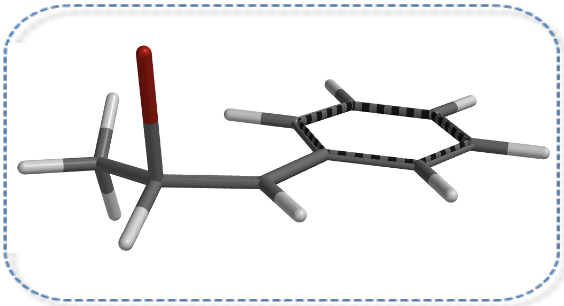
18	H	H10	-0.8915606	0.0960692	-2.5441245
19	H	H14	-0.4188930	-1.2163636	-3.6559917
20	F	F1	0.6889351	-2.7775821	-1.9377179

Cartesian coordinates for geometry minimized *cis*-β-methylstyrene + Cl cation:



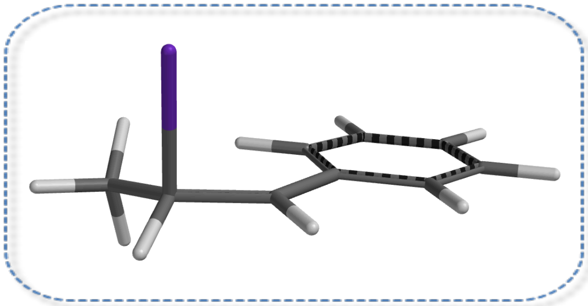
	Atom		X	Y	Z
1	H	H1	-0.0963462	1.2459008	-1.0864510
2	C	C1	-0.0647157	1.1065062	-0.0152871
3	C	C4	0.0356081	0.7524627	2.7927693
4	C	C2	0.0453575	-0.2127516	0.5403547
5	C	C6	-0.1271382	2.2019182	0.8192681
6	C	C5	-0.0778132	2.0280931	2.2163611
7	C	C3	0.0943225	-0.3541759	1.9711455
8	H	H6	-0.2119710	3.2004379	0.4035825
9	H	H5	-0.1272708	2.9013878	2.8611325
10	H	H3	0.1757665	-1.3497128	2.3980117
11	H	H4	0.0731585	0.6416445	3.8712205
12	C	C7	0.1210474	-1.3932821	-0.1967684
13	H	H7	0.2200235	-2.3019809	0.3954807
14	C	C8	0.0444923	-1.6943180	-1.6568612
15	H	H8	0.7119536	-2.5366193	-1.8602527
16	C	C9	0.1760078	-0.6378408	-2.7380225
17	H	H2	-0.6311985	0.0971960	-2.7078397
18	H	H10	1.1451344	-0.1327757	-2.6531436
19	H	H14	0.1401085	-1.1278607	-3.7143236
20	Cl	Cl1	-1.6465270	-2.4342294	-1.6403767

Cartesian coordinates for geometry minimized *cis*-β-methylstyrene + Br cation:



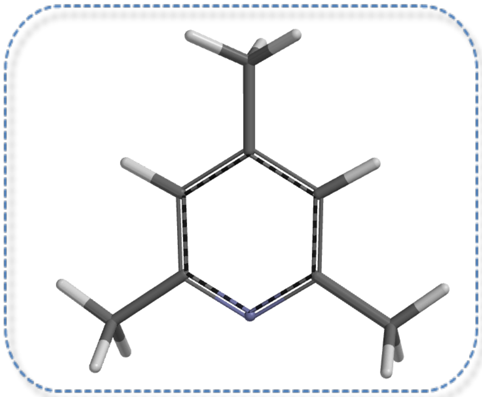
	Atom		X	Y	Z
1	H	H1	-0.1242977	1.2525088	-1.0822717
2	C	C1	-0.0805535	1.1087581	-0.0132837
3	C	C4	0.0438337	0.7574816	2.7966616
4	C	C2	0.0456347	-0.2117892	0.5387691
5	C	C6	-0.1436356	2.2077448	0.8251486
6	C	C5	-0.0823670	2.0375338	2.2248518
7	C	C3	0.1049413	-0.3519290	1.9714021
8	H	H6	-0.2385979	3.2035717	0.4091723
9	H	H5	-0.1326469	2.9086491	2.8698093
10	H	H3	0.1967266	-1.3455523	2.3983420
11	H	H4	0.0897453	0.6443622	3.8729635
12	C	C7	0.1359628	-1.3976990	-0.2044704
13	H	H7	0.2593054	-2.3034865	0.3879168
14	C	C8	0.0964777	-1.6778479	-1.6551731
15	H	H8	0.6841846	-2.5711030	-1.8747749
16	C	C9	0.2170468	-0.6317856	-2.7410982
17	H	H2	-0.5843437	0.1094068	-2.7182471
18	H	H10	1.1862720	-0.1222955	-2.6580732
19	H	H14	0.1860556	-1.1185417	-3.7187228
20	Br	Br1	-1.8597441	-2.4979874	-1.6289216

Cartesian coordinates for geometry minimized *cis* -β-methylstyrene + I cation at the B3LYP/6-31G*/LANL2DZ level:



Atom			X	Y	Z
1	H	H1	-1.2570456	-0.8310066	-0.7161051
2	C	C1	-0.9804834	-0.4643835	0.2609092
3	C	C4	-0.3075297	0.4980664	2.8219562
4	C	C2	0.2425273	0.2419302	0.4558242
5	C	C6	-1.8346219	-0.6719027	1.3230695
6	C	C5	-1.5009766	-0.1977252	2.6008649
7	C	C3	0.5528466	0.7174189	1.7662658
8	H	H6	-2.7678775	-1.2016890	1.1725929
9	H	H5	-2.1809933	-0.3714524	3.4279800
10	H	H3	1.4820386	1.2538936	1.9274982
11	H	H4	-0.0619948	0.8601786	3.8130887
12	C	C7	1.1749812	0.5523158	-0.5538332
13	H	H7	1.9956325	1.1862742	-0.2286387
14	C	C8	1.2384836	0.2443922	-1.9843568
15	H	H8	1.7953812	1.0219839	-2.5039000
16	C	C9	0.1006584	-0.2994382	-2.8159743
17	H	H2	-0.2671061	-1.2667538	-2.4774542
18	H	H10	-0.7254075	0.4203349	-2.8108847
19	H	H14	0.4280237	-0.4139104	-3.8490132
20	I	I1	2.8734633	-1.2785270	-1.6298892

Cartesian coordinates for geometry minimized 2,4,6-trimethyl pyridine (1a):

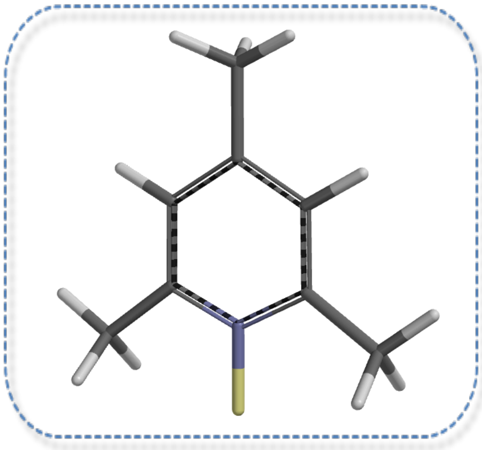


Atom			X	Y	Z
1	C	C1	-1.4244548	-0.0123527	0.0000000
2	N	N1	1.3882477	0.0062446	0.0000000
3	C	C2	-0.6963245	-0.0108158	1.1929154
4	C	C6	-0.6963245	-0.0108158	-1.1929154
5	C	C5	0.7018459	0.0001699	-1.1535693
6	C	C3	0.7018459	0.0001699	1.1535693
7	H	H6	-1.2126451	-0.0200574	-2.1497555
8	H	H3	-1.2126451	-0.0200574	2.1497555
9	C	C4	1.5256542	0.0027114	2.4186636
10	H	H2	2.1824902	-0.8742538	2.4497664
11	H	H4	0.8959480	-0.0014085	3.3136334
12	H	H7	2.1733436	0.8863785	2.4514046
13	C	C7	1.5256542	0.0027114	-2.4186636
14	H	H1	2.1824902	-0.8742538	-2.4497664
15	H	H8	2.1733436	0.8863785	-2.4514046
16	H	H9	0.8959480	-0.0014085	-3.3136334
17	C	C8	-2.9336996	0.0110175	0.0000000
18	H	H5	-3.3427524	-0.4830072	0.8876019
19	H	H10	-3.3427524	-0.4830072	-0.8876019
20	H	H11	-3.3065445	1.0438393	0.0000000

Cartesian coordinates for geometry minimized 2,4,6-trimethyl pyridine (1a) at the B3LYP/6-31G*/SM8 (acetone) level:

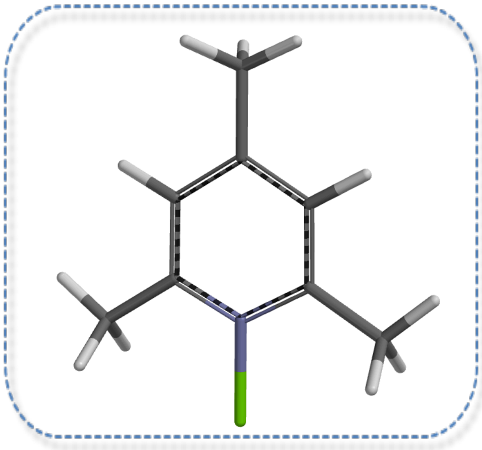
Atom			X	Y	Z
1	C	C1	-1.4232569	-0.0123923	-0.0000003
2	N	N1	1.3924566	0.0055747	0.0000006
3	C	C2	-0.6932652	-0.0105984	1.1928980
4	C	C6	-0.6932644	-0.0105946	-1.1928982
5	C	C5	0.7035880	-0.0000109	-1.1576148
6	C	C3	0.7035875	-0.0000113	1.1576158
7	H	H6	-1.2090640	-0.0188997	-2.1492029
8	H	H3	-1.2090681	-0.0189057	2.1492009
9	C	C4	1.5214692	0.0026874	2.4232737
10	H	H2	2.1790071	-0.8736897	2.4638131
11	H	H4	0.8876639	-0.0014102	3.3143907
12	H	H7	2.1697001	0.8859043	2.4653907
13	C	C7	1.5214683	0.0026782	-2.4232731
14	H	H1	2.1789699	-0.8737259	-2.4638298
15	H	H8	2.1697355	0.8858690	-2.4653754
16	H	H9	0.8876623	-0.0013784	-3.3143898
17	C	C8	-2.9293029	0.0102767	-0.0000001
18	H	H5	-3.3390691	-0.4830526	0.8870475
19	H	H10	-3.3390684	-0.4830271	-0.8870619
20	H	H11	-3.3012808	1.0428893	0.0000153

Cartesian coordinates for geometry minimized 2,4,6-trimethyl pyridine + F cation (1a-F):



Atom			X	Y	Z
1	C	C1	-0.4605306	-0.0037852	-1.3936822
2	N	N1	0.3959968	-0.0043049	1.1699148
3	C	C2	-0.2329322	-1.2069616	-0.7084838
4	C	C6	-0.2268752	1.2011880	-0.7085148
5	C	C5	0.2111258	1.2174310	0.6072769
6	C	C3	0.2061741	-1.2237407	0.6092894
7	H	H2	-0.3969880	-2.1606090	-1.1982709
8	H	H6	-0.3866077	2.1554514	-1.1992386
9	C	C4	0.4775200	-2.4441823	1.4309164
10	C	C10	0.4873300	2.4365565	1.4296020
11	C	C14	-0.9531236	0.0049386	-2.8123576
12	H	H7	-0.3643753	0.6938957	-3.4271886
13	H	H22	-1.9943060	0.3504879	-2.8471818
14	H	H23	-0.9121060	-0.9891229	-3.2627882
15	H	H24	0.2625566	-3.3362828	0.8412759
16	H	H25	1.5244478	-2.4751041	1.7519449
17	H	H26	-0.1455202	-2.4548581	2.3316222
18	H	H27	1.5339301	2.4630265	1.7519018
19	H	H28	-0.1370456	2.4505478	2.3293070
20	H	H29	0.2771937	3.3295574	0.8395081
21	F	F1	0.8341353	-0.0041291	2.4651471

Cartesian coordinates for geometry minimized 2,4,6-trimethyl pyridine + Cl cation (1a-Cl):

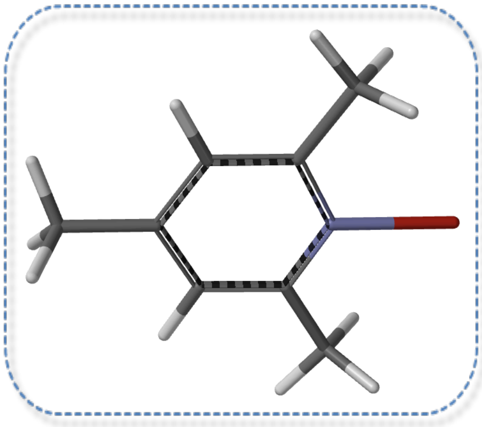


	Atom		X	Y	Z
1	C	C1	-0.4587553	-0.0039247	-1.3860869
2	N	N1	0.4160348	-0.0044046	1.2281940
3	C	C2	-0.2278196	-1.1992827	-0.6959907
4	C	C6	-0.2214938	1.1932565	-0.6962449
5	C	C5	0.2166656	1.2116364	0.6184780
6	C	C3	0.2118328	-1.2180391	0.6205759
7	H	H2	-0.3910220	-2.1538065	-1.1843174
8	H	H6	-0.3799483	2.1484190	-1.1855733
9	Cl	Cl1	0.9620075	-0.0043125	2.8758940
10	C	C4	0.4605612	-2.4885560	1.3717030
11	C	C10	0.4704970	2.4810328	1.3702715
12	C	C14	-0.9549018	0.0046660	-2.8024847
13	H	H7	-0.3678287	0.6934960	-3.4192827
14	H	H22	-1.9957340	0.3518944	-2.8340770
15	H	H23	-0.9166225	-0.9895156	-3.2530373
16	H	H24	0.2497825	-3.3405299	0.7235766
17	H	H25	1.5014445	-2.5568983	1.7067503
18	H	H26	-0.1795422	-2.5589923	2.2580331
19	H	H27	1.5119483	2.5464022	1.7039618
20	H	H28	-0.1685648	2.5536607	2.2571103
21	H	H29	0.2614589	3.3337983	0.7225462

Cartesian coordinates for geometry minimized 2,4,6-trimethyl pyridine + Cl cation (1a-Cl) at the B3LYP/6-31G*/SM8 (acetone) level:

Atom			X	Y	Z
1	C	C1	-0.4559613	-0.0048480	-1.3816389
2	N	N1	0.4159178	-0.0046638	1.2261837
3	C	C2	-0.2255991	-1.2002788	-0.6946727
4	C	C6	-0.2207756	1.1927408	-0.6948392
5	C	C5	0.2164722	1.2125342	0.6191172
6	C	C3	0.2128388	-1.2195999	0.6214042
7	H	H2	-0.3878407	-2.1548634	-1.1818630
8	H	H6	-0.3803688	2.1472686	-1.1837641
9	Cl	Cl1	0.9646636	-0.0041663	2.8807573
10	C	C4	0.4601370	-2.4886766	1.3693577
11	C	C10	0.4678066	2.4808341	1.3675074
12	C	C14	-0.9523920	0.0057120	-2.7959546
13	H	H7	-0.3598737	0.6865478	-3.4158629
14	H	H22	-1.9890795	0.3634138	-2.8301598
15	H	H23	-0.9251701	-0.9887968	-3.2463149
16	H	H24	0.2438912	-3.3368015	0.7188772
17	H	H25	1.5015671	-2.5660677	1.6991569
18	H	H26	-0.1787264	-2.5644022	2.2555277
19	H	H27	1.5095090	2.5557429	1.6968617
20	H	H28	-0.1708472	2.5589875	2.2535668
21	H	H29	0.2538312	3.3293832	0.7167522

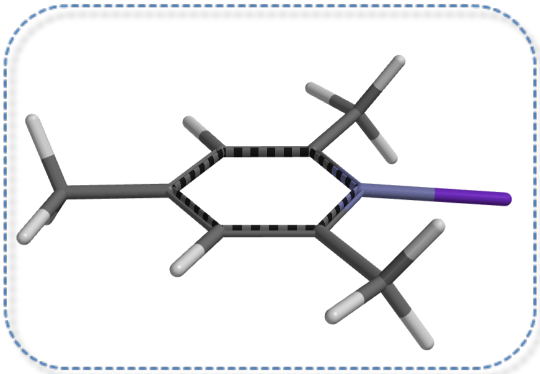
Cartesian coordinates for geometry minimized 2,4,6-trimethyl pyridine + Br cation (1a-Br):



Atom			X	Y	Z
1	C	C1	-0.5085398	-0.0016614	-1.3774365
2	N	N1	0.4439891	-0.0027266	1.2220452

3	C	C2	-0.2527254	-1.2016674	-0.6953799
4	C	C6	-0.2573508	1.1989604	-0.6919287
5	C	C5	0.2215547	1.2155932	0.6154715
6	C	C3	0.2264933	-1.2193070	0.6131688
7	H	H2	-0.4290950	-2.1534307	-1.1806020
8	H	H6	-0.4376370	2.1513820	-1.1749086
9	C	C4	0.4950209	-2.5000639	1.3417112
10	C	C10	0.4859306	2.4951871	1.3478531
11	Br	Br1	1.0961805	-0.0033691	3.0796683
12	C	C14	-1.0170364	0.0034186	-2.7910386
13	H	H7	-0.1929687	0.1941550	-3.4918370
14	H	H22	-1.7590922	0.7930121	-2.9439227
15	H	H23	-1.4667739	-0.9543223	-3.0624677
16	H	H24	1.5341897	2.5731946	1.6573596
17	H	H25	-0.1330370	2.5792812	2.2481237
18	H	H26	0.2594518	3.3428033	0.6997847
19	H	H27	0.2716547	-3.3466338	0.6912466
20	H	H28	1.5434864	-2.5752096	1.6513179
21	H	H29	-0.1236955	-2.5885957	2.2417710

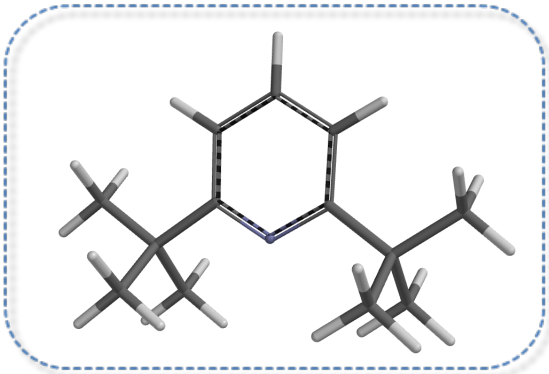
Cartesian coordinates for geometry minimized 2,4,6-trimethyl pyridine + I cation (1a- I) at the B3LYP/6-31G*/LANL2DZ level:



Atom			X	Y	Z
1	C	C1	-0.4641932	0.0083029	-1.3901767
2	N	N1	0.4078970	0.0024977	1.2422231
3	C	C2	-0.2246739	-1.1848352	-0.7031872
4	C	C6	-0.2124777	1.1958822	-0.7038429
5	C	C5	0.2216503	1.2058075	0.6138388
6	C	C3	0.2081600	-1.2008960	0.6119717
7	H	H2	-0.3857530	-2.1375969	-1.1933822
8	H	H6	-0.3631758	2.1506835	-1.1924452
9	C	C4	0.4544323	-2.4921086	1.3277390
10	C	C10	0.4802848	2.4947039	1.3288930
11	I	I1	0.9231693	-0.0014757	3.3228900
12	C	C14	-0.9657914	0.0000599	-2.8025454
13	H	H7	-0.2053585	-0.4068029	-3.4761880

14	H	H22	-1.2260774	0.9993983	-3.1498878
15	H	H23	-1.8481538	-0.6384571	-2.8955120
16	H	H24	1.5141831	2.5577318	1.6788273
17	H	H25	-0.1729783	2.6152442	2.1969467
18	H	H26	0.3028989	3.3319922	0.6561377
19	H	H27	0.2654658	-3.3275621	0.6557852
20	H	H28	1.4884988	-2.5669382	1.6746246
21	H	H29	-0.1980074	-2.6056316	2.1972902

Cartesian coordinates for geometry minimized 2,6-di-*tert*-butyl pyridine (1b):



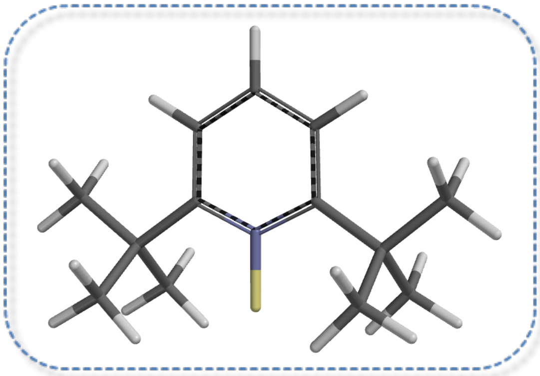
	Atom		X	Y	Z
1	C	C1	-0.7108567	0.0218167	-2.5990573
2	N	N1	0.0215260	-0.0006476	0.0675877
3	C	C2	-0.5264361	-1.1870869	-1.9336875
4	C	C6	-0.5270256	1.2193147	-1.9131182
5	C	C5	-0.1565644	1.1709519	-0.5626801
6	C	C3	-0.1561866	-1.1613723	-0.5824331
7	H	H2	-0.6699041	-2.1246244	-2.4577590
8	H	H6	-0.6712654	2.1654781	-2.4213232
9	H	H4	-0.9980562	0.0308068	-3.6478441
10	C	C4	0.0749097	-2.4292451	0.2564900
11	C	C7	1.5395838	-2.4319098	0.7507208
12	H	H1	1.7605028	-1.5156513	1.3050322
13	H	H8	2.2402534	-2.4997350	-0.0904048
14	H	H9	1.7171826	-3.2910537	1.4092421
15	C	C8	-0.1854748	-3.7185630	-0.5422495
16	H	H3	0.4887314	-3.8089299	-1.4020010
17	H	H10	-1.2179519	-3.7722915	-0.9073025
18	H	H11	-0.0171941	-4.5901615	0.1002301
19	C	C9	-0.8725708	-2.3946492	1.4767446
20	H	H7	-0.7137117	-1.4859947	2.0633833
21	H	H12	-0.6929792	-3.2637641	2.1212907
22	H	H13	-1.9231185	-2.4174559	1.1624936
23	C	C10	0.0748656	2.4241997	0.2977723
24	C	C11	-0.8684097	2.3669328	1.5203620
25	H	H14	-0.7060186	1.4492478	2.0917641
26	H	H16	-1.9200240	2.3928464	1.2099448
27	H	H17	-0.6881079	3.2260124	2.1778977

28	C	C12	1.5411406	2.4208612	0.7870249
29	H	H5	1.7654742	1.4955139	1.3246165
30	H	H18	1.7195087	3.2687133	1.4598032
31	H	H19	2.2389516	2.5044158	-0.0550359
32	C	C13	-0.1913294	3.7272923	-0.4762684
33	H	H15	0.4805734	3.8374473	-1.3355948
34	H	H20	-0.0252224	4.5871480	0.1824438
35	H	H21	-1.2247959	3.7841369	-0.8380848

Cartesian coordinates for geometry minimized 2,6-di-*tert*-butyl pyridine (1b) at the B3LYP/6-31G*/SM8 (acetone) level:

	Atom		X	Y	Z
1	C	C1	-0.6976228	0.0218416	-2.5978550
2	N	N1	0.0232949	-0.0007424	0.0730001
3	C	C2	-0.5164122	-1.1870101	-1.9316710
4	C	C6	-0.5170915	1.2192235	-1.9109971
5	C	C5	-0.1528030	1.1733293	-0.5596962
6	C	C3	-0.1523930	-1.1638580	-0.5795889
7	H	H2	-0.6584949	-2.1235922	-2.4568693
8	H	H6	-0.6600756	2.1644802	-2.4202576
9	H	H4	-0.9805322	0.0308844	-3.6467636
10	C	C4	0.0732644	-2.4368880	0.2555882
11	C	C7	1.5379310	-2.4567669	0.7473401
12	H	H1	1.7757813	-1.5506580	1.3131499
13	H	H8	2.2408825	-2.5243401	-0.0920335
14	H	H9	1.7115489	-3.3232595	1.3968737
15	C	C8	-0.1972043	-3.7203930	-0.5478623
16	H	H3	0.4752553	-3.8167970	-1.4078288
17	H	H10	-1.2298864	-3.7689506	-0.9120559
18	H	H11	-0.0353894	-4.5969813	0.0895222
19	C	C9	-0.8692403	-2.4075368	1.4789386
20	H	H7	-0.7077716	-1.5079568	2.0802919
21	H	H12	-0.6952668	-3.2830763	2.1158943
22	H	H13	-1.9227674	-2.4225039	1.1736151
23	C	C10	0.0731915	2.4317642	0.2971174
24	C	C11	-0.8652168	2.3799751	1.5227846
25	H	H14	-0.6998838	1.4716424	2.1097797
26	H	H16	-1.9197355	2.3972385	1.2210483
27	H	H17	-0.6910147	3.2460906	2.1722965
28	C	C12	1.5393723	2.4456210	0.7843487
29	H	H5	1.7804060	1.5304629	1.3340306
30	H	H18	1.7137353	3.3012601	1.4479078
31	H	H19	2.2395967	2.5283922	-0.0559094
32	C	C13	-0.2029202	3.7290858	-0.4818121
33	H	H15	0.4671020	3.8450745	-1.3413420
34	H	H20	-0.0430390	4.5940425	0.1717877
35	H	H21	-1.2366006	3.7809022	-0.8427725

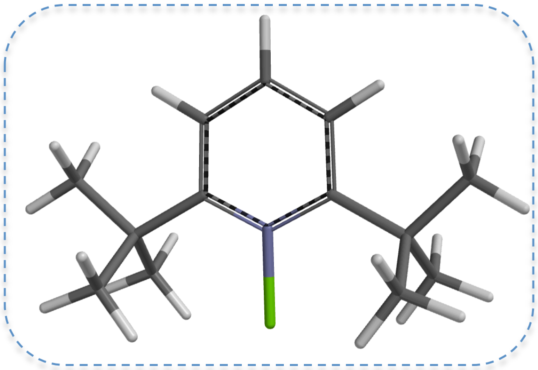
Cartesian coordinates for geometry minimized 2,6-di-*tert*-butyl pyridine + F cation (1b-F):



	Atom		X	Y	Z
1	C	C1	-0.8153856	0.0018584	-2.5292359
2	N	N1	-0.0076080	0.0000015	0.0069609
3	C	C2	-0.6056235	-1.2059500	-1.8717847
4	C	C6	-0.6050219	1.2086951	-1.8701861
5	C	C5	-0.1824163	1.2349054	-0.5444135
6	C	C3	-0.1830476	-1.2340843	-0.5460274
7	H	H2	-0.7676472	-2.1431778	-2.3849468
8	H	H6	-0.7666090	2.1466724	-2.3821219
9	H	H7	-1.1439983	0.0026314	-3.5627262
10	C	C4	0.0811380	-2.5143276	0.2620033
11	C	C7	1.5672427	-2.5733125	0.6994424
12	H	H1	1.8412775	-1.7831052	1.4008763
13	H	H8	2.2362648	-2.5138774	-0.1655373
14	H	H9	1.7544688	-3.5326748	1.1925066
15	C	C8	-0.8663260	-2.5817913	1.4866062
16	H	H4	-0.6904016	-1.7811859	2.2072537
17	H	H10	-0.7120474	-3.5333416	2.0061081
18	H	H11	-1.9167325	-2.5431799	1.1788333
19	C	C9	-0.1962408	-3.7474929	-0.6229126
20	H	H3	0.4620842	-3.7847549	-1.4961540
21	H	H12	-1.2370333	-3.7954905	-0.9578081
22	H	H13	-0.0034497	-4.6496875	-0.0348991
23	C	C10	0.0824153	2.5139597	0.2652872
24	C	C11	1.5686052	2.5716721	0.7026211
25	H	H5	2.2374939	2.5128958	-0.1625067
26	H	H16	1.8423233	1.7805161	1.4031180
27	H	H17	1.7563872	3.5303618	1.1967832
28	C	C12	-0.8648432	2.5802038	1.4901203
29	H	H14	-0.6893206	1.7784212	2.2095554
30	H	H18	-1.9153143	2.5427052	1.1824361
31	H	H19	-0.7098988	3.5308809	2.0110284
32	C	C13	-0.1945323	3.7484215	-0.6179541
33	H	H15	0.4637766	3.7865983	-1.4911685

34	H	H20	-0.0013807	4.6497424	-0.0287237
35	H	H21	-1.2353190	3.7972598	-0.9527469
36	F	F1	0.4167203	-0.0009689	1.3203132

Cartesian coordinates for geometry minimized 2,6-di-*tert*-butyl pyridine + Cl cation (1b-Cl):



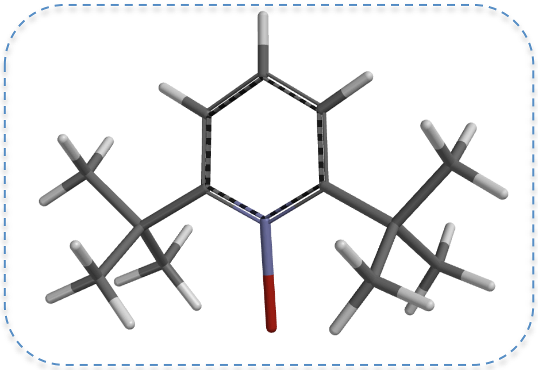
Atom			X	Y	Z
1	C	C1	-0.8375940	0.0018043	-2.4068683
2	N	N1	0.0065405	-0.0001172	0.1780200
3	C	C2	-0.6109334	-1.1967978	-1.7493376
4	C	C6	-0.6104954	1.1994141	-1.7476744
5	C	C5	-0.1742322	1.2384747	-0.4241244
6	C	C3	-0.1747657	-1.2378117	-0.4258099
7	H	H2	-0.7744358	-2.1265625	-2.2710596
8	H	H6	-0.7737061	2.1299383	-2.2681431
9	Cl	Cl1	0.4827766	-0.0013802	1.8545350
10	H	H7	-1.1840302	0.0025913	-3.4357701
11	C	C4	0.0865667	-2.6030961	0.2679741
12	C	C7	1.5771690	-2.7495031	0.6844715
13	H	H1	1.8947323	-2.0798011	1.4816704
14	H	H8	2.2364015	-2.6001653	-0.1775470
15	H	H9	1.7299133	-3.7726734	1.0409613
16	C	C8	-0.8934461	-2.8460161	1.4491616
17	H	H4	-0.7509982	-2.1821728	2.2999487
18	H	H10	-0.7463517	-3.8694111	1.8076945
19	H	H11	-1.9325252	-2.7599699	1.1137842
20	C	C9	-0.1779716	-3.7546293	-0.7376907
21	H	H3	0.4798385	-3.7112225	-1.6117440
22	H	H12	-1.2203331	-3.7947152	-1.0696885
23	H	H13	0.0314141	-4.6984392	-0.2280347
24	C	C10	0.0878939	2.6027141	0.2714171
25	C	C11	1.5786859	2.7477473	0.6876700
26	H	H5	2.2375553	2.5995897	-0.1748268
27	H	H16	1.8961614	2.0764722	1.4835755

28	H	H17	1.7320254	3.7702275	1.0458773
29	C	C12	-0.8916236	2.8446326	1.4532215
30	H	H14	-0.7487756	2.1801028	2.3034017
31	H	H18	-1.9308588	2.7588768	1.1182507
32	H	H19	-0.7443673	3.8677312	1.8125233
33	C	C13	-0.1763397	3.7556886	-0.7326785
34	H	H15	0.4811834	3.7130212	-1.6069781
35	H	H20	0.0337101	4.6987307	-0.2218779
36	H	H21	-1.2187844	3.7967270	-1.0643048

Cartesian coordinates for geometry minimized 2,6-di-*tert*-butyl pyridine + Cl cation (1b-Cl) at the B3LYP/6-31G*/SM8 (acetone) level:

Atom			X	Y	Z
1	C	C1	-0.8403860	0.0018033	-2.4067225
2	N	N1	0.0051419	-0.0001151	0.1761942
3	C	C2	-0.6130383	-1.1961978	-1.7497632
4	C	C6	-0.6125882	1.1988138	-1.7481071
5	C	C5	-0.1763412	1.2371096	-0.4265391
6	C	C3	-0.1768860	-1.2364431	-0.4282175
7	H	H2	-0.7767653	-2.1251510	-2.2730114
8	H	H6	-0.7760135	2.1285285	-2.2701066
9	Cl	Cl1	0.4804495	-0.0013820	1.8588655
10	H	H7	-1.1875700	0.0025877	-3.4343923
11	C	C4	0.0863240	-2.6006941	0.2668197
12	C	C7	1.5742177	-2.7469990	0.6854239
13	H	H1	1.8900100	-2.0834877	1.4890025
14	H	H8	2.2381001	-2.5867091	-0.1709681
15	H	H9	1.7355224	-3.7719481	1.0342031
16	C	C8	-0.8905225	-2.8463750	1.4473577
17	H	H4	-0.7457491	-2.1877271	2.3022757
18	H	H10	-0.7518997	-3.8717997	1.8047519
19	H	H11	-1.9309392	-2.7530957	1.1182573
20	C	C9	-0.1760444	-3.7517532	-0.7380087
21	H	H3	0.4805046	-3.7073350	-1.6121810
22	H	H12	-1.2173957	-3.7937083	-1.0710380
23	H	H13	0.0337907	-4.6981544	-0.2321012
24	C	C10	0.0876613	2.6003121	0.2702526
25	C	C11	1.5757425	2.7452555	0.6886125
26	H	H5	2.2392535	2.5862554	-0.1683051
27	H	H16	1.8914924	2.0800840	1.4908294
28	H	H17	1.7376023	3.7694927	1.0392180
29	C	C12	-0.8886924	2.8449803	1.4514113
30	H	H14	-0.7434706	2.1856836	2.3057492
31	H	H18	-1.9292613	2.7519179	1.1227279
32	H	H19	-0.7499614	3.8701294	1.8095427
33	C	C13	-0.1744052	3.7528130	-0.7330044
34	H	H15	0.4818500	3.7091311	-1.6074280
35	H	H20	0.0361081	4.6984469	-0.2259483
36	H	H21	-1.2158415	3.7957301	-1.0656523

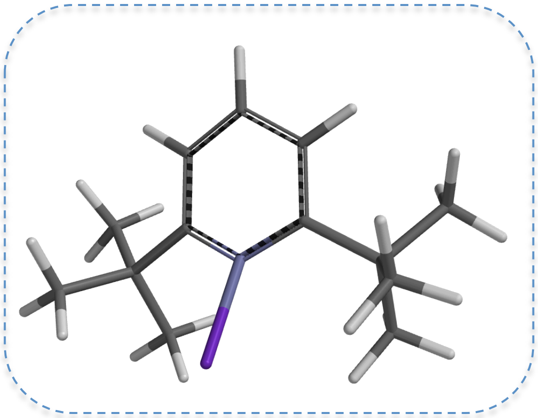
Cartesian coordinates for geometry minimized 2,6-di-*tert*-butyl pyridine + Br cation (1b-Br):



Atom			X	Y	Z
1	C	C1	-0.9251432	0.0017925	-2.3610830
2	N	N1	-0.0335458	-0.0001516	0.2259457
3	C	C2	-0.6738107	-1.1981399	-1.7100091
4	C	C6	-0.6732567	1.2007286	-1.7083771
5	C	C5	-0.2084019	1.2402906	-0.3879434
6	C	C3	-0.2090079	-1.2396769	-0.3896139
7	H	H2	-0.8387886	-2.1263680	-2.2295835
8	H	H6	-0.8378412	2.1297126	-2.2267366
9	H	H7	-1.3016699	0.0025765	-3.3776333
10	C	C4	0.0923253	-2.6258999	0.2613572
11	C	C7	1.5894350	-2.7330317	0.6870791
12	H	H1	1.8860423	-2.0475144	1.4778788
13	H	H8	2.2446075	-2.5730100	-0.1761527
14	H	H9	1.7655337	-3.7493022	1.0531535
15	C	C8	-0.8976335	-2.9522238	1.4228763
16	H	H4	-0.7985797	-2.3104939	2.2950903
17	H	H10	-0.7110853	-3.9802206	1.7493049
18	H	H11	-1.9327860	-2.8982012	1.0688652
19	C	C9	-0.1185754	-3.7601258	-0.7864801
20	H	H3	0.5322622	-3.6527297	-1.6602535
21	H	H12	-1.1599691	-3.8426683	-1.1137469
22	H	H13	0.1407849	-4.7065565	-0.3054912
23	C	C10	0.0936889	2.6255039	0.2648601
24	C	C11	1.5909260	2.7313168	0.6904570
25	H	H5	2.2458728	2.5719686	-0.1730705
26	H	H16	1.8872672	2.0446865	1.4803920
27	H	H17	1.7676420	3.7470566	1.0577039
28	C	C12	-0.8958848	2.9508331	1.4269801
29	H	H14	-0.7966978	2.3082028	2.2985140
30	H	H18	-1.9311508	2.8973885	1.0732164
31	H	H19	-0.7090312	3.9784555	1.7544062
32	C	C13	-0.1168537	3.7611966	-0.7814617

33	H	H15	0.5337950	3.6546504	-1.6554787
34	H	H20	0.1430073	4.7068858	-0.2992960
35	H	H21	-1.1582658	3.8446106	-1.1084467
36	Br	Br1	0.4147886	-0.0015422	2.1627775

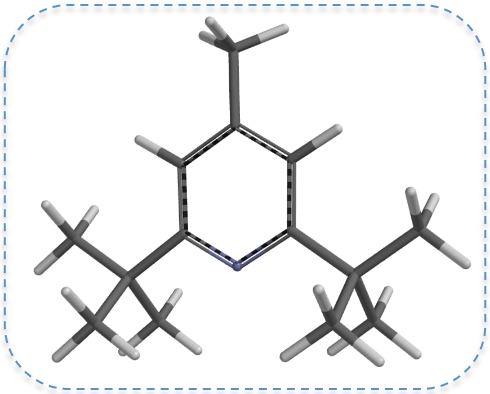
Cartesian coordinates for geometry minimized 2,6-di-*tert*-butyl pyridine + I cation (1b- I) at the B3LYP/6-31G*/LANL2DZ level:



	Atom		X	Y	Z
1	C	C1	-0.4391450	-0.0006867	-2.5328415
2	N	N1	0.4356437	-0.0009252	0.0503267
3	C	C2	-0.3167948	-1.1938785	-1.8414288
4	C	C6	-0.3101791	1.1930383	-1.8432877
5	C	C5	0.1067361	1.2193629	-0.5165189
6	C	C3	0.0999141	-1.2201592	-0.5145197
7	H	H2	-0.5480865	-2.1246544	-2.3341821
8	H	H6	-0.5365337	2.1240960	-2.3378114
9	H	H7	-0.6993825	-0.0007661	-3.5855831
10	C	C4	0.0672006	-2.5630347	0.2659293
11	C	C7	1.4316376	-3.2959964	0.2569615
12	H	H1	2.1949738	-2.8039015	0.8539289
13	H	H8	1.8141320	-3.4082796	-0.7603967
14	H	H9	1.2932110	-4.2979368	0.6686024
15	C	C8	-0.4671951	-2.3587095	1.7037328
16	H	H4	0.1887293	-1.7835733	2.3524893
17	H	H10	-0.5844486	-3.3376336	2.1717722
18	H	H11	-1.4487696	-1.8786890	1.6942843
19	C	C9	-0.9437548	-3.5149194	-0.4289093
20	H	H3	-0.5860813	-3.8934831	-1.3882338
21	H	H12	-1.9231480	-3.0533890	-0.5736734
22	H	H13	-1.0859853	-4.3874804	0.2098904
23	C	C10	0.0806072	2.5630108	0.2628786
24	C	C11	1.4506084	3.2859680	0.2630515
25	H	H5	1.8443961	3.3884109	-0.7510301

26	H	H16	2.2044024	2.7931745	0.8712934
27	H	H17	1.3148758	4.2917513	0.6660488
28	C	C12	-0.4650531	2.3619693	1.6969392
29	H	H14	0.1779998	1.7745244	2.3475798
30	H	H18	-1.4537793	1.8971293	1.6796765
31	H	H19	-0.5700014	3.3409596	2.1678996
32	C	C13	-0.9179861	3.5234145	-0.4376066
33	H	H15	-0.5512549	3.9001146	-1.3943320
34	H	H20	-1.0571797	4.3964343	0.2012276
35	H	H21	-1.9002142	3.0700374	-0.5887869
36	I	I1	2.0999053	-0.0052998	1.4446292

Cartesian coordinates for geometry minimized 4-methyl-2,6-di-*tert*-butyl pyridine (1c):



Atom			X	Y	Z
1	C	C1	-0.6284016	0.0187703	-2.2477325
2	N	N1	0.1242676	-0.0038483	0.4408914
3	C	C2	-0.4366253	-1.1830914	-1.5616066
4	C	C6	-0.4373023	1.2089264	-1.5411106
5	C	C5	-0.0592428	1.1640502	-0.1944256
6	C	C3	-0.0588919	-1.1607703	-0.2141019
7	H	H2	-0.5858641	-2.1236251	-2.0807194
8	H	H6	-0.5874527	2.1580282	-2.0442575
9	C	C4	0.1727253	-2.4328237	0.6190273
10	C	C7	1.6388383	-2.4385614	1.1088571
11	H	H1	1.8622217	-1.5244278	1.6656124
12	H	H8	2.3366234	-2.5036738	0.2650820
13	H	H9	1.8180384	-3.3004130	1.7634867
14	C	C8	-0.0907855	-3.7203686	-0.1815422
15	H	H3	0.5796658	-3.8086575	-1.0444375
16	H	H10	-1.1247757	-3.7735015	-0.5423196
17	H	H11	0.0804665	-4.5932806	0.4584769
18	C	C9	-0.7708848	-2.4013599	1.8423063
19	H	H7	-0.6099456	-1.4942609	2.4307592
20	H	H12	-0.5901002	-3.2723577	2.4841196

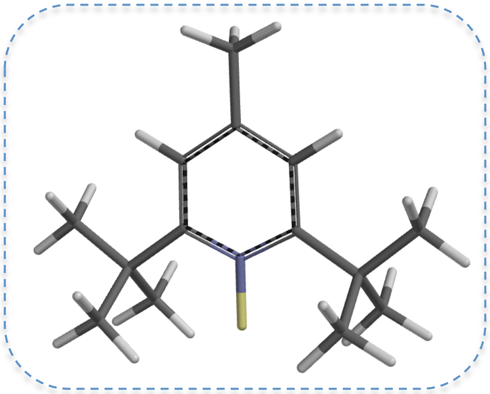
21	H	H13	-1.8223563	-2.4227111	1.5309522
22	C	C10	0.1729022	2.4215834	0.6602370
23	C	C11	-0.7661772	2.3674850	1.8861328
24	H	H14	-0.6015602	1.4513849	2.4594140
25	H	H16	-1.8187813	2.3918852	1.5788629
26	H	H17	-0.5845137	3.2285550	2.5408303
27	C	C12	1.6407279	2.4214186	1.1447604
28	H	H5	1.8677222	1.4981830	1.6847944
29	H	H18	1.8208102	3.2720703	1.8136303
30	H	H19	2.3354283	2.5023099	0.2998326
31	C	C13	-0.0966030	3.7229313	-0.1155867
32	H	H15	0.5712844	3.8310558	-0.9782974
33	H	H20	0.0726761	4.5841527	0.5406414
34	H	H21	-1.1316783	3.7791115	-0.4728246
35	C	C14	-1.0051464	0.0313969	-3.7096556
36	H	H4	-0.1083008	0.0401894	-4.3434377
37	H	H22	-1.5922249	0.9198166	-3.9648506
38	H	H23	-1.5867840	-0.8555718	-3.9818009

Cartesian coordinates for geometry minimized 4-methyl-2,6-di-*tert*-butyl pyridine (1c) at the B3LYP/6-31G*/SM8 (acetone) level:

Atom			X	Y	Z
1	C	C1	-0.6212014	0.0187613	-2.2470346
2	N	N1	0.1241599	-0.0039484	0.4471678
3	C	C2	-0.4309204	-1.1827829	-1.5582805
4	C	C6	-0.4316626	1.2085313	-1.5377253
5	C	C5	-0.0581096	1.1662310	-0.1909117
6	C	C3	-0.0577181	-1.1630742	-0.2106811
7	H	H2	-0.5782762	-2.1229461	-2.0775189
8	H	H6	-0.5800082	2.1572810	-2.0409609
9	C	C4	0.1702272	-2.4405863	0.6178154
10	C	C7	1.6373152	-2.4636483	1.1022307
11	H	H1	1.8791879	-1.5592625	1.6690420
12	H	H8	2.3357535	-2.5297244	0.2589213
13	H	H9	1.8134056	-3.3321755	1.7483926
14	C	C8	-0.1049135	-3.7221002	-0.1872315
15	H	H3	0.5617607	-3.8159295	-1.0519857
16	H	H10	-1.1399494	-3.7703071	-0.5447142
17	H	H11	0.0616943	-4.6001431	0.4469714
18	C	C9	-0.7659766	-2.4148220	1.8461063
19	H	H7	-0.6012597	-1.5170582	2.4492828
20	H	H12	-0.5896234	-3.2924115	2.4796697
21	H	H13	-1.8210542	-2.4282420	1.5459234
22	C	C10	0.1701966	2.4292858	0.6592582
23	C	C11	-0.7623323	2.3813374	1.8895945
24	H	H14	-0.5941020	1.4748336	2.4785829
25	H	H16	-1.8182743	2.3971480	1.5926132
26	H	H17	-0.5857981	3.2496116	2.5356762
27	C	C12	1.6386002	2.4461427	1.1397547

28 H H5	1.8832117	1.5326777	1.6906227
29 H H18	1.8153437	3.3038783	1.7999909
30 H H19	2.3346826	2.5272480	0.2958409
31 C C13	-0.1100037	3.7246628	-0.1214590
32 H H15	0.5544337	3.8378720	-0.9856993
33 H H20	0.0548059	4.5911320	0.5289689
34 H H21	-1.1459397	3.7763282	-0.4759083
35 C C14	-0.9926382	0.0314527	-3.7072396
36 H H4	-0.0936265	0.0408316	-4.3372202
37 H H22	-1.5788784	0.9191163	-3.9652977
38 H H23	-1.5725123	-0.8552012	-3.9825581

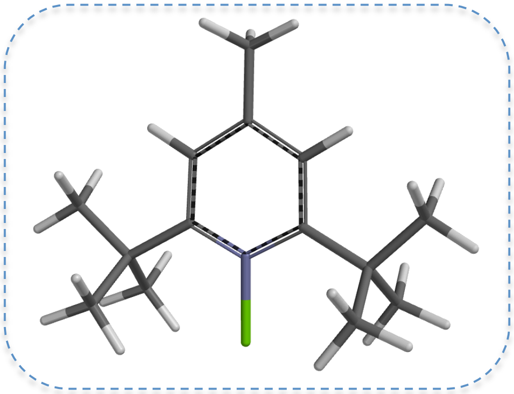
Cartesian coordinates for geometry minimized 4-methyl-2,6-di-*tert*-butyl pyridine + F cation (1c-F):



Atom	X	Y	Z
1 C C1	-0.7321229	-0.0032640	-2.0917719
2 N N1	0.1211046	-0.0033231	0.5206143
3 C C2	-0.4943470	-1.1937572	-1.4096610
4 C C6	-0.4903184	1.1891562	-1.4092914
5 C C5	-0.0579421	1.2312254	-0.0916995
6 C C3	-0.0606379	-1.2352426	-0.0897907
7 H H2	-0.6537221	-2.1269697	-1.9275283
8 H H6	-0.6476660	2.1223756	-1.9286416
9 Cl Cl1	0.5797063	-0.0023829	2.2062999
10 C C4	0.2025965	-2.6016394	0.6019078
11 C C7	1.6878499	-2.7428057	1.0310239
12 H H1	1.9958122	-2.0767939	1.8355615
13 H H8	2.3571422	-2.5813527	0.1790149
14 H H9	1.8503831	-3.7665781	1.3827240
15 C C8	-0.7814430	-2.8524004	1.7753399
16 H H4	-0.6469283	-2.1919951	2.6306486
17 H H10	-0.6403048	-3.8768399	2.1346810
18 H H11	-1.8197373	-2.7645944	1.4380504
19 C C9	-0.0480683	-3.7529742	-0.4053151
20 H H3	0.6125788	-3.7039922	-1.2762015

21	H	H12	-1.0873812	-3.8006228	-0.7438755
22	H	H13	0.1643737	-4.6986449	0.1009725
23	C	C10	0.2083600	2.5969887	0.6003000
24	C	C11	1.6937308	2.7358062	1.0293527
25	H	H5	2.3627276	2.5728707	0.1773745
26	H	H16	2.0005454	2.0693134	1.8339593
27	H	H17	1.8583227	3.7593220	1.3808950
28	C	C12	-0.7752750	2.8504735	1.7734057
29	H	H14	-0.6423313	2.1902089	2.6290965
30	H	H18	-1.8136679	2.7643701	1.4359330
31	H	H19	-0.6324358	3.8748147	2.1323995
32	C	C13	-0.0401574	3.7482461	-0.4075754
33	H	H15	0.6206729	3.6977380	-1.2782550
34	H	H20	0.1735664	4.6939649	0.0980861
35	H	H21	-1.0792947	3.7973129	-0.7465188
36	C	C14	-1.2319662	0.0088306	-3.5045595
37	H	H7	-0.6299916	0.6780400	-4.1282303
38	H	H22	-2.2628047	0.3830097	-3.5379331
39	H	H23	-1.2209295	-0.9878947	-3.9507927

Cartesian coordinates for geometry minimized 4-methyl-2,6-di-*tert*-butyl pyridine + Cl cation (1c-Cl):



	Atom		X	Y	Z
1	C	C1	-0.7323920	-0.0026391	-2.0920847
2	N	N1	0.1203104	-0.0029836	0.5231432
3	C	C2	-0.4948810	-1.1928246	-1.4085605
4	C	C6	-0.4890660	1.1893390	-1.4086707
5	C	C5	-0.0569179	1.2324233	-0.0892231
6	C	C3	-0.0604620	-1.2358068	-0.0872536
7	H	H2	-0.6544210	-2.1266098	-1.9252725
8	H	H6	-0.6437656	2.1236661	-1.9266022
9	Cl	Cl1	0.5782652	-0.0022435	2.2039077
10	C	C4	0.2025356	-2.6029612	0.6030984
11	C	C7	1.6903658	-2.7426481	1.0307164
12	H	H1	1.9988597	-2.0701274	1.8290800

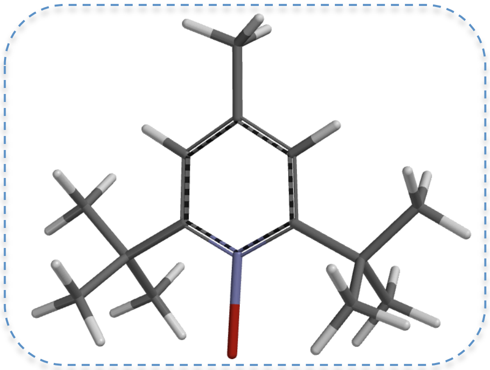
13	H	H8	2.3551595	-2.5906483	0.1733662
14	H	H9	1.8459406	-3.7645438	1.3897467
15	C	C8	-0.7846062	-2.8530097	1.7766097
16	H	H4	-0.6537445	-2.1873803	2.6279506
17	H	H10	-0.6341039	-3.8752895	2.1371058
18	H	H11	-1.8214136	-2.7734362	1.4325988
19	C	C9	-0.0480992	-3.7549937	-0.4051577
20	H	H3	0.6136520	-3.7052260	-1.2759024
21	H	H12	-1.0882781	-3.8022553	-0.7428596
22	H	H13	0.1654840	-4.6979839	0.1044271
23	C	C10	0.2093099	2.5988271	0.6018151
24	C	C11	1.6972887	2.7358603	1.0291259
25	H	H5	2.3616566	2.5828302	0.1716008
26	H	H16	2.0046933	2.0623067	1.8270574
27	H	H17	1.8550046	3.7573071	1.3884918
28	C	C12	-0.7772636	2.8513378	1.7752257
29	H	H14	-0.6475806	2.1859717	2.6269585
30	H	H18	-1.8142100	2.7732288	1.4312590
31	H	H19	-0.6251947	3.8734994	2.1354385
32	C	C13	-0.0395704	3.7512043	-0.4064972
33	H	H15	0.6225718	3.7008092	-1.2769415
34	H	H20	0.1747487	4.6940330	0.1030498
35	H	H21	-1.0795258	3.7995356	-0.7448729
36	C	C14	-1.2332060	0.0072990	-3.5077323
37	H	H7	-0.6379912	0.6844678	-4.1298077
38	H	H22	-2.2690326	0.3687908	-3.5394639
39	H	H23	-1.2101208	-0.9891266	-3.9548706

Cartesian coordinates for geometry minimized 4-methyl-2,6-di-*tert*-butyl pyridine + Cl cation (1c-Cl) at the B3LYP/6-31G*/SM8 (acetone) level:

	Atom		X	Y	Z
1	C	C1	-0.7321229	-0.0032640	-2.0917719
2	N	N1	0.1211046	-0.0033231	0.5206143
3	C	C2	-0.4943470	-1.1937572	-1.4096610
4	C	C6	-0.4903184	1.1891562	-1.4092914
5	C	C5	-0.0579421	1.2312254	-0.0916995
6	C	C3	-0.0606379	-1.2352426	-0.0897907
7	H	H2	-0.6537221	-2.1269697	-1.9275283
8	H	H6	-0.6476660	2.1223756	-1.9286416
9	Cl	Cl1	0.5797063	-0.0023829	2.2062999
10	C	C4	0.2025965	-2.6016394	0.6019078
11	C	C7	1.6878499	-2.7428057	1.0310239
12	H	H1	1.9958122	-2.0767939	1.8355615
13	H	H8	2.3571422	-2.5813527	0.1790149
14	H	H9	1.8503831	-3.7665781	1.3827240
15	C	C8	-0.7814430	-2.8524004	1.7753399
16	H	H4	-0.6469283	-2.1919951	2.6306486
17	H	H10	-0.6403048	-3.8768399	2.1346810
18	H	H11	-1.8197373	-2.7645944	1.4380504

19	C	C9	-0.0480683	-3.7529742	-0.4053151
20	H	H3	0.6125788	-3.7039922	-1.2762015
21	H	H12	-1.0873812	-3.8006228	-0.7438755
22	H	H13	0.1643737	-4.6986449	0.1009725
23	C	C10	0.2083600	2.5969887	0.6003000
24	C	C11	1.6937308	2.7358062	1.0293527
25	H	H5	2.3627276	2.5728707	0.1773745
26	H	H16	2.0005454	2.0693134	1.8339593
27	H	H17	1.8583227	3.7593220	1.3808950
28	C	C12	-0.7752750	2.8504735	1.7734057
29	H	H14	-0.6423313	2.1902089	2.6290965
30	H	H18	-1.8136679	2.7643701	1.4359330
31	H	H19	-0.6324358	3.8748147	2.1323995
32	C	C13	-0.0401574	3.7482461	-0.4075754
33	H	H15	0.6206729	3.6977380	-1.2782550
34	H	H20	0.1735664	4.6939649	0.0980861
35	H	H21	-1.0792947	3.7973129	-0.7465188
36	C	C14	-1.2319662	0.0088306	-3.5045595
37	H	H7	-0.6299916	0.6780400	-4.1282303
38	H	H22	-2.2628047	0.3830097	-3.5379331
39	H	H23	-1.2209295	-0.9878947	-3.9507927

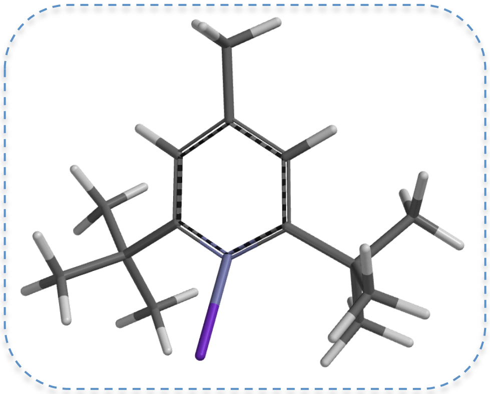
Cartesian coordinates for geometry minimized 4-methyl-2,6-di-*tert*-butyl pyridine + Br cation (1c-Br):



	Atom		X	Y	Z
1	C	C1	-0.8268129	-0.0005627	-2.0434049
2	N	N1	0.0901652	-0.0019158	0.5662924
3	C	C2	-0.5545282	-1.1937201	-1.3711676
4	C	C6	-0.5622387	1.1930933	-1.3666207
5	C	C5	-0.0902469	1.2354396	-0.0538007
6	C	C3	-0.0841465	-1.2371064	-0.0567113
7	H	H2	-0.7162060	-2.1252015	-1.8871348
8	H	H6	-0.7302586	2.1254017	-1.8794595
9	C	C4	0.2264717	-2.6245007	0.5883403
10	C	C7	1.7221046	-2.7199566	1.0204793
11	H	H1	2.0099435	-2.0294907	1.8102307

12	H	H8	2.3799112	-2.5566088	0.1597923
13	H	H9	1.9047864	-3.7337231	1.3903955
14	C	C8	-0.7644797	-2.9636272	1.7451397
15	H	H4	-0.6700909	-2.3267630	2.6215076
16	H	H10	-0.5747408	-3.9929265	2.0657710
17	H	H11	-1.7989347	-2.9111848	1.3888042
18	C	C9	0.0301437	-3.7574104	-0.4634727
19	H	H3	0.6809044	-3.6391760	-1.3359321
20	H	H12	-1.0096640	-3.8498960	-0.7929522
21	H	H13	0.2986435	-4.7027179	0.0148659
22	C	C10	0.2171316	2.6220345	0.5946524
23	C	C11	1.7122773	2.7206109	1.0277159
24	H	H5	2.3707914	2.5565880	0.1676984
25	H	H16	2.0007676	2.0322439	1.8190545
26	H	H17	1.8934405	3.7353857	1.3955073
27	C	C12	-0.7753186	2.9565145	1.7513660
28	H	H14	-0.6830437	2.3148271	2.6244472
29	H	H18	-1.8093279	2.9068986	1.3932001
30	H	H19	-0.5850571	3.9838745	2.0780045
31	C	C13	0.0185905	3.7564639	-0.4552144
32	H	H15	0.6684338	3.6396024	-1.3284809
33	H	H20	0.2871095	4.7013376	0.0239501
34	H	H21	-1.0216900	3.8487668	-0.7836160
35	Br	Br1	0.5184882	-0.0029731	2.5054794
36	C	C14	-1.3481808	0.0047148	-3.4531967
37	H	H7	-0.5308437	0.1915462	-4.1626623
38	H	H22	-2.0898648	0.7960051	-3.5998015
39	H	H23	-1.8044302	-0.9518875	-3.7190667

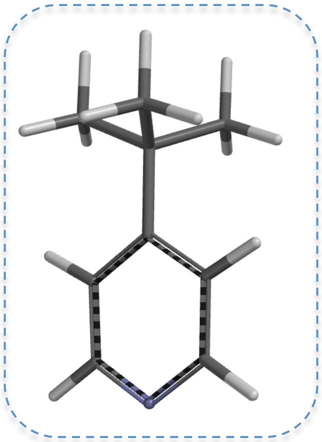
Cartesian coordinates for geometry minimized 4-methyl-2,6-di-*tert*-butyl pyridine + I cation (1c- I) at the B3LYP/6-31G*/LANL2DZ level:



Atom			X	Y	Z
1	C	C1	-0.3656870	-0.0000989	-2.2102900
2	N	N1	0.5022254	-0.0012404	0.4079835

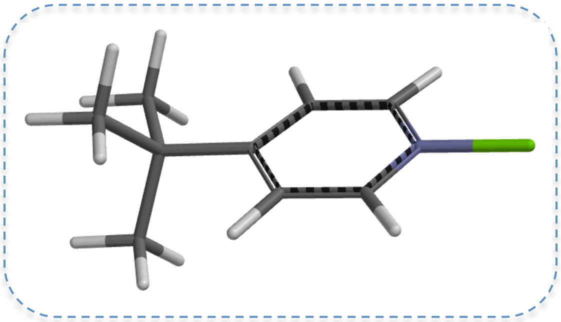
3	C	C2	-0.2514858	-1.1868603	-1.4884587
4	C	C6	-0.2436710	1.1868304	-1.4899658
5	C	C5	0.1702778	1.2151586	-0.1668479
6	C	C3	0.1626493	-1.2162254	-0.1653661
7	H	H2	-0.4941952	-2.1204654	-1.9719039
8	H	H6	-0.4801908	2.1214325	-1.9745711
9	C	C4	0.1241351	-2.5581825	0.6165510
10	C	C7	1.4792944	-3.3066383	0.5820558
11	H	H1	2.2622653	-2.8149741	1.1538343
12	H	H8	1.8349824	-3.4329114	-0.4434773
13	H	H9	1.3418492	-4.3029015	1.0078142
14	C	C8	-0.3761179	-2.3471726	2.0651387
15	H	H4	0.3046516	-1.7844696	2.6992220
16	H	H10	-0.5005094	-3.3243176	2.5351804
17	H	H11	-1.3485646	-1.8490435	2.0779785
18	C	C9	-0.9127685	-3.4971948	-0.0568739
19	H	H3	-0.5788561	-3.8812114	-1.0225426
20	H	H12	-1.8876794	-3.0211431	-0.1836318
21	H	H13	-1.0551328	-4.3673756	0.5853273
22	C	C10	0.1390957	2.5580220	0.6138149
23	C	C11	1.4988105	3.2984513	0.5812490
24	H	H5	1.8589179	3.4189626	-0.4434310
25	H	H16	2.2768526	2.8044417	1.1577008
26	H	H17	1.3656545	4.2970321	1.0028629
27	C	C12	-0.3647605	2.3508979	2.0617100
28	H	H14	0.3107190	1.7828233	2.6966899
29	H	H18	-1.3411058	1.8604126	2.0731828
30	H	H19	-0.4821969	3.3289701	2.5316498
31	C	C13	-0.8908952	3.5029135	-0.0618815
32	H	H15	-0.5530784	3.8845282	-1.0271680
33	H	H20	-1.0290923	4.3741829	0.5797348
34	H	H21	-1.8684414	3.0327026	-0.1901052
35	I	I1	2.1988780	-0.0053861	1.7551371
36	C	C14	-0.6589015	-0.0000189	-3.6793782
37	H	H7	0.2832533	-0.0015435	-4.2397791
38	H	H22	-1.2142006	0.8878465	-3.9847444
39	H	H23	-1.2169808	-0.8862339	-3.9844013

Cartesian coordinates for geometry minimized 4-*tert*-butyl pyridine (1d) at the B3LYP/6-31G*/SM8 (acetone) level:



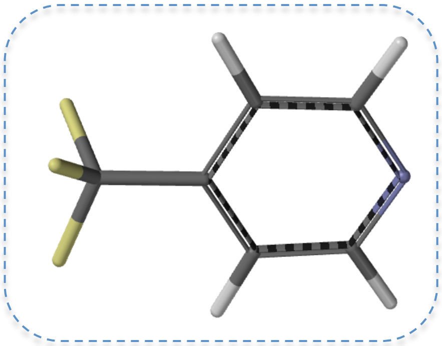
Atom	X	Y	Z
1 C C1	-0.0162441	-0.0280881	0.5708035
2 N N1	0.0243695	-0.0018726	3.4198254
3 C C2	-0.5088386	-1.0960941	1.3311343
4 C C6	0.4993514	1.0556825	1.3013208
5 C C5	0.4975842	1.0242972	2.6915516
6 C C3	-0.4668378	-1.0371726	2.7243038
7 H H2	-0.9283441	-1.9776933	0.8610756
8 H H6	0.9028770	1.9285990	0.7981336
9 H H5	0.8961523	1.8643753	3.2572091
10 H H3	-0.8503401	-1.8678842	3.3141297
11 C C4	-0.0144542	-0.0110348	-0.9661056
12 C C7	-0.7888372	1.2299156	-1.4673411
13 H H4	-0.3446463	2.1649996	-1.1113799
14 H H8	-1.8337108	1.2107073	-1.1370778
15 H H9	-0.7839552	1.2609468	-2.5633546
16 C C8	-0.6719191	-1.2680469	-1.5631408
17 H H7	-0.1363641	-2.1846107	-1.2911561
18 H H10	-0.6661800	-1.2022387	-2.6567102
19 H H11	-1.7163327	-1.3756291	-1.2487450
20 C C9	1.4474883	0.0643320	-1.4656700
21 H H1	2.0287576	-0.8023252	-1.1306587
22 H H12	1.9561794	0.9648568	-1.1064045
23 H H13	1.4742446	0.0839779	-2.5617435

Cartesian coordinates for geometry minimized 4-*tert*-butyl pyridine + Cl cation (1d-Cl) at the B3LYP/6-31G*/SM8 (acetone) level:



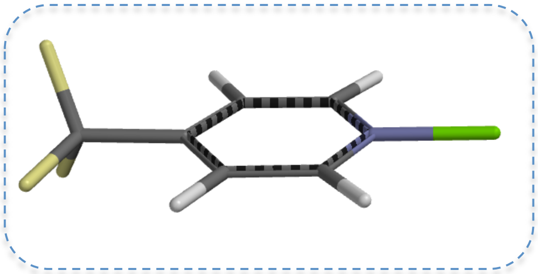
	Atom		X	Y	Z
1	C	C1	-0.0168800	0.0238236	0.3580877
2	N	N1	0.0199414	-0.0655038	3.1236867
3	C	C2	0.4582897	-1.1034779	1.0558977
4	C	C6	-0.4696841	1.1018311	1.1355522
5	C	C5	-0.4476572	1.0494411	2.5159949
6	C	C3	0.4731570	-1.1421331	2.4330715
7	H	H2	0.8264225	-1.9786320	0.5342313
8	H	H6	-0.8519122	2.0086900	0.6850832
9	H	H5	-0.7871592	1.8573793	3.1512649
10	H	H3	0.8276820	-1.9877491	3.0080262
11	Cl	Cl1	0.0414484	-0.1229053	4.8591048
12	C	C4	-0.0173859	0.0407103	-1.1713867
13	C	C7	1.4469948	-0.0881652	-1.6607719
14	H	H1	1.9117556	-1.0226243	-1.3314806
15	H	H8	2.0656503	0.7418628	-1.3027446
16	H	H9	1.4747249	-0.0774781	-2.7560186
17	C	C8	-0.8430916	-1.1638530	-1.6861646
18	H	H7	-0.4247953	-2.1235718	-1.3678808
19	H	H10	-0.8534684	-1.1630856	-2.7815281
20	H	H11	-1.8825476	-1.1179576	-1.3433862
21	C	C9	-0.6223383	1.3366583	-1.7401576
22	H	H4	-0.0491923	2.2254824	-1.4535975
23	H	H12	-1.6639914	1.4785291	-1.4309968
24	H	H13	-0.6159630	1.2927287	-2.8338872

Cartesian coordinates for geometry minimized 4-trifluoromethyl pyridine (1e) at the B3LYP/6-31G*/SM8 (acetone) level:



Atom			X	Y	Z
1	C	C1	-0.0222821	-0.0106755	-0.4744081
2	N	N1	0.0267116	0.0033123	2.3239245
3	C	C2	-0.5036816	-1.1015115	0.2453358
4	C	C6	0.4847055	1.0895113	0.2199553
5	C	C5	0.4861782	1.0448612	1.6120285
6	C	C3	-0.4564999	-1.0422108	1.6391966
7	H	H2	-0.9062120	-1.9736740	-0.2564578
8	H	H6	0.8676625	1.9591618	-0.3035633
9	H	H5	0.8741630	1.8832196	2.1853080
10	H	H3	-0.8256281	-1.8753595	2.2324071
11	C	C4	-0.0139667	-0.0025448	-1.9816058
12	F	F1	-0.6038592	1.1107440	-2.4726993
13	F	F2	-0.6570396	-1.0663946	-2.5049903
14	F	F3	1.2497487	-0.0184396	-2.4644314

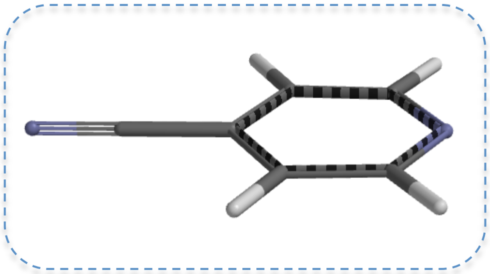
Cartesian coordinates for geometry minimized 4-trifluoromethyl pyridine + Cl cation (1e-Cl) at the B3LYP/6-31G*/SM8 (acetone) level:



Atom			X	Y	Z
1	C	C1	-0.0261847	0.0278727	-0.7328823
2	N	N1	0.0206052	-0.0475513	1.9879863

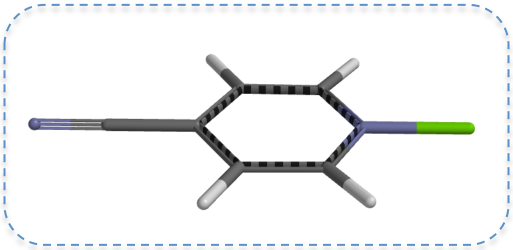
3	C	C2	0.4323894	-1.1143339	-0.0723004
4	C	C6	-0.4605921	1.1288349	0. 0026614
5	C	C5	-0.4317600	1.0768035	1.3869656
6	C	C3	0.4513024	-1.1395095	1.3102452
7	H	H2	0.7774446	-1.9914925	-0.6074554
8	H	H6	-0.8242905	2.0318603	-0.4721054
9	H	H5	-0.7544556	1.8939928	2.0205980
10	H	H3	0.7936729	-1.9894744	1.8878802
11	Cl	Cl1	0.0519635	-0.0957572	3.7226794
12	C	C4	-0.0160889	0.0546331	-2.2475879
13	F	F1	-0.6208038	-1.0415819	-2.7466525
14	F	F2	1.2522653	0.0666041	-2.7050910
15	F	F3	-0.6454677	1.1390992	-2.7349412

Cartesian coordinates for geometry minimized 4-cyanopyridine (1f) at the B3LYP/6-31G*/SM8 (acetone) level:



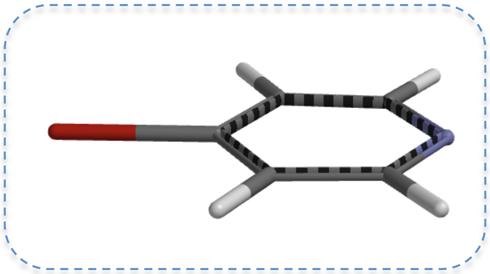
Atom			X	Y	Z
1	N	N1	0.0000000	0.0000000	2.1997659
2	C	C4	0.0000000	0.0000000	-0.5971539
3	C	C2	1.1474557	0.0000000	1.5039004
4	C	C6	-1.1474557	0.0000000	1.5039004
5	C	C5	-1.2094198	0.0000000	0.1121569
6	C	C3	1.2094198	0.0000000	0.1121569
7	H	H2	2.0636346	0.0000000	2.0887390
8	H	H6	-2.0636346	0.0000000	2.0887390
9	H	H5	-2.1624575	0.0000000	-0.4040951
10	H	H3	2.1624575	0.0000000	-0.4040951
11	C	C1	0.0000000	0.0000000	-2.0309621
12	N	N2	0.0000000	0.0000000	-3.1988059

Cartesian coordinates for geometry minimized 4-cyanopyridine + Cl cation (1f-Cl) at the B3LYP/6-31G*/SM8 (acetone) level:



Atom			X	Y	Z
1	N	N1	0.0000000	0.0000000	1.2123809
2	C	C4	0.0000000	0.0000000	-1.5124756
3	C	C2	1.1942669	0.0000000	0.5726390
4	C	C6	-1.1942669	0.0000000	0.5726390
5	C	C5	-1.2129175	0.0000000	-0.8096542
6	C	C3	1.2129175	0.0000000	-0.8096542
7	H	H2	2.0911625	0.0000000	1.1785270
8	H	H6	-2.0911625	0.0000000	1.1785270
9	H	H5	-2.1683554	0.0000000	-1.3199379
10	H	H3	2.1683554	0.0000000	-1.3199379
11	C	C1	0.0000000	0.0000000	-2.9430404
12	N	N2	0.0000000	0.0000000	-4.1101481
13	Cl	Cl1	0.0000000	0.0000000	2.9496747

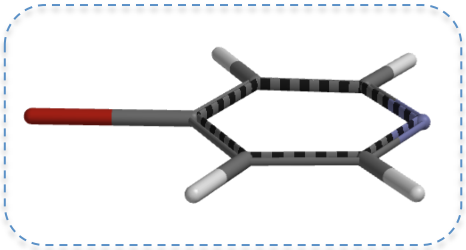
Cartesian coordinates for geometry minimized 4-bromopyridine (1g) at the B3LYP/6-31G*/SM8 (acetone) level:



Atom			X	Y	Z
1	N	N1	0.0000000	0.0000000	2.9013478
2	C	C4	0.0000000	0.0000000	0.1105270
3	C	C2	1.1431628	0.0000000	2.2001341
4	C	C6	-1.1431628	0.0000000	2.2001341
5	C	C5	-1.2058464	0.0000000	0.8057399

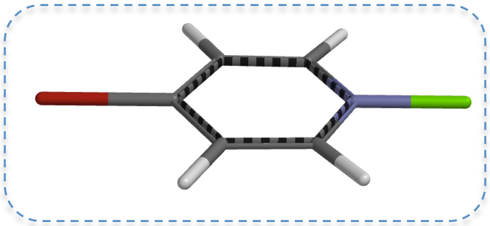
6	C	C3	1.2058464	0.0000000	0.8057399
7	H	H2	2.0633399	0.0000000	2.7801079
8	H	H6	-2.0633399	0.0000000	2.7801079
9	H	H5	-2.1618483	0.0000000	0.2948206
10	H	H3	2.1618483	0.0000000	0.2948206
11	Br	Br1	0.0000000	0.0000000	-1.8055126

Cartesian coordinates for geometry minimized 4-bromopyridine (1g) at the B3LYP/6-31G*/SM8 (acetone) level:



Atom			X	Y	Z
1	N	N1	0.0000000	0.0000000	2.9013478
2	C	C4	0.0000000	0.0000000	0.1105270
3	C	C2	1.1431628	0.0000000	2.2001341
4	C	C6	-1.1431628	0.0000000	2.2001341
5	C	C5	-1.2058464	0.0000000	0.8057399
6	C	C3	1.2058464	0.0000000	0.8057399
7	H	H2	2.0633399	0.0000000	2.7801079
8	H	H6	-2.0633399	0.0000000	2.7801079
9	H	H5	-2.1618483	0.0000000	0.2948206
10	H	H3	2.1618483	0.0000000	0.2948206
11	Br	Br1	0.0000000	0.0000000	-1.8055126

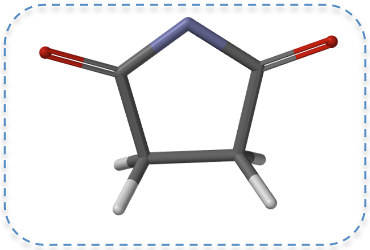
Cartesian coordinates for geometry minimized 4-bromopyridine + Cl (1g-Cl) at the B3LYP/6-31G*/SM8 (acetone) level:



Atom			X	Y	Z
1	N	N1	0.0000000	0.0000000	1.9983709

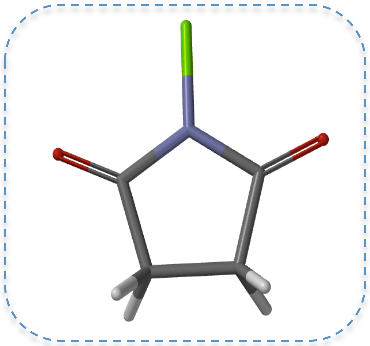
2	C	C4	0.0000000	0.0000000	-0.7248359
3	C	C2	1.1928102	0.0000000	1.3536494
4	C	C6	-1.1928102	0.0000000	1.3536494
5	C	C5	-1.2114857	0.0000000	-0.0279470
6	C	C3	1.2114857	0.0000000	-0.0279470
7	H	H2	2.0911347	0.0000000	1.9583165
8	H	H6	-2.0911347	0.0000000	1.9583165
9	H	H5	-2.1703071	0.0000000	-0.5326010
10	H	H3	2.1703071	0.0000000	-0.5326010
11	Cl	Cl1	0.0000000	0.0000000	3.7332668
12	Br	Br1	0.0000000	0.0000000	-2.6247136

Cartesian coordinates for geometry minimized succinimide anion at the B3LYP/6-31G*/SM8 (acetone) level:



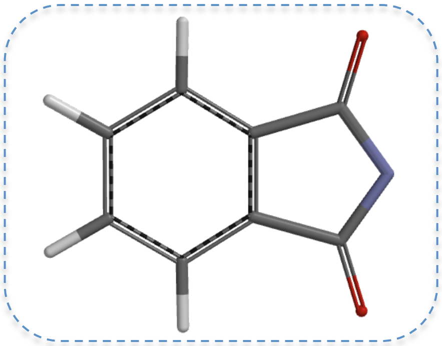
	Atom		X	Y	Z
1	N	N1	0.0000000	-0.0000001	-1.6430693
2	C	C2	1.1154878	0.0000020	-0.8517536
3	C	C3	0.7624587	-0.0000010	0.6543592
4	C	C4	-0.7624590	0.0000015	0.6543592
5	C	C6	-1.1154881	-0.0000019	-0.8517539
6	H	H6	1.2117654	-0.8791951	1.1310469
7	H	H5	1.2117711	0.8791874	1.1310524
8	H	H7	-1.2117663	0.8791950	1.1310476
9	H	H8	-1.2117695	-0.8791875	1.1310528
10	O	O1	-2.2901120	-0.0000053	-1.2431711
11	O	O2	2.2901119	0.0000051	-1.2431703

Cartesian coordinates for geometry minimized *N*-chlorosuccinimide (NCS) at the B3LYP/6-31G*/SM8 (acetone) level:



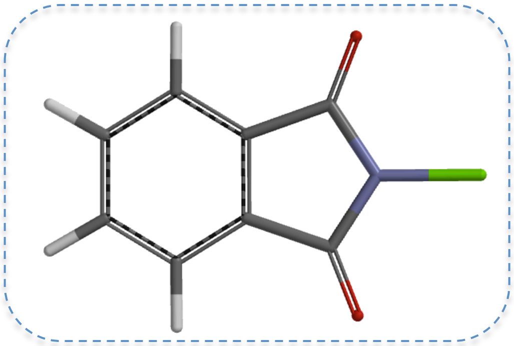
	Atom		X	Y	Z
1	N	N2	0.0000000	0.0000000	0.3164687
2	C	C2	1.1937515	0.0000000	-0.4343312
3	C	C3	0.7701646	0.0000000	-1.8896497
4	C	C4	-0.7701646	0.0000000	-1.8896497
5	C	C6	-1.1937515	0.0000000	-0.4343312
6	H	H6	1.2017538	0.8800770	-2.3749307
7	H	H5	1.2017538	-0.8800770	-2.3749307
8	H	H7	-1.2017538	-0.8800770	-2.3749307
9	H	H8	-1.2017538	0.8800770	-2.3749307
10	O	O1	-2.3092282	0.0000000	0.0392154
11	O	O2	2.3092282	0.0000000	0.0392154
12	Cl	Cl1	0.0000000	0.0000000	2.0320450

Cartesian coordinates for geometry minimized phthalimide anion at the B3LYP/6-31G*/SM8 (acetone) level:



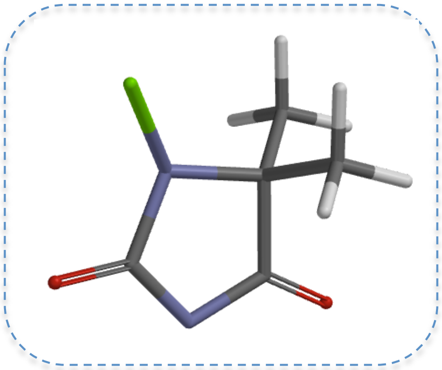
	Atom		X	Y	Z
1	H	H2	-2.5058428	0.0000000	-1.3072244
2	C	C1	-1.4190106	0.0000000	-1.3247221
3	C	C4	1.4190106	0.0000000	-1.3247221
4	C	C2	-0.6956424	0.0000000	-0.1410339
5	C	C6	-0.6998789	0.0000000	-2.5302383
6	C	C5	0.6998789	0.0000000	-2.5302383
7	C	C3	0.6956424	0.0000000	-0.1410339
8	H	H6	-1.2358847	0.0000000	-3.4751863
9	H	H5	1.2358847	0.0000000	-3.4751863
10	H	H4	2.5058428	0.0000000	-1.3072244
11	C	C9	1.1133052	0.0000000	1.3159163
12	O	O2	2.2969444	0.0000000	1.6791531
13	C	C7	-1.1133052	0.0000000	1.3159163
14	O	O3	-2.2969444	0.0000000	1.6791531
15	N	N1	0.0000000	0.0000000	2.1227581

Cartesian coordinates for geometry minimized *N*-chlorophthalimide (NCP) at the B3LYP/6-31G*/SM8 (acetone) level:



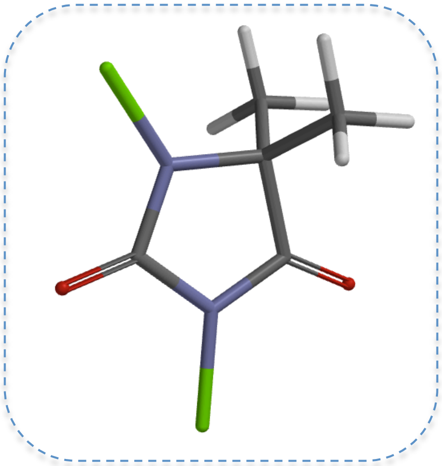
	Atom		X	Y	Z
1	H	H1	-2.5094267	0.0000000	-1.9981670
2	C	C1	-1.4246386	0.0000000	-2.0071608
3	C	C4	1.4246386	0.0000000	-2.0071608
4	C	C2	-0.7003910	0.0000000	-0.8246524
5	C	C6	-0.6994171	0.0000000	-3.2067501
6	C	C5	0.6994171	0.0000000	-3.2067501
7	C	C3	0.7003910	0.0000000	-0.8246524
8	H	H6	-1.2337089	0.0000000	-4.1513571
9	H	H5	1.2337089	0.0000000	-4.1513571
10	H	H4	2.5094267	0.0000000	-1.9981670
11	C	C7	-1.1885780	0.0000000	0.5794528
12	C	C8	1.1885780	0.0000000	0.5794528
13	N	N1	0.0000000	0.0000000	1.3548439
14	O	O1	-2.3178198	0.0000000	1.0194892
15	O	O2	2.3178198	0.0000000	1.0194892
16	Cl	Cl1	0.0000000	0.0000000	3.0595670

Cartesian coordinates for geometry minimized 1-chloro-5,5-dimethylhydantoin anion at the B3LYP/6-31G*/SM8 (acetone) level:



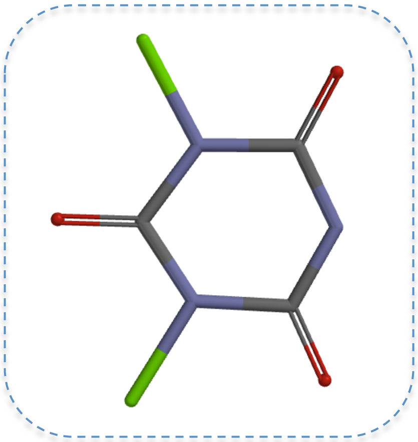
	Atom		X	Y	Z
1	N	N1	0.6348933	0.0196044	0.3935199
2	C	C2	-0.6531504	0.6392987	0.0309234
3	C	C3	-1.5052790	-0.6642301	-0.0227940
4	N	N3	-0.7208693	-1.7740805	-0.0182634
5	C	C7	0.5910462	-1.3817227	0.0862221
6	O	O1	1.6019229	-2.0704046	0.0071321
7	Cl	Cl2	2.1122480	0.8730693	-0.0155140
8	O	O2	-2.7385370	-0.6168048	-0.0837156
9	C	C4	-1.1419147	1.5967263	1.1165117
10	H	H5	-2.1772458	1.8873707	0.9139982
11	H	H6	-0.5224837	2.5002971	1.1491672
12	H	H7	-1.1044665	1.1195958	2.1019300
13	C	C5	-0.6779273	1.3096456	-1.3495440
14	H	H8	-1.7126081	1.5648848	-1.5992339
15	H	H9	-0.2943829	0.6407735	-2.1284128
16	H	H10	-0.0789338	2.2256011	-1.3557543

Cartesian coordinates for geometry minimized 1,3-dichloro-5,5-dimethylhydantoin (DCDMH) at the B3LYP/6-31G*/SM8 (acetone) level:



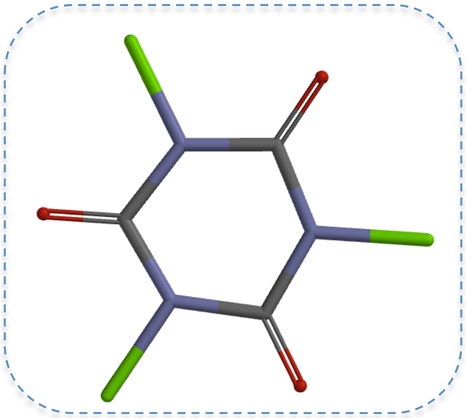
	Atom		X	Y	Z
1	N	N1	0.9282227	-0.4666650	0.1325938
2	C	C2	0.8021885	1.0067936	0.0069192
3	C	C3	-0.7369431	1.1495839	-0.0022491
4	N	N3	-1.2394160	-0.1435735	-0.0110006
5	C	C7	-0.2432908	-1.1677794	0.0380491
6	O	O1	-0.4438673	-2.3600104	0.0133999
7	Cl	Cl1	-2.9051737	-0.5190372	-0.0053392
8	Cl	Cl2	2.4338512	-1.2747265	-0.0064335
9	O	O2	-1.3715844	2.1802447	-0.0088350
10	C	C1	1.3958776	1.7246436	1.2215635
11	H	H2	1.1803832	2.7940166	1.1572922
12	H	H1	2.4811459	1.5890967	1.2404434
13	H	H5	0.9801868	1.3368335	2.1559728
14	C	C4	1.3704076	1.5323056	-1.3174170
15	H	H4	1.1316766	2.5941448	-1.4168392
16	H	H6	0.9534980	0.9969963	-2.1756197
17	H	H7	2.4581197	1.4194055	-1.3299791

Cartesian coordinates for geometry minimized dichloroisocyanuric acid anion at the B3LYP/6-31G*/SM8 (acetone) level:



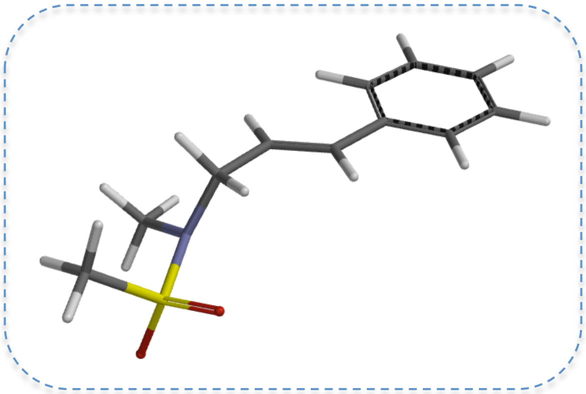
Atom			X	Y	Z
1	N	N2	1.1975822	-0.2247672	0.0000000
2	N	N3	-0.7933257	0.9247690	0.0000000
3	N	N1	-0.8359088	-1.4478491	0.0000000
4	C	C5	-1.5565342	-0.3094036	0.0000000
5	C	C3	0.5102035	-1.5032357	0.0000000
6	C	C1	0.5986729	1.0367859	0.0000000
7	O	O2	1.1895880	-2.5203278	0.0000000
8	O	O3	-2.7770002	-0.2295546	0.0000000
9	O	O4	1.2055501	2.0885643	0.0000000
10	Cl	Cl1	-1.6594540	2.4145250	0.0000000
11	Cl	Cl2	2.9206261	-0.2295063	0.0000000

Cartesian coordinates for geometry minimized trichloroisocyanuric acid (TCCA) at the B3LYP/6-31G*/SM8 (acetone) level:



Atom			X	Y	Z
1	N	N1	1.3469650	0.0000000	0.0000000
2	N	N2	-0.6734825	1.1665059	0.0000000
3	N	N4	-0.6734825	-1.1665059	0.0000000
4	C	C10	-1.4589410	0.0000000	0.0000000
5	C	C8	0.7294705	-1.2634800	0.0000000
6	C	C7	0.7294705	1.2634800	0.0000000
7	O	O1	-2.6624057	0.0000000	0.0000000
8	O	O2	1.3312028	2.3057110	0.0000000
9	O	O3	1.3312028	-2.3057110	0.0000000
10	Cl	Cl1	3.0624432	0.0000000	0.0000000
11	Cl	Cl2	-1.5312216	-2.6521536	0.0000000
12	Cl	Cl3	-1.5312216	2.6521536	0.0000000

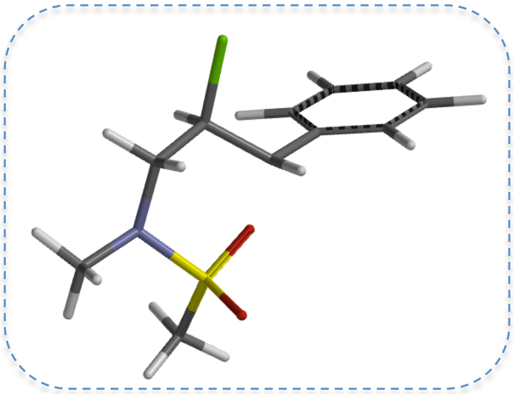
Cartesian coordinates for geometry minimized *N*-cinnamyl-*N*-methylmethanesulfonamide (6):



Atom			X	Y	Z
1	H	H1	-1.0305135	2.8665909	0.2373861
2	C	C1	-0.8216126	2.8025379	1.3014642
3	C	C4	-0.3076293	2.6799012	4.0400905
4	C	C2	-0.5060062	1.5598968	1.8819111
5	C	C6	-0.8759614	3.9582720	2.0742966
6	C	C5	-0.6187115	3.9037641	3.4477374
7	C	C3	-0.2538330	1.5229252	3.2643776
8	H	H6	-1.1218425	4.9072444	1.6048414
9	H	H5	-0.6626065	4.8082310	4.0483011
10	H	H3	-0.0090709	0.5717361	3.7314987
11	H	H4	-0.1065007	2.6241747	5.1065983
12	C	C7	-0.4305058	0.3056322	1.1187739
13	H	H7	-0.2254035	-0.5807294	1.7203402
14	C	C8	-0.5762908	0.1369422	-0.2039278
15	H	H8	-0.7743776	0.9896481	-0.8511283
16	C	C9	-0.4950434	-1.2136049	-0.8658559
17	H	H2	-0.5170834	-1.9941192	-0.1038638

18	H	H10	-1.3644980	-1.3539295	-1.5328648
19	N	N1	0.7563342	-1.3892418	-1.6368630
20	C	C10	0.9018922	-0.5593772	-2.8327703
21	H	H11	0.9017556	0.4918211	-2.5302416
22	H	H12	0.0848355	-0.7145453	-3.5569053
23	H	H13	1.8594506	-0.7765114	-3.3065348
24	S	S1	1.4128934	-2.9387134	-1.6955576
25	O	O1	2.7100099	-2.8249876	-2.3644222
26	O	O2	1.2886646	-3.5048913	-0.3509694
27	C	C11	0.3433312	-3.9201843	-2.7816173
28	H	H9	0.3550429	-3.4891433	-3.7850057
29	H	H16	-0.6699297	-3.9368942	-2.3741136
30	H	H17	0.7532105	-4.9324449	-2.8049756

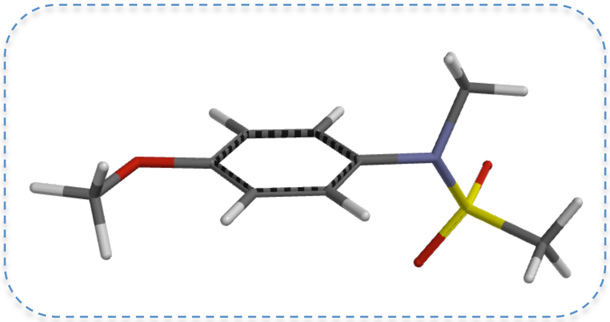
Cartesian coordinates for geometry minimized *N*-cinnamyl-*N*-methylmethanesulfonamide + Cl cation (6-Cl):



Atom	X	Y	Z
1 H	1.696809	0.089600	2.023526
2 C	2.332408	0.307593	1.169557
3 C	3.992070	0.892344	-1.004801
4 C	1.830245	0.221613	-0.138968
5 C	3.655330	0.682201	1.384550
6 C	4.486524	0.971503	0.298089
7 C	2.665650	0.525013	-1.223308
8 H	4.040476	0.745197	2.397573
9 H	5.519885	1.258081	0.469166
10 H	2.281007	0.464077	-2.238175
11 H	4.636648	1.116080	-1.849071
12 C	0.421433	-0.175635	-0.410150
13 H	0.231330	-0.268935	-1.481678
14 C	-0.162246	-1.365370	0.353177
15 C	-1.658009	-1.566799	0.082392
16 H	-1.830369	-1.801693	-0.976270
17 H	-2.021154	-2.406688	0.678479
18 N	-2.475689	-0.389740	0.515604
19 C	-3.939658	-0.642526	0.438464

20	H	-4.145502	-1.492016	1.092740
21	H	-4.269933	-0.869694	-0.580995
22	H	-4.490244	0.218070	0.824109
23	S	-1.995354	1.025254	-0.224353
24	O	-0.443645	1.037550	0.052619
25	O	-2.399642	1.206475	-1.611533
26	C	-2.533132	2.369410	0.830075
27	H	-2.248587	2.146117	1.858739
28	H	-3.613001	2.481820	0.714358
29	H	-2.021382	3.260346	0.456301
30	Cl	0.687011	-2.860690	-0.178562
31	H	0.012926	-1.252804	1.424025

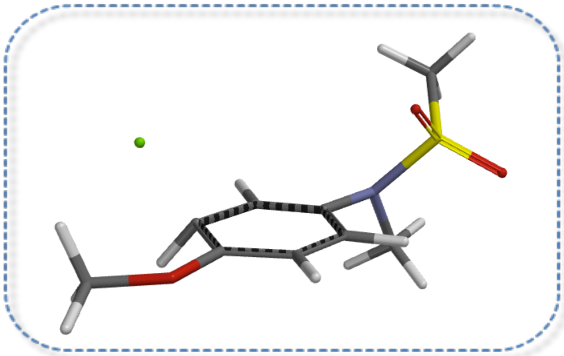
Cartesian coordinates for geometry minimized *N*-(4-methoxyphenyl)-*N*-methylmethanesulfonamide (7):



Atom			X	Y	Z
1	H	H1	-0.8280239	0.7464126	-1.6579833
2	C	C1	-0.5385586	0.8203226	-0.6141097
3	C	C4	0.2194106	0.9770287	2.0610019
4	C	C2	-0.1258567	-0.3300109	0.0536762
5	C	C6	-0.5839693	2.0532117	0.0407250
6	C	C5	-0.2037210	2.1333012	1.3857781
7	C	C3	0.2561821	-0.2422025	1.4006387
8	H	H3	0.5951375	-1.1321139	1.9236242
9	H	H4	0.5187042	1.0646910	3.1005799
10	N	N1	-0.1399570	-1.5884436	-0.6547433
11	S	S1	1.4026110	-2.2684655	-0.9778075
12	C	C8	-1.1403989	-2.5640997	-0.1868703
13	H	H2	-0.9272789	-2.9506061	0.8170278
14	H	H12	-1.1874974	-3.4098397	-0.8787659
15	H	H13	-2.1119680	-2.0640287	-0.1865897
16	O	O2	1.6165569	-3.4481067	-0.1276428
17	O	O3	2.3706445	-1.1724327	-0.9986819
18	C	C9	1.1818779	-2.8512269	-2.6716374
19	H	H11	0.3468644	-3.5529778	-2.7153607
20	H	H14	2.1084281	-3.3572086	-2.9529498
21	H	H15	1.0026214	-1.9882426	-3.3137483
22	H	H9	-0.9097852	2.9325063	-0.5026876

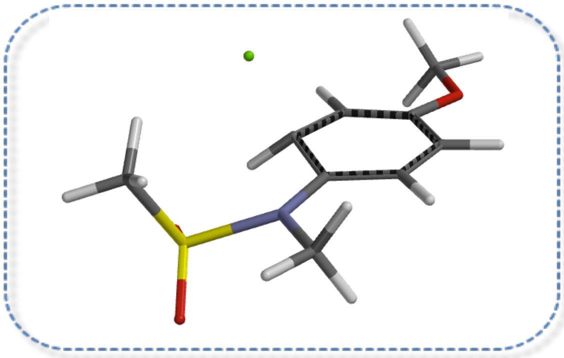
23	O	O1	-0.2093649	3.2782563	2.1253293
24	C	C7	-0.6037831	4.4855130	1.4921983
25	H	H5	0.0569512	4.7336275	0.6512875
26	H	H6	-0.5255599	5.2625426	2.2545830
27	H	H7	-1.6402669	4.4325923	1.1331282

Cartesian coordinates for geometry minimized *N*-(4-methoxyphenyl)-*N*-methylmethanesulfonamide + Cl cation (7-Cl-1):



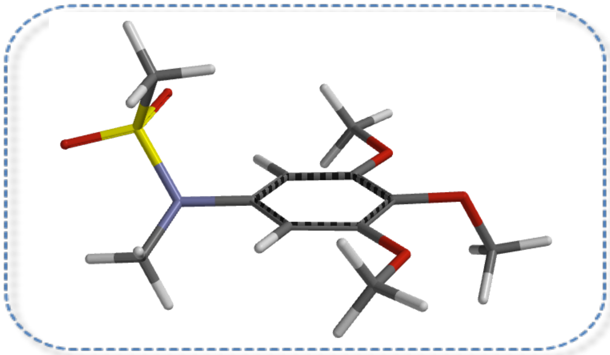
Atom			X	Y	Z
1	H	H1	-1.1679408	0.5393404	-1.6202229
2	C	C1	-0.7071932	0.6233359	-0.6415009
3	C	C4	0.5938769	0.9454410	1.8844954
4	C	C2	-0.1605279	-0.4538131	-0.0349923
5	C	C6	-0.6757176	1.9887666	-0.0350380
6	C	C5	0.0082726	2.0832961	1.3096646
7	C	C3	0.4923162	-0.2733502	1.2515724
8	H	H3	0.9038626	-1.1467847	1.7464521
9	H	H4	1.0860336	1.0455490	2.8458153
10	N	N1	-0.2327809	-1.7339681	-0.6523380
11	S	S1	1.2837435	-2.5734204	-0.7285060
12	C	C8	-1.4212535	-2.5671320	-0.3583811
13	H	H2	-1.4486017	-2.9095966	0.6821118
14	H	H12	-1.4129427	-3.4419995	-1.0106684
15	H	H13	-2.3161982	-1.9823760	-0.5824029
16	O	O2	1.1695434	-3.8118467	0.0372507
17	O	O3	2.2815977	-1.5497212	-0.3886037
18	C	C9	1.4185300	-2.9705831	-2.4755154
19	H	H11	0.5695161	-3.5913106	-2.7678497
20	H	H14	2.3499476	-3.5302390	-2.5933903
21	H	H15	1.4500789	-2.0411476	-3.0452141
22	H	H9	-1.6969950	2.3825780	0.0524142
23	O	O1	0.0497280	3.1756452	2.0069334
24	C	C7	-0.5504572	4.4498204	1.6323065
25	H	H5	0.1334203	4.9750858	0.9663904
26	H	H6	-0.6623669	4.9808296	2.5756889
27	H	H7	-1.5216109	4.2987124	1.1561738
28	Cl	Cl1	0.1841190	3.0888881	-1.2126455

Cartesian coordinates for geometry minimized *N*-(4-methoxyphenyl)-*N*-methylmethanesulfonamide + Cl cation (7-Cl-2):



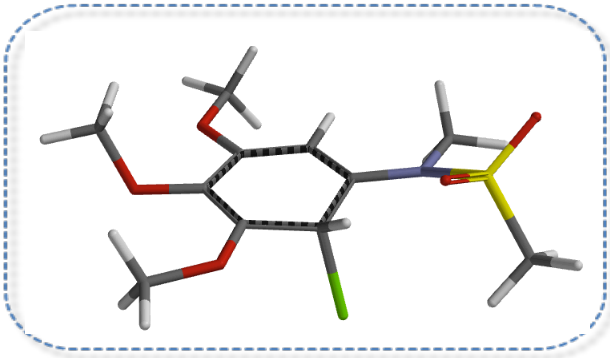
	Atom		X	Y	Z
1	H	H1	0.7545233	0.5200014	-1.4597529
2	C	C1	-0.0171488	0.6432198	-0.7030059
3	C	C4	-0.2950814	1.2157281	2.0530766
4	C	C2	0.0577609	-0.4652841	0.3395080
5	C	C6	-0.0488950	2.0403395	-0.2017802
6	C	C5	-0.1979156	2.3151498	1.1178931
7	C	C3	-0.1857158	-0.0996765	1.6977841
8	H	H3	-0.2395970	-0.8544463	2.4698079
9	H	H4	-0.4455950	1.4789221	3.0969806
10	N	N1	0.2818921	-1.7366073	0.0086877
11	S	S1	1.0417889	-2.3347658	-1.5918841
12	C	C8	0.1865904	-2.8096704	1.0275572
13	H	H2	0.9900449	-2.7123523	1.7627925
14	H	H12	0.2946411	-3.7766796	0.5418474
15	H	H13	-0.7893717	-2.7567642	1.5143265
16	O	O2	1.9001411	-3.4131185	-1.1385160
17	O	O3	1.5596151	-1.1591264	-2.2712309
18	C	C9	-0.3869241	-2.9984357	-2.4562879
19	H	H11	-0.8553384	-3.7604173	-1.8312377
20	H	H14	0.0140180	-3.4519453	-3.3680495
21	H	H15	-1.0684675	-2.1809029	-2.6904622
22	H	H9	0.0142887	2.8116955	-0.9591045
23	O	O1	-0.2622823	3.5162128	1.7088567
24	C	C7	-0.1872241	4.6844471	0.8791927
25	H	H5	0.7691045	4.7145086	0.3449722
26	H	H6	-0.2587461	5.5313609	1.5600164
27	H	H7	-1.0198338	4.7053353	0.1672088
28	Cl	Cl1	-1.6062723	0.3332715	-1.6191967

Cartesian coordinates for geometry minimized *N*-methyl-*N*-(3,4,5-trimethoxyphenyl)methanesulfonamide:



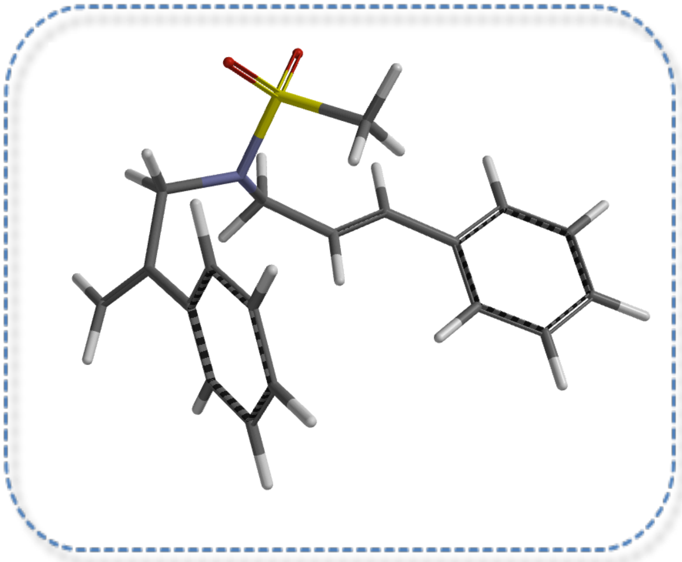
Atom			X	Y	Z
1	C	C1	-1.0309926	-0.1353219	1.3399131
2	C	C4	1.2672646	-0.2438739	-0.2635019
3	C	C2	0.2375798	-0.1321330	1.9427107
4	C	C6	-1.1547915	-0.1516611	-0.0556783
5	C	C5	-0.0017465	-0.2103991	-0.8502877
6	C	C3	1.3836172	-0.1881716	1.1293493
7	H	H6	-2.1333625	-0.1301962	-0.5156833
8	O	O1	-2.0863011	-0.1074981	2.2031059
9	C	C7	-3.3959952	-0.0835119	1.6622379
10	H	H5	-3.5647534	0.8124029	1.0494296
11	H	H8	-4.0714074	-0.0639328	2.5194953
12	H	H9	-3.6033941	-0.9772719	1.0579932
13	O	O2	0.3476819	-0.0293952	3.3049787
14	C	C8	0.5303604	-1.2732688	3.9835550
15	H	H3	-0.3256224	-1.9401431	3.8189956
16	H	H4	0.6017975	-1.0324363	5.0469483
17	H	H7	1.4531692	-1.7686339	3.6598364
18	H	H12	2.1360535	-0.3046660	-0.9015499
19	O	O3	2.5705937	-0.2044372	1.7957345
20	C	C9	3.7687652	-0.2124201	1.0303176
21	H	H1	3.8605057	-1.1293497	0.4338031
22	H	H10	4.5825460	-0.1705282	1.7563869
23	H	H11	3.8254452	0.6572571	0.3645174
24	N	N1	-0.1141312	-0.2770905	-2.2810391
25	C	C10	-1.2980093	-0.9250009	-2.8606351
26	H	H2	-1.1011638	-1.1416912	-3.9093918
27	H	H14	-2.2127137	-0.3170400	-2.7910372
28	H	H15	-1.4578432	-1.8614691	-2.3210899
29	S	S1	0.5770077	0.9726944	-3.2100336
30	O	O4	0.2609094	0.6636564	-4.6058365
31	O	O5	1.9615227	1.1592723	-2.7768471
32	C	C11	-0.3295774	2.4691429	-2.7488351
33	H	H16	0.1200532	3.2962346	-3.3025786
34	H	H18	-0.2250918	2.6290482	-1.6742912
35	H	H19	-1.3779757	2.3518328	-3.0309924

Cartesian coordinates for geometry minimized *N*-methyl-*N*-(3,4,5-trimethoxyphenyl)methanesulfonamide + Cl cation:



	Atom	X	Y	Z
1	C	-0.138405	1.082979	1.305737
2	C	-0.340888	-1.137890	-0.432317
3	C	-0.233881	-0.220594	1.906811
4	C	-0.003333	1.300556	-0.086200
5	C	-0.006754	0.239999	-0.971432
6	C	-0.312871	-1.304612	1.067177
7	H	0.169988	2.306836	-0.435328
8	O	-0.136328	2.066960	2.181463
9	C	-0.076789	3.451629	1.775274
10	H	0.877992	3.664001	1.286200
11	H	-0.154226	4.017311	2.702239
12	H	-0.916787	3.690375	1.117889
13	O	-0.326434	-0.333941	3.261283
14	C	0.888728	-0.121459	4.010964
15	H	1.648936	-0.859964	3.730307
16	H	0.612188	-0.253388	5.057248
17	H	1.275079	0.889413	3.858424
18	O	-0.406258	-2.584299	1.370218
19	C	-0.616412	-3.090793	2.713036
20	H	0.274392	-2.928774	3.322122
21	H	-0.786580	-4.156939	2.569003
22	H	-1.485142	-2.615119	3.166789
23	N	0.156790	0.426542	-2.312556
24	C	0.165627	1.799552	-2.854713
25	H	0.130623	1.759667	-3.941817
26	H	1.074295	2.338836	-2.567688
27	H	-0.721019	2.323165	-2.489781
28	S	0.883255	-0.790652	-3.424970
29	O	1.363667	-1.889502	-2.595545
30	O	1.780538	-0.009760	-4.260439
31	C	-0.530337	-1.326943	-4.396542
32	H	-0.133603	-2.033737	-5.130623
33	H	-0.961701	-0.461553	-4.902453
34	H	-1.252046	-1.809942	-3.737307
35	Cl	-2.048707	-1.519402	-0.986314
36	H	0.286395	-1.908558	-0.876161

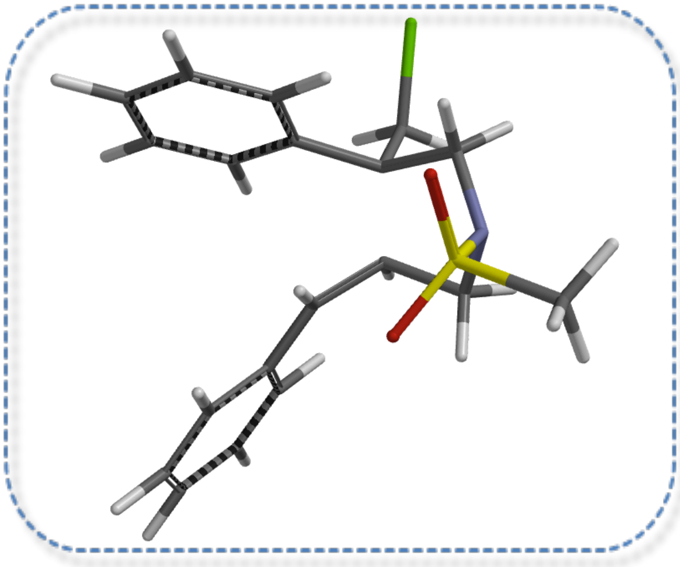
Cartesian coordinates for geometry minimized *N*-cinnamyl-*N*-(2-phenylallyl)methanesulfonamide (9):



	Atom	X	Y	Z
1	H	-3.566164	-1.288921	0.001150
2	C	-3.086618	-1.326162	-0.972973
3	C	-1.823591	-1.353055	-3.451814
4	C	-1.937901	-2.118310	-1.141664
5	C	-3.602261	-0.570975	-2.025066
6	C	-2.974204	-0.583002	-3.271561
7	C	-1.306663	-2.107323	-2.398482
8	H	-4.490656	0.035172	-1.867224
9	H	-3.372990	0.007050	-4.092311
10	H	-0.411133	-2.699010	-2.563266
11	H	-1.326074	-1.371414	-4.418072
12	C	-1.415929	-2.944957	-0.020240
13	C	-2.227222	-3.513929	0.885049
14	H	-1.830236	-4.094874	1.713473
15	H	-3.308773	-3.446626	0.815148
16	C	0.082527	-3.161655	0.076511
17	H	0.304048	-3.798152	0.944391
18	H	0.459573	-3.686248	-0.803156
19	N	0.809548	-1.879215	0.170155
20	S	2.285718	-1.758489	-0.665970
21	C	2.104954	-0.236950	-1.614194
22	H	1.969792	0.596333	-0.924302
23	H	1.245919	-0.342398	-2.277913
24	H	3.028173	-0.118284	-2.186659
25	O	3.384012	-1.560137	0.288852
26	O	2.326176	-2.868048	-1.628568
27	C	0.747034	-1.189784	1.481361
28	H	1.641703	-1.405607	2.077861

29	H	-0.114754	-1.631545	1.995444
30	C	0.534340	0.292513	1.352996
31	H	-0.358485	0.586037	0.802006
32	C	1.366034	1.209648	1.871360
33	H	2.260836	0.849856	2.380749
34	C	1.231407	2.673482	1.816384
35	C	1.089923	5.489955	1.730388
36	C	2.293879	3.468520	2.280515
37	C	0.088644	3.325155	1.315493
38	C	0.021047	4.714377	1.271066
39	C	2.226977	4.860312	2.237305
40	H	3.183920	2.983041	2.674337
41	H	-0.757536	2.740971	0.965341
42	H	-0.871490	5.196276	0.880396
43	H	3.063473	5.451864	2.599836
44	H	1.033023	6.574508	1.695870

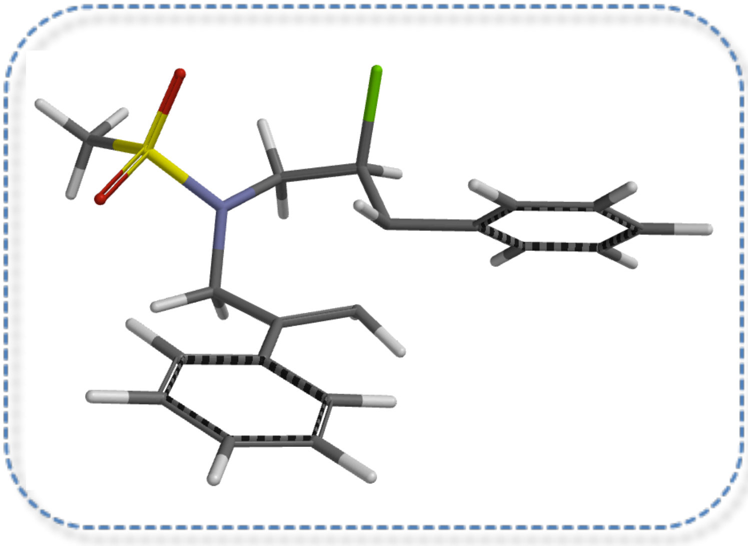
Cartesian coordinates for geometry minimized *N*-cinnamyl-*N*-(2-phenylallyl)methanesulfonamide + Cl cation (11):



Atom	X	Y	Z
1 H H1	0.4549913	2.0183789	1.7077815
2 C C1	0.5066882	1.0313050	2.1604949
3 C C4	0.6975914	-1.4359402	3.4106276
4 C C2	1.1993595	-0.0113499	1.5084218
5 C C6	-0.0786043	0.8433627	3.4143703
6 C C5	0.0158508	-0.3955723	4.0451046
7 C C3	1.2847970	-1.2487676	2.1561092
8 H H6	-0.5923547	1.6691832	3.8978753
9 H H5	-0.4308388	-0.5502060	5.0225903
10 H H3	1.7824480	-2.0921076	1.6947347
11 H H4	0.7759200	-2.4067240	3.8910208

12	C	C7	1.7851769	0.2794130	0.1099132
13	C	C8	2.8139646	1.4281692	0.1885687
14	C	C9	2.4345817	-0.9373404	-0.6425019
15	H	H2	3.3671011	-0.6085093	-1.1123530
16	H	H10	2.6765158	-1.7876940	-0.0128273
17	N	N1	1.5130468	-1.3435279	-1.7137435
18	C	C10	0.8269234	-0.1459969	-2.1619329
19	H	H12	-0.0960951	-0.3784577	-2.6949177
20	H	H13	1.4837303	0.4176882	-2.8350368
21	S	S1	0.5769296	-2.7702330	-1.4858747
22	O	O1	1.1976880	-3.5179864	-0.3930321
23	O	O2	-0.8447235	-2.3823087	-1.4216509
24	C	C11	0.8465008	-3.6522302	-3.0259219
25	H	H9	1.9115313	-3.8709640	-3.1142946
26	H	H16	0.4989974	-3.0365016	-3.8574062
27	H	H17	0.2646101	-4.5753398	-2.9670175
28	Cl	Cl1	4.2727823	0.9555377	1.1415987
29	H	H7	3.1647131	1.7030058	-0.8104295
30	H	H8	2.3999105	2.3137482	0.6722100
31	C	C12	0.6120050	0.7374592	-0.8630435
32	C	C13	-0.7222052	0.4169234	-0.3143275
33	C	C14	-1.8931821	1.1946979	-0.3583255
34	C	C15	-4.3173697	2.5869618	-0.4463631
35	C	C16	-3.1117917	0.5640554	0.0392914
36	C	C17	-1.9296688	2.5524898	-0.7973009
37	C	C18	-3.1308509	3.2333717	-0.8384861
38	C	C19	-4.3094075	1.2550129	-0.0094144
39	H	H11	-3.0830762	-0.4712906	0.3664428
40	H	H18	-1.0151519	3.0569078	-1.0910547
41	H	H19	-3.1635573	4.2663023	-1.1693814
42	H	H20	-5.2349387	0.7720893	0.2859926
43	H	H21	-5.2563291	3.1322903	-0.4824387
44	H	H14	0.6980765	1.7942684	-1.1269414
45	H	H15	-0.8522859	-0.6035739	0.0328690

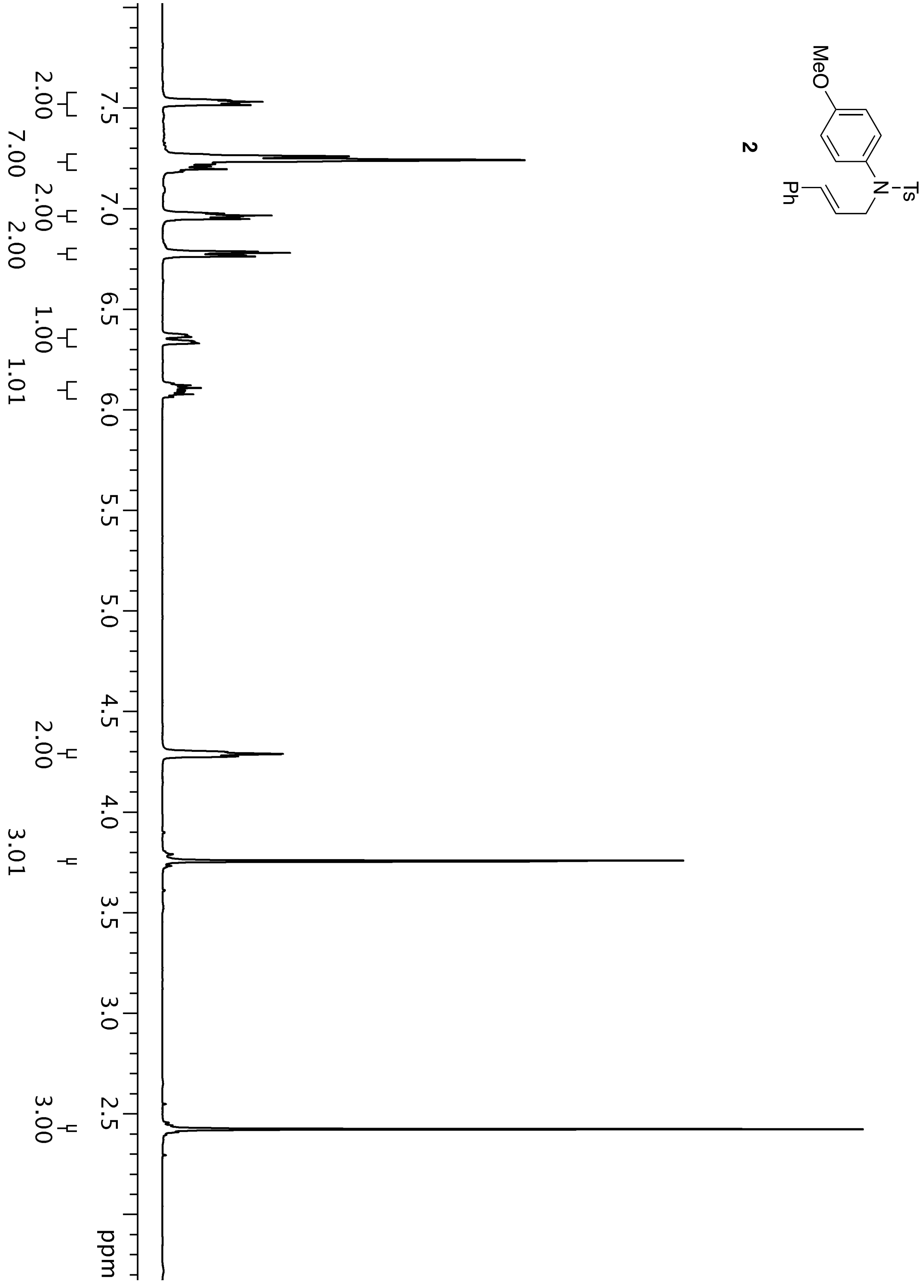
Cartesian coordinates for geometry minimized *N*-cinnamyl-*N*-(2-phenylallyl)methanesulfonamide + Cl cation (11'):



	Atom		X	Y	Z
1	H	H1	-3.2829057	-1.2992582	1.4088336
2	C	C1	-3.1287234	-0.3289719	1.8773291
3	C	C4	-2.7785524	2.1528531	3.1025715
4	C	C2	-1.8923738	0.3259241	1.7693848
5	C	C6	-4.1749707	0.2482735	2.5937201
6	C	C5	-4.0023543	1.4919498	3.2084540
7	C	C3	-1.7317067	1.5755984	2.3822455
8	H	H6	-5.1239514	-0.2734148	2.6760318
9	H	H5	-4.8178121	1.9395918	3.7686355
10	H	H3	-0.7748707	2.0877958	2.3175731
11	H	H4	-2.6333389	3.1150808	3.5848418
12	C	C7	-0.7417111	-0.2802080	0.9891320
13	C	C8	-0.2601987	-1.6293813	1.5575898
14	C	C9	0.6602368	-2.4782880	0.6392513
15	H	H2	1.3005567	-3.0881135	1.2791047
16	H	H10	0.0261732	-3.1684705	0.0640496
17	N	N1	1.4870992	-1.7366961	-0.3134464
18	C	C10	0.9089934	-1.3860597	-1.6110930
19	H	H12	0.2885380	-2.2112378	-1.9902566
20	H	H13	1.7032570	-1.2086742	-2.3301670
21	S	S1	3.1875234	-1.6542560	-0.1189567
22	O	O1	3.6323624	-0.7031560	-1.1422493
23	O	O2	3.4375913	-1.4547759	1.2995091
24	C	C11	3.8006000	-3.2879854	-0.5819418
25	H	H9	3.5274466	-3.4943721	-1.6184087
26	H	H16	3.3884834	-4.0361355	0.0976473
27	H	H17	4.8879798	-3.2509778	-0.4779862
28	Cl	Cl1	0.5478180	-1.3038265	3.1501563
29	H	H8	-1.1241145	-2.2515945	1.8055946

30	C	C12	0.0226030	-0.1709775	-1.4061625
31	C	C13	-1.1648650	-0.4211315	-0.5586246
32	C	C14	0.3592331	1.1164985	-1.8903380
33	C	C15	1.0165054	3.6771755	-2.8664472
34	C	C16	-0.5651384	2.2097330	-1.7909891
35	C	C17	1.6359519	1.3764363	-2.4898543
36	C	C18	1.9509414	2.6376679	-2.9623704
37	C	C19	-0.2398920	3.4598021	-2.2768567
38	H	H14	-1.5440470	2.0644575	-1.3516639
39	H	H18	2.3983170	0.6083964	-2.5087901
40	H	H19	2.9283056	2.8222721	-3.3957091
41	H	H20	-0.9554010	4.2725332	-2.2072737
42	H	H21	1.2676636	4.6637969	-3.2456570
43	H	H15	-1.5636142	-1.4257587	-0.7305025
44	H	H11	-1.9684687	0.2874998	-0.7407650
45	H	H7	0.1048300	0.4103848	1.0348538

VI. NMR spectra



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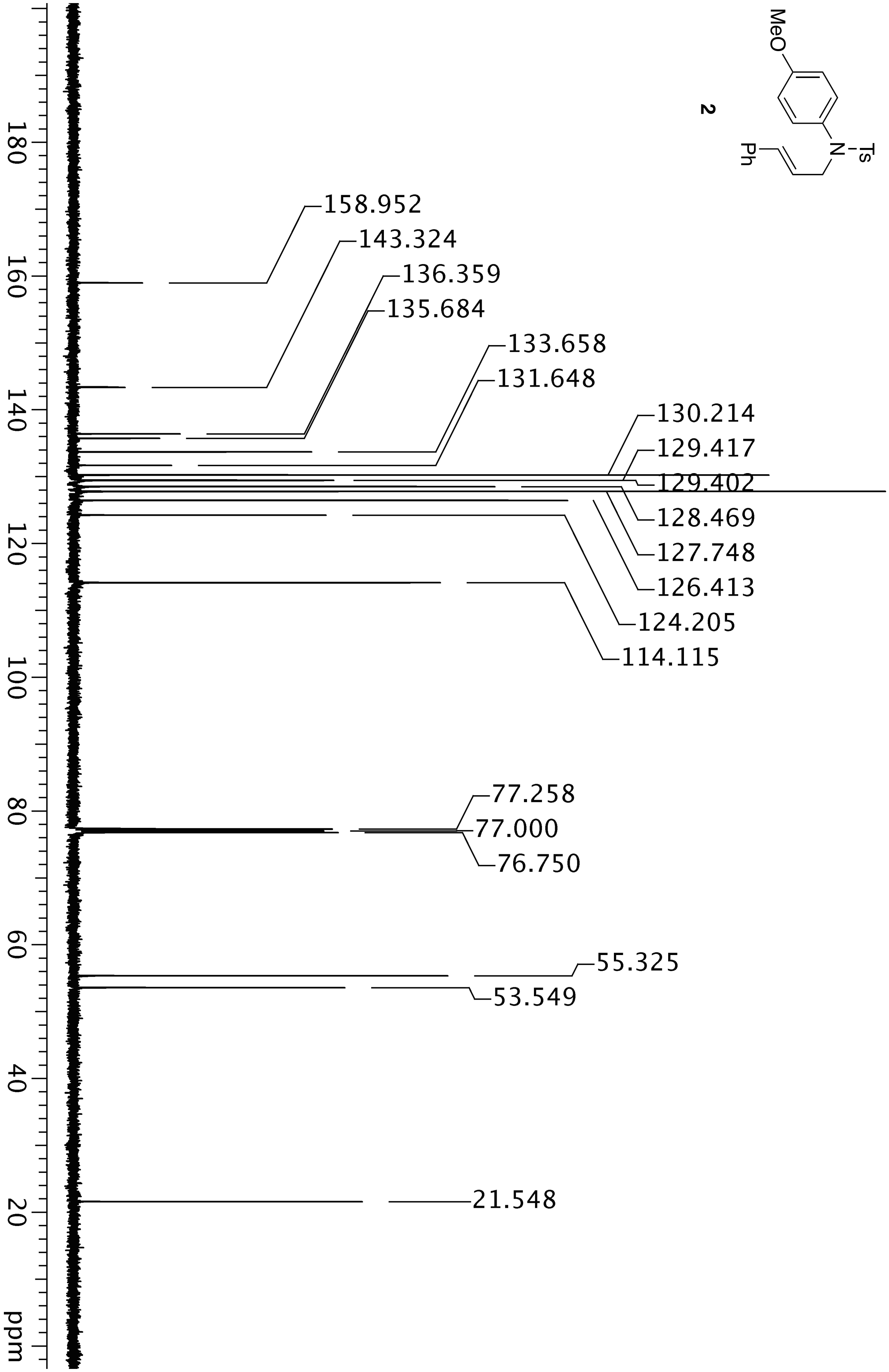
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127.748
126.413
124.205
114.115
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77.000
76.750
55.325
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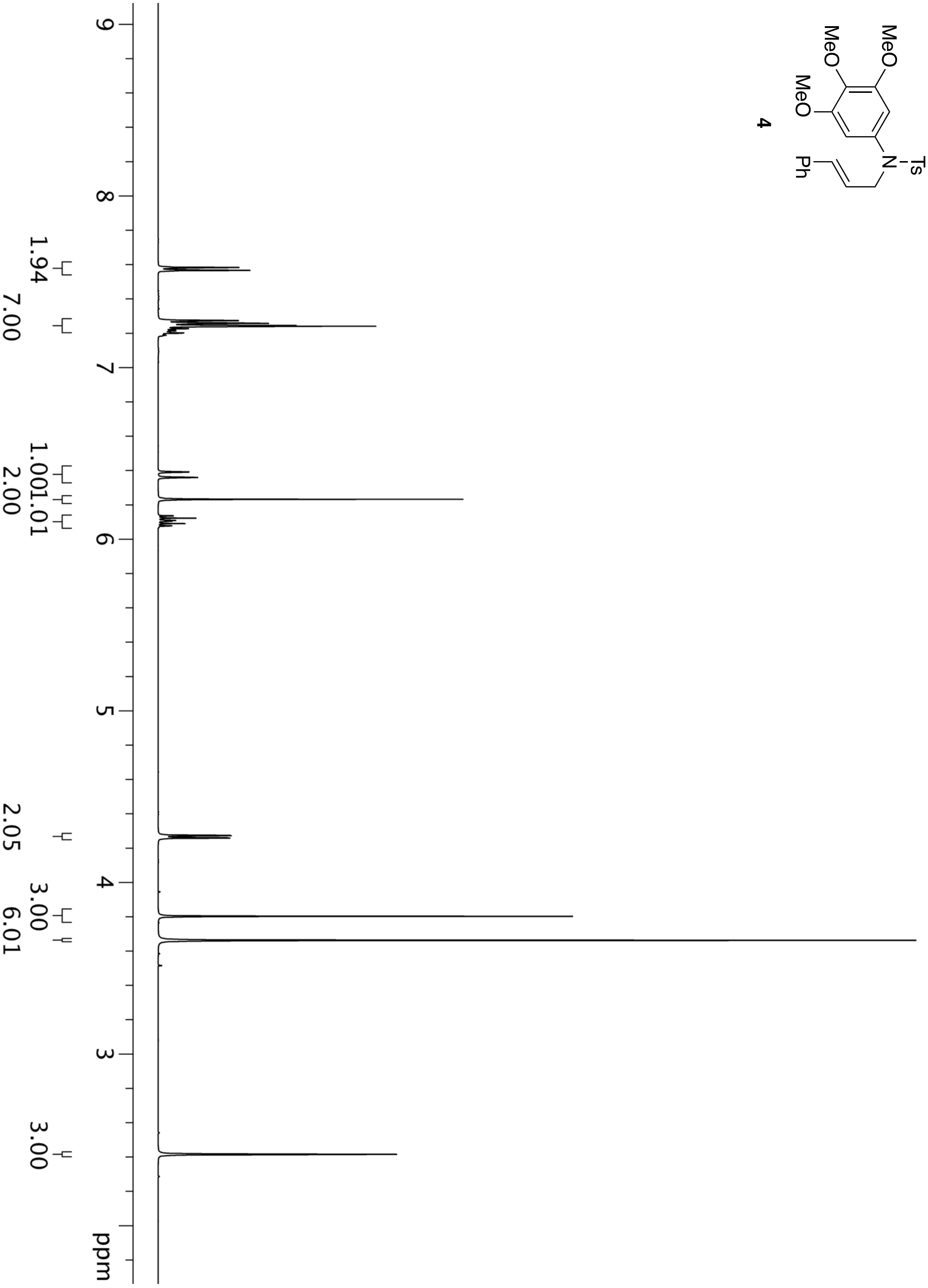
140
120
100
80
60
40
20
ppm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MeO
MeO
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Ts
Ph
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8
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2.00
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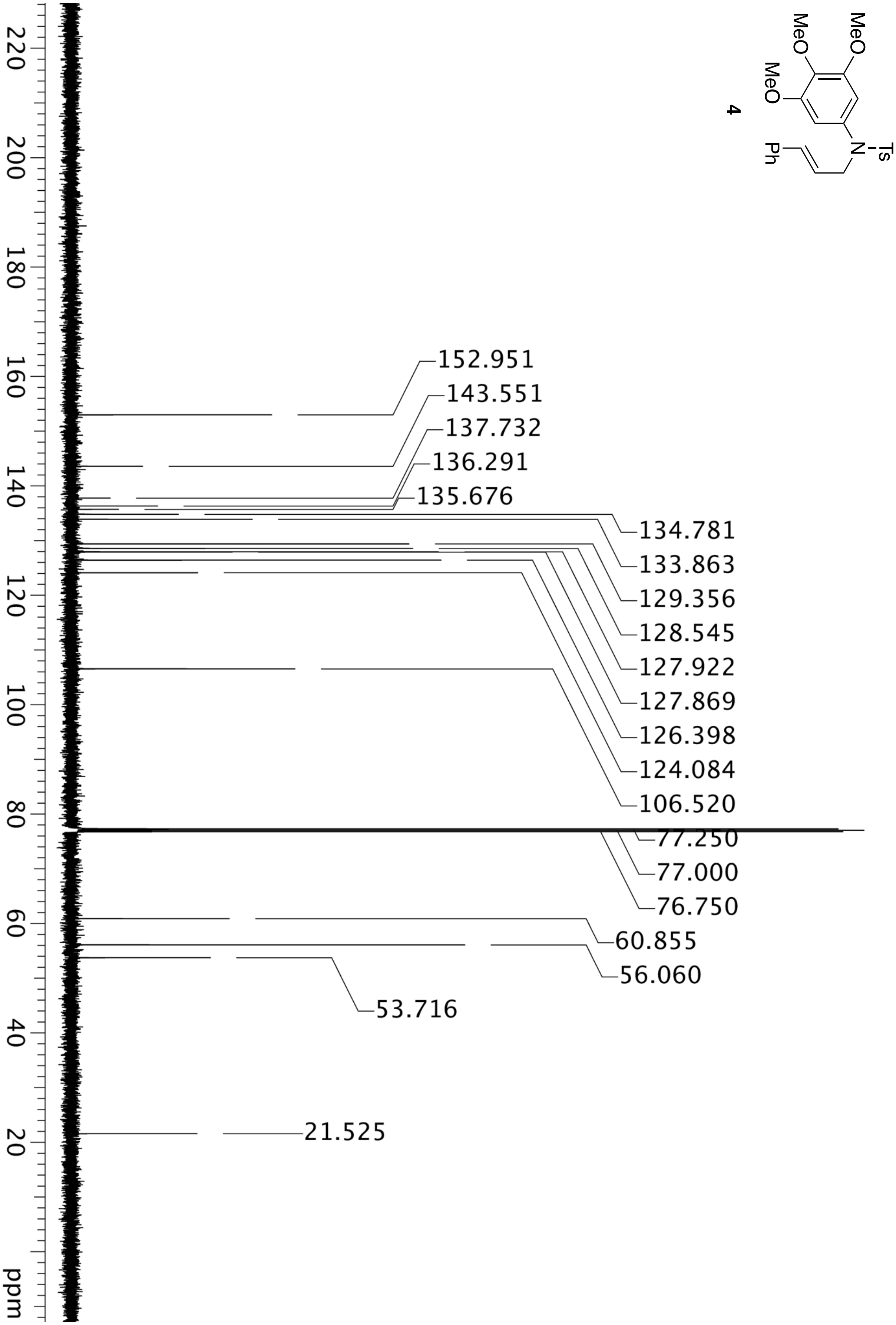
3.00
6.01
3.00

4


4
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MeO
MeO
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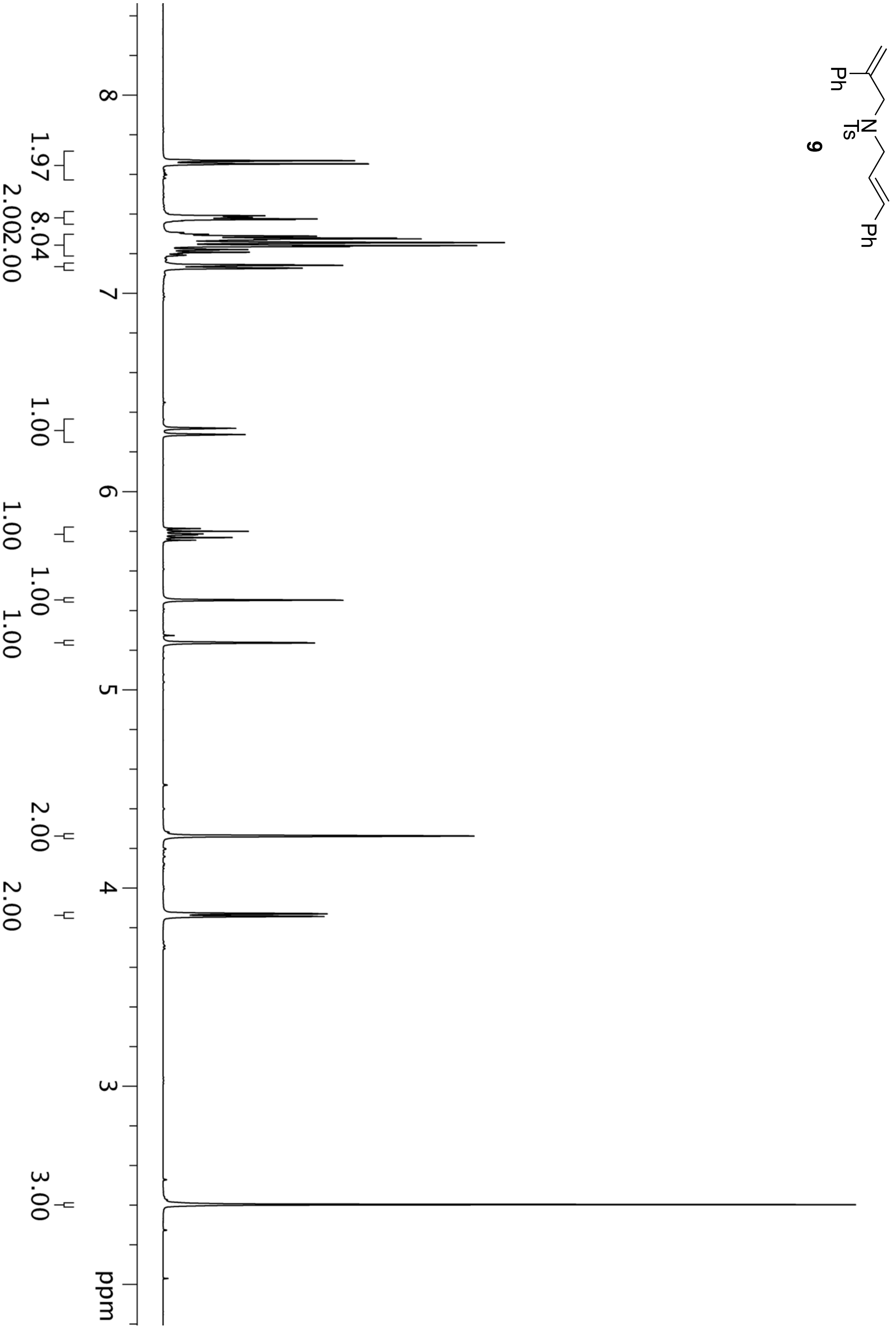
129.356
128.545
127.922
127.869
126.398
124.084
106.520
77.250
77.000
76.750
60.855
56.060
53.716
21.525
220
200
180
160
140
120
100
80
60
40
20
ppm


Ph
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Ts
Ph
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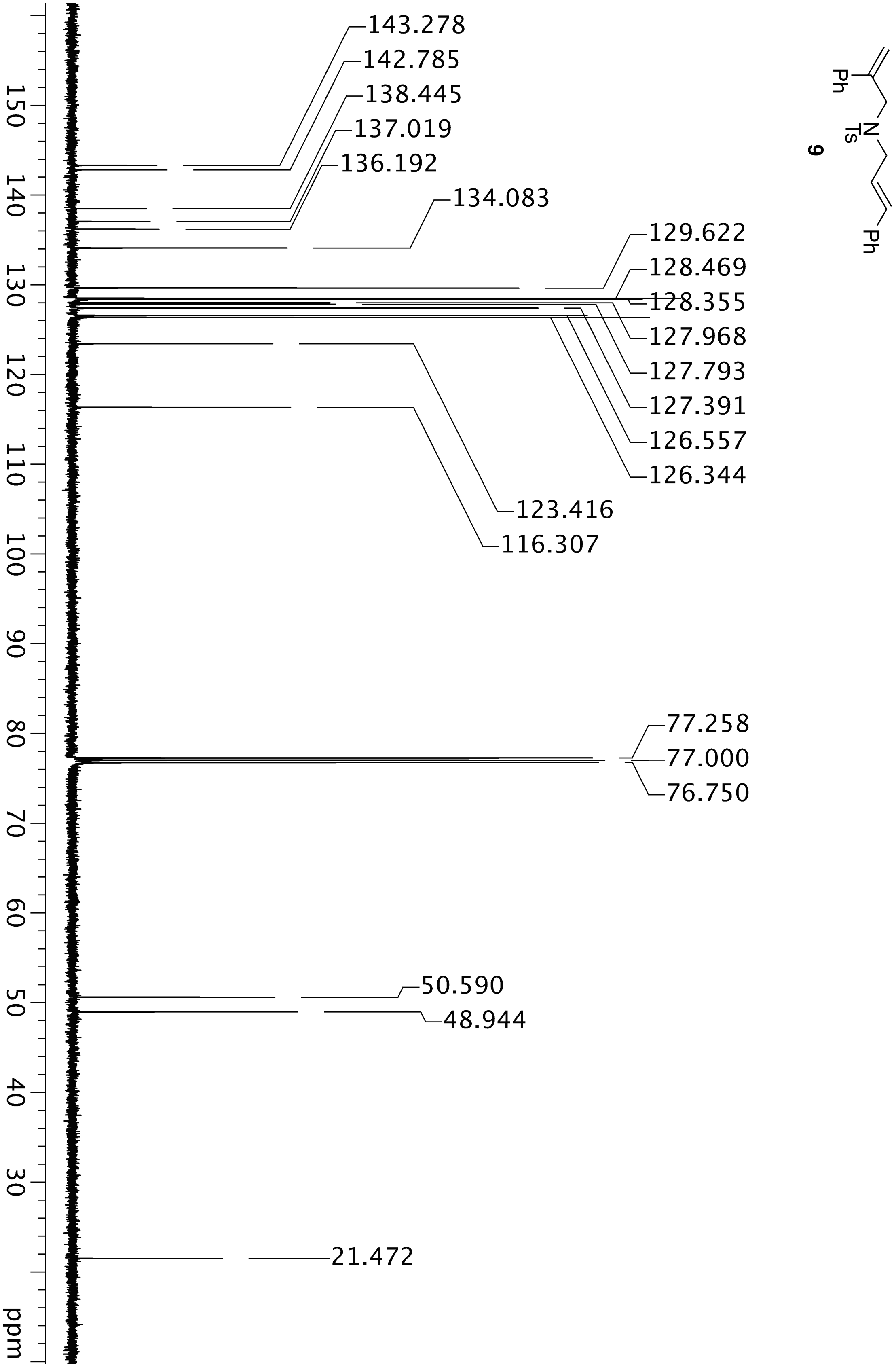
2.00
2.00
3.00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134.083
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128.469
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127.793
127.391
126.557
126.344
123.416
116.307
77.258
77.000
76.750
50.590
48.944
21.472
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm
Ph
N
Ts
Ph
9

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