Supporting Information for:

Singlet oxygen formation vs. photodissociation for light-responsive protic ruthenium anticancer compounds: The oxygenated substituent determines which pathway dominates

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Cellular Studies with 3_A

Experimental Details for Cellular Studies - Breast cancer cell lines MCF7 and MDA-MB-231 (ATCC, Manassas, VA) were cultured in Dulbecco's Modified Eagle's Medium (Gibco, Grand Island, NY) supplemented with 10% fetal bovine serum (Gibco) and 1X penicillin-streptomycin (Corning, Manassas, VA). Cells were treated with 5 μM **3_A** without (dark control) or with blue light irradiation as previously published (using Philips goLITE BLU with broad band blue light centered at 450 nm).[1-2] Singlet oxygen production in cells were measured using Singlet Oxygen Sensor Green (SOSG; Invitrogen, Carsbad, CA) as previously published (n = 3).[3] SOSG luminescence was visualized in using C2+ confocal microscope (Nikon). Late apoptosis was detected using Annexin V and propidium iodide (PI) (FITC Annexin V Apoptosis Kit I; BD Biosciences, San Jose, CA; n = 3) according to manufacturer's protocol. Reactive oxygen species (ROS) production was measured using Total ROS Detection Kit according to manufacturer's protocol (Enzo Life Sciences, Farmingdale, NY; n = 3). Total ROS in cells were measured after irradiation with blue light (sublethal dose). As positive control for ROS detection, cells were treated with 200 μM pyocyanin for 20 min. SOSG, apoptosis, and total ROS were measured quantitatively in Accuri C6 flow cytometer (BD Biosciences). See Figures 1 and 2 in the main text and S1 and S2 below.

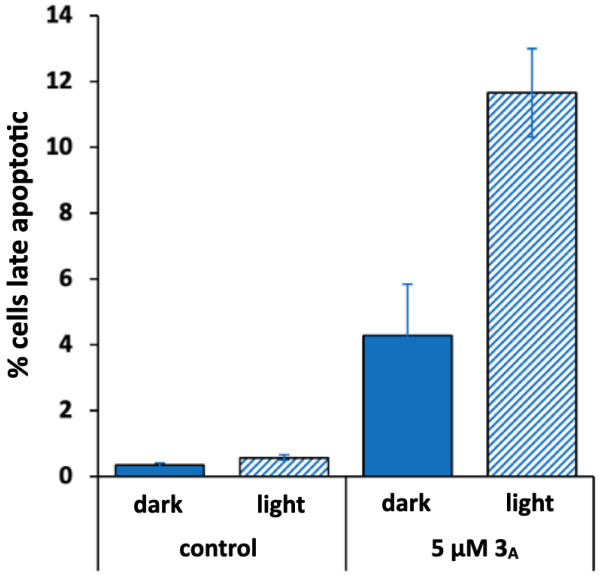


Figure S1. Apoptosis indicators in MDA-MB-231 as measured by Annexin V^+/PI^+. The control uses no ruthenium complex.

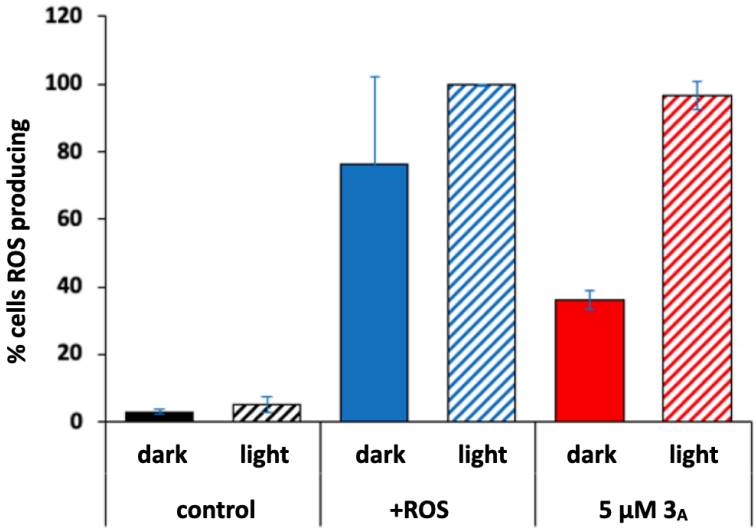


Figure S2. ROS indicators in MDA-MB-231. +ROS is the pyocyanin positive control as an ROS inducer. For both plots, *solid bars* indicate incubation with no ruthenium compound (control), positive control, or $\mathbf{3_A}$ for 48 h in the *dark*. *Striped bars* indicate incubation followed by irradiation with *blue light*.

General Synthetic and Characterization Methods

Complexes $\mathbf{1_A}$, $\mathbf{2_A}$, $\mathbf{3_A}$, **4** and **5** were prepared according to previously published procedures.[1-2, 4] NMR spectra were recorded in a Bruker AVANCE 360 (360 MHz, ^{1}H frequency) or AVANCE 500 (500MHz, ^{1}H frequency) NMR spectrometer. FT-IR spectra were recorded on a Bruker Alpha ATR-IR spectrophotometer. Mass spectra were obtained in a Waters AutoSpec-Ultima NT mass spectrometer or Waters Xero G2-XS QTOF. UV-Vis spectra were recorded with an Ocean Optics FLAME-CHEM-UV-VIS or a Perkin Elmer Lambda 35 instrument using a quartz cuvette of 1 cm path length under ambient atmosphere.

Typical synthesis of the deprotonated complexes ($\mathbf{X_B}$ = $\mathbf{1_B}$, $\mathbf{2_B}$, $\mathbf{3_B}$)

While protected from light, approximately 10-20 mg of the $\mathbf{X_A}$ complex ($\mathbf{1_A}$, $\mathbf{2_A}$, or $\mathbf{3_A}$) was dissolved in a minimum amount of MeOH before adding an excess of NaOH (approximately 4-5 drops of 5M $NaOH_{(aq)}$) until a color change from red-orange to darker purple was observed. The methanol solution was then recrystallized via vapor diffusion with diethyl ether to yield crystals of $\mathbf{X_B}$. The solid was collected by filtration and washed with diethyl ether before drying completely under vacuum. Typical yield was 90%. Purity and identity of the samples was confirmed by ^{1}H NMR, UV-Vis, ESI-MS, and IR.

Characterization Data for 2_B and 3_B

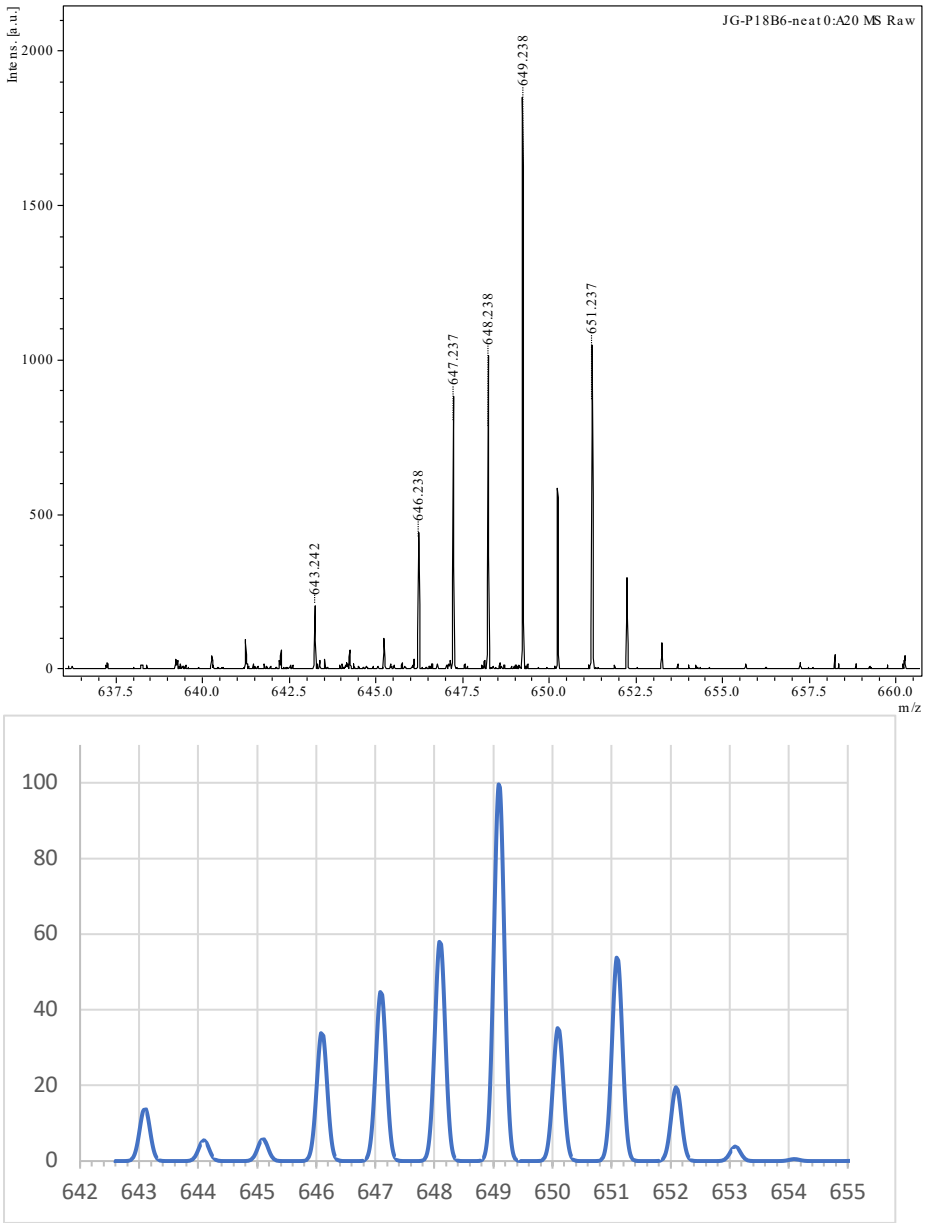


Figure S3. Experimental (top) and simulated (bottom) ESI-MS data for $\mathbf{2_B}$. The ion shown is $[\mathbf{2B}+H^+]^+ = [C_{34}H_{23}N_6O_2Ru]^+$.

UV-Vis Sample Preparation for 2_B: A sample (0.500 mg) of the isolated $\mathbf{2_B}$ was diluted with 5.00 mL MeOH for a concentration of 154 μM. The molar absorptivity for $\mathbf{2_B}$ was measured at ε_{363} = 12,200 $Lmol^{-1}cm^{-1}$ in MeOH. Therefore, as shown in Figure S4, with A_{363} = 1.884 this complex is of similar purity to other samples made by us previously.

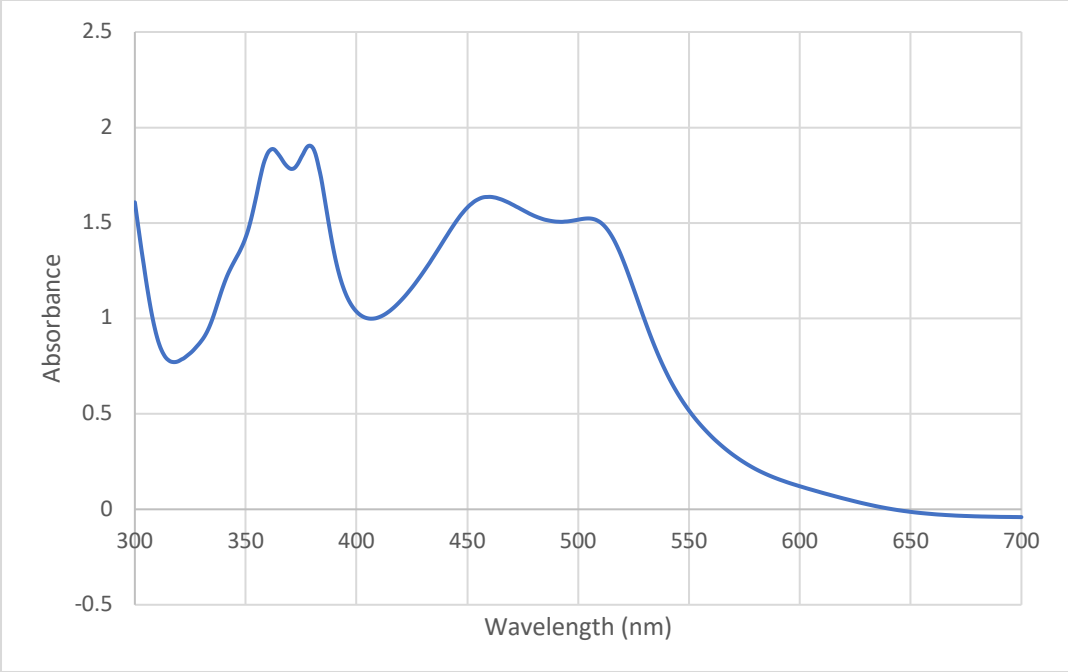


Figure S4. UV-Vis spectrum of $\mathbf{2_B}$ in MeOH.

IR Spectroscopy

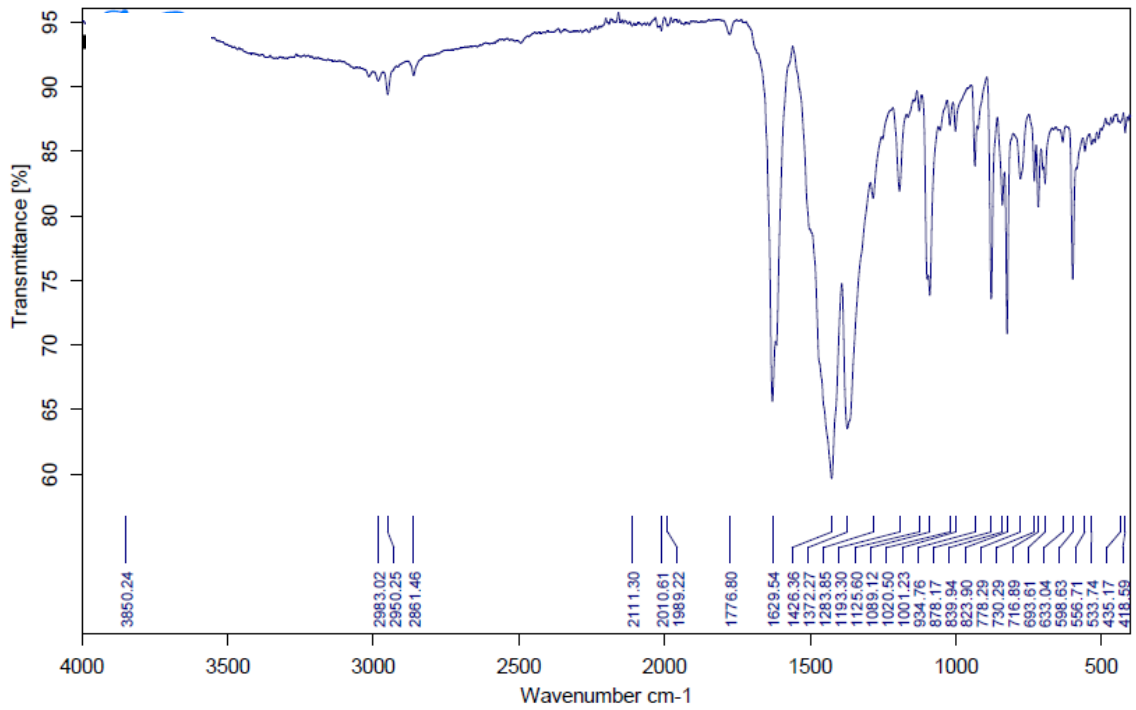


Figure S5. ATR IR spectrum of $\mathbf{2_B}$. The peak at 1630 cm^{-1} shows the C=O bond of the deprotonated ligand. This peak is absent for $\mathbf{2_A}$.

UV-Vis Sample Preparation for 3_B: A sample (0.500 mg) of the isolated $\mathbf{3_B}$ was diluted with 9.30 mL MeOH for a concentration of 70.3 μM. The molar absorptivity was measured at ε_{341} = 15,500 $Lmol^{-1}cm^{-1}$ in MeOH. Therefore, as shown in Figure S6, with A_{341} = 1.0787 this complex is of similar purity to other samples made by us previously.

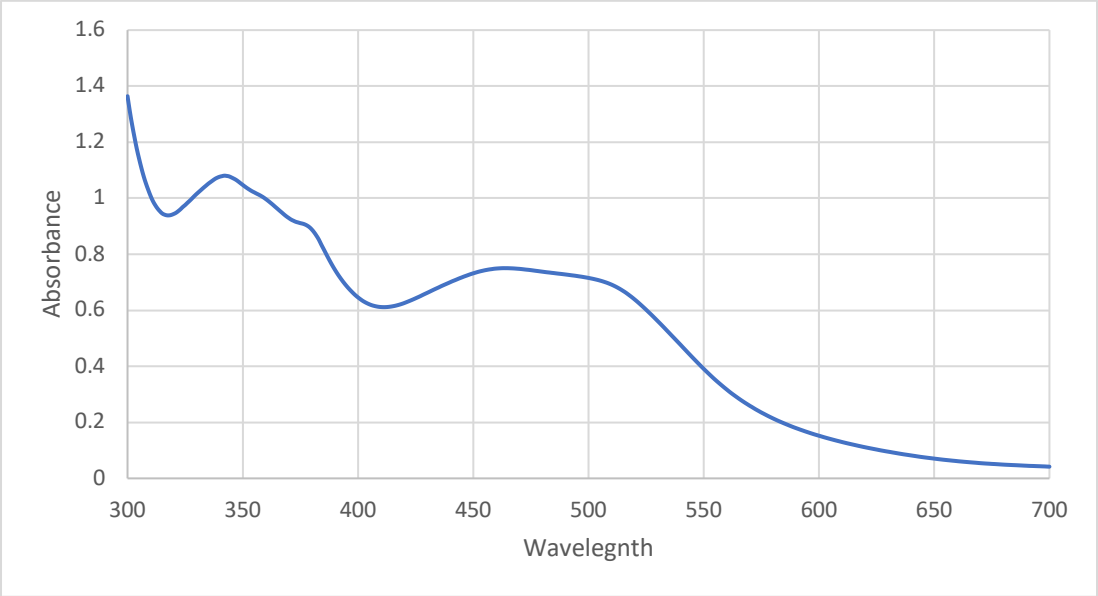


Figure S6. UV-Vis spectrum of $\mathbf{3_B}$ in MeOH.

Singlet Oxygen Quantum Yield Measurements

Singlet oxygen quantum yields (Φ_Δ) were measured by the emissive actinometric method that has worked well in the past with other polypyridyl-type Ru(II) complexes.[5-7] A PTI Quantamaster spectrometer equipped with a Hamamatsu R5509-42 near-infrared detector (cooled to −80 °C) was used to measure the intensity of the $^1O_2$ emission that occurs at around 1276 nm. The quantum yield was calculated by the relative actinometric method in Equation 1, using $[Ru(bpy)_3](PF_6)_2$ as the standard (Φ_Δ = 0.56 in aerated MeCN)[8]

$$\Phi_\Delta = \Phi_{\Delta,S}\left(\frac{I}{I_S}\right)\left(\frac{A_S}{A}\right)\left(\frac{\eta^2}{\eta_S^2}\right) \quad (1)$$

where *I* is the emission integration, *A* is the absorption of the solution at the excitation wavelength, and η is the refractive index of the solvent. The standard is indicated by the subscript *S*. The samples were measured in deuterated methanol solution, and the standard in acetonitrile. The excitation wavelength was the longest in the excitation spectrum to maximize the emission at 1276 nm. The emission spectrum was recorded between 1200–1350 nm with a 1000 nm long pass filter, and internally corrected for variations in the illumination source and detector output. The spectra were signal averaged over multiple scans to reduce noise and were baseline corrected.

Computational Methods

All computations were carried out using Revision C.01 of the Gaussian 16[9] suite of programs with default (10^{-8}) SCF convergence criteria. Either the PBE0 functional[10] in conjunction with Grimme's D3 empirical dispersion[11] and Becke-Johnson damping[12] [EMP=GD3BJ] or the B3LYP functional[13-14] were used for all computations. The basis set combinations are defined as follows: BS1 is the Couty and Hall modification[15] (mod-LANL2DZ) to the valence basis set of LANL2DZ+ECP combination for Ru[16] and for C, H, N, and O the 6-31G(d')[17-19] basis sets (the 6-31G(d') basis sets have the d polarization functions taken from the 6-311G(d)[20] basis sets rather than the default value of 0.8[21] for C, N, and O); BS2 is the SDD triple-ζ quality Stuttgart valence (2f,g) basis set with the Stuttgart/Köln quasi-relativistic small core ECP (SDD(2f,g)) for Ru,[22-23] and the jul-cc-pVDZ basis sets for C, H, N, and O [24-25] (the jul- augmentation scheme uses the corresponding aug-cc-pV*X*Z basis but removes the diffuse functions from H and He). Spherical harmonic d functions were used throughout; *i.e.* there are 5 angular basis functions per *d* function. Excited state optimizations were carried out as variational triplets, ^{1}TD-DFT, and ^{3}TD-DFT. Optimizations with TD-DFT were carried out using analytical gradients and the first 3 excitations were solved iteratively [TD(SINGLETS,ROOT=1) or TD(TRIPLETS,ROOT=1)]. All stationary points were confirmed to be minima by an analytical frequency computation at the same level of theory. Free energies used for comparisons were obtained directly from optimizations with either PBE0-D3BJ/BS1 or B3LYP/BS1. Free energies from B3LYP/BS2 single-point computations on B3LYP/BS1 (B3LYP/BS2//B3LYP-BS1) were obtained by applying the thermodynamic corrections from the BS1 geometries to the electronic energies from the BS2. UV-VIS absorption spectra were simulated using TD-DFT[26] single points on the PBE0-D3BJ/BS1 optimized geometries (TD-DFT//PBE0-D3BJ/BS1). To simulate the absorption spectra, the first 30 vertical excitations were solved iteratively [TD(ROOT=1,NSTATES=30)]. Simulated absorption spectra were generated using an in-house Fortran program by convoluting[27] the computed excitation energies and oscillator strengths with a Gaussian line-shape and a broadening of 20 nm. Orbital images were generated in Chemcraft[28] using an isovalue of 0.02.

Comparison to X-Ray Structures

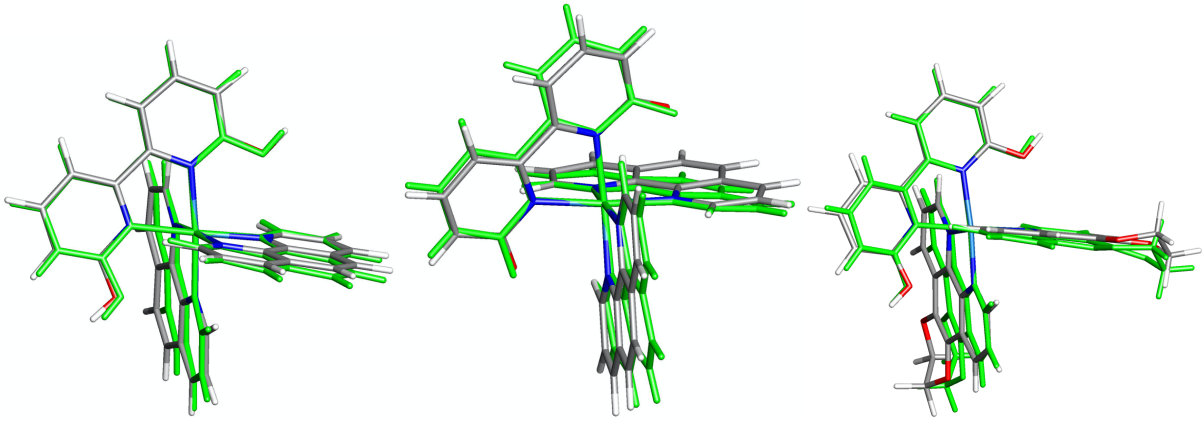


Figure S7: Overlay of experimental crystal structures[2] (green) to PBE0-D3BJ/BS1 optimized geometries ("normal" colors). Structures are matched to the central Ru and the six coordinated N atoms. Complex $\mathbf{2_A}$ is on the left, $\mathbf{2_B}$ is in the middle, and $\mathbf{3_A}$ is on the right.

Both the crystal structure and DFT optimized geometries have distortions in the ligands. These distortions were previously believed to be perhaps influenced to crystal packing forces. However, observing similar distortions in the DFT optimized geometries indicates that these distortions are instead features of these complexes. It should be noted that the crystal structure and DFT geometries do not overlap incredibly well against all heavy atoms see Table S1, indicating that while these distortions are inherently present, crystal packing likely does have an effect.

Table S1: RMSDs (Å) of the DFT optimized geometries from the crystal structure

	All Heavy Atoms	**Ru-N_6**
2A	0.192	0.034
2B	0.357	0.058
3A	0.354	0.060

Relative Energies of Various Computed States

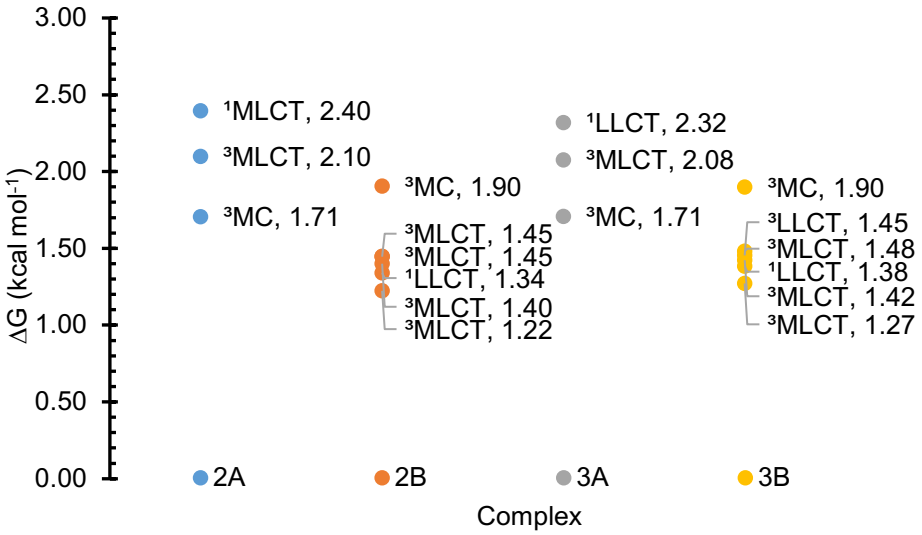


Figure S8: Relative free energies (eV) of the Ru complexes studied from PBE0-D3BJ/BS1.

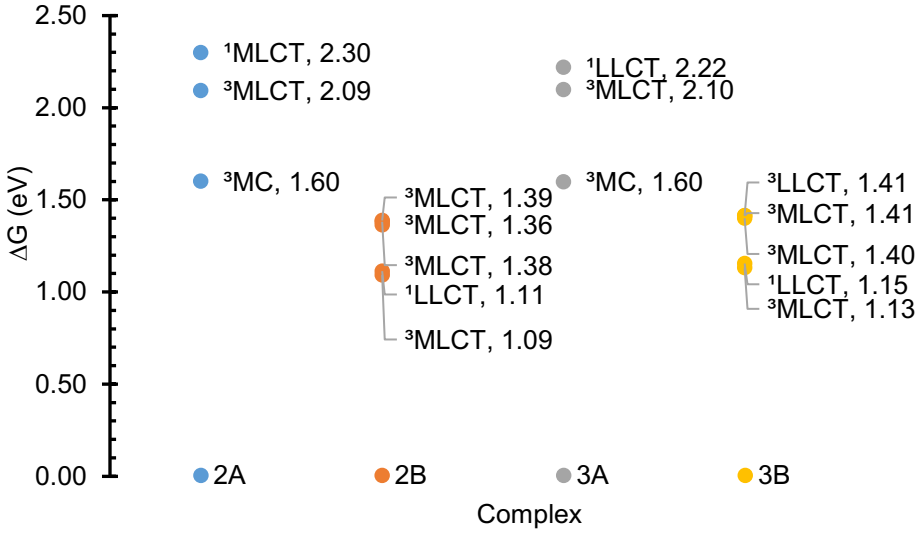


Figure S9: Relative free energies (eV) of the Ru complexes studied from B3LYP/BS1. MC states were not computed for **2B** and **3B** because other states aligned well with the trends from PBE0-D3BJ/BS1.

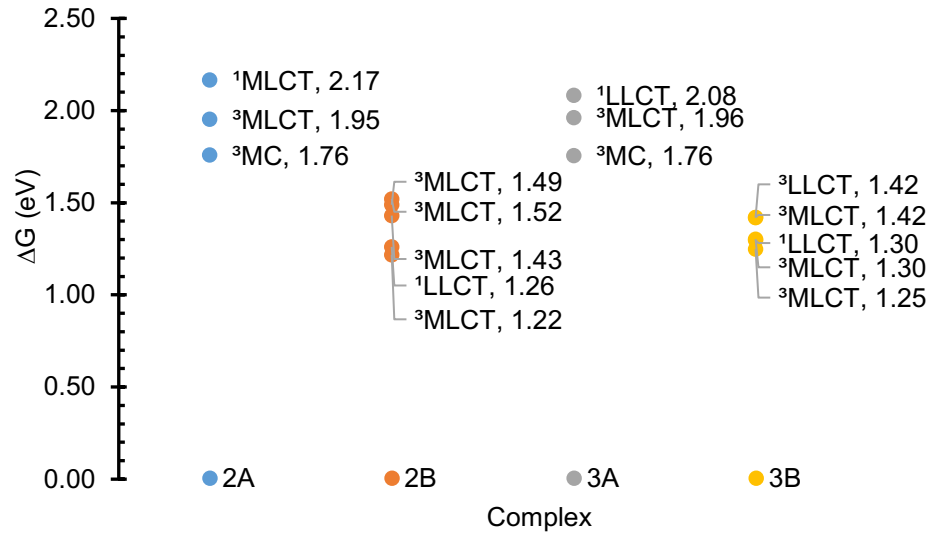


Figure S10: Relative free energies (eV) of the Ru complexes studied from B3LYP/BS2//B3LYP/BS1. Thermodynamic corrections from the B3LYP/BS1 optimizations were applied to the electronic energy of the B3LYP/BS2//B3LYP/BS1 single-point computations. MC states were not computed for **2B** and **3B** because other states aligned well with the trends from PBE0-D3BJ/BS1.

Table S2: Absolute (Hartrees) and relative (eV) electronic (E_{el}) and free (G) energies for the ground and various excited states of each complex from PBE0-D3BJ/BS1.

File Designation	Spin State	Primary Character	E_{el}	G	ΔE_{el}	ΔG
2a						
td-sing--vsing-1001	^{1}TD-^{1}DFT	^{1}MLCT	–1880.60371	–1880.14440	2.46	2.39
td-trip--vsing-1001	^{3}TD-^{1}DFT	^{3}MLCT	–1880.61288	–1880.15536	2.21	2.10
gs-triplet	^{3}DFT	^{3}MC	–1880.62542	–1880.16973	1.87	1.70
gs-singlet	^{1}DFT	^{1}GS	–1880.69421	–1880.23242	0.00	0.00
2b						
td-sing--vsing-1001	^{1}TD-^{1}DFT	^{1}LLCT	–1879.86909	–1879.44035	1.49	1.34
td-sing--vtrip-1001	^{1}TD-^{3}DFT	^{3}LMCT	–1879.86733	–1879.43641	1.54	1.45
td-trip--vsing-1001	^{3}TD-^{1}DFT	^{3}MLCT	–1879.87549	–1879.44459	1.31	1.22
td-trip--vtrip-1001	^{3}TD-^{3}DFT	^{3}LMCT	–1879.86653	–1879.43645	1.56	1.44
gs-triplet-mc	^{3}DFT	^{3}MC	–1879.84756	–1879.41960	2.08	1.90
gs-triplet	^{3}DFT	^{3}MLCT	–1879.86787	–1879.43810	1.52	1.40
gs-singlet	^{1}DFT	^{1}GS	–1879.92383	–1879.48958	0.00	0.00
3a						
td-sing--vsing-1001	^{1}TD-^{1}DFT	^{1}MLCT	–2335.85023	–2335.30713	2.39	2.32
td-trip--vsing-1001	^{3}TD-^{1}DFT	^{3}MLCT	–2335.85877	–2335.31605	2.16	2.08
gs-triplet	^{3}DFT	^{3}MC	–2335.86954	–2335.32959	1.87	1.71
gs-singlet	^{1}DFT	^{1}GS	–2335.93817	–2335.39234	0.00	0.00
3b						
td-sing--vsing-1001	^{1}TD-^{1}DFT	^{1}LLCT	–2335.09847	–2334.58504	1.52	1.38
td-sing--vtrip-1001	^{1}TD-^{3}DFT	^{3}MLCT	–2335.09734	–2334.58143	1.55	1.48
td-trip--vsing-1001	^{3}TD-^{1}DFT	^{3}MLCT	–2335.10498	–2334.58915	1.34	1.27
td-trip--vtrip-1001	^{3}TD-^{3}DFT	^{3}LLCT	–2335.09665	–2334.58245	1.57	1.45
gs-triplet-mc	^{3}DFT	^{3}MC	–2335.07863	–2334.56613	2.06	1.90
gs-triplet	^{3}DFT	^{3}MLCT	–2335.09798	–2334.58361	1.54	1.42
gs-singlet	^{1}DFT	^{1}GS	–2335.15435	–2334.63586	0.00	0.00

Table S3: Absolute (Hartrees) electronic (E_{el}) and free (G) energies and relative free energies (eV) for the ground and various excited states of each complex from B3LYP/BS1 and B3LYP/BS2//B3LYP/BS1.

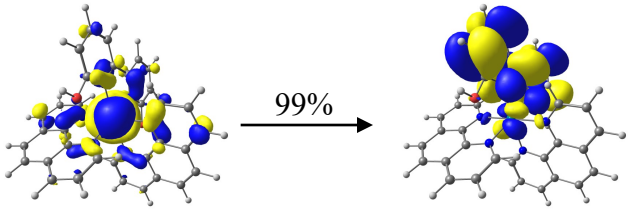
			BS1			BS2//BS1		
File Designation	**Spin State**	**Primary Character**	**E_{el}**	**G**	**ΔG**	**E_{el}**	**G**	**ΔG**
2a								
td-sing--vsing-1001	^{1}TD-^{1}DFT	^{1}MLCT	–1880.60371	–1880.14440	2.30	–1883.82757	–1883.37350	2.17
td-trip--vsing-1001	^{3}TD-^{1}DFT	^{3}MLCT	–1880.61288	–1880.15536	2.09	–1883.83342	–1883.38128	1.95
gs-triplet	^{3}DFT	^{3}MC	–1880.62542	–1880.16973	1.60	–1883.83735	–1883.38841	1.76
gs-singlet	^{1}DFT	^{1}GS	–1880.69421	–1880.23242	0.00	–1883.90826	–1883.45307	0.00
2b								
td-sing--vsing-1001	^{1}TD-^{1}DFT	^{1}LLCT	–1879.86909	–1879.44035	1.11	–1883.09450	–1882.67112	1.26
td-sing--vtrip-1001	^{1}TD-^{3}DFT	^{3}LMCT	–1879.86733	–1879.43641	1.36	–1883.08536	–1882.66158	1.52
td-trip--vsing-1001	^{3}TD-^{1}DFT	^{3}MLCT	–1879.87549	–1879.44459	1.09	–1883.09678	–1882.67273	1.22
td-trip--vtrip-1001	^{3}TD-^{3}DFT	^{3}LMCT	–1879.86653	–1879.43645	1.39	–1883.08686	–1882.66274	1.49
gs-triplet	^{3}DFT	^{3}MLCT	–1879.86787	–1879.43810	1.38	–1883.08803	–1882.66487	1.43
gs-singlet	^{1}DFT	^{1}GS	–1879.92383	–1879.48958	0.00	–1883.14555	–1882.71744	0.00
3a								
td-sing--vsing-1001	^{1}TD-^{1}DFT	^{1}MLCT	–2335.85023	–2335.30713	2.22	–2339.59777	–2339.06127	2.08
td-trip--vsing-1001	^{3}TD-^{1}DFT	^{3}MLCT	–2335.85877	–2335.31605	2.10	–2339.60293	–2339.06572	1.96
gs-triplet	^{3}DFT	^{3}MC	–2335.86954	–2335.32959	1.60	–2339.60486	–2339.07329	1.76
gs-singlet	^{1}DFT	^{1}GS	–2335.93817	–2335.39234	0.00	–2339.67560	–2339.13784	0.00
3b								
td-sing--vsing-1001	^{1}TD-^{1}DFT	^{1}LLCT	–2335.09847	–2334.58504	1.15	–2338.84676	–2338.34011	1.30
td-sing--vtrip-1001	^{1}TD-^{3}DFT	^{3}MLCT	–2335.09734	–2334.58143	1.41	–2338.84309	–2338.33564	1.42
td-trip--vsing-1001	^{3}TD-^{1}DFT	^{3}MLCT	–2335.10498	–2334.58915	1.13	–2338.84938	–2338.34192	1.25
td-trip--vtrip-1001	^{3}TD-^{3}DFT	^{3}LLCT	–2335.09665	–2334.58245	1.41	–2338.84309	–2338.33564	1.42
gs-triplet	^{3}DFT	^{3}MLCT	–2335.09798	–2334.58361	1.40	–2338.84638	–2338.33992	1.30
gs-singlet	^{1}DFT	^{1}GS	–2335.15435	–2334.63586	0.00	–2338.89897	–2338.38779	0.00

State Assignments

Character of the various excited states was determined by examining either the HOMO or the natural transition orbitals (NTOs) for the lowest excitation (root 1). For DFT optimized geometries, examining the nature of the HOMO is a good indication as to the state. For TD-DFT optimized geometries, each was optimized with respect to the lowest excitation (root 1). Therefore, examining the NTOs for this excitation will be a good indication as to the nature of the optimized state. The orbitals used for each assignment are shown below.

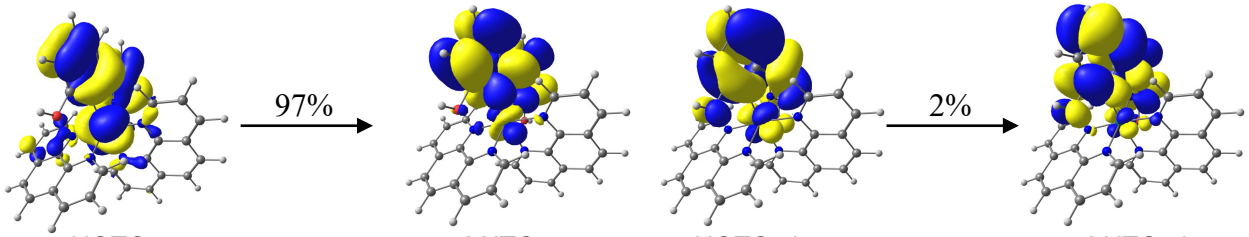
Complex 2_A

td-sing--vsing-1001

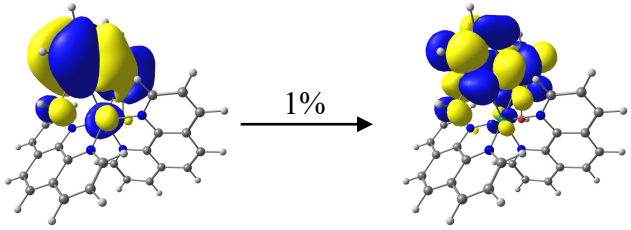


HOTO LUTO

td-trip--vsing-1001

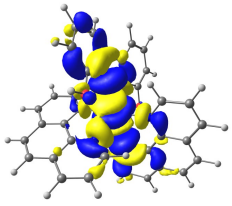


HOTO LUTO HOTO–1 LUTO+1



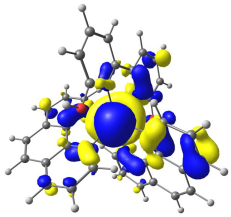
HOTO–2 LUTO+2

gs-triplet



HOMO

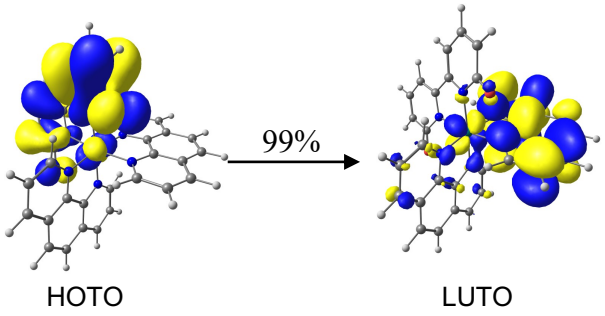
gs-singlet



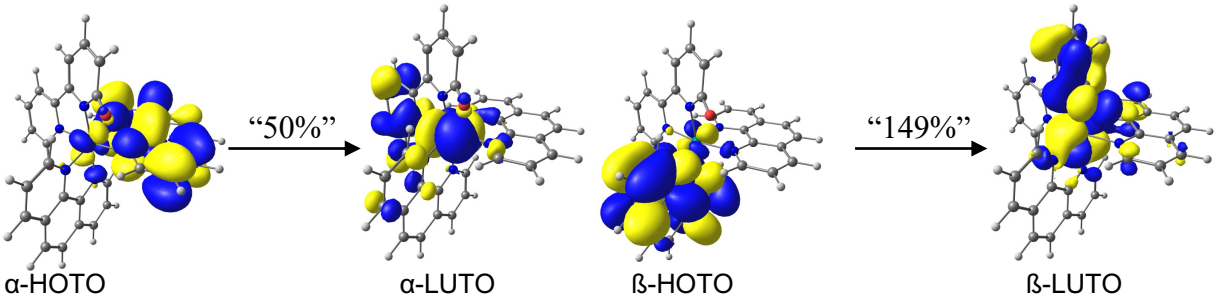
HOMO

Complex 2_B

td-sing--vsing-1001



td-sing--vtrip-1001



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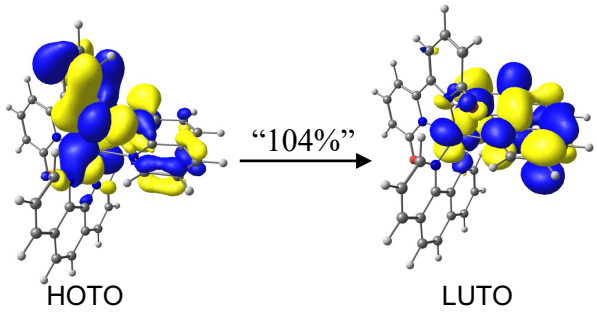

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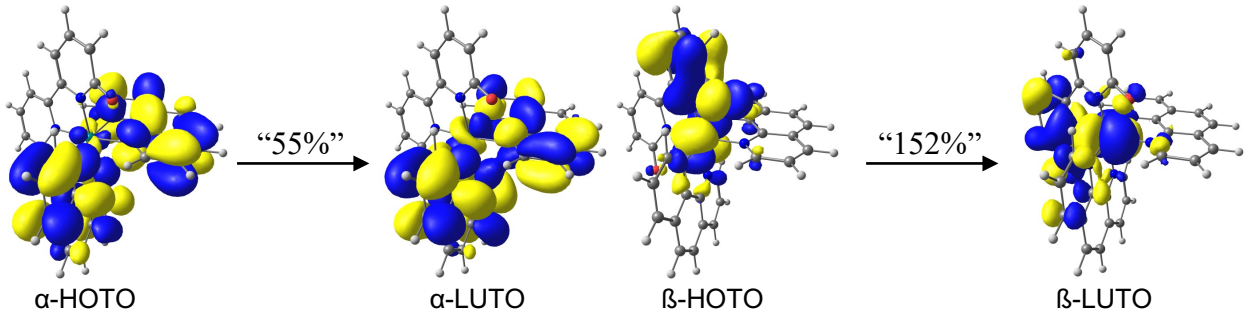

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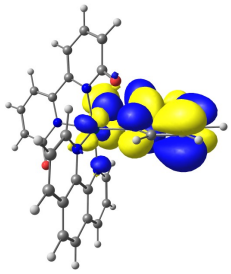

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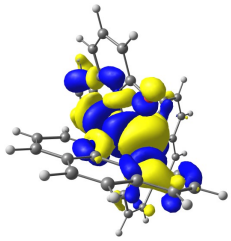

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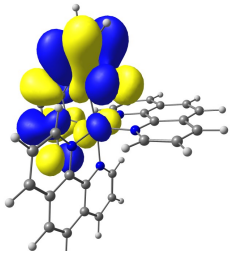

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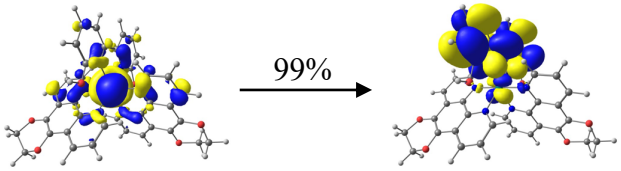

HOTO LUTO

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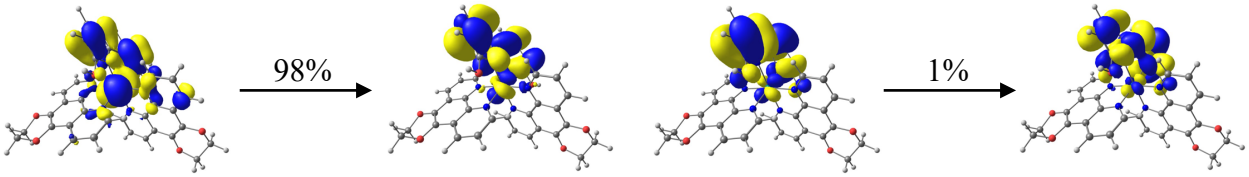
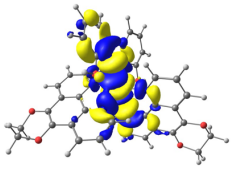


HOTO LUTO HOTO–1 LUTO+1

gs-triplet



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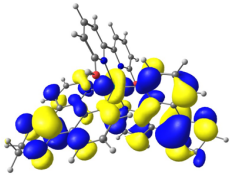

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Complex 3_B

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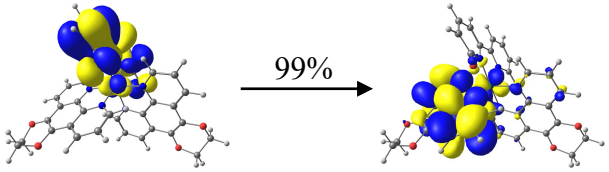

HOTO LUTO

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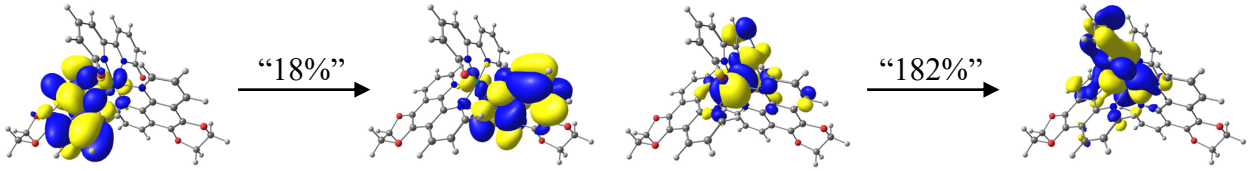

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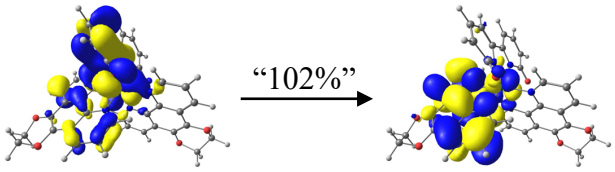

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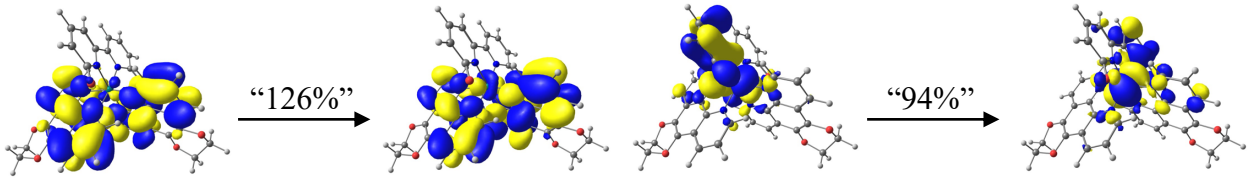

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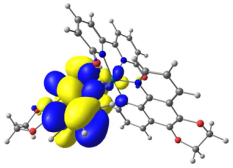
gs-triplet



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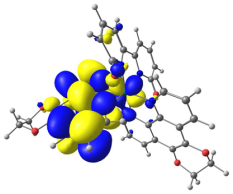

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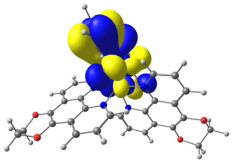

HOMO

Simulated Ground State Absorption Spectra

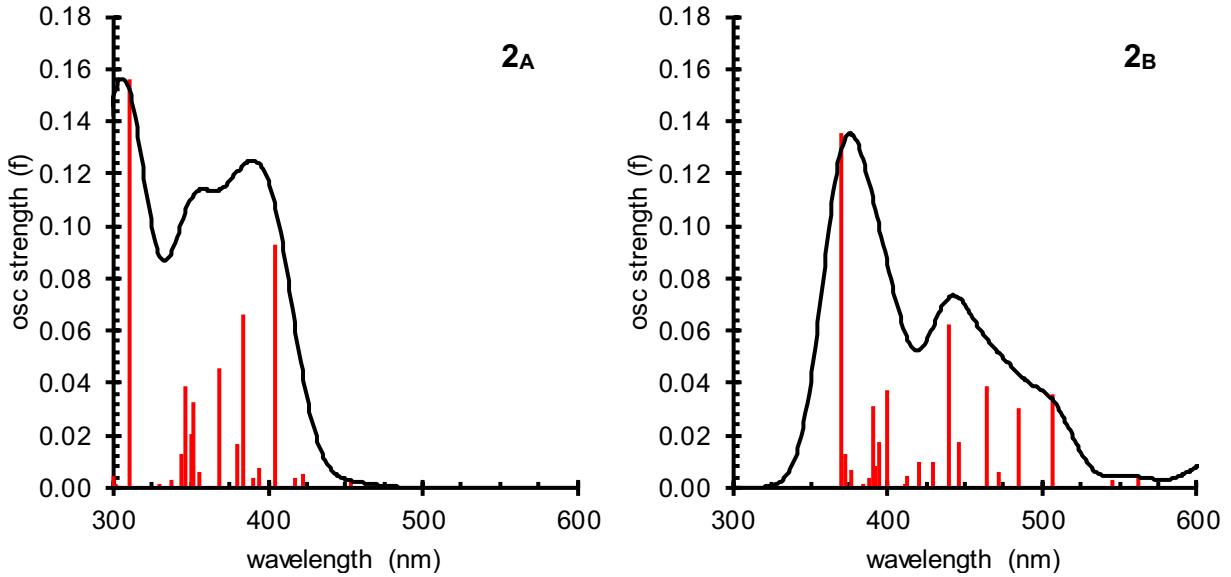

Figure S11: Simulated absorption spectra (black curve) with computed excitations (red sticks) of complex $\mathbf{2_A}$ (left) and $\mathbf{2_B}$ (right) PBE0-D3BJ/BS1.

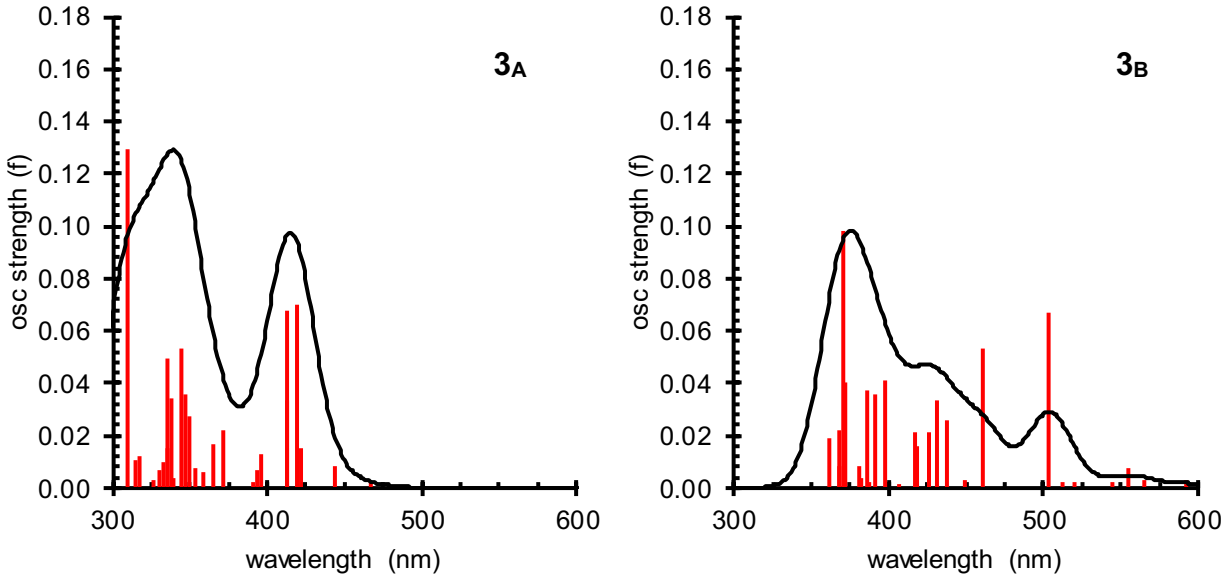

Figure S12: Simulated absorption spectra (black curve) with computed excitations (red sticks) of complex $\mathbf{3_A}$ (left) and $\mathbf{3_B}$ (right) PBE0-D3BJ/BS1.

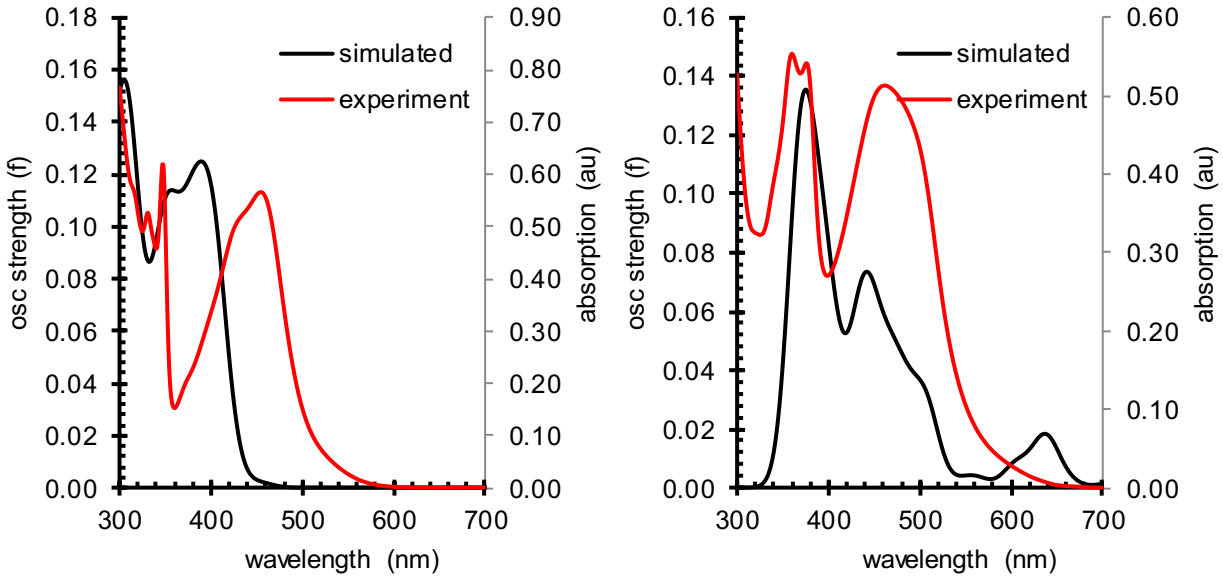

Figure S13: Simulated absorption spectra (black curve) with experimental absorption (red curve) of complex $\mathbf{2_A}$ (left) and $\mathbf{2_B}$ (right) PBE0-D3BJ/BS1.

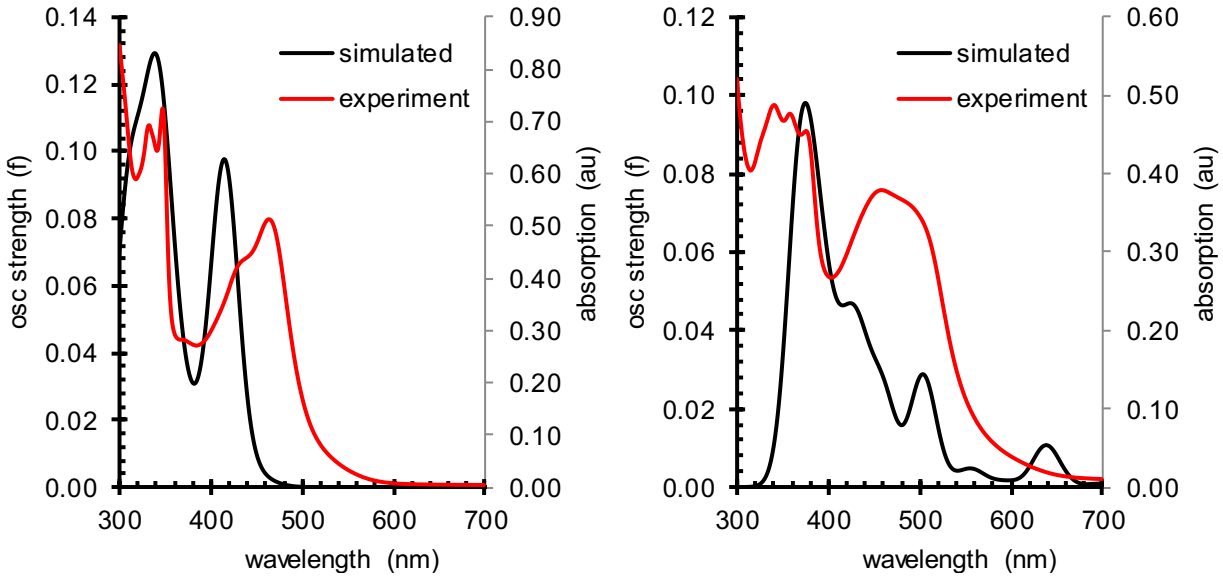

Figure S14: Simulated absorption spectra (black curve) with experimental absorption (red curve) of complex $\mathbf{3_A}$ (left) and $\mathbf{3_B}$ (right) PBE0-D3BJ/BS1.

Phosphorescence Experiments

Note that due to logistical constraints Figure S15 was obtained on a fluorimeter in Prof. McFarland's lab at University of Texas at Arlington, and Figures S16-S19 were obtained on a fluorimeter in Prof. Bonizzoni's lab at the University of Alabama. This explains the differences in the appearance of the spectra, specifically that Figure S15 shows emission into the near IR at 1100 nm. A variety of solvents were used with complexes $\mathbf{2_A}$ and $\mathbf{2_B}$ to demonstrate that each form of the complex shows similar luminescence wavelengths across different solvents (see Figures S16-18, Table S4). For $\mathbf{2_A}$, the luminescence wavelengths are 610 to 628 nm, and for $\mathbf{2_B}$, they are 696 to 710 nm. For $\mathbf{1_A}$/$\mathbf{1_B}$ and $\mathbf{3_A}$/$\mathbf{3_B}$ the solvent which gave the best spectra are shown in Figures S15 and S19 which were taken in aqueous and acetonitrile solution, respectively. Table S4 shows that the A forms consistently shift to higher wavelength upon deprotonation to the B forms for **1**-**3**.

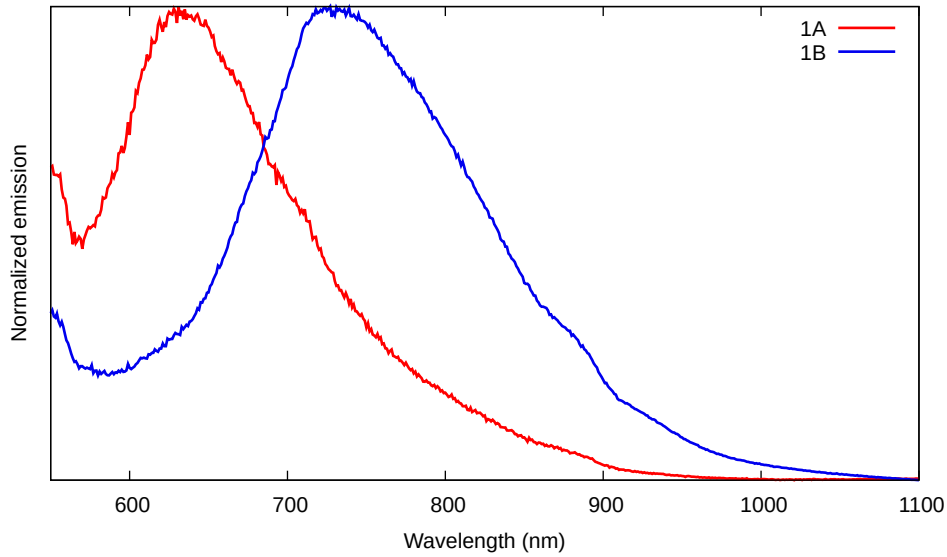

Figure S15: Phosphorescence (normalized emission) of $\mathbf{1_A}$ and $\mathbf{1_B}$ in water.

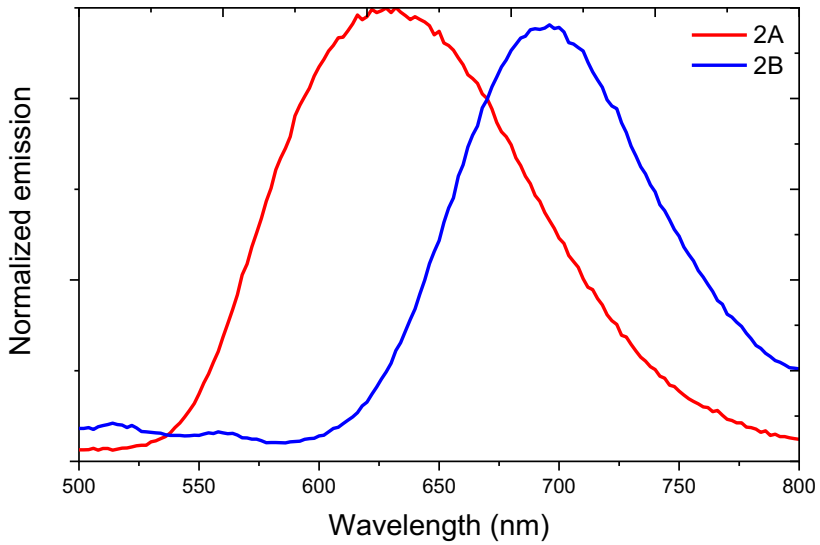

Figure S16: Phosphorescence (normalized emission) of $\mathbf{2_A}$ and $\mathbf{2_B}$ in water.

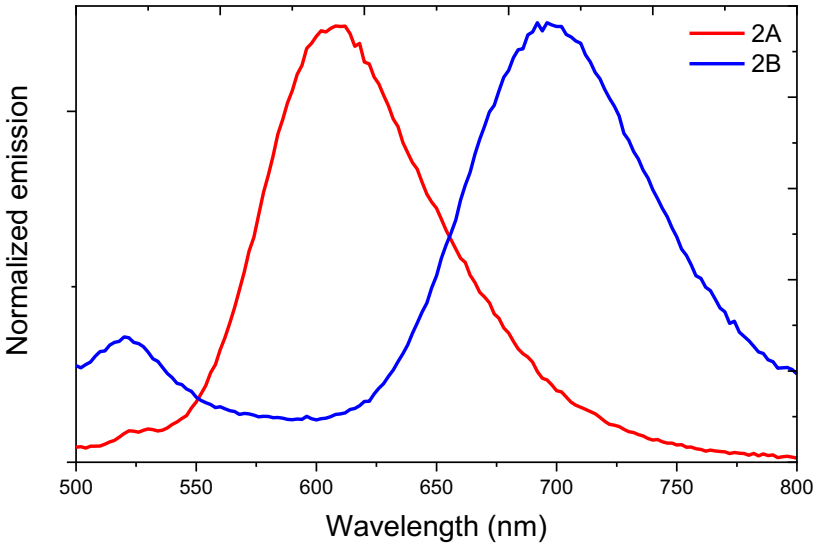

Figure S17: Phosphorescence (normalized emission) of $\mathbf{2_A}$ and $\mathbf{2_B}$ in methanol.

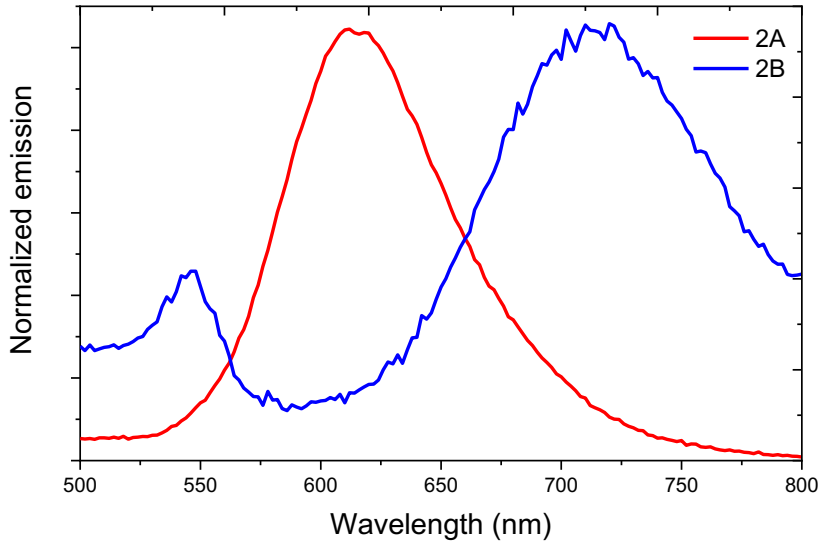

Figure S18: Phosphorescence (normalized emission) of $\mathbf{2_A}$ and $\mathbf{2_B}$ in acetonitrile.

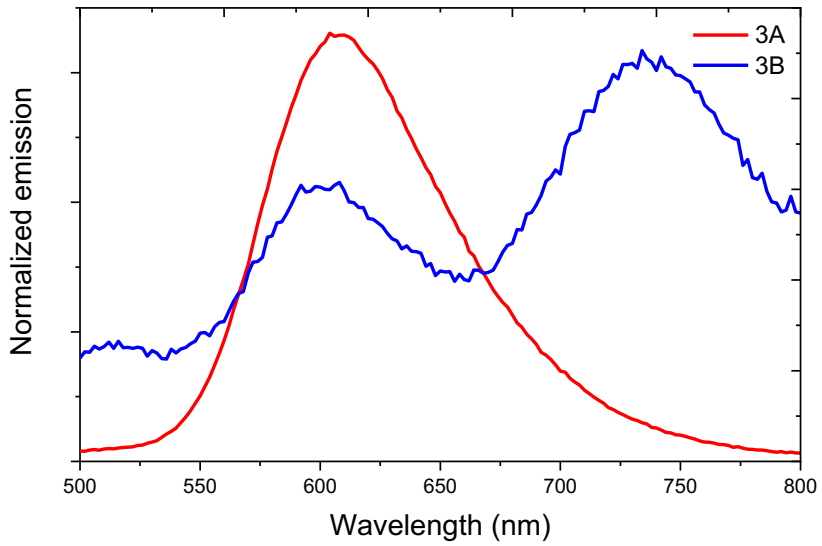

Figure S19: Phosphorescence (normalized emission) of $\mathbf{3_A}$ and $\mathbf{3_B}$ in acetonitrile. $\mathbf{3_B}$ (as prepared by *in situ* deprotonation) appears to be a mixture of $\mathbf{3_A}$ and $\mathbf{3_B}$.

Table S4: Emission wavelength (maxima) of each compound in each solvent. Excitation: 470 nm.

Solvent	**Compound (acidic forms)**	**Emission wavelength (nm)**	**Compound (basic forms)**	**Emission wavelength (nm)**
Water	$\mathbf{1_A}$	630	$\mathbf{1_B}$	727
	$\mathbf{2_A}$	628	$\mathbf{2_B}$	696
Acetonitrile	$\mathbf{2_A}$	612	$\mathbf{2_B}$	710
	$\mathbf{3_A}$	610	$\mathbf{3_B}$	734
Methanol	$\mathbf{2_A}$	610	$\mathbf{2_B}$	698

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Molecular Coordinates

pbe0-d3bj-bs1-2a--td-sing--vsing-1001

Ru	-0.000032	0.187524	0.000051
O	-2.026814	0.512697	2.475733
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H	2.658175	0.578271	-3.201840
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H	-3.602765	1.627780	-3.483499
C	-4.243849	-0.081628	-2.339994
H	-5.208334	-0.172535	-2.835017
C	-3.895273	-0.984141	-1.313364
C	-2.634046	-0.811533	-0.711822
C	-2.221190	-1.664046	0.351475
C	-3.064570	-2.702579	0.791804
C	-2.590102	-3.509167	1.846866
H	-3.203841	-4.324525	2.223600
C	-1.347398	-3.251967	2.390766
H	-0.954572	-3.853732	3.204886
C	-0.579013	-2.190994	1.888864
H	0.396276	-1.954610	2.304921
C	-4.738846	-2.045949	-0.850164
H	-5.710995	-2.180231	-1.318227
C	-4.338143	-2.872621	0.156996
H	-4.986759	-3.675315	0.499461
C	0.579488	-2.190721	-1.888954
H	-0.395843	-1.954510	-2.305012
C	1.348099	-3.251503	-2.390915
H	0.955414	-3.853288	-3.205087
C	2.590845	-3.508486	-1.847008
H	3.204759	-4.323691	-2.223789
C	3.065131	-2.701870	-0.791885
C	2.221532	-1.663540	-0.351500
C	2.634196	-0.811011	0.711859
C	3.895455	-0.983390	1.313399
C	4.243837	-0.080860	2.340080
H	5.208338	-0.171593	2.835103
C	3.357743	0.915621	2.701952
H	3.602396	1.628360	3.483665
C	2.119861	1.012772	2.051368
H	1.395933	1.781406	2.303941
C	4.338731	-2.871689	-0.157072
H	4.987517	-3.674228	-0.499579
C	4.739253	-2.044995	0.850142
H	5.711424	-2.179103	1.318206

total energy= -1880.60370608
zpe= -1880.080939
th energy= -1880.048543
th enthalpy= -1880.047599
free energy= -1880.144396

pbe0-d3bj-bs1-2a--td-trip--vsing-1001

Ru	0.017775	0.238790	0.025717
O	-1.538576	-0.188654	2.834797
H	-2.045921	-0.375477	3.634346
O	2.191912	1.620375	-1.883827
H	2.810073	1.993152	-2.524052
N	-1.256972	1.383965	1.246854
N	0.256083	2.077179	-0.799368
N	-1.712314	-0.188141	-1.088621
N	-0.487022	-1.676453	0.756448
N	1.367255	-0.858722	-1.133297
N	1.742045	0.464242	1.146051
C	-1.907662	1.004014	2.342092
C	-2.896307	1.778312	2.960476
H	-3.384150	1.426080	3.865199
C	-3.222787	3.016109	2.384873
H	-3.990125	3.637773	2.837918
C	-2.552010	3.445601	1.264321
H	-2.772389	4.415609	0.834362
C	-1.538370	2.627404	0.692242
C	-0.751273	3.001628	-0.412069
C	-0.884257	4.233626	-1.109966
H	-1.705052	4.901136	-0.873359
C	0.041634	4.584115	-2.053083
H	-0.039262	5.527899	-2.584519
C	1.139438	3.716788	-2.320357
H	1.915230	3.999567	-3.026375
C	1.198004	2.500143	-1.672782
C	-2.292044	0.574575	-2.010350
H	-1.794034	1.509563	-2.246758
C	-3.480488	0.197988	-2.652857
H	-3.910475	0.859107	-3.399265
C	-4.079071	-1.002301	-2.329184
H	-5.000718	-1.314557	-2.815379

```
C    -3.480947 -1.834004 -1.360151
C    -2.289897 -1.375229 -0.761926
C    -1.628830 -2.174019  0.218595
C    -2.159165 -3.428947  0.580685
C    -1.443935 -4.179327  1.536301
H    -1.814236 -5.154210  1.845947
C    -0.276027 -3.666374  2.063434
H     0.301275 -4.220348  2.797690
C     0.171894 -2.404802  1.647178
H     1.076838 -1.967498  2.058145
C    -4.009860 -3.105300 -0.964827
H    -4.930999 -3.451199 -1.427542
C    -3.374103 -3.872096 -0.035393
H    -3.780463 -4.838816  0.252064
C     1.143297 -1.497202 -2.272096
H     0.144830 -1.404727 -2.690364
C     2.137218 -2.248893 -2.918374
H     1.901031 -2.750707 -3.852009
C     3.395587 -2.335247 -2.358821
H     4.181958 -2.910627 -2.842443
C     3.660377 -1.663564 -1.146878
C     2.600817 -0.936571 -0.571186
C     2.806141 -0.218779  0.643077
C     4.068510 -0.223042  1.266956
C     4.202807  0.532232  2.450912
H     5.159917  0.561070  2.967341
C     3.117598  1.234375  2.939555
H     3.194659  1.830291  3.843973
C     1.894754  1.177551  2.257377
H     1.016402  1.712774  2.605099
C     4.932780 -1.670961 -0.487087
H     5.746198 -2.238305 -0.933073
C     5.130271 -0.977579  0.669481
H     6.102514 -0.983906  1.156277
 total energy= -1880.61288144
          zpe= -1880.092609
    th energy= -1880.060076
  th enthalpy= -1880.059132
  free energy= -1880.155357

pbe0-d3bj-bs1-2a--gs-triplet
Ru   -0.007650  0.140865 -0.130539
O    -2.093352  0.101449  2.704778
H    -2.765715 -0.103565  3.366057
O     1.832357  1.418043 -2.211611
H     2.497914  1.689439 -2.856397
N    -1.480495  1.647219  1.203212
N     0.175497  2.173517 -0.903529
N    -1.757115 -0.362724 -1.161013
N    -0.527991 -1.698841  0.788109
N     1.715010 -1.294246 -1.015168
N     1.761506  0.548184  0.982498
C    -2.386018  1.258624  2.092520
C    -3.545087  1.995639  2.367695
H    -4.263532  1.654038  3.109516
C    -3.748126  3.170510  1.662409
H    -4.643086  3.762155  1.837224
C    -2.802616  3.587208  0.724812
H    -2.963139  4.491523  0.147893
C    -1.672339  2.797796  0.533745
C    -0.609707  3.172266 -0.425591
C    -0.416402  4.494027 -0.809931
H    -1.024242  5.282873 -0.381264
C     0.591123  4.797013 -1.723716
H     0.761452  5.824615 -2.034104
C     1.378134  3.777361 -2.229341
H     2.169051  3.975748 -2.948600
C     1.134537  2.475047 -1.785010
C    -2.346733  0.322416 -2.138132
H    -1.859941  1.246583 -2.436583
C    -3.527750 -0.109806 -2.755887
H    -3.961690  0.489044 -3.551070
C    -4.119232 -1.287327 -2.342940
H    -5.037037 -1.642317 -2.806480
C    -3.521305 -2.034906 -1.308447
C    -2.331221 -1.527785 -0.747387
C    -1.675012 -2.238098  0.299254
C    -2.217482 -3.446785  0.781752
C    -1.521625 -4.095112  1.822060
H    -1.902110 -5.030809  2.226093
C    -0.360580 -3.532556  2.314726
H     0.198519 -4.007344  3.115570
C     0.107174 -2.329494  1.767959
H     1.019272 -1.862766  2.129310
C    -4.052961 -3.266863 -0.805461
H    -4.969915 -3.653979 -1.243321
C    -3.427940 -3.943836  0.198112
H    -3.840235 -4.878236  0.571569
C     1.661903 -2.190508 -1.984193
H     0.692542 -2.329190 -2.460751
C     2.780482 -2.934788 -2.395758
H     2.684150 -3.657489 -3.200923
C     3.986033 -2.728999 -1.757867
H     4.872958 -3.288852 -2.047296
C     4.068880 -1.782573 -0.714980
C     2.886779 -1.082740 -0.381489
C     2.912610 -0.108721  0.674679
C     4.121144  0.137262  1.365561
C     4.105669  1.097992  2.396553
H     5.019321  1.310489  2.947565
C     2.929892  1.754566  2.694156
H     2.880364  2.498249  3.483849
C     1.776327  1.449640  1.961135
H     0.826700  1.936416  2.167017
C     5.277635 -1.510741  0.002074
H     6.178507 -2.057743 -0.266329
C     5.301781 -0.587466  1.001382
H     6.221766 -0.384229  1.544360
    el energy= -1880.62542369
          zpe= -1880.103090
    th energy= -1880.070004
  th enthalpy= -1880.069060
  free energy= -1880.169728
```

pbe0-d3bj-bs1-2a--gs-singlet

Ru	-0.008885	0.236449	0.028205
O	-1.688717	0.065837	2.774855
H	-2.242271	-0.067341	3.554539
O	2.028869	1.320700	-2.217406
H	2.650728	1.590139	-2.904900
N	-1.197052	1.576352	1.169780
N	0.361363	2.103357	-0.909105
N	-1.719445	-0.181850	-1.095818
N	-0.601465	-1.564412	0.883287
N	1.253467	-1.002476	-1.062616
N	1.744254	0.415683	1.132151
C	-1.910420	1.279187	2.263116
C	-2.819853	2.170080	2.843047
H	-3.383684	1.877500	3.725832
C	-2.982861	3.416449	2.268645
H	-3.688612	4.127869	2.688905
C	-2.219648	3.753120	1.153916
H	-2.326713	4.732984	0.705023
C	-1.328025	2.820885	0.636909
C	-0.430217	3.127796	-0.488819
C	-0.363046	4.393291	-1.059550
H	-0.997905	5.197966	-0.709633
C	0.551072	4.629338	-2.082814
H	0.621609	5.610729	-2.544019
C	1.378053	3.601497	-2.493996
H	2.114632	3.750458	-3.280179
C	1.255872	2.352985	-1.874331
C	-2.260178	0.532911	-2.078303
H	-1.743278	1.449849	-2.346232
C	-3.426908	0.137378	-2.748307
H	-3.820890	0.763092	-3.543721
C	-4.050658	-1.040597	-2.389854
H	-4.954208	-1.371015	-2.897361
C	-3.500952	-1.822890	-1.353737
C	-2.330389	-1.343016	-0.731031
C	-1.720598	-2.090499	0.321016
C	-2.282382	-3.316354	0.732266
C	-1.624592	-4.015207	1.764745
H	-2.019571	-4.967182	2.112500
C	-0.479891	-3.477417	2.316930
H	0.056267	-3.989984	3.110278
C	0.000515	-2.245436	1.849712
H	0.887736	-1.790175	2.278918
C	-4.059608	-3.066102	-0.912162
H	-4.963150	-3.430589	-1.395021
C	-3.473005	-3.783549	0.086349
H	-3.902268	-4.729000	0.409515
C	0.973028	-1.702096	-2.153943
H	-0.025101	-1.576596	-2.563249
C	1.905536	-2.554118	-2.764753
H	1.618650	-3.102631	-3.657130
C	3.168489	-2.679942	-2.223494
H	3.909564	-3.332921	-2.679167
C	3.494621	-1.948162	-1.063183
C	2.492199	-1.122424	-0.516720
C	2.762105	-0.350764	0.652735
C	4.032504	-0.405131	1.260738
C	4.235432	0.389831	2.407511
H	5.200427	0.380747	2.909380
C	3.200161	1.173028	2.877337
H	3.322971	1.799338	3.756009
C	1.965484	1.158234	2.212226
H	1.128595	1.757272	2.559325
C	4.776088	-1.996263	-0.423340
H	5.544491	-2.638365	-0.847449
C	5.035519	-1.254199	0.689443
H	6.013194	-1.295844	1.163659

el energy= -1880.69420844
zpe= -1880.169806
th energy= -1880.137860
th enthalpy= -1880.136916
free energy= -1880.232423

pbe0-d3bj-bs1-2b--td-sing--vsing-1001

Ru	-0.010156	0.241891	0.074319
O	1.565729	0.182630	3.035040
O	-2.136062	1.562619	-2.076327
N	1.235913	1.524116	1.211945
N	-0.283723	2.109141	-0.840049
N	-1.263830	-0.888482	-1.084577
N	-1.748300	0.430830	1.148342
N	1.695826	-0.213798	-1.077295
N	0.540544	-1.588145	0.921250
C	1.900313	1.174536	2.390772
C	2.974210	2.041102	2.841822
H	3.524735	1.705736	3.715482
C	3.245671	3.227769	2.207801
H	4.040692	3.882047	2.558949
C	2.469732	3.594095	1.105275
H	2.647588	4.535295	0.600994
C	1.471721	2.708708	0.645751
C	0.591327	3.061345	-0.477156
C	0.642665	4.324833	-1.076091
H	1.360987	5.068738	-0.755678
C	-0.272078	4.619589	-2.098935
H	-0.247026	5.590919	-2.589121
C	-1.196464	3.675801	-2.456577
H	-1.939096	3.853725	-3.228962
C	-1.259509	2.380953	-1.799838
C	-0.986734	-1.522145	-2.216686
H	0.028442	-1.407965	-2.584493
C	-1.938441	-2.290741	-2.901795
H	-1.649431	-2.788532	-3.823045
C	-3.218934	-2.406036	-2.398333
H	-3.974968	-2.996268	-2.911956
C	-3.541112	-1.741909	-1.200187
C	-2.522193	-0.992913	-0.580839
C	-2.787121	-0.278352	0.621936
C	-4.067831	-0.318921	1.208412
C	-4.262626	0.417919	2.391957
H	-5.235304	0.414015	2.879365
C	-3.204288	1.138002	2.915028

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H    -3.315078  1.715672  3.828437
C    -1.962995  1.120857  2.266562
H    -1.104417  1.658711  2.656332
C    -4.833608 -1.778978 -0.583212
H    -5.618036 -2.362783 -1.060756
C    -5.086586 -1.098893  0.569675
H    -6.074308 -1.133044  1.024936
C     2.276150  0.484488 -2.066732
H     1.797757  1.427963 -2.314286
C     3.391258  0.046835 -2.758967
H     3.802500  0.659659 -3.555068
C     3.963701 -1.199880 -2.423309
H     4.837795 -1.576124 -2.949655
C     3.389930 -1.954008 -1.399435
C     2.247252 -1.431445 -0.731250
C     1.637656 -2.153786  0.307837
C     2.147354 -3.421214  0.722111
C     1.503343 -4.075939  1.774940
H     1.873233 -5.044058  2.109377
C     0.406859 -3.481158  2.387843
H    -0.111370 -3.954615  3.215424
C    -0.029482 -2.230516  1.921501
H    -0.870562 -1.727022  2.390424
C     3.881749 -3.236940 -0.973207
H     4.754526 -3.643080 -1.481918
C     3.289227 -3.935815  0.036154
H     3.685154 -4.903240  0.341187
 total energy= -1879.86909072
          zpe= -1879.376839
    th energy= -1879.344617
  th enthalpy= -1879.343673
  free energy= -1879.440351

pbe0-d3bj-bs1-2b--td-sing--vtrip-
1001
Ru    0.025313  0.265893  0.111533
O     0.929405  0.497854  3.223316
O    -2.207622  1.182971 -2.092554
N     0.950841  1.629761  1.237936
N    -0.441511  2.011332 -0.896391
N    -1.147130 -1.093948 -1.029714
N    -1.798009  0.281351  1.155217
N     1.604478 -0.103676 -1.135712
N     0.819666 -1.446837  1.042788
C     1.438741  1.379914  2.529510
C     2.512179  2.237895  2.979034
H     2.980940  1.977645  3.923311
C     2.840121  3.362740  2.279257
H     3.617816  4.029781  2.647924
C     2.152243  3.693551  1.086900
H     2.374095  4.613056  0.557020
C     1.209993  2.816594  0.602723
C     0.369526  3.052277 -0.583684
C     0.359123  4.240585 -1.289756
H     1.011527  5.061299 -1.013875
C    -0.543854  4.356718 -2.365058
H    -0.565580  5.274540 -2.951311
C    -1.400642  3.330876 -2.660608
H    -2.122156  3.396231 -3.470219
C    -1.409093  2.106279 -1.891476
C    -0.781914 -1.770338 -2.105835
H     0.241368 -1.622365 -2.436354
C    -1.666069 -2.615562 -2.794588
H    -1.313283 -3.143341 -3.675763
C    -2.961779 -2.753727 -2.347937
H    -3.669826 -3.396791 -2.866564
C    -3.370285 -2.046296 -1.199786
C    -2.414377 -1.225575 -0.574774
C    -2.766761 -0.483164  0.593124
C    -4.067093 -0.575209  1.126315
C    -4.340656  0.166194  2.292691
H    -5.333866  0.126640  2.735536
C    -3.340109  0.926040  2.859775
H    -3.511648  1.501172  3.764886
C    -2.070547  0.959659  2.261954
H    -1.246630  1.517963  2.691820
C    -4.689513 -2.117118 -0.646808
H    -5.423676 -2.750728 -1.139915
C    -5.025082 -1.411869  0.468332
H    -6.029705 -1.473702  0.880974
C     2.020561  0.615350 -2.218736
H     1.398819  1.465823 -2.479705
C     3.129362  0.273643 -2.949394
H     3.402610  0.876435 -3.810515
C     3.895507 -0.866342 -2.585475
H     4.774782 -1.155499 -3.155730
C     3.506423 -1.615530 -1.471142
C     2.354001 -1.207294 -0.749889
C     1.927635 -1.922146  0.375938
C     2.629735 -3.080162  0.827245
C     2.147231 -3.732250  1.964414
H     2.660829 -4.619429  2.331848
C     1.025473 -3.236521  2.620889
H     0.635093 -3.709805  3.516270
C     0.405107 -2.080826  2.126467
H    -0.446247 -1.640972  2.635940
C     4.200139 -2.784344 -1.003938
H     5.086626 -3.101892 -1.550449
C     3.781757 -3.485900  0.089558
H     4.329237 -4.366670  0.421014
 total energy= -1879.86732688
          zpe= -1879.373128
    th energy= -1879.341173
  th enthalpy= -1879.340229
  free energy= -1879.436408

pbe0-d3bj-bs1-2b--td-trip--vsing-
1001
Ru    0.013305  0.257090  0.116811
O     0.991974  0.387709  3.222746
O    -2.297670  1.313290 -1.944573
N     1.000062  1.557046  1.257730
N    -0.450940  2.047043 -0.809419
N    -1.196761 -1.022499 -1.073300
```

```
N    -1.784692  0.221348  1.199663
N     1.574004 -0.073714 -1.147827
N     0.823267 -1.504939  0.978642
C     1.514078  1.263293  2.532069
C     2.629397  2.071605  2.975687
H     3.107832  1.773481  3.903486
C     2.976797  3.201052  2.294339
H     3.785018  3.834327  2.655769
C     2.263699  3.582984  1.132188
H     2.499473  4.508787  0.619495
C     1.276742  2.752498  0.649790
C     0.404642  3.053042 -0.496895
C     0.399264  4.266921 -1.156612
H     1.085223  5.059769 -0.880247
C    -0.549819  4.447032 -2.182100
H    -0.572669  5.386189 -2.733549
C    -1.451354  3.458031 -2.471546
H    -2.208079  3.576033 -3.242198
C    -1.462760  2.205097 -1.749445
C    -0.861403 -1.625710 -2.200830
H     0.156034 -1.463459 -2.541798
C    -1.768578 -2.416407 -2.924034
H    -1.441003 -2.884877 -3.847325
C    -3.054308 -2.577454 -2.455927
H    -3.778803 -3.180361 -2.999584
C    -3.431140 -1.946578 -1.254101
C    -2.454686 -1.174273 -0.599820
C    -2.773278 -0.502846  0.617939
C    -4.061125 -0.618964  1.175719
C    -4.302500  0.054282  2.389300
H    -5.285376 -0.004645  2.852417
C    -3.282695  0.774487  2.975394
H    -3.428957  1.298038  3.915564
C    -2.027799  0.835403  2.350955
H    -1.190480  1.362261  2.794602
C    -4.737187 -2.044226 -0.674883
H    -5.488286 -2.640059 -1.189102
C    -5.040292 -1.408313  0.490241
H    -6.035405 -1.489246  0.922151
C     1.955881  0.656520 -2.248610
H     1.319384  1.501165 -2.489027
C     3.049054  0.335613 -3.005075
H     3.292429  0.950797 -3.866587
C     3.849819 -0.794653 -2.670615
H     4.721941 -1.063231 -3.260004
C     3.484818 -1.566858 -1.553801
C     2.343112 -1.183519 -0.809593
C     1.938168 -1.938733  0.298149
C     2.660704 -3.095761  0.717365
C     2.194369 -3.778617  1.847246
H     2.724735 -4.665754  2.190814
C     1.073912 -3.318306  2.521588
H     0.697381 -3.816660  3.409118
C     0.426570 -2.164023  2.049035
H    -0.435589 -1.756709  2.567730
C     4.198071 -2.733330 -1.121381
H     5.080364 -3.026604 -1.688073
C     3.807721 -3.469412 -0.035959
H     4.373024 -4.348456  0.268216
 total energy= -1879.87549063
          zpe= -1879.382450
    th energy= -1879.350377
  th enthalpy= -1879.349433
  free energy= -1879.444590

pbe0-d3bj-bs1-2b--td-trip--vtrip-
1001
Ru    0.055480  0.316624  0.070950
O     1.029615  0.120902  3.154056
O    -1.838686  1.849741 -2.081331
N     1.317988  1.403595  1.290017
N     0.106978  2.081745 -0.884245
N    -1.293181 -0.670020 -1.177300
N    -1.692428  0.697600  1.076768
N     1.736865 -0.424387 -0.950724
N     0.282819 -1.583633  0.959571
C     1.663323  1.013821  2.578179
C     2.771090  1.729516  3.170798
H     3.097025  1.393129  4.151045
C     3.345092  2.800271  2.540345
H     4.163046  3.340390  3.015378
C     2.866813  3.230354  1.285812
H     3.271877  4.114827  0.807261
C     1.846534  2.501960  0.703739
C     1.168255  2.885901 -0.549411
C     1.515650  3.978181 -1.310569
H     2.363617  4.593788 -1.032247
C     0.738700  4.295564 -2.452039
H     1.022182  5.144217 -3.072520
C    -0.369430  3.562005 -2.749996
H    -1.017206  3.793678 -3.590195
C    -0.783334  2.451788 -1.911984
C    -1.067246 -1.295406 -2.321709
H    -0.040670 -1.278140 -2.678283
C    -2.077806 -1.949697 -3.038661
H    -1.830085 -2.454328 -3.967479
C    -3.372767 -1.945145 -2.541926
H    -4.177788 -2.445678 -3.076554
C    -3.646295 -1.280827 -1.338657
C    -2.564914 -0.645764 -0.681282
C    -2.775574  0.078240  0.514477
C    -4.067745  0.163143  1.084106
C    -4.211856  0.910975  2.260346
H    -5.190220  0.998163  2.728046
C    -3.095168  1.540016  2.815312
H    -3.174496  2.122296  3.728260
C    -1.856604  1.411226  2.197390
H    -0.955312  1.857698  2.603352
C    -4.944532 -1.198354 -0.741009
H    -5.776113 -1.694084 -1.238071
C    -5.145624 -0.511841  0.418246
H    -6.139308 -0.453203  0.857945
C     2.482620  0.188279 -1.881519
H     2.219641  1.218945 -2.100019
```

```
C     3.521252 -0.444014 -2.550240
H     4.082312  0.107752 -3.298436
C     3.825290 -1.778612 -2.251415
H     4.635286 -2.296632 -2.759934
C     3.078573 -2.441212 -1.274595
C     2.031178 -1.727781 -0.635419
C     1.265386 -2.337041  0.378390
C     1.536206 -3.668692  0.795030
C     0.767960 -4.193211  1.837245
H     0.946949 -5.210837  2.179456
C    -0.206502 -3.399642  2.434716
H    -0.810726 -3.767766  3.257748
C    -0.406823 -2.097519  1.969012
H    -1.137161 -1.441418  2.429512
C     3.313948 -3.798169 -0.864079
H     4.110354 -4.351706 -1.357936
C     2.582247 -4.381059  0.124921
H     2.787558 -5.405524  0.430126
 total energy= -1879.86652593
          zpe= -1879.373304
    th energy= -1879.341456
  th enthalpy= -1879.340512
  free energy= -1879.436452

pbe0-d3bj-bs1-2b--gs-triplet-mc
Ru   -0.059098  0.018938 -0.108393
O    -2.453946  0.323422  2.227261
O     1.912022  0.545837 -2.226172
N    -1.199528  1.756287  0.977648
N     0.586526  1.845150 -0.940515
N    -1.789967 -0.125716 -1.248311
N    -1.012281 -1.689179  0.737647
N     1.650573 -1.889492 -0.626688
N     1.729063  0.220676  1.099757
C    -2.245064  1.485947  1.840138
C    -3.042265  2.624626  2.241048
H    -3.857530  2.439315  2.936044
C    -2.788358  3.875449  1.738792
H    -3.411147  4.718245  2.039465
C    -1.738129  4.085146  0.822355
H    -1.557082  5.062452  0.387845
C    -0.973246  2.983740  0.471917
C     0.134496  3.044733 -0.511531
C     0.678324  4.224222 -0.996065
H     0.328601  5.185147 -0.635447
C     1.704687  4.135207 -1.954335
H     2.148153  5.050343 -2.346441
C     2.151903  2.915322 -2.400707
H     2.940335  2.824328 -3.142837
C     1.582574  1.699523 -1.886752
C    -2.146454  0.678989 -2.247665
H    -1.399264  1.405037 -2.554761
C    -3.406231  0.605667 -2.853509
H    -3.641025  1.287058 -3.666127
C    -4.330818 -0.319205 -2.405376
H    -5.319203 -0.387133 -2.855175
C    -3.983735 -1.177297 -1.346209
C    -2.690739 -1.043561 -0.801786
C    -2.272969 -1.877561  0.273405
C    -3.153851 -2.838197  0.807761
C    -2.682027 -3.618295  1.878316
H    -3.330691 -4.366908  2.328732
C    -1.398070 -3.415516  2.346864
H    -1.003342 -3.997258  3.174886
C    -0.593466 -2.438527  1.748215
H     0.420376 -2.247965  2.089212
C    -4.862098 -2.163916 -0.789985
H    -5.861743 -2.261373 -1.208276
C    -4.464706 -2.958000  0.242364
H    -5.143851 -3.697665  0.661368
C     1.598222 -2.847470 -1.528246
H     0.603363 -3.114344 -1.884063
C     2.739765 -3.505880 -2.018067
H     2.639414 -4.283705 -2.770265
C     3.971940 -3.151448 -1.512485
H     4.881170 -3.645740 -1.850080
C     4.056197 -2.131345 -0.544102
C     2.848506 -1.507362 -0.154619
C     2.882730 -0.428761  0.801475
C     4.115892 -0.071189  1.394635
C     4.113575  0.960424  2.352428
H     5.049075  1.256929  2.823141
C     2.925850  1.581093  2.671726
H     2.879671  2.381549  3.404278
C     1.754426  1.187754  2.012091
H     0.798232  1.672245  2.197058
C     5.290680 -1.722897  0.052359
H     6.209164 -2.216552 -0.259297
C     5.315599 -0.743923  0.995289
H     6.253459 -0.440425  1.456129
    el energy= -1879.84755763
          zpe= -1879.352565
    th energy= -1879.319804
  th enthalpy= -1879.318860
  free energy= -1879.419601

pbe0-d3bj-bs1-2b--gs-triplet
Ru    0.006600  0.249250  0.125430
O     0.999399  0.200130  3.233987
O    -2.259965  1.511659 -1.881429
N     1.053531  1.463996  1.327267
N    -0.371240  2.094990 -0.726084
N    -1.254656 -0.898971 -1.132407
N    -1.771510  0.198537  1.230010
N     1.577046 -0.082570 -1.157435
N     0.744910 -1.559998  0.909949
C     1.547089  1.095702  2.586062
C     2.687351  1.846106  3.063982
H     3.147325  1.497391  3.983815
C     3.095597  2.978517  2.420248
H     3.928972  3.560443  2.810852
C     2.417894  3.429664  1.263003
H     2.697555  4.362315  0.785967
C     1.398474  2.658983  0.752544
```

```
C     0.547447  3.037545 -0.387864
C     0.623603  4.259654 -1.027674
H     1.358781  5.000339 -0.733969
C    -0.305403  4.522399 -2.054349
H    -0.261398  5.471078 -2.587966
C    -1.270561  3.602943 -2.364931
H    -2.015320  3.785403 -3.134634
C    -1.368284  2.340575 -1.665183
C    -0.956790 -1.426464 -2.308302
H     0.062139 -1.277961 -2.652343
C    -1.900359 -2.127922 -3.074554
H    -1.601029 -2.539165 -4.034058
C    -3.185887 -2.277720 -2.600548
H    -3.938218 -2.812448 -3.176700
C    -3.524704 -1.725717 -1.349897
C    -2.512880 -1.040177 -0.653364
C    -2.792046 -0.449384  0.613683
C    -4.075806 -0.562674  1.182089
C    -4.276927  0.027899  2.444763
H    -5.254821 -0.031551  2.918303
C    -3.223953  0.667959  3.065739
H    -3.338983  1.124162  4.044559
C    -1.975853  0.732509  2.428712
H    -1.110278  1.186911  2.898219
C    -4.825749 -1.821226 -0.759248
H    -5.604278 -2.350338 -1.304715
C    -5.090562 -1.265263  0.455245
H    -6.082148 -1.344779  0.895528
C     1.991588  0.681511 -2.205855
H     1.389500  1.561503 -2.409585
C     3.085628  0.357577 -2.970197
H     3.361901  1.002838 -3.798898
C     3.832973 -0.812096 -2.676468
H     4.702135 -1.085143 -3.269823
C     3.436460 -1.616714 -1.605147
C     2.297537 -1.227776 -0.852041
C     1.852295 -2.006744  0.222145
C     2.532846 -3.201894  0.600901
C     2.039516 -3.914544  1.695208
H     2.537357 -4.831421  2.006900
C     0.924019 -3.440979  2.381489
H     0.524669 -3.962120  3.245708
C     0.320471 -2.251977  1.956187
H    -0.529336 -1.836195  2.487550
C     4.107410 -2.826086 -1.213613
H     4.984608 -3.128771 -1.783000
C     3.677659 -3.582981 -0.163262
H     4.207856 -4.492923  0.112785
    el energy= -1879.86786772
          zpe= -1879.374433
    th energy= -1879.342365
  th enthalpy= -1879.341421
  free energy= -1879.438102

pbe0-d3bj-bs1-2b--gs-singlet
Ru   -0.023035  0.166446  0.058262
O     1.206695 -0.002405  3.048406
O    -2.169077  1.323893 -2.126668
N     1.026434  1.456338  1.293020
N    -0.430690  2.018859 -0.798032
N    -1.297523 -0.990539 -1.117057
N    -1.725163  0.195309  1.208702
N     1.647478 -0.042361 -1.139169
N     0.789516 -1.591492  0.823820
C     1.547068  1.071743  2.524505
C     2.467239  1.996210  3.138877
H     2.929707  1.675426  4.068367
C     2.697010  3.234204  2.597714
H     3.373223  3.930543  3.093096
C     2.042397  3.625377  1.416303
H     2.168827  4.623797  1.014261
C     1.211424  2.705936  0.798475
C     0.402127  3.016702 -0.397396
C     0.464645  4.236518 -1.050276
H     1.144943  5.012147 -0.718672
C    -0.387088  4.442012 -2.150448
H    -0.349062  5.387185 -2.691745
C    -1.269269  3.465556 -2.530342
H    -1.954161  3.597247 -3.363661
C    -1.352240  2.205262 -1.828557
C    -1.050451 -1.574205 -2.280265
H    -0.042806 -1.455301 -2.668476
C    -2.024638 -2.286483 -2.993882
H    -1.760904 -2.734921 -3.947568
C    -3.299788 -2.397128 -2.480271
H    -4.077315 -2.938555 -3.015097
C    -3.590716 -1.792632 -1.242135
C    -2.548768 -1.097161 -0.600657
C    -2.781259 -0.457879  0.652028
C    -4.047933 -0.529712  1.263744
C    -4.200496  0.105552  2.511762
H    -5.163063  0.078617  3.018481
C    -3.116625  0.750491  3.072665
H    -3.192985  1.244433  4.037118
C    -1.889507  0.775939  2.393721
H    -1.010588  1.256903  2.807587
C    -4.874511 -1.844854 -0.609142
H    -5.677800 -2.379673 -1.111855
C    -5.094066 -1.241144  0.591917
H    -6.073828 -1.288235  1.062854
C     2.043197  0.749179 -2.135850
H     1.396913  1.594169 -2.353911
C     3.217804  0.511472 -2.861400
H     3.488898  1.196434 -3.659763
C     4.011235 -0.576154 -2.551335
H     4.930141 -0.776673 -3.098338
C     3.614924 -1.434482 -1.508353
C     2.418528 -1.122456 -0.830472
C     1.951178 -1.958263  0.226714
C     2.690914 -3.097230  0.608618
C     2.174353 -3.880126  1.656446
H     2.709807 -4.768784  1.984206
C     0.990561 -3.496856  2.256573
H     0.565901 -4.068043  3.077018
```

```
C     0.334184 -2.339523  1.821393
H    -0.573264 -1.989010  2.300232
C     4.350119 -2.595722 -1.102433
H     5.276153 -2.829900 -1.623460
C     3.907862 -3.389909 -0.088076
H     4.477000 -4.267545  0.211908
    el energy= -1879.92382684
          zpe= -1879.427219
    th energy= -1879.395660
  th enthalpy= -1879.394716
  free energy= -1879.489578

pbe0-d3bj-bs1-3a--td-sing--vsing-
1001
Ru   -0.002214  0.723835  0.001799
O     1.861446  1.076421 -2.593503
O    -1.827429  1.024613  2.629299
H    -2.399600  1.081401  3.403794
N     0.748718  2.351985 -1.092544
N    -0.780215  2.330607  1.107882
N     1.825351  0.702915  0.981547
N     0.946876 -0.873430 -0.974029
N    -0.929028 -0.894374  0.964422
N    -1.829263  0.685040 -0.979341
C     1.566032  2.314377 -2.155491
C     2.061804  3.444737 -2.782868
H     2.703915  3.355176 -3.654295
C     1.703920  4.699406 -2.255852
H     2.084963  5.607371 -2.715229
C     0.880984  4.771969 -1.159407
H     0.620409  5.736977 -0.741175
C     0.387686  3.587750 -0.562665
C    -0.465738  3.575510  0.570043
C    -1.000829  4.744444  1.161082
H    -0.778629  5.715698  0.735198
C    -1.813376  4.648676  2.263345
H    -2.225544  5.544807  2.719054
C    -2.118052  3.385088  2.802999
H    -2.746879  3.277838  3.682088
C    -1.585354  2.269892  2.179177
C     2.236254  1.543392  1.926792
H     1.534198  2.317728  2.219460
C     3.503171  1.424054  2.515309
H     3.794401  2.126026  3.290759
C     4.360052  0.419936  2.106785
H     5.344958  0.303060  2.550012
C     3.948403 -0.464358  1.088598
C     2.661706 -0.277418  0.550451
C     2.187041 -1.124469 -0.487480
C     3.002698 -2.159748 -0.981987
C     2.480283 -2.956943 -2.020942
H     3.082422 -3.761533 -2.433155
C     1.209994 -2.694135 -2.492509
H     0.776489 -3.287940 -3.291709
C     0.466156 -1.638556 -1.942110
H    -0.529241 -1.397762 -2.304073
C     4.765590 -1.527977  0.587814
C     4.309923 -2.344206 -0.427909
C    -0.431899 -1.669683  1.915942
H     0.560330 -1.418644  2.279586
C    -1.152784 -2.752435  2.443587
H    -0.703452 -3.358311  3.224778
C    -2.418652 -3.030202  1.968758
H    -2.999978 -3.861184  2.357821
C    -2.963828 -2.213853  0.956776
C    -2.167971 -1.155001  0.479772
C    -2.653250 -0.308154 -0.553336
C    -3.945545 -0.495936 -1.078033
C    -4.379849  0.406686 -2.070311
H    -5.374561  0.297747 -2.493183
C    -3.532172  1.418212 -2.479725
H    -3.839245  2.131831 -3.238244
C    -2.256616  1.534070 -1.909653
H    -1.563036  2.316220 -2.201660
C    -4.267309 -2.413769  0.399379
C    -4.752568 -1.566938 -0.576902
O     5.055422 -3.331232 -0.956373
O     5.973274 -1.680946  1.158719
C     6.441090 -3.245270 -0.616452
C     6.596260 -2.930874  0.855411
O    -4.973597 -3.454360  0.875693
O    -5.986390 -1.688095 -1.097489
C    -6.108413 -3.791657  0.074865
C    -6.847363 -2.536375 -0.334763
H     6.877882 -4.215045 -0.865830
H     6.909420 -2.464491 -1.230167
H     7.647560 -2.823584  1.132403
H     6.134698 -3.715543  1.469323
H    -7.195697 -1.985990  0.549146
H    -7.699033 -2.766453 -0.979071
H    -5.766588 -4.345126 -0.809697
H    -6.734903 -4.441148  0.690621
H     2.438400  1.150298 -3.362972
 total energy= -2335.85022546
          zpe= -2335.235596
    th energy= -2335.196633
  th enthalpy= -2335.195689
  free energy= -2335.307132

pbe0-d3bj-bs1-3a--td-trip--vsing-
1001
Ru    0.027601  0.771920  0.035471
O    -1.397308  0.752855  2.943057
O     2.336672  1.673108 -1.993805
H     2.970617  1.896320 -2.685905
N    -0.964741  2.176673  1.251592
N     0.540712  2.498327 -0.883589
N    -1.807823  0.617690 -0.984661
N    -0.770221 -0.994584  0.881496
N     1.093840 -0.593315 -1.134106
N     1.810585  0.714338  1.078002
C    -1.604019  1.964301  2.400112
C    -2.417069  2.917973  3.014422
H    -2.904422  2.699345  3.960522
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C    -2.568773  4.160158  2.379760
H    -3.198587  4.923104  2.829173
C    -1.899419  4.416394  1.205668
H    -1.981639  5.386859  0.730149
C    -1.067536  3.416693  0.639676
C    -0.285257  3.595029 -0.520377
C    -0.256800  4.781043 -1.295516
H    -0.946852  5.587058 -1.071872
C     0.660711  4.916098 -2.302866
H     0.699494  5.824885 -2.896409
C     1.596120  3.870849 -2.552485
H     2.374032  3.984358 -3.302205
C     1.499114  2.710054 -1.821906
C    -2.285328  1.427294 -1.924121
H    -1.645414  2.250096 -2.225815
C    -3.547594  1.229493 -2.504218
H    -3.889441  1.917789 -3.271327
C    -4.330217  0.168195 -2.099396
H    -5.309450 -0.012922 -2.533019
C    -3.840172 -0.701736 -1.104188
C    -2.563671 -0.433252 -0.572429
C    -2.007203 -1.294702  0.416009
C    -2.736742 -2.410890  0.870663
C    -2.132627 -3.232475  1.843626
H    -2.669754 -4.098060  2.220596
C    -0.865477 -2.918856  2.291451
H    -0.366984 -3.532447  3.035961
C    -0.210566 -1.786853  1.785198
H     0.777899 -1.504647  2.134227
C    -4.572018 -1.838032 -0.632765
C    -4.041374 -2.661203  0.338041
C     0.703034 -1.218497 -2.234306
H    -0.278227 -0.955473 -2.619080
C     1.511852 -2.168941 -2.878301
H     1.145890 -2.654417 -3.778114
C     2.754881 -2.472947 -2.362284
H     3.401913 -3.205281 -2.836417
C     3.190550 -1.811593 -1.195444
C     2.313601 -0.877951 -0.612922
C     2.700382 -0.174464  0.561162
C     3.968233 -0.389028  1.133132
C     4.303972  0.370523  2.272824
H     5.277850  0.236727  2.735244
C     3.389280  1.276726  2.774968
H     3.621752  1.880331  3.647089
C     2.143224  1.425609  2.150711
H     1.396234  2.126733  2.509400
C     4.467166 -2.045248 -0.589651
C     4.852721 -1.341025  0.532449
O    -4.702810 -3.722989  0.833745
O    -5.775782 -2.054916 -1.192908
C    -6.095556 -3.727548  0.514424
C    -6.296364 -3.361111 -0.939924
O     5.250278 -2.971635 -1.171463
O     6.058432 -1.493961  1.109992
C     6.350357 -3.384020 -0.358275
C     7.002262 -2.179360  0.284961
H    -6.454523 -4.737654  0.725080
H    -6.612353 -3.012142  1.167766
H    -7.356880 -3.323408 -1.199561
H    -5.785257 -4.080206 -1.593720
H     7.374515 -1.486039 -0.480861
H     7.825414 -2.473076  0.940438
H     5.984232 -4.080094  0.408012
H     7.042984 -3.906165 -1.022508
H    -1.881885  0.690134  3.775067
 total energy= -2335.85876870
          zpe= -2335.245774
    th energy= -2335.206794
  th enthalpy= -2335.205850
  free energy= -2335.316050

pbe0-d3bj-bs1-3a--gs-triplet
Ru   -0.035800  0.661989 -0.147164
O    -1.878548  1.026657  2.832718
O     1.902271  1.563600 -2.337383
H     2.568486  1.701926 -3.022256
N    -1.072004  2.426910  1.281525
N     0.513516  2.624289 -0.932791
N    -1.916979  0.547076 -1.058728
N    -0.859011 -1.044706  0.805868
N     1.276265 -1.086803 -1.160911
N     1.848282  0.670810  0.841683
C    -1.979141  2.219513  2.227788
C    -2.954299  3.166943  2.565127
H    -3.678405  2.969766  3.352499
C    -2.968357  4.360710  1.862169
H    -3.719300  5.114354  2.084989
C    -2.018977  4.588203  0.865579
H    -2.035106  5.507607  0.290331
C    -1.077685  3.594019  0.614298
C    -0.023147  3.756125 -0.410987
C     0.408044  5.015833 -0.810336
H    -0.001781  5.906285 -0.346970
C     1.398799  5.118327 -1.784747
H     1.753592  6.093395 -2.108262
C     1.932475  3.965750 -2.333781
H     2.702349  4.007378 -3.100450
C     1.458826  2.734723 -1.871664
C    -2.415380  1.348261 -1.997433
H    -1.773466  2.160860 -2.325193
C    -3.693271  1.161815 -2.542120
H    -4.047043  1.841805 -3.311377
C    -4.481563  0.118967 -2.097399
H    -5.474589 -0.054085 -2.501790
C    -3.980022 -0.737342 -1.097279
C    -2.682687 -0.484929 -0.608114
C    -2.118853 -1.329379  0.388465
C    -2.864925 -2.406158  0.907513
C    -2.262102 -3.195200  1.907098
H    -2.811188 -4.029704  2.333632
C    -0.980791 -2.888508  2.321061
H    -0.485425 -3.476537  3.088032
C    -0.306036 -1.803450  1.743609
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H     0.703495 -1.538584  2.044790
C    -4.722210 -1.844078 -0.573839
C    -4.186945 -2.645369  0.411878
C     0.966601 -1.940442 -2.120193
H    -0.034481 -1.853421 -2.539651
C     1.865161 -2.915206 -2.586315
H     1.563865 -3.594667 -3.378478
C     3.120599 -2.993376 -2.020249
H     3.844483 -3.735154 -2.345196
C     3.469213 -2.090943 -0.994317
C     2.498092 -1.145968 -0.595084
C     2.801055 -0.219437  0.458082
C     4.075538 -0.249685  1.067094
C     4.348046  0.681954  2.088319
H     5.324244  0.679503  2.564284
C     3.365069  1.574816  2.460661
H     3.535461  2.304600  3.246546
C     2.123808  1.537462  1.813010
H     1.318963  2.216529  2.081008
C     4.749279 -2.113611 -0.354917
C     5.048735 -1.206973  0.635809
O    -4.860037 -3.674887  0.960041
O    -5.945442 -2.053428 -1.098308
C    -6.256772 -3.667625  0.664044
C    -6.477508 -3.343605 -0.797699
O     5.618419 -3.056848 -0.767863
O     6.250907 -1.161975  1.245647
C     6.722422 -3.239233  0.117794
C     7.262926 -1.895667  0.557669
H    -6.627949 -4.664618  0.913107
H    -6.752515 -2.923690  1.301972
H    -7.541795 -3.300956 -1.040937
H    -5.986354 -4.089901 -1.436389
H     7.598653 -1.313570 -0.311196
H     8.091621 -2.009219  1.260718
H     6.390450 -3.823250  0.986679
H     7.471181 -3.808779 -0.437967
H    -2.537399  0.953205  3.533825
    el energy= -2335.86954384
          zpe= -2335.255161
    th energy= -2335.215571
  th enthalpy= -2335.214627
  free energy= -2335.329592

pbe0-d3bj-bs1-3a--gs-singlet
Ru    0.006930  0.793893  0.037311
O    -1.493646  0.989221  2.882601
O     2.081517  1.467643 -2.329909
H     2.695475  1.610193 -3.060892
N    -0.885565  2.342446  1.180950
N     0.616842  2.544978 -0.989865
N    -1.802813  0.628079 -0.996380
N    -0.822770 -0.860194  0.988254
N     0.987677 -0.668741 -1.067377
N     1.819369  0.710130  1.055924
C    -1.564046  2.200956  2.326301
C    -2.290240  3.242687  2.913149
H    -2.834729  3.074527  3.839450
C    -2.298480  4.476502  2.290184
H    -2.860536  5.303650  2.715275
C    -1.563630  4.649108  1.120544
H    -1.546705  5.616372  0.633479
C    -0.858001  3.571138  0.599152
C     0.008606  3.692846 -0.584619
C     0.227705  4.908396 -1.222321
H    -0.264226  5.812377 -0.884925
C     1.109164  4.961097 -2.298475
H     1.296105  5.899768 -2.812994
C     1.755223  3.805192 -2.694008
H     2.462454  3.808846 -3.520210
C     1.486230  2.616888 -2.006119
C    -2.265988  1.383608 -1.987839
H    -1.624435  2.196990 -2.313733
C    -3.507078  1.148054 -2.597766
H    -3.832370  1.795757 -3.406570
C    -4.291599  0.096154 -2.170168
H    -5.253241 -0.118421 -2.626904
C    -3.824181 -0.716919 -1.118196
C    -2.568773 -0.407126 -0.557751
C    -2.036864 -1.210157  0.492666
C    -2.770161 -2.309898  0.980123
C    -2.196236 -3.071632  2.017250
H    -2.735713 -3.924565  2.418379
C    -0.952045 -2.712862  2.494601
H    -0.473135 -3.279077  3.288154
C    -0.293585 -1.597735  1.955545
H     0.676156 -1.281495  2.326925
C    -4.558329 -1.837756 -0.614664
C    -4.052097 -2.603803  0.413103
C     0.538660 -1.344722 -2.116364
H    -0.443222 -1.064888 -2.486324
C     1.284696 -2.364044 -2.727852
H     0.866415 -2.887350 -3.582711
C     2.532689 -2.688867 -2.236997
H     3.133756 -3.474429 -2.685373
C     3.030702 -1.978808 -1.126061
C     2.212551 -0.977007 -0.569616
C     2.663776 -0.232466  0.558041
C     3.936870 -0.480076  1.107718
C     4.338730  0.303057  2.208481
H     5.317158  0.142944  2.651748
C     3.472819  1.261032  2.696681
H     3.747980  1.884216  3.542501
C     2.217338  1.435996  2.095744
H     1.511970  2.177331  2.459302
C     4.314600 -2.235964 -0.545560
C     4.761903 -1.496770  0.528294
O    -4.718817 -3.649321  0.939072
O    -5.741823 -2.098932 -1.204183
C    -6.096803 -3.692378  0.568699
C    -6.247680 -3.400314 -0.908548
O     5.040958 -3.225540 -1.101489
O     5.977058 -1.676902  1.082530
C     6.136297 -3.650918 -0.291323
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C     6.862797 -2.448943  0.272658
H    -6.449450 -4.696564  0.815840
H    -6.649661 -2.954180  1.165006
H    -7.297934 -3.397233 -1.209767
H    -5.698707 -4.141137 -1.505291
H     7.247764 -1.816597 -0.538675
H     7.688811 -2.749485  0.921672
H     5.754926 -4.285432  0.519958
H     6.786362 -4.242664 -0.940230
H    -2.010592  0.971727  3.697572
    el energy= -2335.93816887
          zpe= -2335.321807
    th energy= -2335.283315
  th enthalpy= -2335.282370
  free energy= -2335.392339

pbe0-d3bj-bs1-3b--td-sing--vsing-
1001
Ru    0.027681  0.801280  0.087602
O    -1.309413  1.269519  3.131690
O     2.284733  1.541034 -2.208693
N    -0.874547  2.375314  1.177333
N     0.620091  2.512855 -0.966854
N    -1.782615  0.631716 -0.980450
N    -0.840960 -0.822323  1.081779
N     0.972712 -0.632124 -1.033814
N     1.815038  0.695984  1.091271
C    -1.510383  2.248073  2.415110
C    -2.383345  3.329225  2.835328
H    -2.934837  3.169241  3.756856
C    -2.466691  4.496129  2.117950
H    -3.105967  5.312184  2.448212
C    -1.699553  4.630655  0.957058
H    -1.725898  5.551389  0.388230
C    -0.915011  3.540982  0.528305
C    -0.043682  3.637020 -0.651994
C     0.111360  4.839908 -1.350474
H    -0.441390  5.726823 -1.067608
C     1.013468  4.880853 -2.424731
H     1.143783  5.800430 -2.992042
C     1.730368  3.756643 -2.734397
H     2.455618  3.734264 -3.542624
C     1.585424  2.526293 -1.974855
C    -2.245765  1.357461 -2.002062
H    -1.604226  2.173050 -2.324673
C    -3.447262  1.097030 -2.647030
H    -3.756849  1.722114 -3.478500
C    -4.234775  0.009536 -2.217267
H    -5.175797 -0.235200 -2.699474
C    -3.783778 -0.762970 -1.152239
C    -2.543636 -0.434083 -0.535927
C    -2.046695 -1.194827  0.531254
C    -2.779416 -2.302589  1.048401
C    -2.259885 -2.999530  2.135552
H    -2.811635 -3.841261  2.544025
C    -1.042070 -2.590730  2.685948
H    -0.608920 -3.098328  3.541701
C    -0.380054 -1.496176  2.123540
H     0.557697 -1.138025  2.539280
C    -4.503093 -1.896548 -0.636789
C    -4.027649 -2.626767  0.420845
C     0.520167 -1.270735 -2.105730
H    -0.468493 -0.979647 -2.446921
C     1.265955 -2.260789 -2.759099
H     0.840024 -2.753599 -3.628533
C     2.520997 -2.602055 -2.292910
H     3.121220 -3.367229 -2.775583
C     3.020949 -1.930969 -1.163423
C     2.206121 -0.953003 -0.565684
C     2.662544 -0.236720  0.576621
C     3.936736 -0.491964  1.117183
C     4.340110  0.259540  2.235344
H     5.319152  0.090750  2.673191
C     3.466235  1.200960  2.749049
H     3.735683  1.797646  3.616101
C     2.213413  1.392387  2.154218
H     1.495541  2.108728  2.540551
C     4.309009 -2.194229 -0.592691
C     4.755580 -1.492173  0.499418
O    -4.708959 -3.688710  0.945273
O    -5.678046 -2.195803 -1.268622
C    -6.060714 -3.728803  0.537085
C    -6.156884 -3.486843 -0.956445
O     5.047041 -3.168831 -1.190308
O     5.986314 -1.691483  1.048349
C     6.138779 -3.601635 -0.399134
C     6.858722 -2.405935  0.191829
H    -6.441775 -4.718371  0.808802
H    -6.635128 -2.958688  1.074215
H    -7.194002 -3.530471 -1.304165
H    -5.563284 -4.244451 -1.491105
H     7.207447 -1.744044 -0.614655
H     7.712505 -2.714493  0.802403
H     5.773009 -4.253060  0.408394
H     6.793586 -4.177572 -1.059840
 total energy= -2335.09847051
          zpe= -2334.513323
    th energy= -2334.474633
  th enthalpy= -2334.473689
  free energy= -2334.585039

pbe0-d3bj-bs1-3b--td-sing--vtrip-
1001
Ru   -0.009591  0.817764  0.118527
O    -0.761165  1.426549  3.223522
O     2.244953  1.253772 -2.210963
N    -0.710387  2.378540  1.146301
N     0.639486  2.398152 -1.049064
N    -1.674217  0.563684 -1.049127
N    -0.976362 -0.697387  1.214685
N     0.925289 -0.778849 -0.933317
N     1.838318  0.681213  1.104882
C    -1.180436  2.303003  2.466533
C    -2.123533  3.325229  2.863517
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H    -2.589219  3.206407  3.837270
C    -2.331184  4.420430  2.076371
H    -3.006387  5.209842  2.403089
C    -1.647891  4.559633  0.844176
H    -1.770811  5.452132  0.240978
C    -0.840392  3.531681  0.416538
C    -0.019897  3.557986 -0.806572
C     0.116240  4.673247 -1.612068
H    -0.415494  5.591797 -1.391016
C     0.987045  4.582185 -2.715899
H     1.104105  5.438067 -3.379596
C     1.694961  3.432845 -2.943599
H     2.388825  3.337226 -3.774157
C     1.576208  2.285038 -2.071672
C    -2.029151  1.224560 -2.180723
H    -1.322428  1.973807 -2.524072
C    -3.187085  0.949764 -2.867050
H    -3.410251  1.501819 -3.774986
C    -4.068160 -0.059612 -2.394425
H    -4.983972 -0.303656 -2.922435
C    -3.737784 -0.740782 -1.226455
C    -2.530849 -0.413469 -0.554178
C    -2.152021 -1.083374  0.612119
C    -2.970454 -2.105652  1.176249
C    -2.549607 -2.717609  2.353587
H    -3.162941 -3.494853  2.800763
C    -1.350268 -2.310388  2.942610
H    -0.997974 -2.753295  3.868844
C    -0.608283 -1.290551  2.342651
H     0.305811 -0.918950  2.794279
C    -4.551158 -1.781607 -0.656945
C    -4.188623 -2.429952  0.496960
C     0.430062 -1.495132 -1.929117
H    -0.576072 -1.240683 -2.246420
C     1.166003 -2.515314 -2.550943
H     0.711948 -3.072460 -3.365219
C     2.448175 -2.791384 -2.127787
H     3.046174 -3.571376 -2.589261
C     2.987276 -2.035685 -1.069369
C     2.178450 -1.038471 -0.499652
C     2.670698 -0.252230  0.585490
C     3.969909 -0.462742  1.081973
C     4.399014  0.338155  2.157214
H     5.400541  0.206592  2.555853
C     3.527575  1.269386  2.682713
H     3.816104  1.897691  3.520296
C     2.245614  1.415631  2.132651
H     1.520452  2.114097  2.534136
C     4.307671 -2.239557 -0.552835
C     4.787973 -1.469833  0.477326
O    -4.960910 -3.401248  1.066767
O    -5.695806 -2.081873 -1.338942
C    -6.284933 -3.409754  0.571878
C    -6.271074 -3.308939 -0.940578
O     5.037192 -3.228941 -1.131769
O     6.045394 -1.611519  0.976339
C     6.181837 -3.590751 -0.378092
C     6.895830 -2.347696  0.113683
H    -6.739309 -4.347279  0.907461
H    -6.845630 -2.562525  0.995036
H    -7.284576 -3.329367 -1.353617
H    -5.691745 -4.145619 -1.360552
H     7.185594 -1.718565 -0.740489
H     7.785964 -2.602070  0.696236
H     5.876491 -4.210058  0.478044
H     6.818101 -4.181457 -1.043516
 total energy= -2335.09733859
          zpe= -2334.510405
    th energy= -2334.472018
  th enthalpy= -2334.471074
  free energy= -2334.581434

pbe0-d3bj-bs1-3b--td-trip--vsing-
1001
Ru    0.001577  0.795960  0.125841
O    -0.821768  1.358621  3.233729
O     2.335365  1.366263 -2.102083
N    -0.778227  2.313356  1.155742
N     0.630572  2.418520 -0.994912
N    -1.659584  0.554226 -1.046062
N    -0.969739 -0.762469  1.183472
N     0.984518 -0.732658 -0.970377
N     1.823467  0.642498  1.149385
C    -1.265652  2.215914  2.470693
C    -2.257704  3.194794  2.863123
H    -2.724034  3.051998  3.833045
C    -2.501578  4.283230  2.078092
H    -3.212547  5.043544  2.396462
C    -1.801387  4.454857  0.859804
H    -1.948463  5.346139  0.260173
C    -0.941055  3.465230  0.435730
C    -0.091892  3.543617 -0.764262
C     0.019369  4.675243 -1.549667
H    -0.560892  5.566271 -1.337740
C     0.936068  4.638387 -2.618712
H     1.038665  5.506994 -3.268177
C     1.708194  3.527401 -2.829489
H     2.438187  3.477535 -3.632728
C     1.612853  2.362410 -1.977503
C    -2.002195  1.209659 -2.190998
H    -1.289173  1.953174 -2.532535
C    -3.154812  0.944066 -2.884875
H    -3.364609  1.497903 -3.794951
C    -4.056560 -0.054358 -2.418422
H    -4.971701 -0.287870 -2.951019
C    -3.732421 -0.742297 -1.248254
C    -2.527837 -0.426875 -0.571225
C    -2.155095 -1.119399  0.583323
C    -2.982321 -2.139759  1.138371
C    -2.564334 -2.767737  2.309726
H    -3.185898 -3.543101  2.749184
C    -1.360898 -2.383059  2.900399
H    -1.011404 -2.839605  3.820803
C    -0.605901 -1.369666  2.302360
```

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H     0.319760 -1.022117  2.750309
C    -4.554625 -1.781279 -0.690163
C    -4.201642 -2.446220  0.458776
C     0.524481 -1.401207 -2.014789
H    -0.479111 -1.146009 -2.339044
C     1.291941 -2.375004 -2.671659
H     0.867081 -2.894666 -3.525397
C     2.568193 -2.654260 -2.231310
H     3.189293 -3.399887 -2.718498
C     3.070110 -1.948085 -1.122335
C     2.231983 -0.994052 -0.522072
C     2.684818 -0.253334  0.609383
C     3.974961 -0.467382  1.127057
C     4.366351  0.288954  2.247535
H     5.360480  0.155070  2.663391
C     3.466902  1.181702  2.793643
H     3.725378  1.775927  3.665240
C     2.196297  1.333572  2.220173
H     1.451111  2.000797  2.638027
C     4.381096 -2.156910 -0.584103
C     4.823247 -1.431826  0.494282
O    -4.984265 -3.417449  1.016810
O    -5.700308 -2.066146 -1.377098
C    -6.306955 -3.406761  0.519284
C    -6.288009 -3.291169 -0.992015
O     5.141117 -3.104077 -1.193636
O     6.071022 -1.578026  1.016167
C     6.275468 -3.482829 -0.432874
C     6.954374 -2.253667  0.137363
H    -6.772266 -4.342626  0.844432
H    -6.859991 -2.557726  0.949096
H    -7.300537 -3.298049 -1.407961
H    -5.715719 -4.129489 -1.418382
H     7.250715 -1.576755 -0.677111
H     7.836156 -2.521248  0.726668
H     5.963213 -4.150168  0.383779
H     6.937569 -4.027482 -1.112252
 total energy= -2335.10498127
          zpe= -2334.519149
    th energy= -2334.480641
  th enthalpy= -2334.479697
  free energy= -2334.589148

pbe0-d3bj-bs1-3b--td-trip--vtrip-
1001
Ru    0.003628  0.889762  0.078789
O    -0.928777  1.205600  3.171964
O     2.266948  1.643889 -2.137898
N    -0.843874  2.387073  1.222249
N     0.488595  2.525309 -0.982821
N    -1.841458  0.652211 -0.900414
N    -0.786035 -0.785441  1.088170
N     0.957142 -0.532913 -1.111279
N     1.802216  0.766361  1.063482
C    -1.272819  2.206276  2.531543
C    -2.107037  3.259890  3.065702
H    -2.507175  3.102526  4.063439
C    -2.339071  4.410073  2.361015
H    -2.950443  5.201771  2.792341
C    -1.768260  4.592536  1.084953
H    -1.892927  5.524710  0.545608
C    -1.023121  3.553176  0.560579
C    -0.275841  3.632495 -0.709564
C    -0.285374  4.727673 -1.542494
H    -0.904494  5.587403 -1.312259
C     0.538457  4.720492 -2.694949
H     0.517443  5.572767 -3.372391
C     1.370896  3.669205 -2.933916
H     2.049534  3.640073 -3.781207
C     1.440915  2.543406 -2.020791
C    -2.365626  1.397502 -1.881584
H    -1.792943  2.272761 -2.173373
C    -3.559508  1.076081 -2.513850
H    -3.926843  1.717652 -3.309074
C    -4.267330 -0.067771 -2.121597
H    -5.201956 -0.348456 -2.596723
C    -3.752392 -0.850608 -1.089266
C    -2.524987 -0.465923 -0.491231
C    -1.970081 -1.218335  0.560031
C    -2.641260 -2.359488  1.073008
C    -2.070032 -3.033408  2.151378
H    -2.567813 -3.906344  2.563111
C    -0.873802 -2.556835  2.687957
H    -0.404787 -3.044168  3.536868
C    -0.273763 -1.427665  2.132463
H     0.639828 -1.013155  2.544019
C    -4.402028 -2.030530 -0.589893
C    -3.878269 -2.744162  0.457324
C     0.526205 -1.123972 -2.216997
H    -0.452795 -0.812808 -2.571589
C     1.272145 -2.097772 -2.888824
H     0.863412 -2.558267 -3.783126
C     2.517451 -2.467400 -2.395613
H     3.121137 -3.223197 -2.889099
C     3.000292 -1.842421 -1.240656
C     2.183331 -0.869946 -0.619845
C     2.628485 -0.185314  0.532607
C     3.896926 -0.462289  1.090329
C     4.297323  0.267648  2.214985
H     5.269464  0.077170  2.659300
C     3.434785  1.231836  2.739240
H     3.710269  1.810911  3.615356
C     2.199209  1.453413  2.138781
H     1.484895  2.172759  2.524332
C     4.275438 -2.133547 -0.653924
C     4.710240 -1.463585  0.461999
O    -4.496308 -3.840745  0.979194
O    -5.562968 -2.382781 -1.213046
C    -5.851125 -3.947825  0.585300
C    -5.977160 -3.699414 -0.904673
O     5.014300 -3.100440 -1.264318
O     5.929908 -1.689329  1.025486
C     6.090286 -3.561920 -0.468433
C     6.810047 -2.387665  0.164278
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H    -6.175577 -4.958190  0.852281
H    -6.456056 -3.213576  1.137930
H    -7.015240 -3.787646 -1.239628
H    -5.355478 -4.421919 -1.454823
H     7.175942 -1.707893 -0.619446
H     7.652193 -2.718612  0.779353
H     5.707730 -4.230939  0.316773
H     6.750864 -4.126059 -1.133691
 total energy= -2335.09665450
          zpe= -2334.511136
    th energy= -2334.472713
  th enthalpy= -2334.471768
  free energy= -2334.582447

pbe0-d3bj-bs1-3b--gs-triplet-mc
Ru   -0.083114  0.404963 -0.137103
O    -2.370688  0.892284  2.285821
O     1.865241  0.796072 -2.319202
N    -1.011103  2.220333  1.028680
N     0.708142  2.179502 -0.957907
N    -1.876111  0.465030 -1.188411
N    -1.154530 -1.228303  0.717466
N     1.397214 -1.648190 -0.782061
N     1.765908  0.399314  0.987956
C    -2.057549  2.035963  1.912848
C    -2.732205  3.237708  2.352771
H    -3.542584  3.117785  3.067658
C    -2.376667  4.467299  1.859910
H    -2.910014  5.359671  2.188507
C    -1.337121  4.591777  0.916622
H    -1.079235  5.553654  0.486528
C    -0.687027  3.429237  0.532192
C     0.392554  3.405389 -0.483781
C     1.038167  4.539221 -0.952485
H     0.798081  5.518278 -0.553088
C     2.022598  4.377845 -1.944508
H     2.544691  5.255653 -2.325224
C     2.331651  3.133353 -2.436855
H     3.085551  2.985898 -3.205415
C     1.658725  1.964508 -1.938118
C    -2.202407  1.328821 -2.148439
H    -1.403676  1.985660 -2.480147
C    -3.493302  1.393218 -2.684089
H    -3.703100  2.113590 -3.469547
C    -4.482988  0.552965 -2.206858
H    -5.495052  0.585369 -2.598782
C    -4.161403 -0.356211 -1.184800
C    -2.836249 -0.369919 -0.710442
C    -2.447485 -1.275101  0.316587
C    -3.390404 -2.152144  0.883011
C    -2.955454 -3.001508  1.913751
H    -3.660861 -3.680121  2.383908
C    -1.632338 -2.943592  2.310679
H    -1.259531 -3.582229  3.106405
C    -0.761401 -2.042299  1.688398
H     0.283079 -1.964025  1.976807
C    -5.108615 -1.262028 -0.604855
C    -4.738781 -2.120262  0.400491
C     1.205726 -2.584232 -1.688580
H     0.176375 -2.729342 -2.015122
C     2.249026 -3.364474 -2.214294
H     2.038422 -4.121043 -2.965523
C     3.530962 -3.160151 -1.748537
H     4.369145 -3.748869 -2.109774
C     3.754483 -2.161649 -0.781739
C     2.642054 -1.409822 -0.343834
C     2.828083 -0.361614  0.628630
C     4.113720 -0.141244  1.170532
C     4.271202  0.872734  2.132576
H     5.254955  1.061375  2.551834
C     3.167007  1.605276  2.512582
H     3.240267  2.396942  3.252559
C     1.931158  1.344570  1.909366
H     1.038854  1.920178  2.144594
C     5.049697 -1.904018 -0.230211
C     5.221080 -0.928263  0.715354
O    -5.618139 -2.968917  0.998978
O    -6.372167 -1.216983 -1.107690
C    -6.968365 -2.616935  0.753710
C    -7.165177 -2.324853 -0.720520
O     6.071459 -2.680969 -0.682426
O     6.436461 -0.635487  1.256614
C     7.231193 -2.599735  0.126522
C     7.510706 -1.156195  0.494456
H    -7.576295 -3.466801  1.077501
H    -7.231144 -1.731219  1.350273
H    -8.202793 -2.057346 -0.941388
H    -6.882452 -3.205827 -1.315762
H     7.639806 -0.555509 -0.417883
H     8.406399 -1.068625  1.116441
H     7.085084 -3.195105  1.040060
H     8.049932 -3.029967 -0.457989
    el energy= -2335.07863002
          zpe= -2334.491309
    th energy= -2334.452100
  th enthalpy= -2334.451156
  free energy= -2334.566125

pbe0-d3bj-bs1-3b--gs-triplet
Ru    0.004912  0.788202  0.132492
O    -0.843870  1.265512  3.254856
O     2.353344  1.483916 -2.056771
N    -0.814735  2.276012  1.201391
N     0.592955  2.445532 -0.951761
N    -1.667983  0.547856 -1.048840
N    -0.938126 -0.790154  1.156563
N     1.027757 -0.664881 -1.017889
N     1.799373  0.602233  1.191014
C    -1.293228  2.140638  2.510958
C    -2.299529  3.096790  2.919253
H    -2.757126  2.934065  3.890602
C    -2.585480  4.183280  2.143989
H    -3.314910  4.919124  2.479148
C    -1.909966  4.386013  0.917465
```

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H    -2.084068  5.281041  0.330731
C    -1.026759  3.423233  0.484458
C    -0.183341  3.536875 -0.717889
C    -0.128594  4.666441 -1.511293
H    -0.750392  5.529092 -1.300116
C     0.784075  4.672271 -2.585617
H     0.838481  5.542636 -3.238512
C     1.612823  3.603420 -2.793800
H     2.344197  3.587373 -3.597089
C     1.579006  2.439513 -1.934580
C    -2.016826  1.220852 -2.171382
H    -1.315108  1.982408 -2.497971
C    -3.172670  0.953601 -2.869431
H    -3.393629  1.522305 -3.767568
C    -4.053279 -0.060714 -2.415418
H    -4.969007 -0.295384 -2.947991
C    -3.722181 -0.764121 -1.261571
C    -2.515248 -0.447565 -0.582789
C    -2.125824 -1.150506  0.559793
C    -2.942359 -2.183155  1.105311
C    -2.517471 -2.823122  2.265339
H    -3.130270 -3.608764  2.698055
C    -1.311579 -2.432601  2.856807
H    -0.955152 -2.897661  3.770426
C    -0.567404 -1.408429  2.273173
H     0.354703 -1.057709  2.724629
C    -4.532588 -1.818362 -0.713586
C    -4.165309 -2.490553  0.424573
C     0.604775 -1.274427 -2.113869
H    -0.394973 -1.015588 -2.448277
C     1.401478 -2.197313 -2.807146
H     1.004668 -2.672151 -3.699662
C     2.670621 -2.486644 -2.351071
H     3.313499 -3.194784 -2.865158
C     3.135195 -1.841346 -1.190405
C     2.269186 -0.935308 -0.555360
C     2.684344 -0.254472  0.625495
C     3.963731 -0.483253  1.164001
C     4.316640  0.214003  2.334047
H     5.301340  0.068140  2.768000
C     3.391613  1.064573  2.906058
H     3.620046  1.610136  3.816976
C     2.133772  1.234768  2.310661
H     1.362828  1.858182  2.749981
C     4.434740 -2.065838 -0.631351
C     4.839513 -1.400613  0.499243
O    -4.934549 -3.473996  0.976702
O    -5.678234 -2.106137 -1.398914
C    -6.259961 -3.474659  0.485271
C    -6.250404 -3.342472 -1.024817
O     5.222638 -2.966576 -1.275242
O     6.074979 -1.563444  1.044545
C     6.340510 -3.378013 -0.507047
C     6.989435 -2.177712  0.152541
H    -6.711701 -4.419760  0.802595
H    -6.820814 -2.637362  0.927476
H    -7.265004 -3.355848 -1.435389
H    -5.670790 -4.169014 -1.463880
H     7.299928 -1.451281 -0.612492
H     7.857971 -2.470578  0.749451
H     6.014291 -4.095382  0.260244
H     7.026982 -3.874974 -1.198693
    el energy= -2335.09797595
          zpe= -2334.511994
    th energy= -2334.473439
  th enthalpy= -2334.472494
  free energy= -2334.583609

pbe0-d3bj-bs1-3b--gs-singlet
Ru    0.020045  0.657748  0.069947
O    -1.097796  0.911572  3.100337
O     2.206683  1.341806 -2.271995
N    -0.807228  2.175037  1.212957
N     0.616685  2.361313 -0.966721
N    -1.718576  0.558782 -1.044241
N    -0.961541 -0.913659  1.023144
N     1.080206 -0.754833 -1.038698
N     1.767119  0.571110  1.150178
C    -1.320668  1.970107  2.489983
C    -2.091810  3.055912  3.043457
H    -2.550730  2.880261  4.012684
C    -2.189145  4.260141  2.396510
H    -2.752173  5.078263  2.845333
C    -1.542425  4.457905  1.163797
H    -1.561814  5.424222  0.673572
C    -0.858304  3.388719  0.609674
C    -0.068997  3.487615 -0.635046
C    -0.008501  4.643573 -1.395919
H    -0.573915  5.524968 -1.116951
C     0.814810  4.641965 -2.536003
H     0.869815  5.532620 -3.161854
C     1.554577  3.532658 -2.849611
H     2.215229  3.502822 -3.711933
C     1.513042  2.339622 -2.035408
C    -2.060016  1.300848 -2.097850
H    -1.327887  2.037138 -2.415295
C    -3.283992  1.140348 -2.758991
H    -3.506940  1.775653 -3.611560
C    -4.188298  0.189194 -2.325174
H    -5.144714  0.043369 -2.817961
C    -3.847038 -0.605567 -1.216163
C    -2.596012 -0.385280 -0.607981
C    -2.183529 -1.180506  0.501330
C    -3.036062 -2.177428  1.015250
C    -2.581230 -2.924980  2.114325
H    -3.214050 -3.698025  2.539518
C    -1.329744 -2.644415  2.629982
H    -0.943581 -3.190905  3.485629
C    -0.553685 -1.625490  2.067080
H     0.411396 -1.352537  2.478973
C    -4.700570 -1.626501 -0.685162
C    -4.314422 -2.375556  0.398723
C     0.702942 -1.408340 -2.128195
H    -0.298671 -1.193996 -2.489899
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C     1.542413 -2.309508 -2.796533
H     1.177981 -2.811624 -3.688403
C     2.817291 -2.541497 -2.321702
H     3.494783 -3.230613 -2.816495
C     3.237768 -1.857643 -1.166514
C     2.329169 -0.974065 -0.558782
C     2.700960 -0.259757  0.616977
C     3.979555 -0.428053  1.178615
C     4.286022  0.299357  2.343671
H     5.267870  0.200393  2.796694
C     3.316997  1.122924  2.882765
H     3.508971  1.694406  3.786472
C     2.064706  1.236306  2.262964
H     1.274081  1.860800  2.663040
C     4.536838 -2.020195 -0.584739
C     4.899310 -1.321020  0.539664
O    -5.109592 -3.332936  0.947806
O    -5.892898 -1.806529 -1.317508
C    -6.460339 -3.231332  0.532686
C    -6.526375 -3.023815 -0.967182
O     5.370355 -2.900123 -1.203890
O     6.134386 -1.426593  1.103198
C     6.494187 -3.250190 -0.416661
C     7.083415 -2.012625  0.230310
H    -6.948808 -4.163965  0.829835
H    -6.941115 -2.387625  1.049077
H    -7.560522 -2.948834 -1.316169
H    -6.028827 -3.859547 -1.481391
H     7.369600 -1.285735 -0.543971
H     7.958431 -2.257827  0.839435
H     6.190743 -3.967626  0.360334
H     7.210052 -3.729368 -1.091199
    el energy= -2335.15435038
          zpe= -2334.565494
    th energy= -2334.527421
  th enthalpy= -2334.526477
  free energy= -2334.635856

b3lyp-bs1-2a--td-sing--vsing-1001
Ru    0.000011  0.179221  0.000021
O    -2.012109  0.560396  2.544114
H    -2.630312  0.640007  3.284736
O     2.012422  0.561130 -2.543737
H     2.630696  0.640967 -3.284275
N    -0.842169  1.836219  1.064069
N     0.841723  1.836530 -1.063928
N    -1.791922  0.138506 -1.118895
N    -1.045895 -1.441502  0.914507
N     1.046286 -1.441181 -0.914654
N     1.791938  0.138809  1.118866
C    -1.715750  1.804515  2.089586
C    -2.268623  2.937185  2.672284
H    -2.951503  2.847727  3.512207
C    -1.910829  4.193521  2.140072
H    -2.337518  5.100648  2.559346
C    -1.025786  4.264536  1.088156
H    -0.765300  5.228671  0.668595
C    -0.467123  3.080339  0.538105
C     0.466132  3.080516 -0.538027
C     1.024315  4.264921 -1.088109
H     0.763387  5.228968 -0.668619
C     1.909479  4.194232 -2.139948
H     2.335801  5.101522 -2.559241
C     2.267887  2.938023 -2.672041
H     2.950928  2.848809 -3.511858
C     1.715440  1.805146 -2.089337
C    -2.143023  0.966870 -2.105947
H    -1.420170  1.730346 -2.373088
C    -3.378455  0.857986 -2.767857
H    -3.613830  1.553682 -3.567685
C    -4.272223 -0.129230 -2.388911
H    -5.233561 -0.228690 -2.888245
C    -3.932354 -1.012582 -1.337759
C    -2.669242 -0.833864 -0.725808
C    -2.268001 -1.678078  0.356054
C    -3.129458 -2.706592  0.807028
C    -2.673656 -3.507829  1.879427
H    -3.301558 -4.310336  2.260248
C    -1.430207 -3.258948  2.433097
H    -1.051883 -3.854266  3.258868
C    -0.641526 -2.212703  1.921083
H     0.332328 -1.988490  2.345538
C    -4.789967 -2.063352 -0.862837
H    -5.758666 -2.198446 -1.337698
C    -4.403476 -2.877053  0.164126
H    -5.060673 -3.668948  0.515167
C     0.642109 -2.212363 -1.921321
H    -0.331775 -1.988304 -2.345790
C     1.431017 -3.258404 -2.433403
H     1.052843 -3.853714 -3.259250
C     2.674490 -3.507101 -1.879706
H     3.302560 -4.309453 -2.260578
C     3.130096 -2.705874 -0.807215
C     2.268420 -1.677570 -0.356185
C     2.669465 -0.833361  0.725753
C     3.932592 -1.011866  1.337734
C     4.272250 -0.128506  2.388945
H     5.233587 -0.227806  2.888313
C     3.378278  0.858522  2.767910
H     3.613497  1.554223  3.567780
C     2.142847  0.967203  2.105969
H     1.419838  1.730529  2.373117
C     4.404123 -2.876135 -0.164276
H     5.061490 -3.667873 -0.515352
C     4.790421 -2.062438  0.862762
H     5.759130 -2.197384  1.337645
    el energy= -1882.60777204
 total energy= -1882.53124697
          zpe= -1882.013976
    th energy= -1881.981253
  th enthalpy= -1881.980309
  free energy= -1882.077175

b3lyp-bs1-2a--td-trip--vsing-1001
```

Ru	0.015144	0.214114	0.018710
O	-1.693307	0.058048	2.802640
H	-2.240761	-0.039507	3.595201
O	2.166419	1.249862	-2.193810
H	2.790562	1.530567	-2.878568
N	-1.141832	1.568651	1.197880
N	0.442396	2.034815	-0.920383
N	-1.770493	-0.109066	-1.105370
N	-0.697132	-1.644595	0.821916
N	1.316625	-1.094412	-1.060473
N	1.786849	0.373397	1.140715
C	-1.876396	1.299504	2.288966
C	-2.748110	2.211823	2.881192
H	-3.296748	1.945290	3.780237
C	-2.879914	3.484368	2.286670
H	-3.562986	4.213289	2.714128
C	-2.131078	3.800112	1.176280
H	-2.220685	4.780967	0.725262
C	-1.228759	2.843789	0.627167
C	-0.372465	3.107112	-0.471626
C	-0.271152	4.378380	-1.102568
H	-0.910680	5.190937	-0.779277
C	0.654248	4.588786	-2.094574
H	0.740934	5.561250	-2.571012
C	1.519034	3.532192	-2.484151
H	2.274746	3.677040	-3.251041
C	1.376833	2.301588	-1.867245
C	-2.281897	0.675371	-2.057238
H	-1.712879	1.564031	-2.307743
C	-3.490855	0.374931	-2.709874
H	-3.858439	1.047907	-3.478782
C	-4.188014	-0.768219	-2.362392
H	-5.125535	-1.019340	-2.853579
C	-3.671741	-1.618736	-1.357398
C	-2.449098	-1.241689	-0.751265
C	-1.873908	-2.060714	0.272261
C	-2.522814	-3.254951	0.669889
C	-1.897807	-4.029173	1.674395
H	-2.360795	-4.954351	2.010512
C	-0.699935	-3.598769	2.216299
H	-0.192953	-4.169920	2.988470
C	-0.129005	-2.396449	1.762604
H	0.801866	-2.029124	2.183041
C	-4.315314	-2.830165	-0.929952
H	-5.254969	-3.112190	-1.398651
C	-3.763238	-3.615861	0.040984
H	-4.257163	-4.532443	0.354268
C	1.056196	-1.805200	-2.154193
H	0.065979	-1.689136	-2.584811
C	2.005736	-2.660222	-2.744919
H	1.737784	-3.214888	-3.639370
C	3.262105	-2.775536	-2.178384
H	4.013406	-3.428183	-2.617555
C	3.569895	-2.030274	-1.016109
C	2.552037	-1.199109	-0.490913
C	2.806866	-0.411587	0.676215
C	4.076784	-0.451139	1.298861
C	4.267600	0.370952	2.434193
H	5.229103	0.372931	2.943116
C	3.229740	1.170516	2.883495
H	3.350001	1.816128	3.748287
C	1.997678	1.148202	2.208613
H	1.161278	1.760938	2.528285
C	4.847188	-2.067034	-0.358154
H	5.623071	-2.710644	-0.765727
C	5.092063	-1.307693	0.750529
H	6.064737	-1.337992	1.235444

el energy= -1882.60618388
total energy= -1882.53686732
zpe= -1882.021098
th energy= -1881.988220
th enthalpy= -1881.987275
free energy= -1882.084733

b3lyp-bs1-2a--gs-triplet

Ru	-0.033143	0.119452	-0.128941
O	-2.117802	0.369887	2.768039
H	-2.764276	0.260570	3.480791
O	1.654359	1.221260	-2.465686
H	2.278601	1.420548	-3.179277
N	-1.437063	1.810096	1.171599
N	0.176915	2.150243	-1.037488
N	-1.771052	-0.443594	-1.204365
N	-0.640746	-1.674876	0.901870
N	1.699720	-1.394037	-0.951876
N	1.772932	0.529439	1.003532
C	-2.311668	1.553244	2.144093
C	-3.345149	2.435616	2.500380
H	-4.035798	2.192681	3.304773
C	-3.457262	3.622152	1.788774
H	-4.252837	4.325382	2.021405
C	-2.542606	3.906125	0.769643
H	-2.638927	4.820138	0.195110
C	-1.532407	2.979088	0.498762
C	-0.506011	3.226429	-0.549320
C	-0.249471	4.516967	-1.016341
H	-0.763775	5.367948	-0.585973
C	0.696697	4.710921	-2.025105
H	0.907970	5.710519	-2.395935
C	1.363668	3.613706	-2.549947
H	2.097686	3.721439	-3.344822
C	1.069297	2.350569	-2.020173
C	-2.310388	0.172112	-2.261718
H	-1.811417	1.076250	-2.596381
C	-3.458773	-0.304709	-2.915831
H	-3.847457	0.239508	-3.771552
C	-4.075178	-1.455591	-2.456624
H	-4.967328	-1.842553	-2.943914
C	-3.534113	-2.133033	-1.340434
C	-2.369711	-1.588008	-0.745258
C	-1.772160	-2.236073	0.381327
C	-2.352558	-3.415654	0.909634
C	-1.720787	-4.005741	2.027893
H	-2.133067	-4.912558	2.465106

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C    -0.581180 -3.420817  2.552293
H    -0.072455 -3.849147  3.411011
C    -0.069554 -2.254104  1.958151
H     0.825842 -1.776660  2.344550
C    -4.100984 -3.333015 -0.789224
H    -4.994545 -3.744866 -1.252116
C    -3.535712 -3.946953  0.291311
H    -3.973749 -4.854114  0.700807
C     1.645402 -2.318108 -1.903125
H     0.677299 -2.466832 -2.378426
C     2.762506 -3.080009 -2.298259
H     2.660785 -3.822298 -3.084899
C     3.971959 -2.864832 -1.664178
H     4.855500 -3.437296 -1.938717
C     4.061203 -1.889642 -0.643208
C     2.880071 -1.168401 -0.323128
C     2.918342 -0.160986  0.709418
C     4.138071  0.085621  1.394929
C     4.142680  1.071921  2.406952
H     5.062098  1.281833  2.949178
C     2.976254  1.754766  2.694939
H     2.940893  2.516256  3.468483
C     1.812843  1.453418  1.968489
H     0.877597  1.966278  2.169836
C     5.277712 -1.611447  0.066090
H     6.172399 -2.173635 -0.191320
C     5.312974 -0.663542  1.045682
H     6.235808 -0.457285  1.582623
    el energy= -1882.55173007
          zpe= -1882.035406
    th energy= -1882.001787
  th enthalpy= -1882.000843
  free energy= -1882.102789

b3lyp-bs1-2a--gs-singlet
Ru   -0.001517  0.216922  0.006578
O    -1.936362  0.506342  2.632886
H    -2.541068  0.528551  3.389304
O     2.026406  0.832683 -2.489337
H     2.648661  0.957674 -3.221097
N    -0.940679  1.850333  1.091403
N     0.722232  1.987505 -1.025702
N    -1.775395  0.007014 -1.145144
N    -0.924765 -1.435109  0.954497
N     1.095854 -1.286215 -0.999804
N     1.784445  0.164252  1.152357
C    -1.763700  1.750402  2.151326
C    -2.403472  2.853285  2.737177
H    -3.062413  2.711223  3.590642
C    -2.178271  4.110595  2.202461
H    -2.663153  4.986024  2.626031
C    -1.314305  4.236577  1.113960
H    -1.131705  5.215961  0.690754
C    -0.703930  3.098844  0.584364
C     0.245315  3.177991 -0.548117
C     0.640649  4.401130 -1.091436
H     0.265346  5.335367 -0.694019
C     1.542880  4.422408 -2.155659
H     1.861972  5.366175 -2.589685
C     2.026566  3.221912 -2.647687
H     2.731350  3.192745 -3.475474
C     1.591991  2.028058 -2.051998
C    -2.186593  0.742347 -2.181587
H    -1.529574  1.550877 -2.487063
C    -3.395405  0.499403 -2.857749
H    -3.673402  1.133903 -3.694291
C    -4.206079 -0.544150 -2.448065
H    -5.144383 -0.755001 -2.956223
C    -3.802494 -1.344827 -1.354990
C    -2.572825 -1.024729 -0.728568
C    -2.111050 -1.800616  0.384140
C    -2.881949 -2.893412  0.850577
C    -2.375152 -3.628537  1.946616
H    -2.933805 -4.477473  2.334407
C    -1.168550 -3.254159  2.509253
H    -0.746661 -3.796447  3.350550
C    -0.473830 -2.149028  1.985249
H     0.467254 -1.827381  2.419663
C    -4.567810 -2.455089 -0.858864
H    -5.510559 -2.694707 -1.344886
C    -4.124651 -3.198861  0.196762
H    -4.709917 -4.039621  0.561685
C     0.728875 -2.001599 -2.062250
H    -0.238309 -1.763199 -2.493257
C     1.538499 -3.007334 -2.620709
H     1.181279 -3.556774 -3.486929
C     2.773114 -3.276994 -2.059011
H     3.419333 -4.048133 -2.472430
C     3.193875 -2.535710 -0.931071
C     2.310846 -1.547272 -0.432261
C     2.685506 -0.765719  0.708697
C     3.940333 -0.975449  1.331560
C     4.256471 -0.170260  2.449874
H     5.210457 -0.297998  2.956528
C     3.342061  0.772546  2.884810
H     3.552101  1.408537  3.739837
C     2.115675  0.908960  2.210382
H     1.378233  1.637091  2.534025
C     4.458523 -2.733633 -0.277783
H     5.129473 -3.496147 -0.666352
C     4.818073 -1.984031  0.805198
H     5.778909 -2.140779  1.289606
    el energy= -1882.61681914
          zpe= -1882.097968
    th energy= -1882.065629
  th enthalpy= -1882.064685
  free energy= -1882.161630

b3lyp-bs1-2b--td-sing--vsing-1001
Ru   -0.018716  0.217628  0.058366
O     1.819817  0.353347  2.922706
O    -2.239531  1.320498 -2.191528
N     1.151696  1.680632  1.163966
N    -0.494068  2.084197 -0.889217
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N	-1.236393	-1.047734	-1.054362
N	-1.781728	0.290971	1.181291
N	1.728609	-0.143768	-1.136215
N	0.727341	-1.570519	0.940532
C	1.929420	1.417860	2.308597
C	2.851341	2.449124	2.764810
H	3.471385	2.191656	3.618036
C	2.909429	3.677330	2.148177
H	3.593993	4.449191	2.494055
C	2.058029	3.925674	1.066430
H	2.077547	4.889304	0.575678
C	1.189455	2.899140	0.610282
C	0.248152	3.143467	-0.502677
C	0.123298	4.420104	-1.076142
H	0.729422	5.250089	-0.738375
C	-0.823818	4.616183	-2.097699
H	-0.930935	5.596145	-2.559628
C	-1.607485	3.561892	-2.489145
H	-2.363703	3.654971	-3.263355
C	-1.489230	2.247726	-1.868235
C	-0.945196	-1.685994	-2.187428
H	0.050114	-1.514452	-2.583808
C	-1.859711	-2.529014	-2.842246
H	-1.556991	-3.022182	-3.761928
C	-3.122586	-2.718412	-2.309113
H	-3.849032	-3.365192	-2.796952
C	-3.465003	-2.051961	-1.113277
C	-2.482648	-1.223270	-0.521739
C	-2.779061	-0.503225	0.677096
C	-4.053469	-0.618831	1.283364
C	-4.288959	0.128521	2.457598
H	-5.254923	0.066855	2.954672
C	-3.277312	0.933870	2.956025
H	-3.420230	1.523226	3.857773
C	-2.041069	0.989468	2.291899
H	-1.225363	1.601372	2.663561
C	-4.746894	-2.163852	-0.474057
H	-5.497267	-2.807095	-0.929820
C	-5.029390	-1.479180	0.672698
H	-6.006515	-1.569666	1.143227
C	2.235196	0.571069	-2.163045
H	1.669749	1.456964	-2.437273
C	3.383640	0.216488	-2.854905
H	3.727273	0.835756	-3.678156
C	4.079633	-0.958043	-2.479246
H	4.981806	-1.266662	-3.002494
C	3.590725	-1.727344	-1.417712
C	2.402831	-1.294492	-0.750249
C	1.877766	-2.040319	0.325261
C	2.520296	-3.242826	0.772477
C	1.955933	-3.931441	1.854094
H	2.426739	-4.846844	2.210136
C	0.807623	-3.434655	2.465863
H	0.348397	-3.935385	3.312486
C	0.239504	-2.244895	1.969476
H	-0.645440	-1.823056	2.438281
C	4.215835	-2.942088	-0.953818
H	5.120221	-3.275770	-1.460451
C	3.705034	-3.664017	0.087584
H	4.198914	-4.576442	0.418858

el energy= -1881.83028491
total energy= -1881.79716968
zpe= -1881.310135
th energy= -1881.277576
th enthalpy= -1881.276632
free energy= -1881.373791

b3lyp-bs1-2b--td-sing--vtrip-1001

Ru	0.016752	0.289697	0.053759
O	1.243229	0.134103	3.121538
O	-2.075162	1.716689	-2.068162
N	1.235661	1.500969	1.275461
N	-0.143259	2.109035	-0.862853
N	-1.320449	-0.809052	-1.174651
N	-1.751890	0.487916	1.141927
N	1.764942	-0.282760	-1.045448
N	0.498882	-1.613439	0.912637
C	1.712890	1.123673	2.537613
C	2.752267	1.963618	3.104494
H	3.171798	1.639092	4.052764
C	3.145228	3.124724	2.489441
H	3.909964	3.755727	2.940974
C	2.543658	3.521888	1.275015
H	2.811540	4.463371	0.809741
C	1.591645	2.681422	0.710338
C	0.818346	3.026868	-0.508225
C	1.001878	4.201880	-1.217384
H	1.774797	4.902142	-0.922857
C	0.164240	4.493651	-2.324213
H	0.324778	5.409006	-2.891575
C	-0.850400	3.640385	-2.647683
H	-1.547740	3.833792	-3.457318
C	-1.093996	2.433786	-1.869755
C	-1.096218	-1.405299	-2.342687
H	-0.088046	-1.313352	-2.737470
C	-2.082265	-2.120190	-3.040801
H	-1.829930	-2.592210	-3.985815
C	-3.362441	-2.213534	-2.501911
H	-4.148241	-2.760781	-3.019396
C	-3.641512	-1.586206	-1.277208
C	-2.583239	-0.882714	-0.634953
C	-2.810684	-0.199380	0.585494
C	-4.096409	-0.217774	1.193744
C	-4.267215	0.492213	2.392879
H	-5.238254	0.498457	2.883642
C	-3.181010	1.188565	2.940492
H	-3.279531	1.743305	3.869011
C	-1.949361	1.161838	2.289967
H	-1.077843	1.666864	2.691712
C	-4.928796	-1.606524	-0.640533
H	-5.737131	-2.151302	-1.125082
C	-5.145561	-0.955963	0.539520
H	-6.128453	-0.976152	1.006786
C	2.412915	0.404675	-2.003696

```
H     2.017916  1.389525 -2.231837
C     3.518542 -0.097121 -2.686923
H     3.989208  0.511455 -3.453799
C     4.002386 -1.375229 -2.373988
H     4.865414 -1.790159 -2.890122
C     3.363269 -2.117418 -1.370672
C     2.236474 -1.537514 -0.719016
C     1.571804 -2.234683  0.318686
C     2.028273 -3.519154  0.740069
C     1.350857 -4.140771  1.798530
H     1.671900 -5.122440  2.142279
C     0.281834 -3.483952  2.404714
H    -0.258053 -3.927682  3.235714
C    -0.100917 -2.219844  1.935464
H    -0.911673 -1.673645  2.403954
C     3.788157 -3.427907 -0.949557
H     4.644209 -3.875290 -1.451507
C     3.154520 -4.093587  0.059028
H     3.499610 -5.077973  0.370588
    el energy= -1881.77841498
 total energy= -1881.78835529
          zpe= -1881.300937
    th energy= -1881.268652
  th enthalpy= -1881.267708
  free energy= -1881.364574

b3lyp-bs1-2b--td-trip--vsing-1001
Ru   -0.018796  0.222490  0.083829
O     1.441673  0.458626  3.138191
O    -2.245963  1.347636 -2.149136
N     1.099661  1.659160  1.207738
N    -0.452525  2.071658 -0.893041
N    -1.230111 -1.044781 -1.053194
N    -1.798207  0.289005  1.185434
N     1.713771 -0.140786 -1.125865
N     0.754976 -1.559213  0.978943
C     1.751852  1.425281  2.435825
C     2.757720  2.381223  2.875264
H     3.301687  2.126780  3.779515
C     2.943914  3.565367  2.200072
H     3.673510  4.297508  2.539565
C     2.157401  3.828288  1.071824
H     2.266714  4.766105  0.543021
C     1.240574  2.849426  0.608800
C     0.351813  3.104302 -0.545039
C     0.315238  4.351858 -1.176667
H     0.971266  5.158457 -0.874895
C    -0.613093  4.548945 -2.218605
H    -0.654743  5.507628 -2.733462
C    -1.461083  3.529176 -2.564903
H    -2.202075  3.634420 -3.352511
C    -1.437387  2.243897 -1.878267
C    -0.923647 -1.691532 -2.176723
H     0.085128 -1.544559 -2.547555
C    -1.841176 -2.510908 -2.857373
H    -1.526591 -3.010504 -3.769544
C    -3.121958 -2.666483 -2.359308
H    -3.852092 -3.293086 -2.867565
C    -3.478804 -1.993382 -1.171036
C    -2.492472 -1.190064 -0.552742
C    -2.800270 -0.473985  0.646509
C    -4.089205 -0.570794  1.223892
C    -4.331686  0.158611  2.408281
H    -5.309915  0.111579  2.882499
C    -3.310971  0.923251  2.947464
H    -3.456985  1.494044  3.860542
C    -2.059783  0.963035  2.309696
H    -1.235753  1.538884  2.716804
C    -4.778883 -2.078551 -0.565782
H    -5.532850 -2.699422 -1.045874
C    -5.072043 -1.398457  0.580674
H    -6.061559 -1.469909  1.027901
C     2.192188  0.557876 -2.174256
H     1.621508  1.441594 -2.444380
C     3.321501  0.193913 -2.895423
H     3.641776  0.803826 -3.734665
C     4.026265 -0.976629 -2.524986
H     4.914081 -1.291813 -3.068941
C     3.565302 -1.734311 -1.445901
C     2.394953 -1.295508 -0.748539
C     1.892399 -2.033594  0.339366
C     2.543862 -3.233445  0.779776
C     2.007155 -3.915987  1.876120
H     2.485786 -4.829563  2.225897
C     0.869640 -3.413670  2.514204
H     0.432612 -3.909197  3.375443
C     0.291618 -2.230707  2.026152
H    -0.581254 -1.804466  2.512734
C     4.200974 -2.946630 -0.989579
H     5.092334 -3.285018 -1.515944
C     3.714866 -3.659449  0.067413
H     4.215178 -4.570403  0.393173
    el energy= -1881.83192829
 total energy= -1881.79865811
          zpe= -1881.311393
    th energy= -1881.278869
  th enthalpy= -1881.277925
  free energy= -1881.374608

b3lyp-bs1-2b--td-trip--vtrip-1001
Ru    0.028064  0.271333  0.092727
O     1.007632  0.574278  3.233003
O    -2.139078  1.159752 -2.270849
N     0.939219  1.690007  1.218684
N    -0.460412  2.036471 -0.959581
N    -1.160539 -1.126747 -1.043951
N    -1.822501  0.270688  1.154341
N     1.672476 -0.117483 -1.136812
N     0.859358 -1.440091  1.069809
C     1.458218  1.477274  2.521689
C     2.489740  2.395624  2.973025
H     2.968459  2.158450  3.918424
C     2.749346  3.542626  2.277329
H     3.486583  4.256404  2.641527
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C     2.031093  3.829346  1.087794
H     2.201663  4.760260  0.559415
C     1.131789  2.900680  0.595805
C     0.287184  3.115035 -0.601522
C     0.223840  4.329482 -1.272963
H     0.823091  5.175696 -0.957314
C    -0.661561  4.441007 -2.367383
H    -0.722037  5.379916 -2.916735
C    -1.447303  3.375868 -2.724416
H    -2.151345  3.426499 -3.550449
C    -1.400708  2.118620 -1.998498
C    -0.815998 -1.787980 -2.143053
H     0.190988 -1.615618 -2.507651
C    -1.694605 -2.657883 -2.814682
H    -1.349597 -3.175252 -3.705294
C    -2.977356 -2.835015 -2.329775
H    -3.681010 -3.497556 -2.830029
C    -3.375567 -2.139797 -1.168802
C    -2.422598 -1.289918 -0.554576
C    -2.775189 -0.548732  0.616795
C    -4.072750 -0.673360  1.173600
C    -4.364356  0.082164  2.328765
H    -5.350451  0.013472  2.783623
C    -3.384351  0.902181  2.866500
H    -3.569926  1.494325  3.758128
C    -2.124482  0.970184  2.252168
H    -1.328260  1.581059  2.660502
C    -4.682424 -2.250422 -0.585770
H    -5.407471 -2.907536 -1.061933
C    -5.016399 -1.550624  0.537326
H    -6.010564 -1.641558  0.970199
C     2.106560  0.581718 -2.221595
H     1.505281  1.443865 -2.491041
C     3.219403  0.217937 -2.954268
H     3.506054  0.812527 -3.817003
C     3.961881 -0.930191 -2.579437
H     4.839111 -1.237277 -3.144374
C     3.557050 -1.667755 -1.460192
C     2.402713 -1.236639 -0.740968
C     1.968897 -1.933161  0.402348
C     2.672935 -3.089426  0.870302
C     2.201990 -3.722673  2.026718
H     2.715464 -4.606018  2.403323
C     1.086725 -3.206374  2.689534
H     0.702005 -3.664732  3.595558
C     0.461343 -2.058479  2.178871
H    -0.386380 -1.614936  2.689813
C     4.242819 -2.842188 -0.981183
H     5.122564 -3.178192 -1.527797
C     3.821751 -3.519782  0.127621
H     4.361537 -4.400681  0.471830
    el energy= -1881.77793542
 total energy= -1881.78782694
          zpe= -1881.300089
    th energy= -1881.267785
  th enthalpy= -1881.266841
  free energy= -1881.363709
```

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b3lyp-bs1-2b--gs-triplet
Ru    0.005131  0.270775  0.096470
O     1.086149  0.137545  3.221856
O    -2.184456  1.722592 -1.932559
N     1.157157  1.458927  1.338589
N    -0.244857  2.141204 -0.754463
N    -1.324506 -0.791927 -1.194409
N    -1.771136  0.274602  1.224954
N     1.681721 -0.174878 -1.128915
N     0.633720 -1.622417  0.886350
C     1.616994  1.078202  2.611849
C     2.714425  1.858714  3.153711
H     3.130660  1.516181  4.096920
C     3.148014  2.998149  2.529727
H     3.951581  3.591642  2.964210
C     2.529367  3.435768  1.334413
H     2.818306  4.375774  0.878185
C     1.534017  2.650011  0.777883
C     0.724924  3.047047 -0.396259
C     0.872267  4.258430 -1.050897
H     1.641807  4.959542 -0.748669
C    -0.020763  4.582923 -2.100595
H     0.096206  5.527475 -2.630508
C    -1.038576  3.727828 -2.423100
H    -1.766590  3.952437 -3.197422
C    -1.227879  2.473737 -1.712050
C    -1.087999 -1.272325 -2.412549
H    -0.081901 -1.128959 -2.794487
C    -2.065629 -1.932348 -3.173995
H    -1.805780 -2.312372 -4.157705
C    -3.343302 -2.087845 -2.653336
H    -4.122055 -2.592811 -3.221563
C    -3.631816 -1.576917 -1.374406
C    -2.582832 -0.928260 -0.672514
C    -2.819756 -0.363766  0.610403
C    -4.101727 -0.463067  1.212022
C    -4.275515  0.116622  2.482232
H    -5.245436  0.062449  2.972447
C    -3.197253  0.749982  3.096173
H    -3.293162  1.198462  4.080712
C    -1.962021  0.805672  2.440873
H    -1.088567  1.249561  2.903894
C    -4.920621 -1.671022 -0.746899
H    -5.722212 -2.173958 -1.284420
C    -5.144840 -1.141500  0.490589
H    -6.126711 -1.217580  0.953671
C     2.207176  0.563314 -2.132788
H     1.712536  1.508080 -2.333111
C     3.303163  0.154048 -2.879663
H     3.671620  0.794433 -3.675834
C     3.916073 -1.082560 -2.594987
H     4.777896 -1.424109 -3.164052
C     3.405035 -1.873203 -1.558647
C     2.274976 -1.392657 -0.832649
C     1.727339 -2.147448  0.224885
C     2.305918 -3.397573  0.606135
```

```
C     1.738425 -4.082849  1.686798
H     2.155689 -5.038984  1.997908
C     0.649941 -3.522574  2.360143
H     0.193466 -4.018534  3.211259
C     0.143357 -2.289998  1.932091
H    -0.682676 -1.819384  2.452287
C     3.958799 -3.146785 -1.173529
H     4.819389 -3.519133 -1.726644
C     3.437568 -3.870734 -0.141015
H     3.878454 -4.826091  0.138867
    el energy= -1881.78712628
          zpe= -1881.299985
    th energy= -1881.267511
  th enthalpy= -1881.266566
  free energy= -1881.363963

b3lyp-bs1-2b--gs-singlet
Ru   -0.014564  0.164210  0.044290
O     1.314435  0.187745  3.039635
O    -2.160303  1.132761 -2.283155
N     0.974245  1.586863  1.241118
N    -0.525457  1.991795 -0.896041
N    -1.279337 -1.123627 -1.081612
N    -1.748861  0.162014  1.212097
N     1.692974 -0.039580 -1.163438
N     0.907896 -1.555600  0.887501
C     1.547612  1.279093  2.482986
C     2.392248  2.298004  3.068606
H     2.890090  2.038796  3.999292
C     2.507456  3.540990  2.496744
H     3.125816  4.306059  2.966522
C     1.807116  3.845560  1.311693
H     1.849811  4.841492  0.887126
C     1.046730  2.845001  0.717585
C     0.206685  3.071420 -0.484352
C     0.141892  4.300479 -1.130345
H     0.735277  5.140625 -0.789883
C    -0.727630  4.435109 -2.231974
H    -0.788227  5.389239 -2.755942
C    -1.500718  3.374745 -2.632695
H    -2.193422  3.444910 -3.467235
C    -1.447860  2.096431 -1.951184
C    -1.023222 -1.758055 -2.222686
H    -0.026108 -1.622993 -2.631022
C    -1.976538 -2.543784 -2.893198
H    -1.702489 -3.029438 -3.825854
C    -3.245782 -2.675775 -2.361595
H    -4.006581 -3.272137 -2.861190
C    -3.551352 -2.018680 -1.149808
C    -2.527974 -1.250974 -0.546176
C    -2.782136 -0.561704  0.682343
C    -4.050929 -0.654324  1.302732
C    -4.231654  0.032220  2.523857
H    -5.193808 -0.010169  3.030557
C    -3.173336  0.746130  3.057362
H    -3.271280  1.280187  3.998495
C    -1.944102  0.788649  2.375772
H    -1.090140  1.326076  2.770730
C    -4.833963 -2.090234 -0.507124
H    -5.617359 -2.679019 -0.980409
C    -5.073870 -1.437801  0.667577
H    -6.049911 -1.499828  1.144812
C     2.060987  0.726194 -2.197745
H     1.386845  1.539311 -2.445697
C     3.243008  0.503112 -2.923092
H     3.485318  1.164764 -3.750211
C     4.078459 -0.544343 -2.573196
H     5.001596 -0.733707 -3.117279
C     3.718340 -1.375487 -1.490577
C     2.508995 -1.082641 -0.813298
C     2.083697 -1.895854  0.286028
C     2.878710 -2.991809  0.705852
C     2.408409 -3.757230  1.792995
H     2.986429 -4.608721  2.146571
C     1.214063 -3.401863  2.396385
H     0.824177 -3.958744  3.243899
C     0.500841 -2.289105  1.923305
H    -0.415517 -1.965926  2.403472
C     4.505529 -2.492345 -1.045107
H     5.435971 -2.709662 -1.565914
C     4.103721 -3.264108  0.006608
H     4.710495 -4.105600  0.335536
    el energy= -1881.84281633
          zpe= -1881.351665
    th energy= -1881.319681
  th enthalpy= -1881.318736
  free energy= -1881.414709

b3lyp-bs1-3a--td-sing--vsing-1001
Ru   -0.002418  0.713398  0.000674
O     1.826926  1.107025 -2.675645
O    -1.832255  1.088803  2.678204
H    -2.395002  1.165610  3.461852
N     0.759846  2.377238 -1.116574
N    -0.776690  2.369853  1.120293
N     1.852687  0.674577  1.006500
N     0.983253 -0.905169 -0.982877
N    -0.976890 -0.914150  0.980749
N    -1.856741  0.663233 -1.005873
C     1.556159  2.349427 -2.201743
C     2.059337  3.485007 -2.824383
H     2.681481  3.398286 -3.710490
C     1.732233  4.739418 -2.269189
H     2.121411  5.648874 -2.718944
C     0.924050  4.806336 -1.156807
H     0.686741  5.769520 -0.721625
C     0.414368  3.619025 -0.566971
C    -0.440698  3.614989  0.572624
C    -0.959258  4.797445  1.164508
H    -0.729482  5.763132  0.730832
C    -1.766252  4.722534  2.277254
H    -2.162080  5.628285  2.728688
C    -2.083281  3.464797  2.830852
H    -2.703936  3.371964  3.717383
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C    -1.571812  2.334087  2.206105
C     2.261293  1.497949  1.975919
H     1.561037  2.268041  2.280552
C     3.526695  1.370043  2.574737
H     3.809929  2.058356  3.365396
C     4.390731  0.374133  2.151853
H     5.372720  0.252561  2.599208
C     3.986466 -0.495916  1.112951
C     2.696645 -0.304979  0.564758
C     2.231356 -1.146390 -0.490010
C     3.062469 -2.174346 -0.994715
C     2.553617 -2.968491 -2.048385
H     3.165989 -3.762719 -2.464514
C     1.281605 -2.713412 -2.528023
H     0.859389 -3.302712 -3.336716
C     0.521070 -1.669482 -1.968761
H    -0.473417 -1.439826 -2.338538
C     4.815478 -1.551056  0.600485
C     4.371449 -2.357135 -0.432188
C    -0.504791 -1.684846  1.956895
H     0.486974 -1.447516  2.329132
C    -1.249593 -2.748826  2.499336
H    -0.817262 -3.346664  3.296327
C    -2.517069 -3.016200  2.014434
H    -3.114285 -3.831064  2.412275
C    -3.041231 -2.207513  0.979524
C    -2.223730 -1.162255  0.488096
C    -2.693836 -0.323355 -0.566441
C    -3.989057 -0.511145 -1.103066
C    -4.409027  0.374173 -2.122587
H    -5.399840  0.262615 -2.552760
C    -3.548830  1.372125 -2.548571
H    -3.842731  2.069866 -3.326979
C    -2.275753  1.493450 -1.965002
H    -1.579426  2.266762 -2.270457
C    -4.346372 -2.402337  0.412144
C    -4.813456 -1.568432 -0.587808
O     5.132962 -3.340016 -0.968597
O     6.029759 -1.706364  1.178211
C     6.529148 -3.261874 -0.618091
C     6.679192 -2.954043  0.863227
O    -5.077038 -3.429939  0.905393
O    -6.050615 -1.692552 -1.123147
C    -6.221716 -3.780950  0.102467
C    -6.944018 -2.524092 -0.356182
H     6.958971 -4.234306 -0.870381
H     7.003550 -2.482719 -1.228718
H     7.728209 -2.827356  1.141720
H     6.232086 -3.748841  1.474348
H    -7.311465 -1.948648  0.503364
H    -7.779489 -2.761799 -1.019110
H    -5.881521 -4.371537 -0.758075
H    -6.859117 -4.399396  0.739112
H     2.389321  1.189830 -3.458918
    el energy= -2338.30618026
 total energy= -2338.23218955
          zpe= -2337.624480
```

```
    th energy= -2337.585084
  th enthalpy= -2337.584140
  free energy= -2337.695691

b3lyp-bs1-3a--td-trip--vsing-1001
Ru    0.013696  0.737630  0.014736
O    -1.634919  0.984956  2.822607
O     1.998771  1.260136 -2.514656
H     2.591379  1.390438 -3.268765
N    -0.819050  2.323435  1.175006
N     0.682554  2.425881 -1.061954
N    -1.854189  0.652767 -0.999163
N    -0.925688 -0.944460  0.956411
N     1.029384 -0.828519 -1.035642
N     1.857816  0.684501  1.028133
C    -1.564582  2.230670  2.291143
C    -2.201789  3.312704  2.889687
H    -2.766022  3.179682  3.808526
C    -2.080138  4.578270  2.275225
H    -2.583327  5.439777  2.705630
C    -1.319947  4.712959  1.137122
H    -1.228212  5.681249  0.660120
C    -0.658469  3.581939  0.580357
C     0.185445  3.648493 -0.559553
C     0.559803  4.870509 -1.183818
H     0.186913  5.809550 -0.793049
C     1.415191  4.867526 -2.258584
H     1.707740  5.800168 -2.732904
C     1.930010  3.638846 -2.740478
H     2.606286  3.604035 -3.590006
C     1.544139  2.469355 -2.104698
C    -2.289861  1.469040 -1.961866
H    -1.611981  2.257807 -2.268913
C    -3.555555  1.314654 -2.555101
H    -3.859417  2.001730 -3.339214
C    -4.390958  0.294269 -2.136463
H    -5.371891  0.149925 -2.579125
C    -3.955257 -0.575500 -1.110150
C    -2.667864 -0.355447 -0.565646
C    -2.171072 -1.206090  0.469135
C    -2.968876 -2.269232  0.955650
C    -2.428340 -3.077282  1.982298
H    -3.015383 -3.898193  2.382795
C    -1.157674 -2.802449  2.454197
H    -0.710183 -3.402676  3.241003
C    -0.432375 -1.723719  1.915581
H     0.559237 -1.477510  2.281966
C    -4.751401 -1.661859 -0.611147
C    -4.277551 -2.475773  0.400951
C     0.587673 -1.564897 -2.050753
H    -0.400845 -1.326485 -2.431503
C     1.356293 -2.597514 -2.621534
H     0.946609 -3.168434 -3.449662
C     2.617672 -2.867962 -2.123845
H     3.233628 -3.658020 -2.542537
C     3.111211 -2.093730 -1.047975
C     2.270116 -1.080406 -0.530486
```

```
C     2.713699 -0.274013  0.561547
C     4.003938 -0.463638  1.109834
C     4.397899  0.388517  2.167521
H     5.384585  0.273924  2.606338
C     3.518530  1.357917  2.620323
H     3.792976  2.029247  3.428501
C     2.251628  1.482119  2.025473
H     1.537969  2.231425  2.350653
C     4.410239 -2.292364 -0.467475
C     4.850781 -1.489803  0.569117
O    -5.006799 -3.491243  0.922342
O    -5.965679 -1.839636 -1.183768
C    -6.406613 -3.446445  0.582038
C    -6.575362 -3.112266 -0.891627
O     5.162982 -3.290805 -0.987154
O     6.082002 -1.616790  1.118802
C     6.300758 -3.655150 -0.180798
C     6.998012 -2.406124  0.334664
H    -6.806639 -4.435941  0.816506
H    -6.899581 -2.694146  1.211435
H    -7.629529 -3.011476 -1.161215
H    -6.108766 -3.880694 -1.521699
H     7.368984 -1.794167 -0.497795
H     7.827717 -2.656579  1.000172
H     5.956973 -4.281850  0.652370
H     6.956255 -4.240698 -0.830086
H    -2.170858  1.017268  3.627960
    el energy= -2338.30514704
 total energy= -2338.23739014
          zpe= -2337.631054
    th energy= -2337.592372
  th enthalpy= -2337.591427
  free energy= -2337.700172

b3lyp-bs1-3a--gs-triplet
Ru   -0.051374  0.651255 -0.152359
O    -1.830537  1.287529  2.894441
O     1.689021  1.424952 -2.581725
H     2.296894  1.503396 -3.331808
N    -0.971037  2.578813  1.257787
N     0.530657  2.613384 -1.055162
N    -1.936388  0.499132 -1.111613
N    -0.961012 -0.991611  0.908550
N     1.242355 -1.177073 -1.112792
N     1.868641  0.634021  0.855626
C    -1.816343  2.493546  2.284582
C    -2.621874  3.564138  2.707298
H    -3.295048  3.456965  3.554912
C    -2.532793  4.758169  2.004857
H    -3.150883  5.606163  2.288543
C    -1.645273  4.862574  0.929397
H    -1.587314  5.784297  0.362014
C    -0.866176  3.751530  0.594072
C     0.122566  3.798520 -0.516346
C     0.617283  5.016060 -0.988240
H     0.322074  5.946470 -0.518004
C     1.519552  5.027715 -2.053930
H     1.914622  5.967930 -2.429782
C     1.905970  3.825823 -2.628671
H     2.596194  3.793006 -3.468152
C     1.383979  2.641967 -2.090890
C    -2.394993  1.233620 -2.130272
H    -1.737992  2.018862 -2.490640
C    -3.654168  1.014968 -2.714591
H    -3.970502  1.640969 -3.543851
C    -4.470701  0.009543 -2.227477
H    -5.448238 -0.184273 -2.658160
C    -4.016100 -0.779073 -1.146521
C    -2.731058 -0.501805 -0.619516
C    -2.215467 -1.285386  0.457781
C    -3.000643 -2.320602  1.021209
C    -2.449627 -3.050488  2.098670
H    -3.028191 -3.846883  2.556886
C    -1.178899 -2.733413  2.546187
H    -0.724637 -3.274729  3.371052
C    -0.461512 -1.697150  1.923128
H     0.538534 -1.430156  2.250778
C    -4.794059 -1.843243 -0.575777
C    -4.308742 -2.579957  0.487030
C     0.918312 -2.046322 -2.061869
H    -0.084580 -1.959579 -2.476154
C     1.805741 -3.037941 -2.524007
H     1.489969 -3.725701 -3.303481
C     3.068010 -3.120488 -1.966361
H     3.780361 -3.874515 -2.287138
C     3.436767 -2.203917 -0.954155
C     2.477036 -1.236258 -0.556944
C     2.805010 -0.289422  0.478905
C     4.090930 -0.332115  1.080135
C     4.391268  0.610962  2.088790
H     5.370917  0.597442  2.556325
C     3.426825  1.529057  2.458281
H     3.617599  2.266114  3.232883
C     2.177032  1.508590  1.818042
H     1.395336  2.212192  2.086015
C     4.726746 -2.232362 -0.324755
C     5.047599 -1.314872  0.653004
O    -5.023107 -3.569655  1.077708
O    -6.007537 -2.078445 -1.134498
C    -6.420005 -3.576956  0.728622
C    -6.587189 -3.343298 -0.764743
O     5.588758 -3.196036 -0.735985
O     6.263753 -1.283109  1.256743
C     6.713531 -3.389901  0.140554
C     7.275639 -2.044884  0.574094
H    -6.801531 -4.556962  1.026015
H    -6.933634 -2.795289  1.303780
H    -7.641887 -3.287249 -1.045480
H    -6.097875 -4.140219 -1.340148
H     7.626219 -1.472843 -0.295296
H     8.096994 -2.164690  1.285132
H     6.388686 -3.973778  1.011922
H     7.447079 -3.965653 -0.429498
H    -2.439098  1.303336  3.647421
```

```
    el energy= -2338.25010494
          zpe= -2337.643163
    th energy= -2337.602919
  th enthalpy= -2337.601975
  free energy= -2337.718533

b3lyp-bs1-3a--gs-singlet
Ru    0.004656  0.773840  0.008641
O    -1.750993  1.168219  2.743628
O     1.925531  1.281198 -2.591676
H     2.508598  1.372794 -3.359555
N    -0.801696  2.454411  1.126010
N     0.744275  2.502677 -1.079398
N    -1.835265  0.632996 -1.048288
N    -0.935240 -0.829440  1.022269
N     0.974855 -0.785956 -1.042092
N     1.845151  0.647870  1.059984
C    -1.561814  2.398725  2.234942
C    -2.122879  3.532200  2.842575
H    -2.733800  3.425393  3.735971
C    -1.882899  4.773763  2.278079
H    -2.307850  5.672077  2.717775
C    -1.081383  4.853693  1.138948
H    -0.886230  5.820301  0.692624
C    -0.547670  3.686808  0.589805
C     0.337427  3.716020 -0.595627
C     0.744509  4.916647 -1.179501
H     0.424031  5.869136 -0.777463
C     1.586944  4.890367 -2.291237
H     1.914336  5.815740 -2.757475
C     2.001053  3.666231 -2.788778
H     2.658213  3.599781 -3.652795
C     1.558015  2.497340 -2.151328
C    -2.265240  1.371780 -2.074409
H    -1.593600  2.151037 -2.420841
C    -3.511825  1.162342 -2.691000
H    -3.804860  1.794098 -3.524557
C    -4.341697  0.154596 -2.233486
H    -5.306691 -0.037236 -2.692328
C    -3.915593 -0.640441 -1.145118
C    -2.648101 -0.361358 -0.578314
C    -2.162330 -1.146191  0.515239
C    -2.954896 -2.195851  1.038969
C    -2.433700 -2.938087  2.122987
H    -3.017605 -3.748036  2.549139
C    -1.182800 -2.611923  2.614276
H    -0.745910 -3.161376  3.443265
C    -0.462572 -1.549514  2.038605
H     0.513251 -1.265667  2.418926
C    -4.704231 -1.713115 -0.606479
C    -4.243590 -2.459283  0.460268
C     0.516133 -1.493307 -2.073544
H    -0.459279 -1.211528 -2.456777
C     1.246003 -2.546137 -2.655094
H     0.817590 -3.089554 -3.492424
C     2.492610 -2.874583 -2.154683
H     3.079931 -3.682836 -2.579355
C     3.005476 -2.135893 -1.064153
C     2.202539 -1.097975 -0.533422
C     2.671829 -0.329065  0.578212
C     3.947832 -0.589156  1.134409
C     4.370425  0.211801  2.219802
H     5.346418  0.041786  2.663751
C     3.524089  1.198876  2.692304
H     3.813678  1.833567  3.524831
C     2.267723  1.386889  2.088823
H     1.584046  2.151771  2.443699
C     4.290709 -2.399268 -0.477840
C     4.754669 -1.638873  0.577422
O    -4.967493 -3.462064  1.017577
O    -5.900501 -1.949190 -1.202197
C    -6.354099 -3.472133  0.631020
C    -6.482290 -3.221188 -0.863388
O     5.006181 -3.420588 -1.012378
O     5.975243 -1.832105  1.138033
C     6.109629 -3.854346 -0.196145
C     6.859901 -2.649794  0.350702
H    -6.738470 -4.457511  0.906278
H    -6.887470 -2.699983  1.201134
H    -7.529384 -3.167937 -1.171924
H    -5.973010 -4.008812 -1.434404
H     7.270245 -2.043689 -0.467874
H     7.669514 -2.952195  1.019702
H     5.723269 -4.475646  0.622626
H     6.745926 -4.462153 -0.844336
H    -2.305474  1.222509  3.535846
    el energy= -2338.31501806
          zpe= -2337.705598
    th energy= -2337.666612
  th enthalpy= -2337.665667
  free energy= -2337.777253

b3lyp-bs1-3b--td-sing--vsing-1001
Ru    0.031113  0.771058  0.069851
O    -1.567760  1.294737  3.038324
O     2.288001  1.480067 -2.304615
N    -0.874073  2.424884  1.156380
N     0.701128  2.515399 -0.987040
N    -1.803721  0.607713 -1.033620
N    -0.907886 -0.861064  1.068038
N     1.010985 -0.694275 -1.035281
N     1.838724  0.645645  1.114355
C    -1.601356  2.323801  2.358296
C    -2.373267  3.480209  2.792344
H    -2.969701  3.347198  3.689781
C    -2.322063  4.670276  2.104523
H    -2.891503  5.536530  2.435500
C    -1.507654  4.755856  0.970012
H    -1.438899  5.687515  0.424818
C    -0.795092  3.608271  0.534476
C     0.111110  3.676233 -0.631620
C     0.360863  4.896498 -1.282189
H    -0.125145  5.810624 -0.968179
C     1.275640  4.921935 -2.350580
```

```
H     1.476797  5.855929 -2.872581
C     1.909972  3.761259 -2.710653
H     2.636011  3.721079 -3.517641
C     1.665757  2.506199 -2.009436
C    -2.248696  1.333445 -2.071689
H    -1.583970  2.124695 -2.407075
C    -3.462045  1.102805 -2.712784
H    -3.752397  1.724151 -3.554465
C    -4.288291  0.048483 -2.262001
H    -5.237780 -0.169147 -2.739947
C    -3.862349 -0.724406 -1.181403
C    -2.604710 -0.429641 -0.567318
C    -2.134521 -1.194092  0.516823
C    -2.910808 -2.274573  1.048857
C    -2.415884 -2.983139  2.145186
H    -2.997551 -3.800196  2.561582
C    -1.180808 -2.615998  2.693593
H    -0.766355 -3.133408  3.553199
C    -0.476635 -1.548210  2.120213
H     0.474844 -1.228838  2.536469
C    -4.624590 -1.826434 -0.645747
C    -4.174180 -2.560884  0.422837
C     0.579380 -1.335920 -2.121305
H    -0.401880 -1.047305 -2.482916
C     1.337873 -2.325976 -2.767298
H     0.926538 -2.816321 -3.645506
C     2.588582 -2.667366 -2.281014
H     3.196464 -3.430366 -2.756867
C     3.072324 -1.995059 -1.139986
C     2.245478 -1.013832 -0.547860
C     2.692323 -0.294625  0.603636
C     3.968702 -0.550031  1.157347
C     4.367571  0.205482  2.279820
H     5.343106  0.036297  2.724628
C     3.492130  1.153722  2.786273
H     3.758781  1.754348  3.651854
C     2.240445  1.346120  2.180816
H     1.530038  2.072724  2.561343
C     4.358215 -2.258222 -0.552534
C     4.794566 -1.554871  0.546027
O    -4.899427 -3.600651  0.960513
O    -5.822054 -2.093216 -1.272931
C    -6.263882 -3.607602  0.555491
C    -6.362122 -3.368039 -0.945894
O     5.111722 -3.236767 -1.146903
O     6.028197 -1.760299  1.111122
C     6.209959 -3.677823 -0.349208
C     6.924025 -2.481285  0.265800
H    -6.666195 -4.587738  0.832825
H    -6.816837 -2.823836  1.095396
H    -7.403834 -3.361751 -1.284099
H    -5.812495 -4.155490 -1.484487
H     7.297394 -1.816753 -0.527238
H     7.760416 -2.795670  0.897891
H     5.843209 -4.345686  0.444214
H     6.870646 -4.239599 -1.016946
   el energy= -2337.51543977
```

```
 total energy= -2337.48070657
          zpe= -2336.902169
    th energy= -2336.863033
  th enthalpy= -2336.862088
  free energy= -2336.974058

b3lyp-bs1-3b--td-sing--vtrip-1001
Ru   -0.010363  0.820306  0.100896
O    -0.823953  1.450657  3.244790
O     2.193625  1.303981 -2.351181
N    -0.710238  2.405951  1.151758
N     0.649417  2.444798 -1.077932
N    -1.727892  0.559606 -1.060881
N    -1.009599 -0.709735  1.212646
N     0.964742 -0.778372 -0.975979
N     1.862472  0.660222  1.112847
C    -1.202099  2.343485  2.480499
C    -2.114734  3.397676  2.889319
H    -2.584157  3.280974  3.861592
C    -2.273097  4.514823  2.118543
H    -2.917246  5.328418  2.448623
C    -1.567960  4.638443  0.893454
H    -1.654521  5.543678  0.303540
C    -0.790845  3.584791  0.447822
C     0.034937  3.621835 -0.780821
C     0.211212  4.773363 -1.537281
H    -0.282719  5.700261 -1.269373
C     1.071868  4.711221 -2.655163
H     1.217955  5.597879 -3.271349
C     1.727782  3.544323 -2.951304
H     2.409925  3.460839 -3.792962
C     1.567015  2.352875 -2.136061
C    -2.099673  1.222923 -2.186417
H    -1.405273  1.982325 -2.530976
C    -3.266936  0.944954 -2.872088
H    -3.500746  1.503017 -3.774119
C    -4.135837 -0.071985 -2.399969
H    -5.054258 -0.316297 -2.923223
C    -3.792751 -0.761935 -1.235474
C    -2.577015 -0.431184 -0.565775
C    -2.193154 -1.099110  0.608461
C    -3.018372 -2.119919  1.179697
C    -2.603184 -2.727948  2.366514
H    -3.217311 -3.502543  2.816202
C    -1.403796 -2.314799  2.960212
H    -1.053831 -2.755767  3.888777
C    -0.654366 -1.299622  2.355202
H     0.260000 -0.935124  2.810531
C    -4.604960 -1.807337 -0.661928
C    -4.239845 -2.449911  0.496844
C     0.502687 -1.464066 -2.016364
H    -0.491347 -1.198934 -2.359746
C     1.249141 -2.473338 -2.649067
H     0.813542 -3.005995 -3.489690
C     2.520754 -2.772696 -2.193440
H     3.125006 -3.545028 -2.659036
C     3.035803 -2.048618 -1.099169
```

```
C     2.215266 -1.055242 -0.514891
C     2.692742 -0.292321  0.597060
C     3.988508 -0.524467  1.117657
C     4.416068  0.261051  2.207801
H     5.407874  0.109183  2.621986
C     3.551210  1.212245  2.725440
H     3.838781  1.832036  3.570044
C     2.280702  1.384257  2.154180
H     1.571307  2.100488  2.550693
C     4.344724 -2.277493 -0.552065
C     4.807559 -1.536495  0.509632
O    -5.016277 -3.429012  1.071646
O    -5.760376 -2.114866 -1.342850
C    -6.352086 -3.455895  0.577536
C    -6.346647 -3.348845 -0.942022
O     5.088941 -3.264709 -1.141455
O     6.060279 -1.709822  1.039518
C     6.222604 -3.666014 -0.371397
C     6.938567 -2.441971  0.184120
H    -6.788132 -4.403131  0.911651
H    -6.924908 -2.621417  1.009577
H    -7.363346 -3.356951 -1.348780
H    -5.778556 -4.187678 -1.372628
H     7.273995 -1.794383 -0.639022
H     7.800316 -2.725833  0.796029
H     5.894664 -4.316916  0.452383
H     6.867985 -4.236006 -1.046917
    el energy= -2337.46222189
 total energy= -2337.47197900
          zpe= -2336.892958
    th energy= -2336.854076
  th enthalpy= -2336.853132
  free energy= -2336.964529

b3lyp-bs1-3b--td-trip--vsing-1001
Ru    0.031445  0.768416  0.096657
O    -1.231862  1.391589  3.183540
O     2.324651  1.439781 -2.251381
N    -0.826137  2.406976  1.161075
N     0.682530  2.475911 -1.006999
N    -1.779562  0.591596 -1.034982
N    -0.951624 -0.830702  1.126123
N     1.003775 -0.726523 -0.999259
N     1.848265  0.640446  1.133452
C    -1.448307  2.341554  2.425595
C    -2.302950  3.447205  2.832094
H    -2.835141  3.325336  3.770263
C    -2.361375  4.600134  2.083999
H    -2.974336  5.442870  2.396573
C    -1.594328  4.684683  0.915254
H    -1.601794  5.593609  0.327815
C    -0.833105  3.566604  0.488627
C     0.035779  3.628113 -0.706660
C     0.213893  4.816409 -1.420846
H    -0.317354  5.721917 -1.155927
C     1.121410  4.818635 -2.499590
H     1.270292  5.727822 -3.080440
C     1.814671  3.674514 -2.798656
H     2.533619  3.629512 -3.612123
C     1.648761  2.451168 -2.024648
C    -2.185340  1.283697 -2.112907
H    -1.503370  2.056951 -2.454716
C    -3.379756  1.040321 -2.782807
H    -3.637671  1.634672 -3.653976
C    -4.230908  0.009484 -2.321686
H    -5.167753 -0.215108 -2.821002
C    -3.845126 -0.731417 -1.205460
C    -2.602937 -0.428320 -0.562298
C    -2.167611 -1.168043  0.551187
C    -2.966449 -2.228200  1.090862
C    -2.504639 -2.915157  2.214295
H    -3.103470 -3.717111  2.635544
C    -1.276539 -2.547381  2.782959
H    -0.888277 -3.048754  3.664053
C    -0.550142 -1.500440  2.204172
H     0.393570 -1.178237  2.635124
C    -4.632352 -1.810539 -0.659512
C    -4.217384 -2.518736  0.440488
C     0.558551 -1.390789 -2.064987
H    -0.434067 -1.122956 -2.410611
C     1.320111 -2.376533 -2.714828
H     0.899110 -2.884773 -3.578100
C     2.586530 -2.687586 -2.252176
H     3.198707 -3.444772 -2.731834
C     3.082196 -1.993019 -1.129177
C     2.251337 -1.018836 -0.532231
C     2.706601 -0.285767  0.608347
C     3.994682 -0.521765  1.142292
C     4.397922  0.237071  2.261381
H     5.383554  0.083638  2.689380
C     3.513513  1.164389  2.787357
H     3.781418  1.764490  3.652862
C     2.249642  1.338214  2.200810
H     1.530957  2.045254  2.600174
C     4.383813 -2.229986 -0.566403
C     4.828016 -1.513196  0.519902
O    -4.966302 -3.536384  0.987939
O    -5.815110 -2.084543 -1.310387
C    -6.319164 -3.544691  0.545761
C    -6.374590 -3.345927 -0.963721
O     5.142103 -3.199271 -1.169242
O     6.074745 -1.694439  1.063449
C     6.264542 -3.615113 -0.391650
C     6.967622 -2.402183  0.203611
H    -6.736818 -4.513768  0.838794
H    -6.880415 -2.742267  1.048472
H    -7.406599 -3.340841 -1.330388
H    -5.817125 -4.151879 -1.465529
H     7.312249 -1.734204 -0.599373
H     7.822061 -2.697591  0.820478
H     5.926584 -4.286053  0.411886
H     6.922433 -4.167313 -1.070023
    el energy= -2337.51713421
 total energy= -2337.48237589
```

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          zpe= -2336.903742
    th energy= -2336.864654
  th enthalpy= -2336.863710
  free energy= -2336.974921

b3lyp-bs1-3b--td-trip--vtrip-1001
Ru   -0.010243  0.820084  0.100917
O    -0.824094  1.449697  3.244987
O     2.194781  1.305345 -2.349762
N    -0.710933  2.405179  1.152014
N     0.649115  2.444992 -1.077329
N    -1.727599  0.559184 -1.061095
N    -1.009409 -0.710428  1.212289
N     0.965369 -0.778104 -0.976287
N     1.862505  0.660260  1.112954
C    -1.202637  2.342406  2.480765
C    -2.115688  3.396220  2.889745
H    -2.584847  3.279355  3.862127
C    -2.274859  4.513204  2.118922
H    -2.919441  5.326442  2.449036
C    -1.570019  4.637121  0.893700
H    -1.657165  5.542289  0.303758
C    -0.792264  3.583930  0.448070
C     0.033585  3.621533 -0.780477
C     0.209112  4.773112 -1.537052
H    -0.285704  5.699624 -1.269430
C     1.070070  4.711508 -2.654735
H     1.215513  5.598184 -3.271042
C     1.727091  3.545138 -2.950493
H     2.409520  3.462078 -3.791960
C     1.567102  2.353703 -2.135091
C    -2.099252  1.222452 -2.186725
H    -1.404751  1.981742 -2.531325
C    -3.266536  0.944610 -2.872399
H    -3.500241  1.502634 -3.774483
C    -4.135631 -0.072147 -2.400239
H    -5.054096 -0.316319 -2.923479
C    -3.792632 -0.762120 -1.235726
C    -2.576836 -0.431540 -0.566061
C    -2.193023 -1.099615  0.608109
C    -3.018338 -2.120344  1.179330
C    -2.603131 -2.728532  2.366070
H    -3.217336 -3.503087  2.815725
C    -1.403655 -2.315613  2.959722
H    -1.053662 -2.756727  3.888206
C    -0.654169 -1.300420  2.354772
H     0.260187 -0.935953  2.810152
C    -4.604995 -1.807388 -0.662157
C    -4.239921 -2.450073  0.496581
C     0.503554 -1.463640 -2.016902
H    -0.490460 -1.198515 -2.360360
C     1.250262 -2.472671 -2.649668
H     0.814933 -3.005229 -3.490497
C     2.521868 -2.771904 -2.193896
H     3.126311 -3.544049 -2.659551
C     3.036642 -2.047938 -1.099424
C     2.215850 -1.054818 -0.515084
C     2.693037 -0.291982  0.597085
C     3.988804 -0.523959  1.117752
C     4.416099  0.261478  2.208059
H     5.407875  0.109736  2.622362
C     3.550990  1.212407  2.725773
H     3.838384  1.832130  3.570489
C     2.280501  1.384243  2.154423
H     1.570978  2.100364  2.550900
C     4.345559 -2.276644 -0.552213
C     4.808126 -1.535722  0.509638
O    -5.016509 -3.429032  1.071414
O    -5.760510 -2.114691 -1.343002
C    -6.352363 -3.455631  0.577411
C    -6.347026 -3.348551 -0.942136
O     5.090034 -3.263610 -1.141703
O     6.060833 -1.708885  1.039620
C     6.223761 -3.664754 -0.371663
C     6.939369 -2.440617  0.184126
H    -6.788569 -4.402790  0.911538
H    -6.924977 -2.621050  1.009529
H    -7.363763 -3.356413 -1.348803
H    -5.779157 -4.187494 -1.372816
H     7.274662 -1.792783 -0.638879
H     7.801165 -2.724356  0.796023
H     5.895962 -4.315894  0.451986
H     6.869325 -4.234453 -1.047255
    el energy= -2337.46222844
 total energy= -2337.47197877
          zpe= -2336.892956
    th energy= -2336.854074
  th enthalpy= -2336.853130
  free energy= -2336.964527

b3lyp-bs1-3b--gs-triplet
Ru    0.013240  0.815562  0.101665
O    -0.939038  1.218900  3.250271
O     2.363037  1.631378 -2.101752
N    -0.852825  2.321518  1.231875
N     0.564772  2.509328 -0.951796
N    -1.773765  0.575228 -1.025407
N    -0.914946 -0.836171  1.106035
N     1.067135 -0.599220 -1.100536
N     1.806362  0.603882  1.182188
C    -1.317392  2.170142  2.549838
C    -2.232284  3.192793  3.024410
H    -2.661942  3.036041  4.009890
C    -2.481119  4.318651  2.285127
H    -3.145407  5.092657  2.667966
C    -1.846624  4.504292  1.033902
H    -1.980495  5.427004  0.480791
C    -1.033724  3.493374  0.548353
C    -0.215695  3.608155 -0.680223
C    -0.173426  4.747388 -1.466168
H    -0.795488  5.603601 -1.231567
C     0.720862  4.790248 -2.563218
H     0.749850  5.676442 -3.196167
C     1.560892  3.737946 -2.803960
```

```
H     2.286927  3.743335 -3.612008
C     1.557154  2.556901 -1.955540
C    -2.192706  1.285935 -2.093434
H    -1.541170  2.094456 -2.408570
C    -3.374829  1.009771 -2.768679
H    -3.651278  1.617078 -3.625649
C    -4.193695 -0.052309 -2.336833
H    -5.121921 -0.292761 -2.844688
C    -3.792541 -0.802369 -1.227778
C    -2.565525 -0.472057 -0.580129
C    -2.116605 -1.205574  0.535334
C    -2.897621 -2.273998  1.071646
C    -2.427842 -2.940061  2.206861
H    -3.008429 -3.753189  2.631754
C    -1.217781 -2.531881  2.780950
H    -0.825877 -3.015572  3.670549
C    -0.507389 -1.475366  2.206795
H     0.417011 -1.120967  2.647417
C    -4.556144 -1.902792 -0.695375
C    -4.135247 -2.597487  0.412675
C     0.688961 -1.153666 -2.250891
H    -0.290921 -0.866562 -2.619426
C     1.493271 -2.062674 -2.953637
H     1.123692 -2.493576 -3.879684
C     2.744985 -2.400927 -2.453392
H     3.392195 -3.101446 -2.971878
C     3.176512 -1.812429 -1.251886
C     2.300428 -0.909842 -0.598365
C     2.692116 -0.273272  0.610194
C     3.962768 -0.535263  1.182861
C     4.304675  0.130977  2.372685
H     5.274630 -0.045026  2.827076
C     3.381630  1.003395  2.945175
H     3.604399  1.525709  3.871093
C     2.143510  1.212402  2.327313
H     1.383033  1.848167  2.765297
C     4.456514 -2.079754 -0.653838
C     4.838296 -1.458268  0.511659
O    -4.864067 -3.627093  0.956374
O    -5.722441 -2.205277 -1.357071
C    -6.214860 -3.667514  0.502776
C    -6.262114 -3.476853 -1.007776
O     5.259480 -2.977953 -1.307506
O     6.062872 -1.669535  1.092319
C     6.355068 -3.445333 -0.521031
C     7.006839 -2.281138  0.213545
H    -6.611652 -4.644674  0.796572
H    -6.795935 -2.876152  0.999429
H    -7.290909 -3.491030 -1.382155
H    -5.685855 -4.272955 -1.503175
H     7.373108 -1.536831 -0.508625
H     7.838923 -2.618194  0.839532
H     5.996162 -4.192665  0.202028
H     7.053017 -3.922209 -1.216326
   el energy= -2337.47148959
        zpe= -2336.893085
   th energy= -2336.854039
  th enthalpy= -2336.853095
  free energy= -2336.965032

b3lyp-bs1-3b--gs-singlet
Ru    0.014258  0.661615  0.052516
O    -1.185527  1.000352  3.087081
O     2.145648  1.274515 -2.407858
N    -0.781030  2.246273  1.191104
N     0.654874  2.369745 -1.024151
N    -1.762543  0.550914 -1.066986
N    -1.021540 -0.909139  1.044250
N     1.091145 -0.814270 -1.037904
N     1.796734  0.562341  1.142648
C    -1.330088  2.073825  2.470064
C    -2.043952  3.207274  3.018986
H    -2.523753  3.056691  3.982552
C    -2.062478  4.417973  2.371756
H    -2.582129  5.268715  2.813136
C    -1.389003  4.576846  1.143577
H    -1.354106  5.543556  0.655533
C    -0.755578  3.470408  0.589011
C     0.048116  3.538822 -0.656602
C     0.201252  4.714118 -1.383322
H    -0.294105  5.627474 -1.076340
C     1.030324  4.695365 -2.523329
H     1.157781  5.604940 -3.110875
C     1.681695  3.542198 -2.881986
H     2.341165  3.492998 -3.744553
C     1.538898  2.319859 -2.115719
C    -2.104923  1.282486 -2.134647
H    -1.371091  2.011186 -2.462352
C    -3.333161  1.122910 -2.795643
H    -3.552204  1.748280 -3.656884
C    -4.245787  0.182061 -2.346922
H    -5.203064  0.037682 -2.837840
C    -3.910005 -0.602104 -1.223443
C    -2.651438 -0.384995 -0.613574
C    -2.249873 -1.169203  0.515086
C    -3.120780 -2.152363  1.043768
C    -2.681078 -2.890483  2.160752
H    -3.325345 -3.649419  2.593465
C    -1.427661 -2.616719  2.683227
H    -1.053997 -3.154747  3.550132
C    -0.633411 -1.614094  2.107080
H     0.331805 -1.352170  2.524764
C    -4.777603 -1.609349 -0.676670
C    -4.402183 -2.347184  0.421687
C     0.715146 -1.493887 -2.118752
H    -0.281501 -1.281943 -2.493929
C     1.550081 -2.420293 -2.765116
H     1.183712 -2.940198 -3.646316
C     2.824435 -2.651788 -2.279525
H     3.496528 -3.358253 -2.756334
C     3.249316 -1.942098 -1.136617
C     2.343295 -1.032513 -0.546344
C     2.723786 -0.294484  0.619495
C     4.008299 -0.463776  1.185423
```

```
C     4.327510  0.285751  2.337982
H     5.309270  0.185309  2.790205
C     3.368293  1.133276  2.865485
H     3.570340  1.721209  3.756686
C     2.112186  1.247298  2.245885
H     1.335254  1.892659  2.638331
C     4.550680 -2.103906 -0.548135
C     4.920768 -1.382929  0.562981
O    -5.216086 -3.296577  0.982159
O    -5.981016 -1.787407 -1.310146
C    -6.577530 -3.196580  0.563328
C    -6.644926 -2.997192 -0.945102
O     5.385132 -3.008757 -1.151772
O     6.163408 -1.494183  1.132938
C     6.519310 -3.360933 -0.360041
C     7.121965 -2.115504  0.276813
H    -7.063150 -4.129350  0.866290
H    -7.058957 -2.352388  1.078087
H    -7.678683 -2.898615 -1.290754
H    -6.170423 -3.846624 -1.458474
H     7.433424 -1.405444 -0.503136
H     7.982856 -2.363978  0.905222
H     6.215367 -4.072943  0.421625
H     7.228320 -3.848842 -1.036259
    el energy= -2337.52767577
          zpe= -2336.945606
    th energy= -2336.907038
  th enthalpy= -2336.906093
  free energy= -2337.016487
```