Synthesis, Computational, and Spectroscopic Analysis of Tunable Highly Fluorescent BN-1,2-Azaborine Derivatives Containing the N-BOH Moiety

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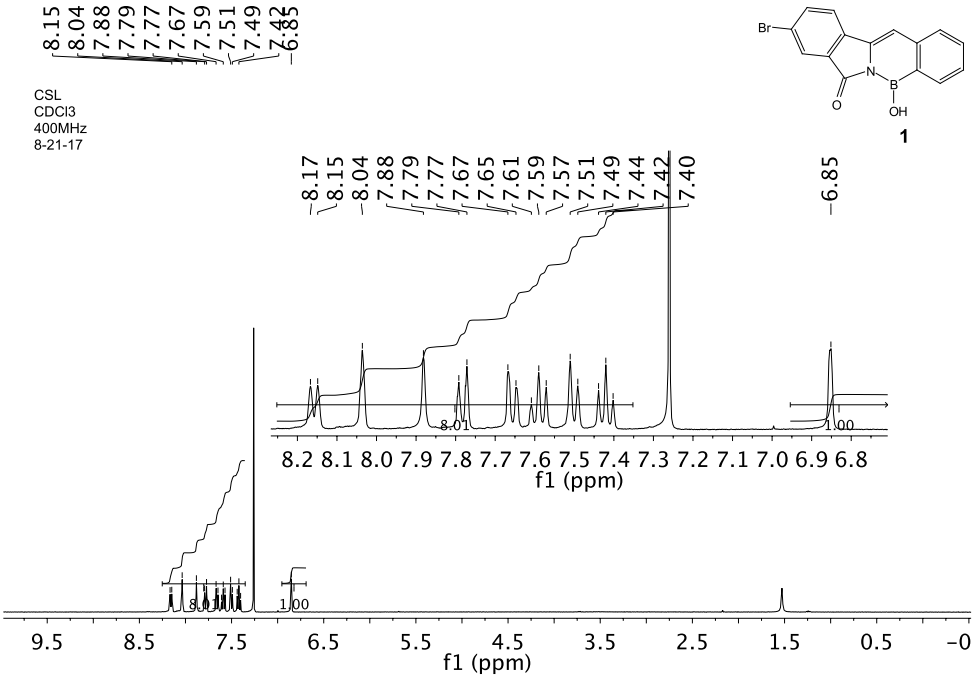
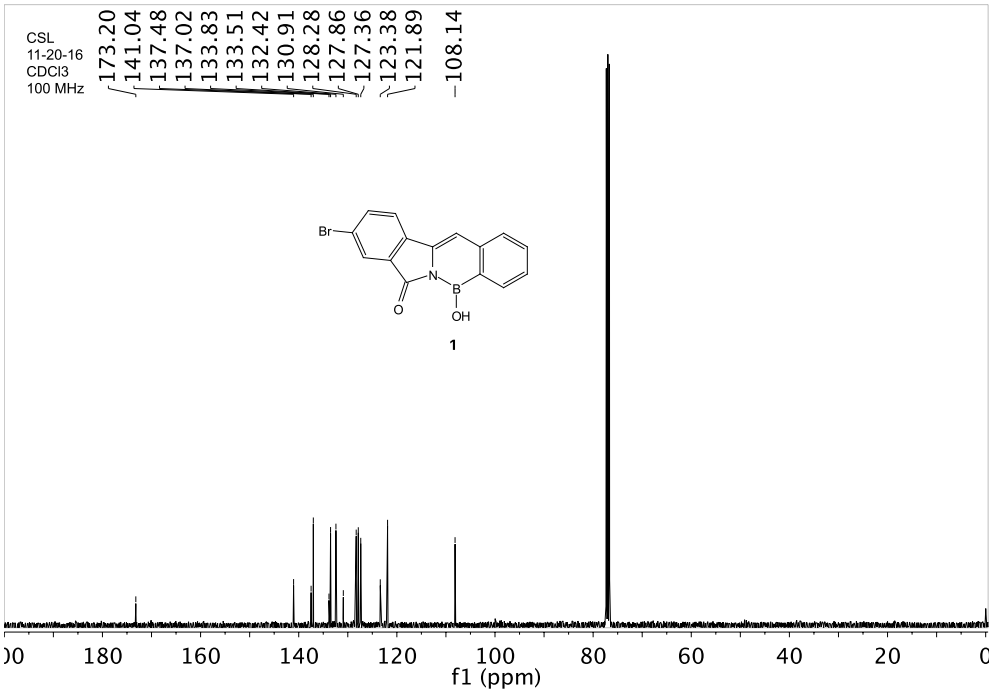
† Electronic supplementary information (ESI) available. See DOI:

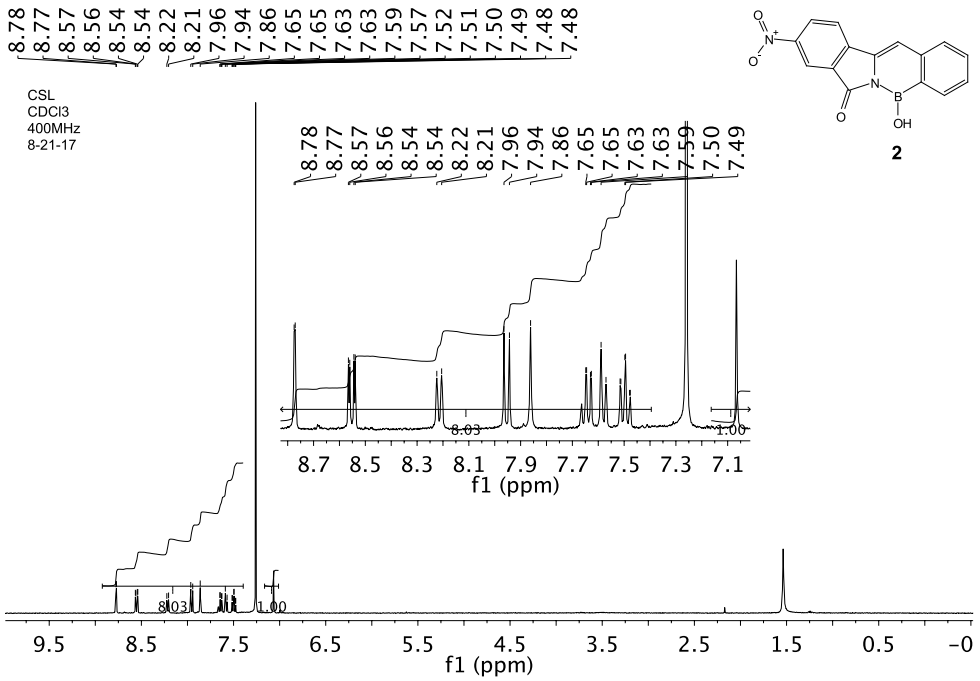
^{1}H NMR/^{13}C NMR



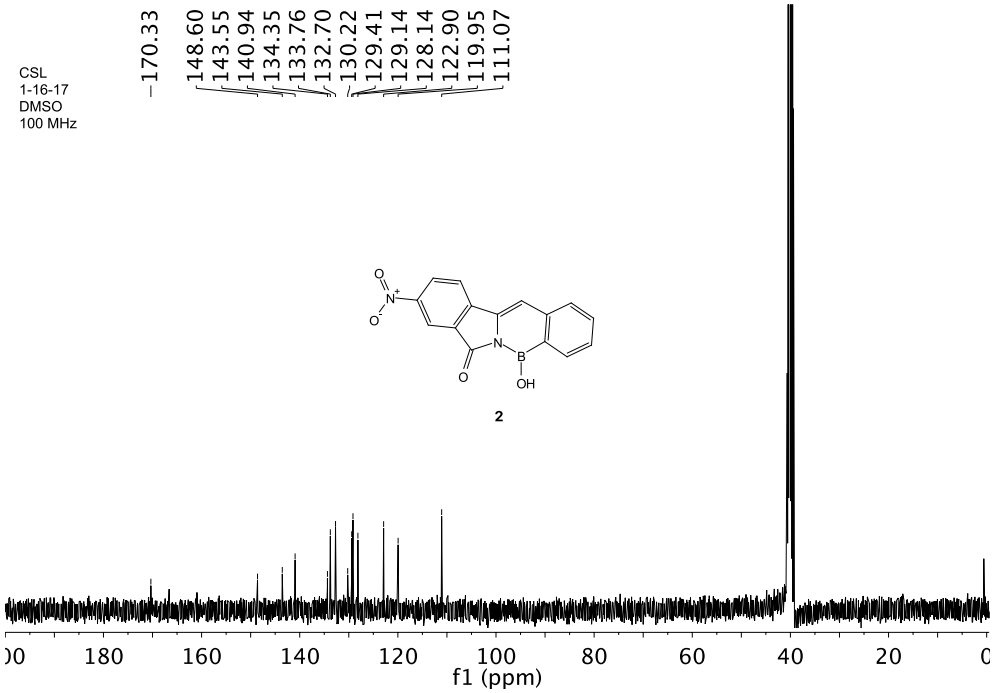
^{1}H NMR spectrum (400 MHz) of **1** in $CDCl_3$



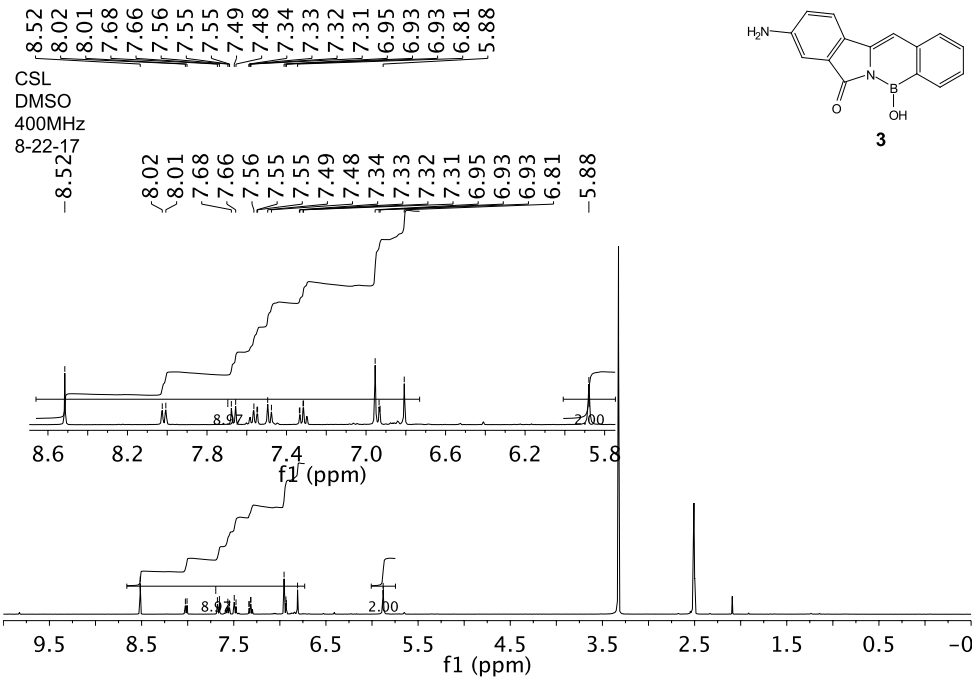
^{13}C NMR spectrum (100 MHz) of **1** in $CDCl_3$



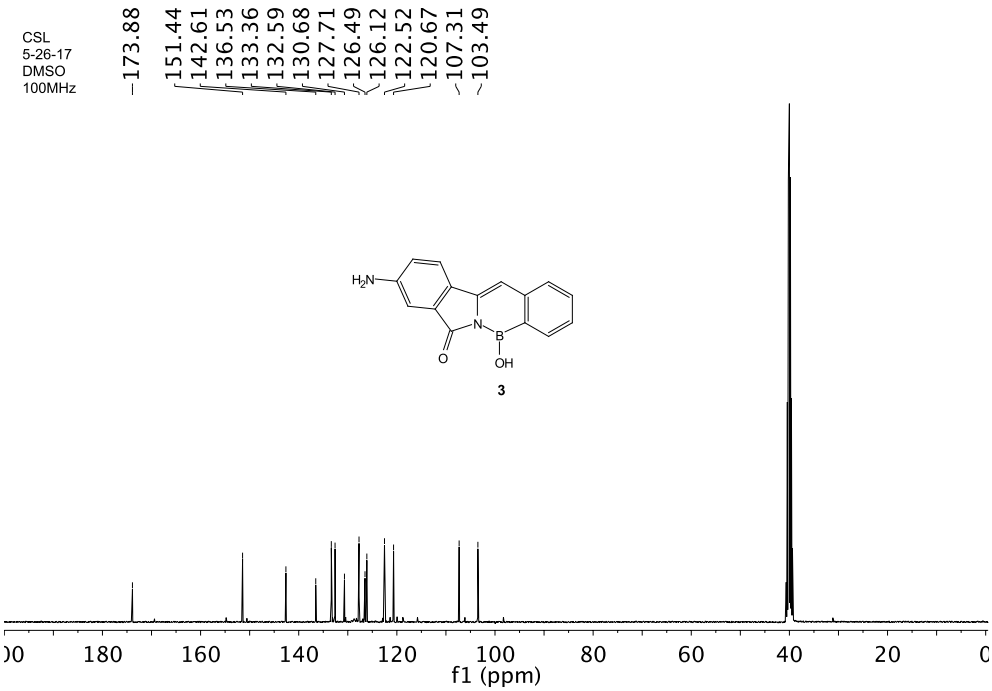
^{1}H NMR spectrum (400 MHz) of **2** in $CDCl_3$



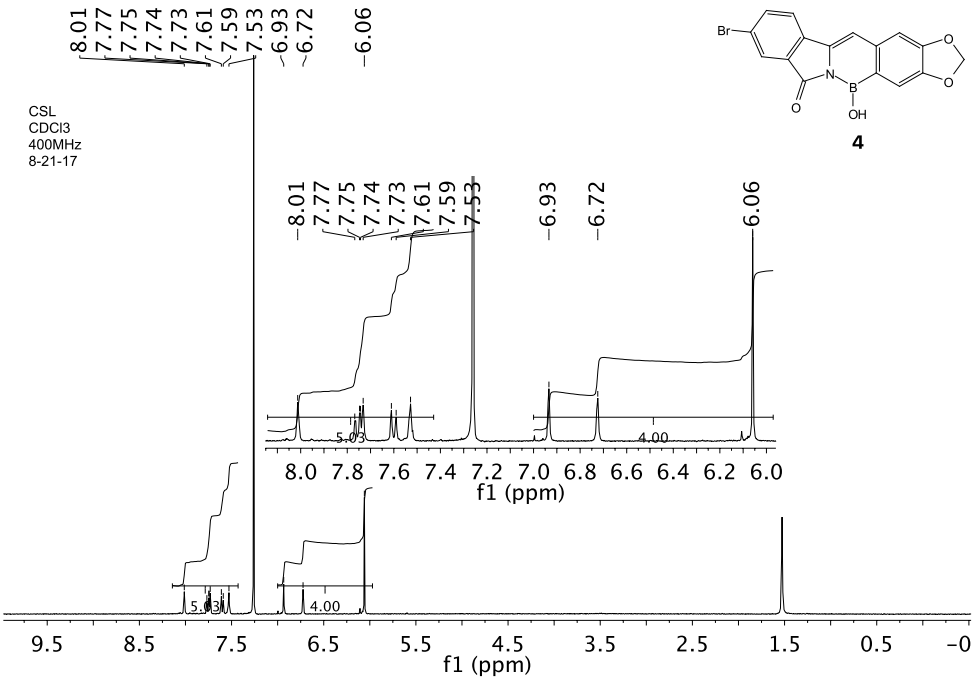
^{13}C NMR spectrum (100 MHz) of **2** in DMSO



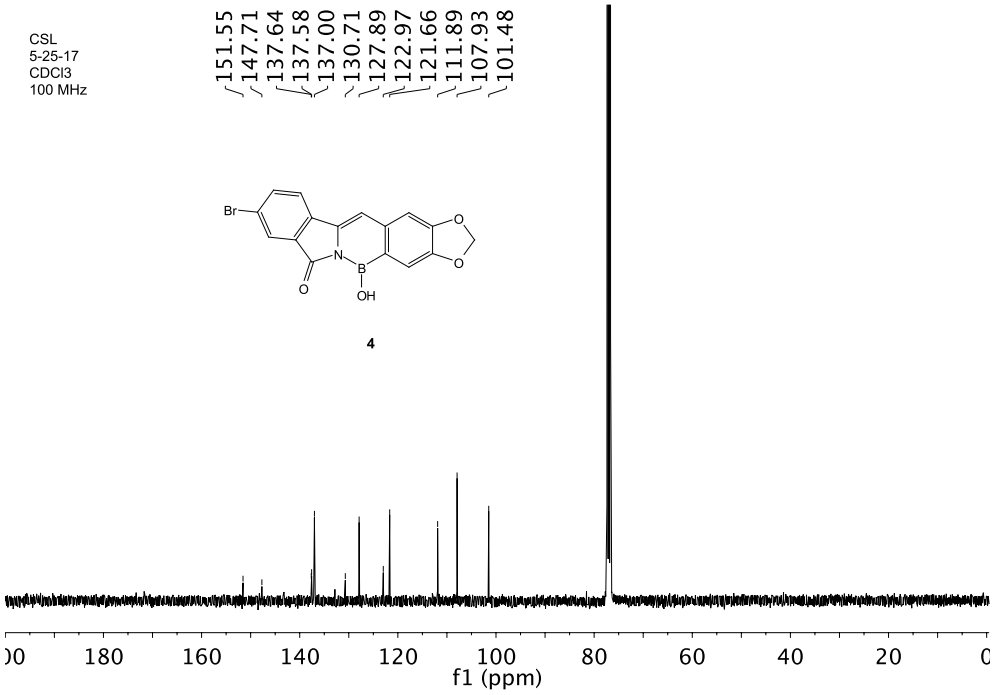
^{1}H NMR spectrum (400 MHz) of **3** in DMSO



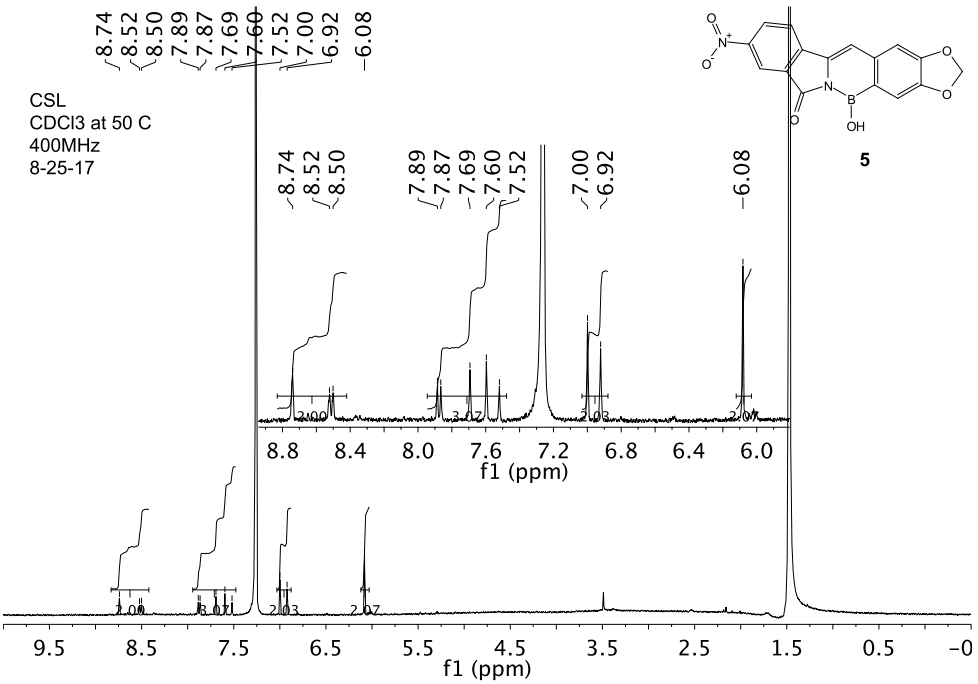
^{13}C NMR spectrum (100 MHz) of **3** in DMSO



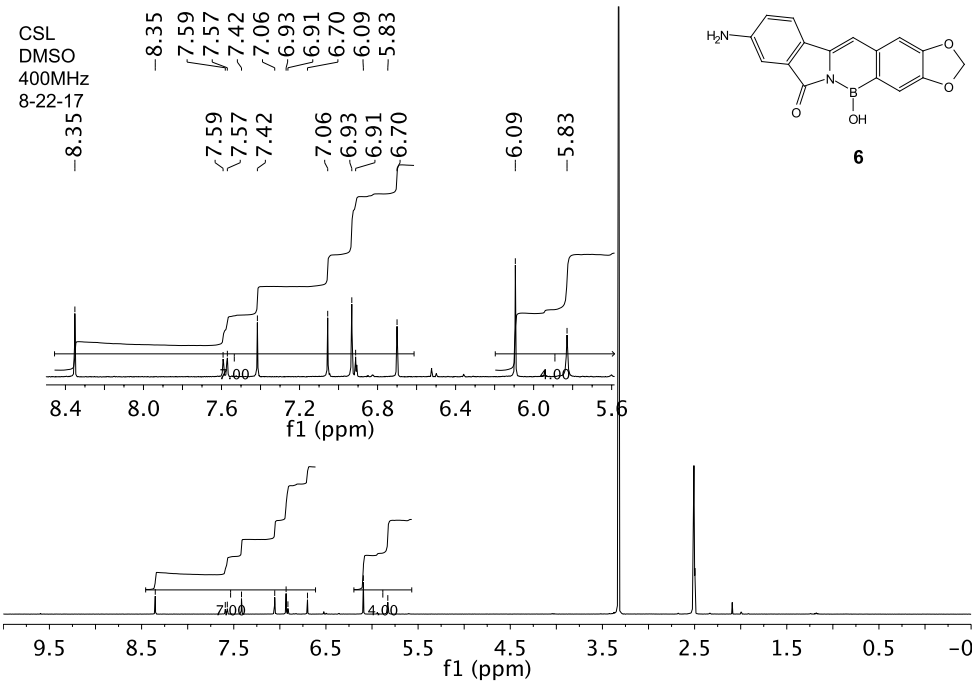
^{1}H NMR spectrum (400 MHz) of **4** in $CDCl_3$



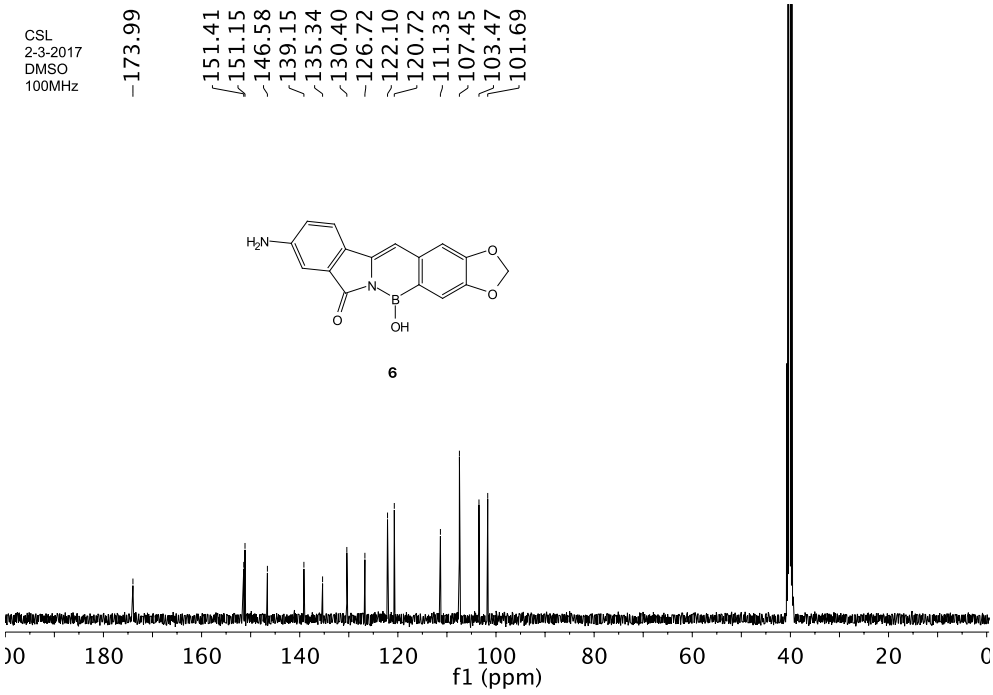
^{13}C NMR spectrum (100 MHz) of **4** in $CDCl_3$



^{1}H NMR spectrum (400 MHz) of **5** in $CDCl_3$ at 50 °C



^{1}H NMR spectrum (400 MHz) of **6** in DMSO



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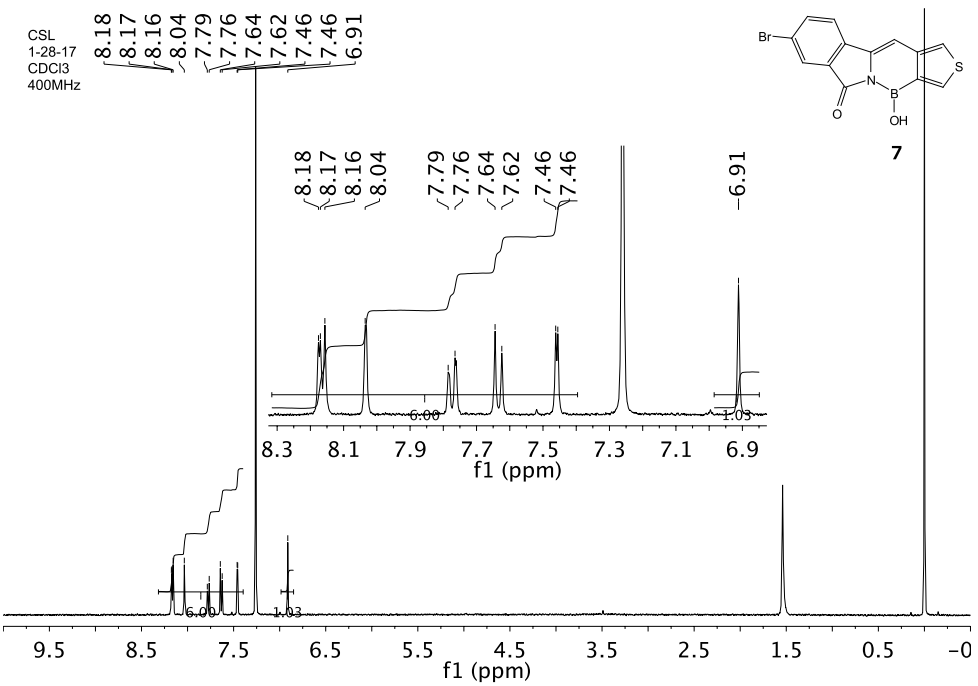
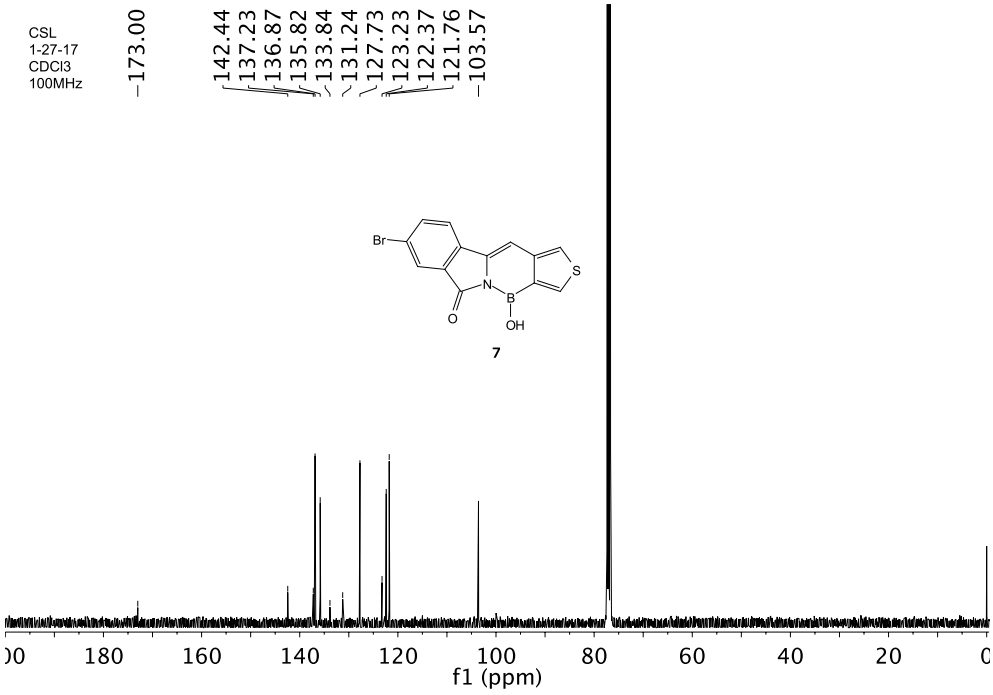
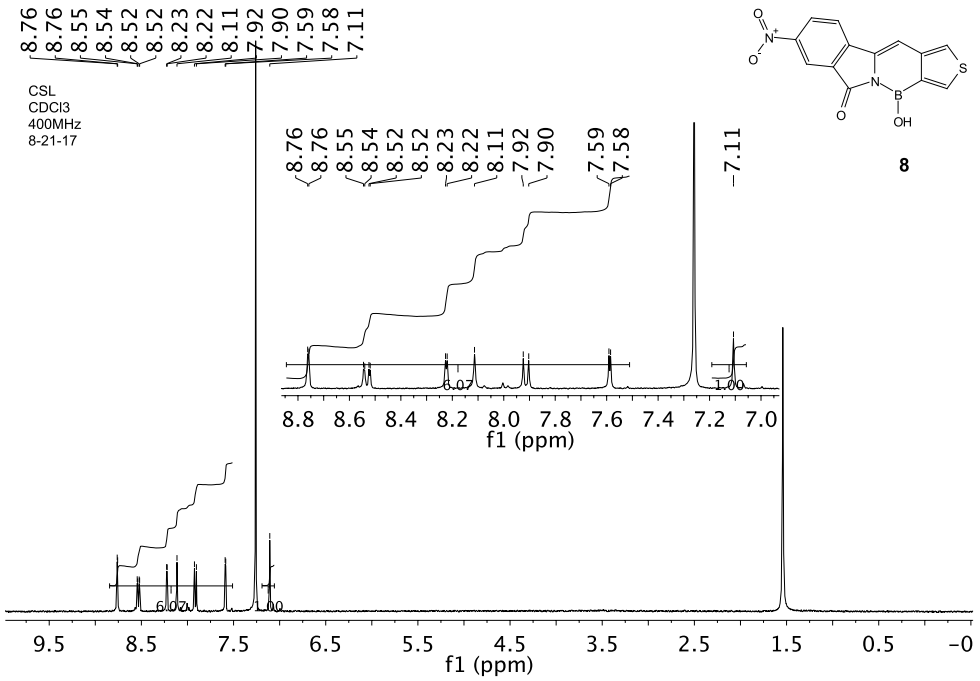


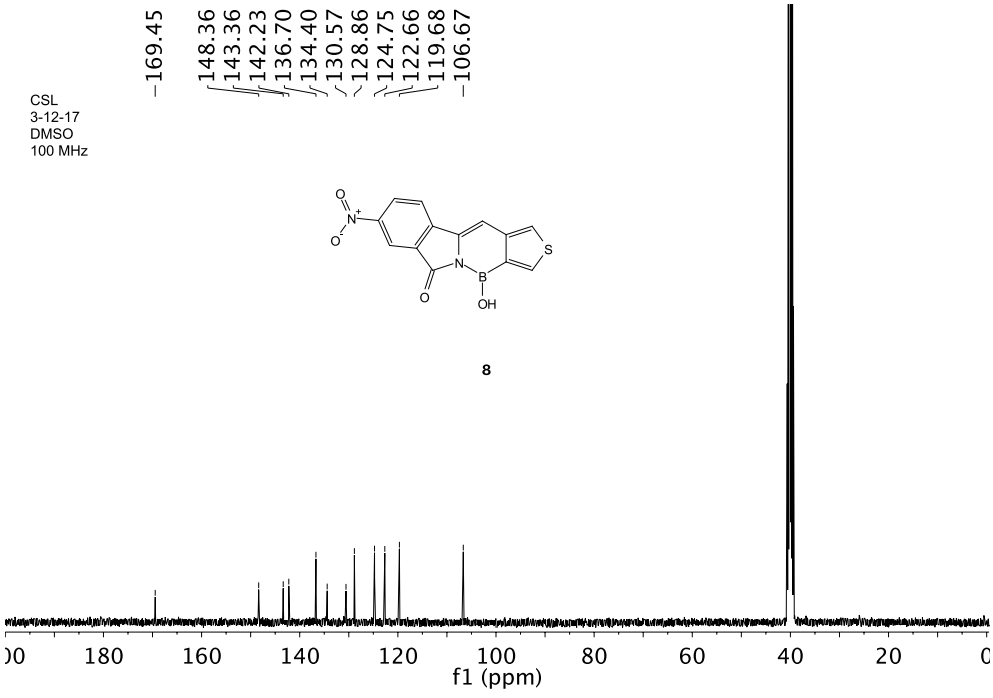
^{1}H NMR spectrum (400 MHz) of **7** in $CDCl_3$



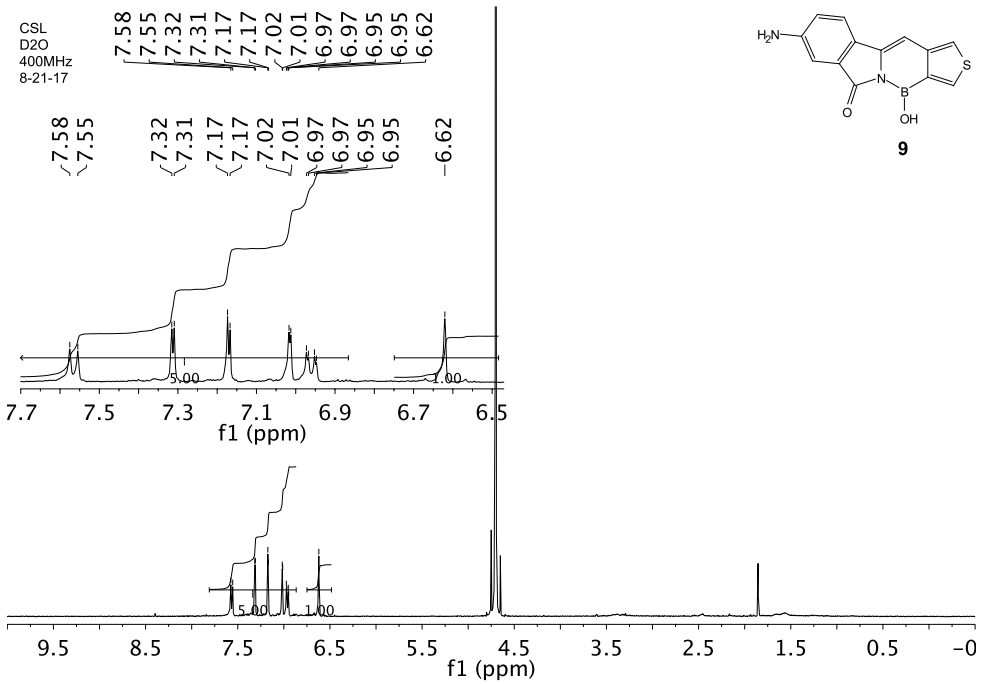
^{13}C NMR spectrum (100 MHz) of **7** in $CDCl_3$



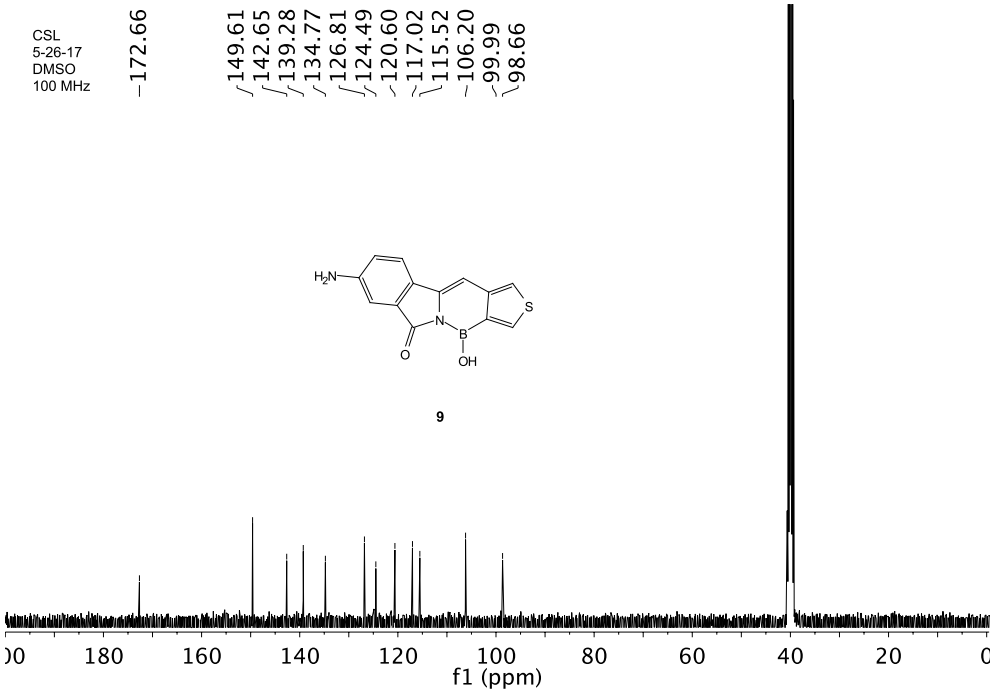
^{1}H NMR spectrum (400 MHz) of **8** in $CDCl_3$



^{13}C NMR spectrum (100 MHz) of **8** in DMSO

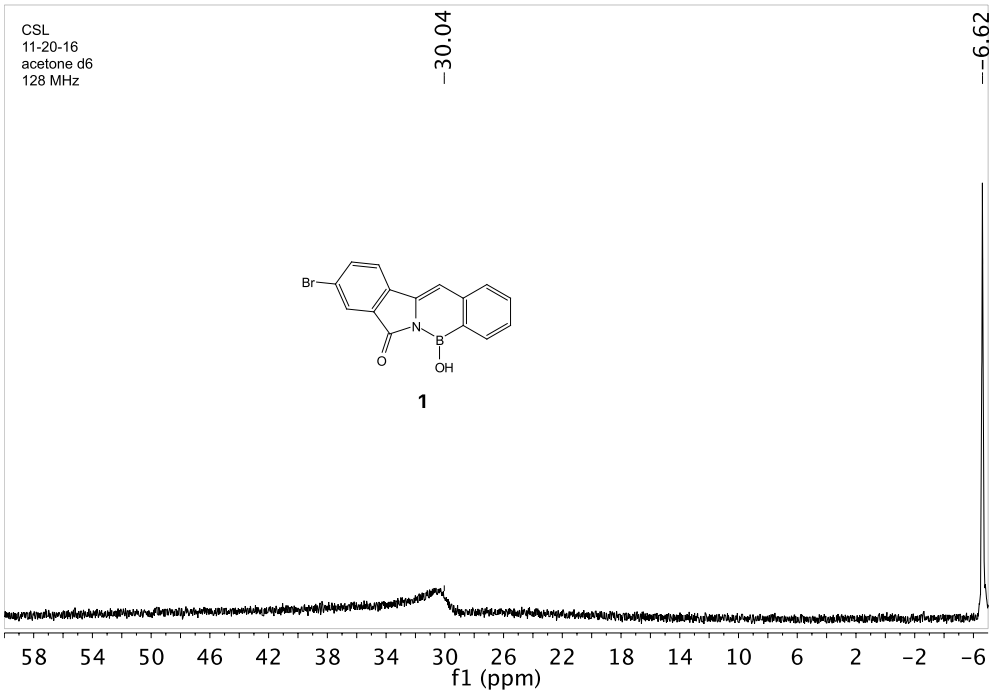


^{1}H NMR spectrum (400 MHz) of **9** in D_2O

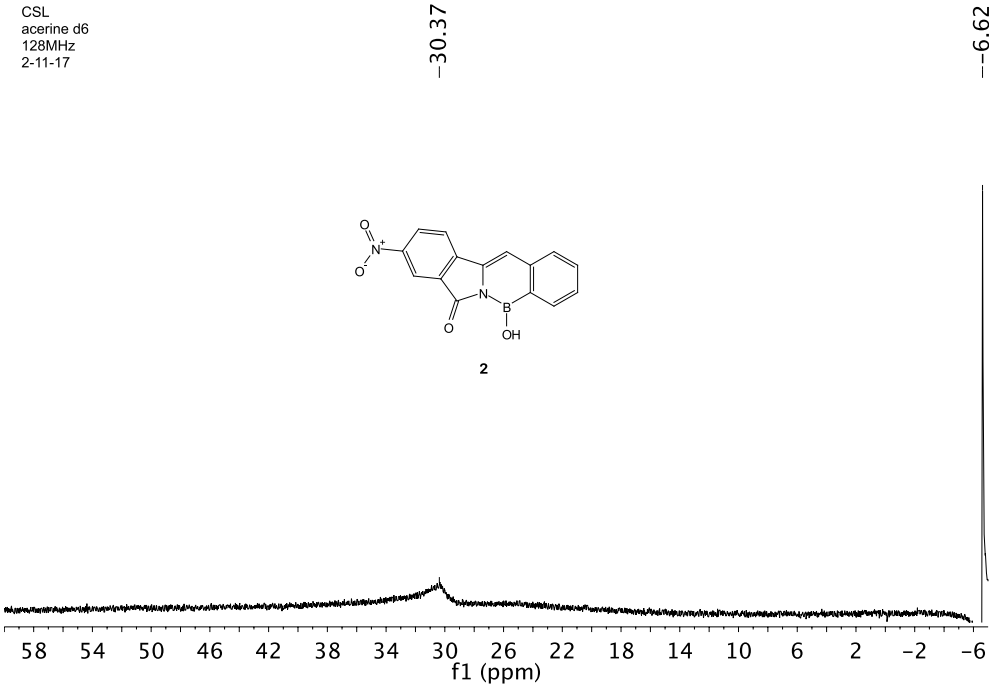


^{13}C NMR spectrum (100 MHz) of **9** in DMSO

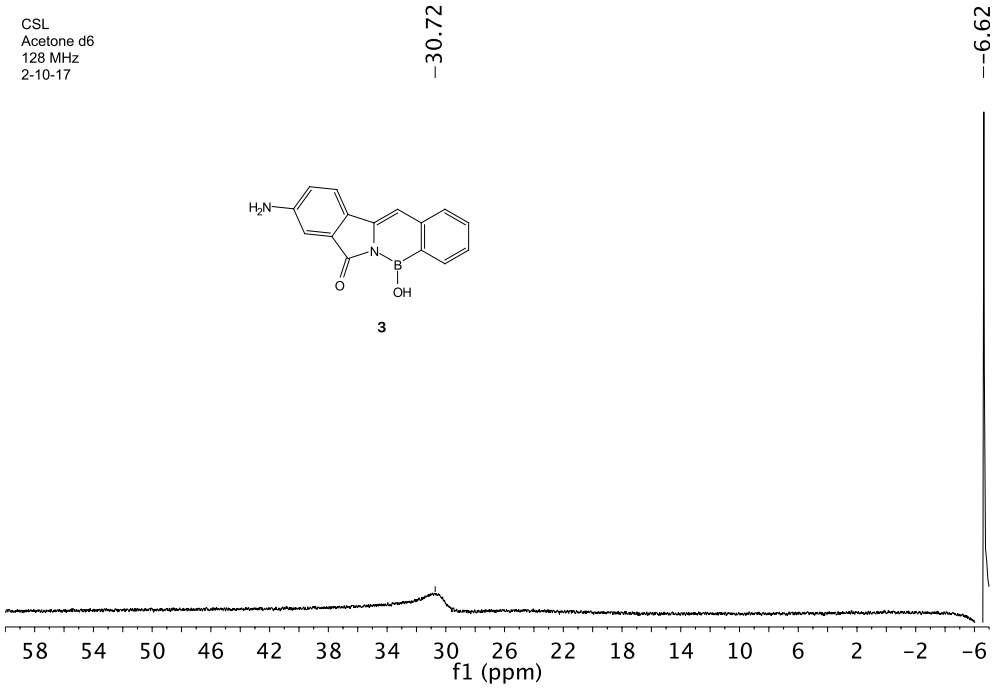
^{11}B NMR



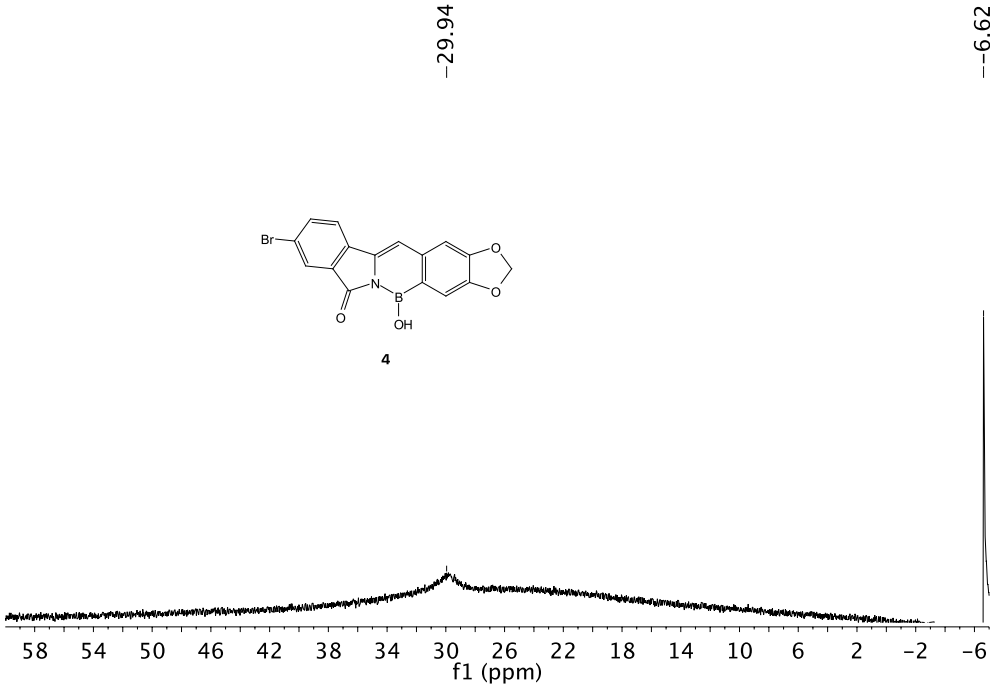
^{11}B NMR spectrum (128 MHz) of **1** in acetone d_6



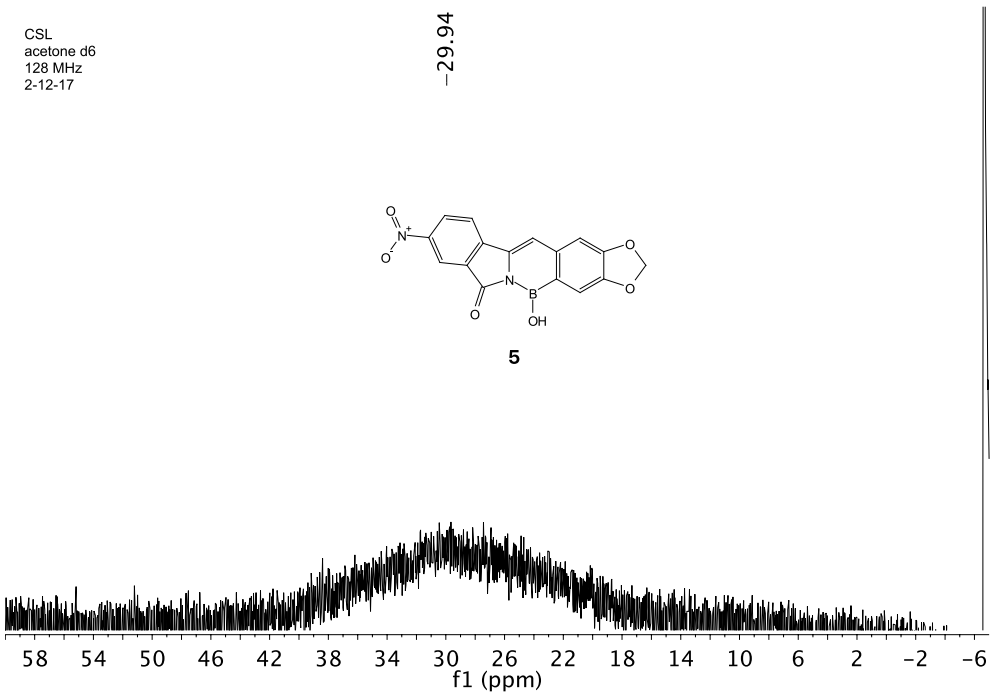
^{11}B NMR spectrum (128 MHz) of **2** in acetone d_6



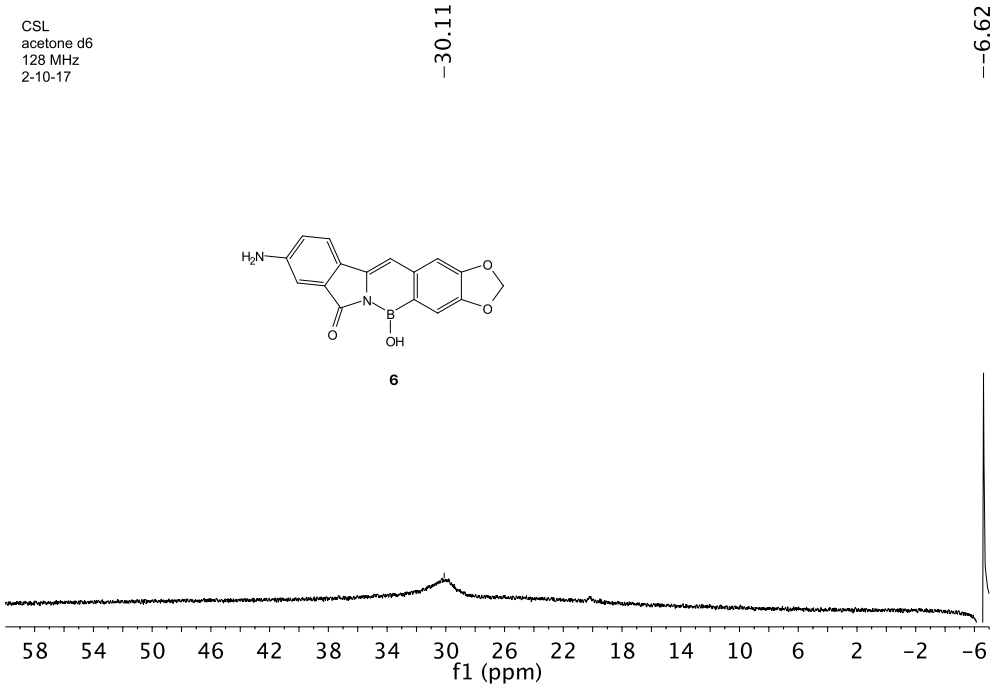
^{11}B NMR spectrum (128 MHz) of **3** in acetone d_6



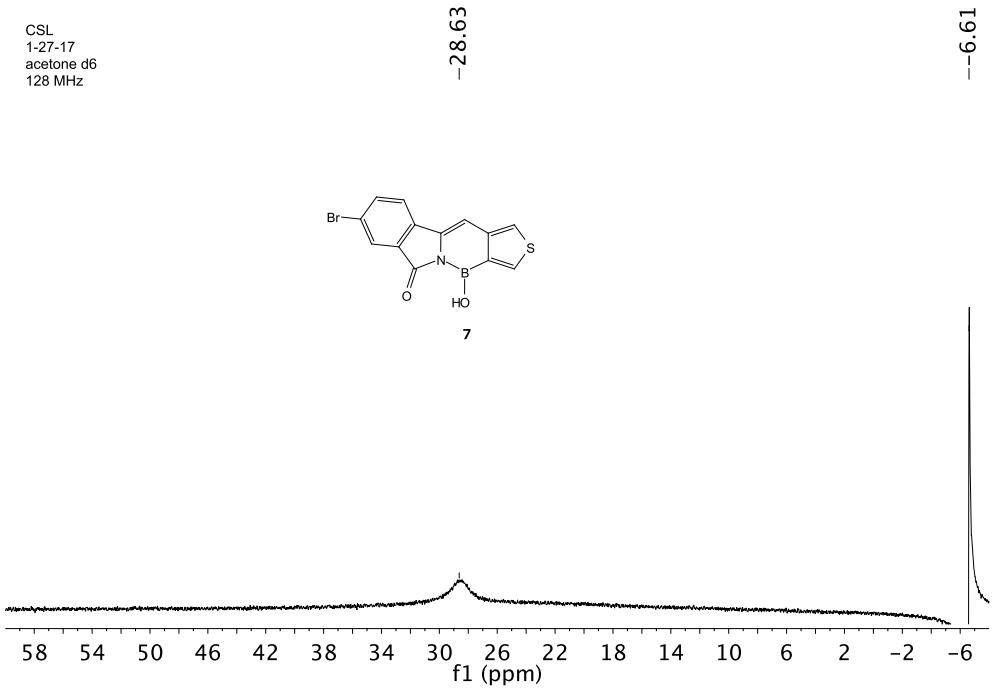
^{11}B NMR spectrum (128 MHz) of **4** in acetone d_6



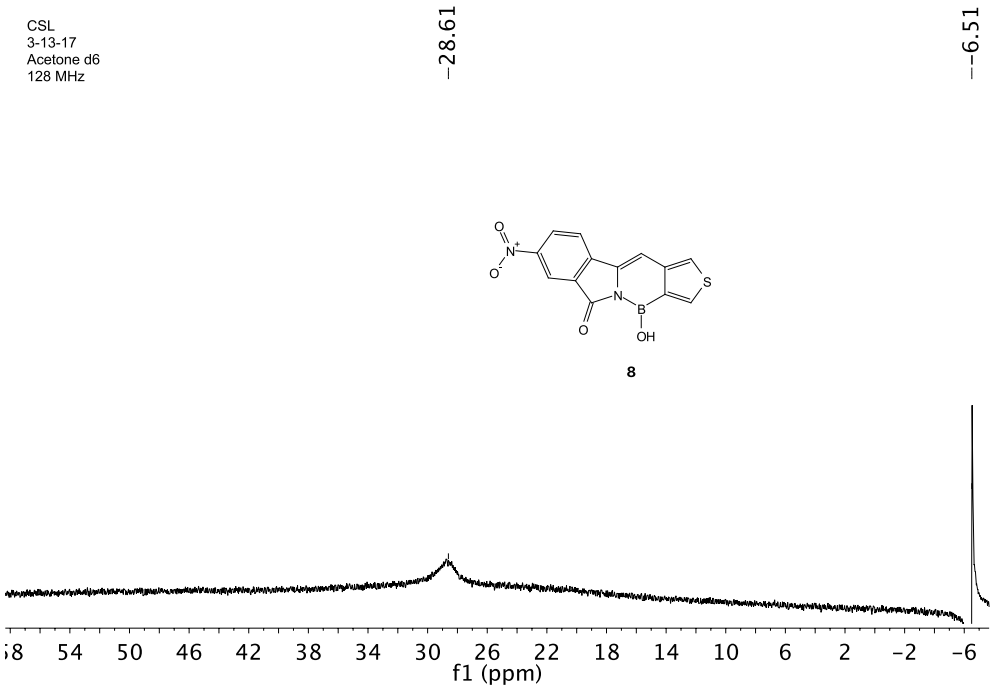
^{11}B NMR spectrum (128 MHz) of **5** in acetone d_6



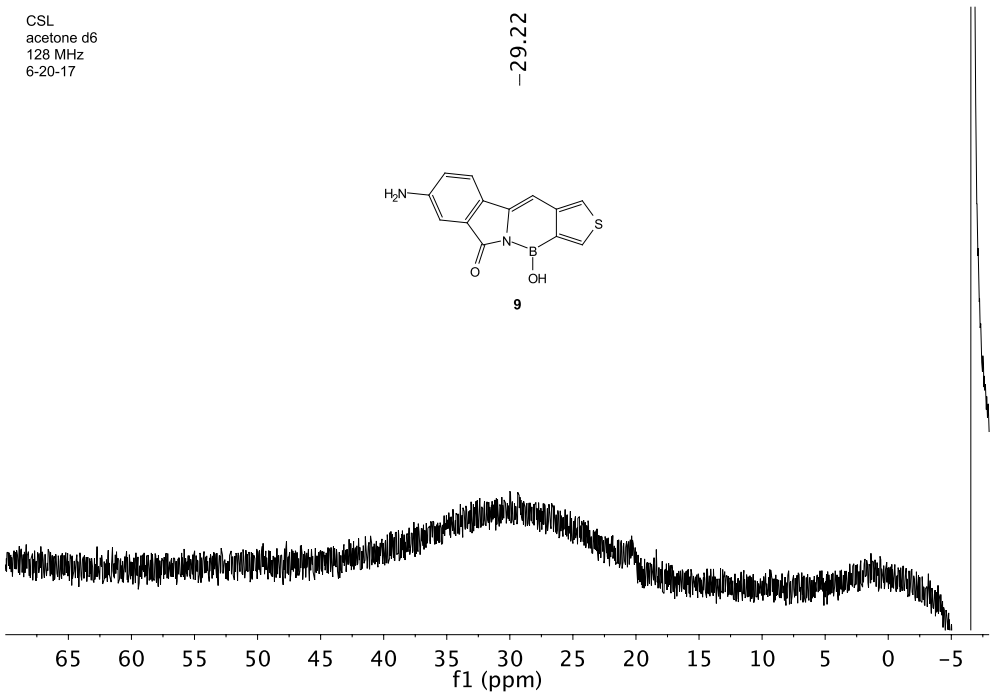
^{11}B NMR spectrum (128 MHz) of **6** in acetone d_6



^{11}B NMR spectrum (128 MHz) of **7** in acetone d_6

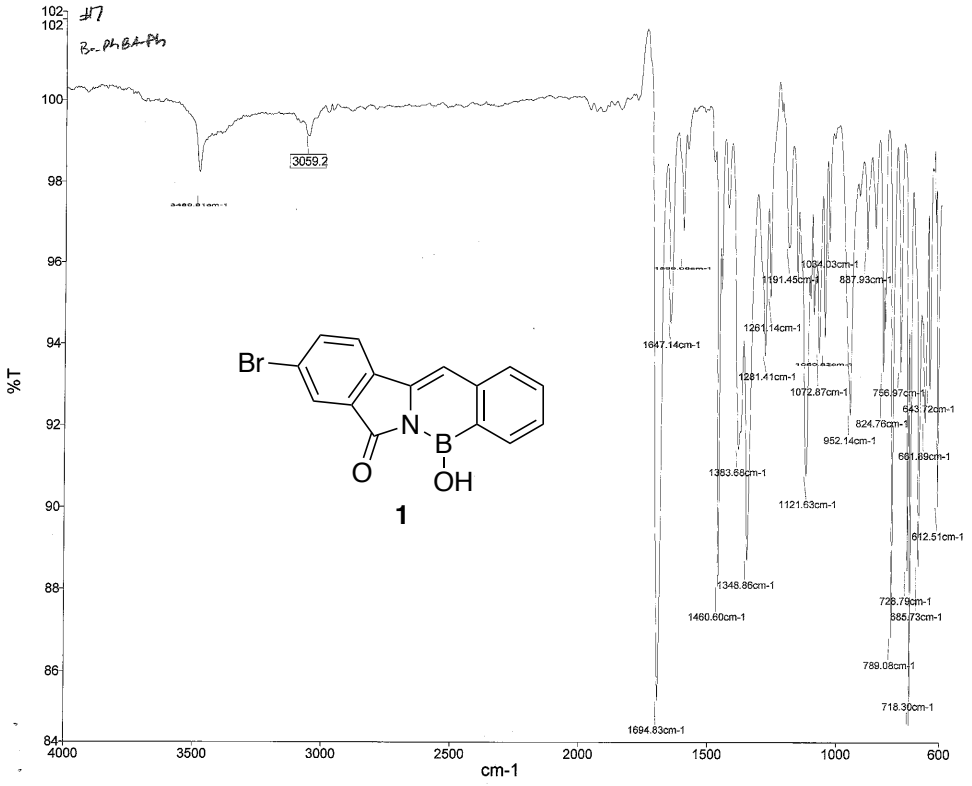


^{11}B NMR spectrum (128 MHz) of **8** in acetone d_6



^{11}B NMR spectrum (128 MHz) of **9** in acetone d_6

FT-IR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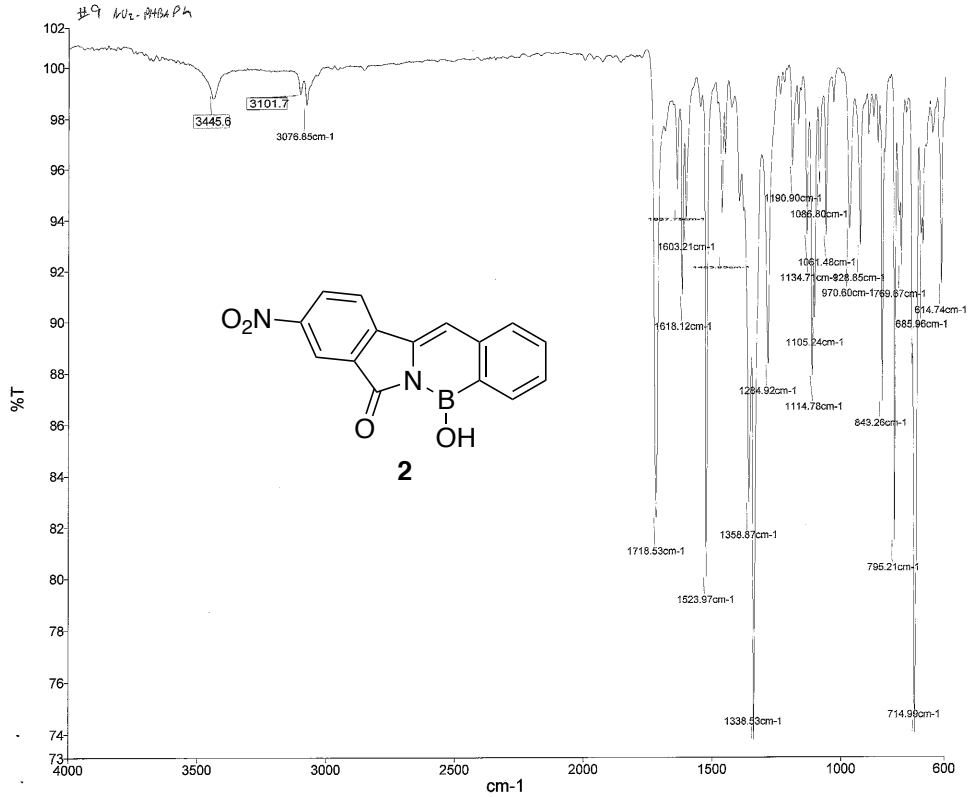
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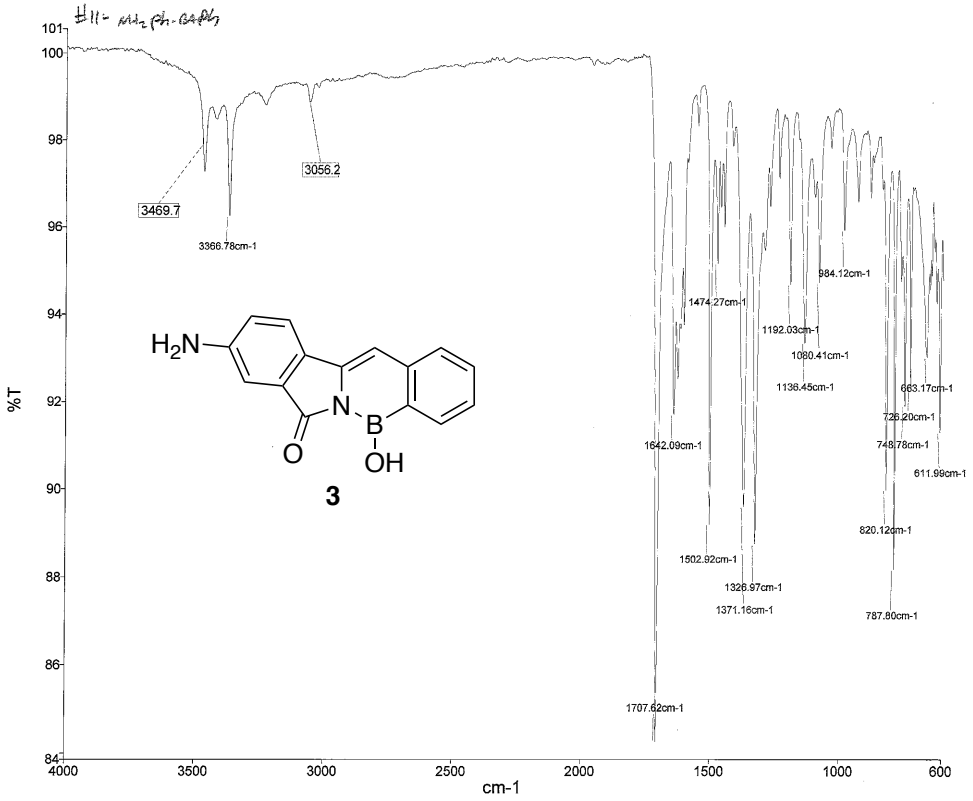
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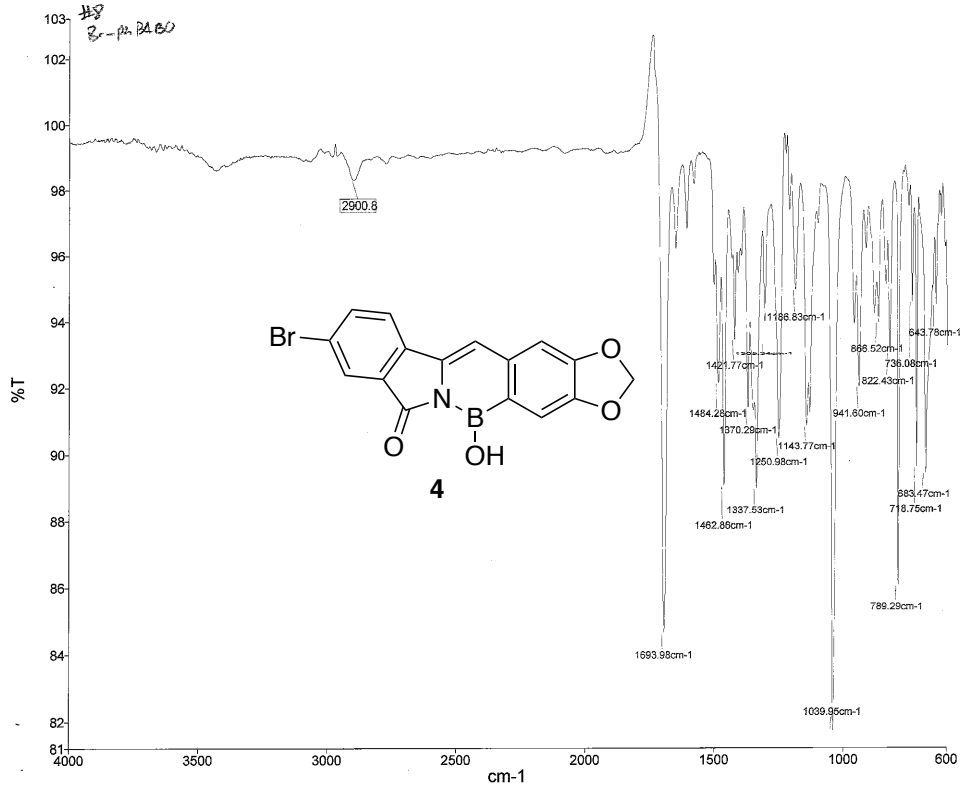
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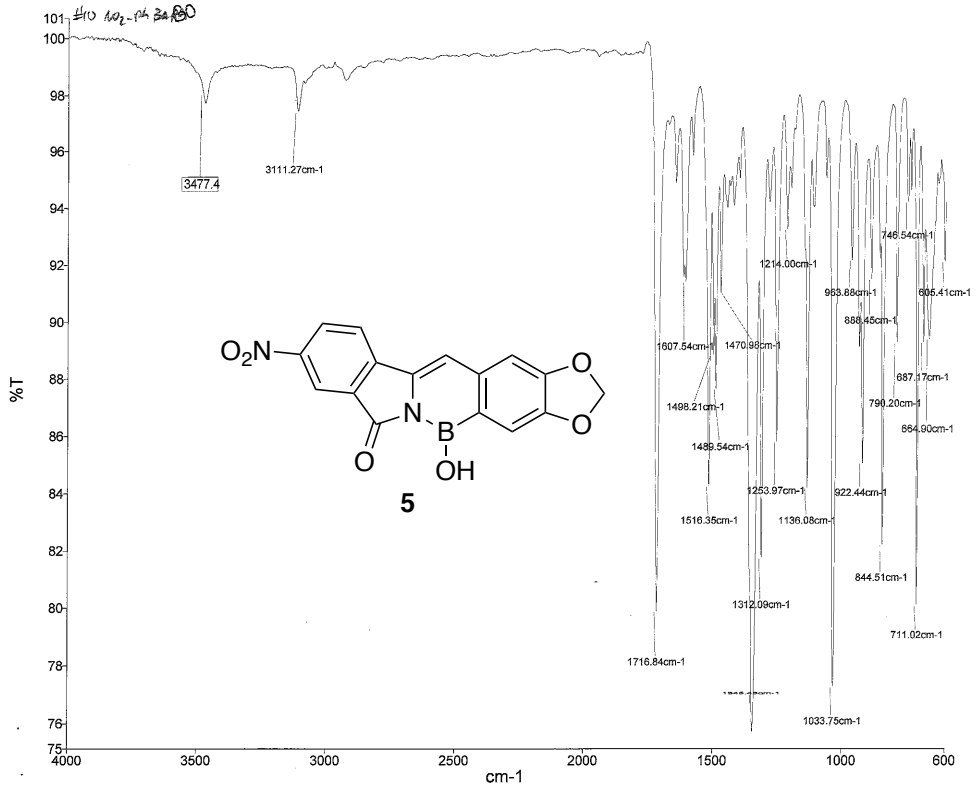
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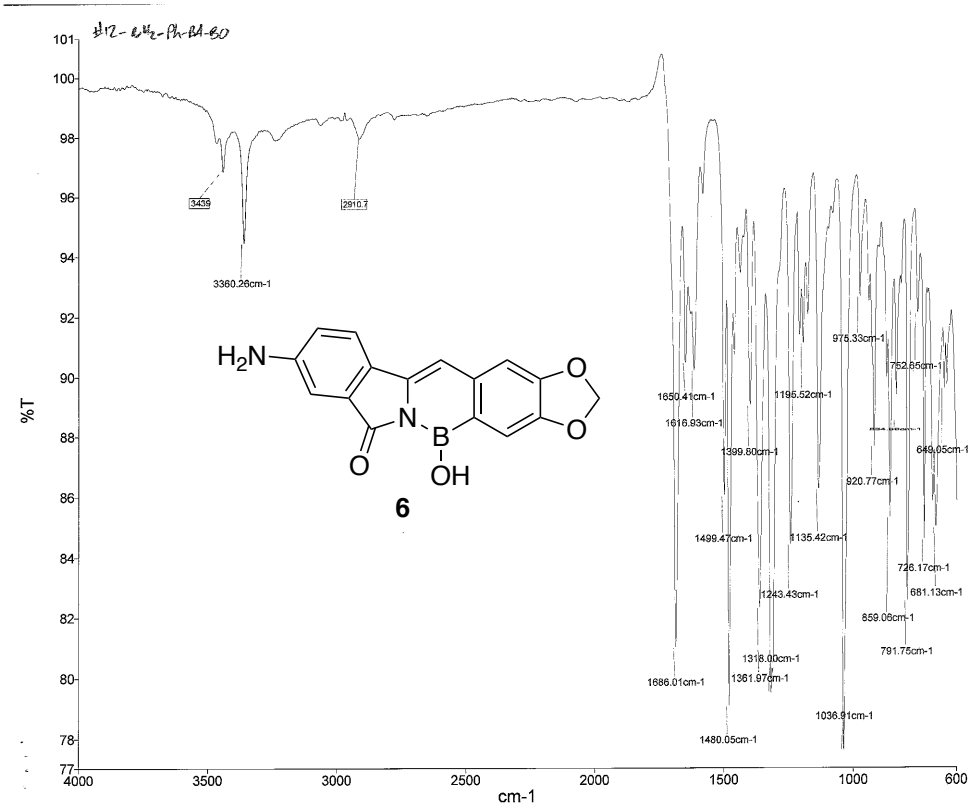
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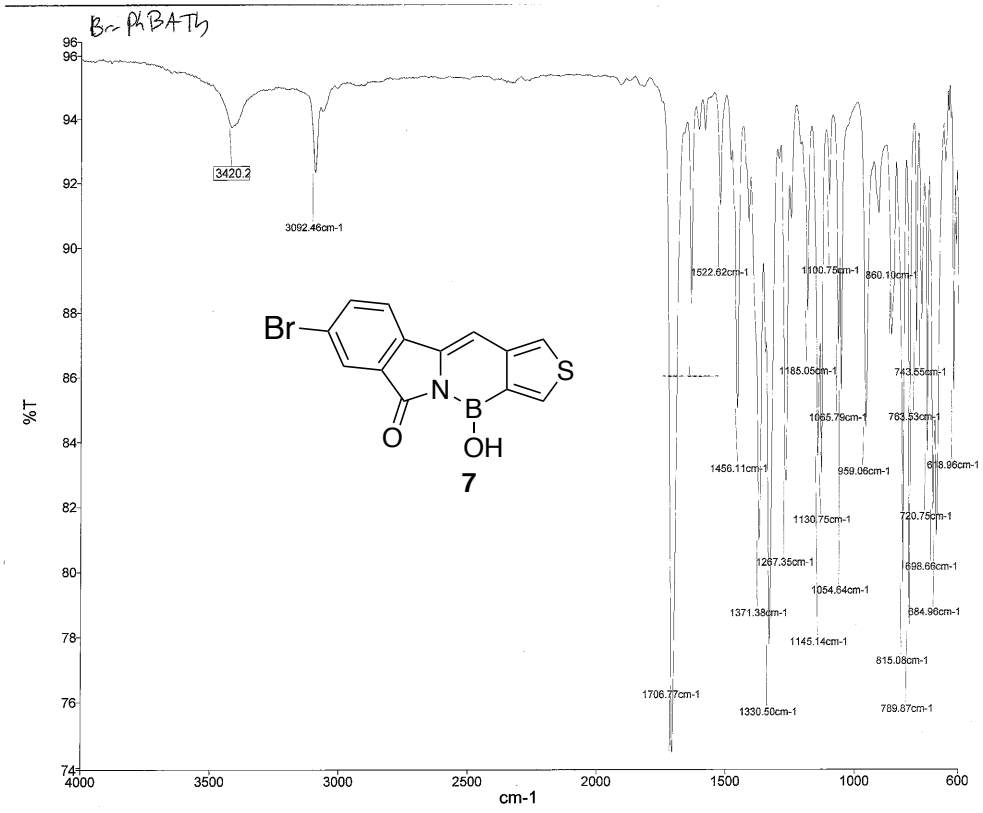
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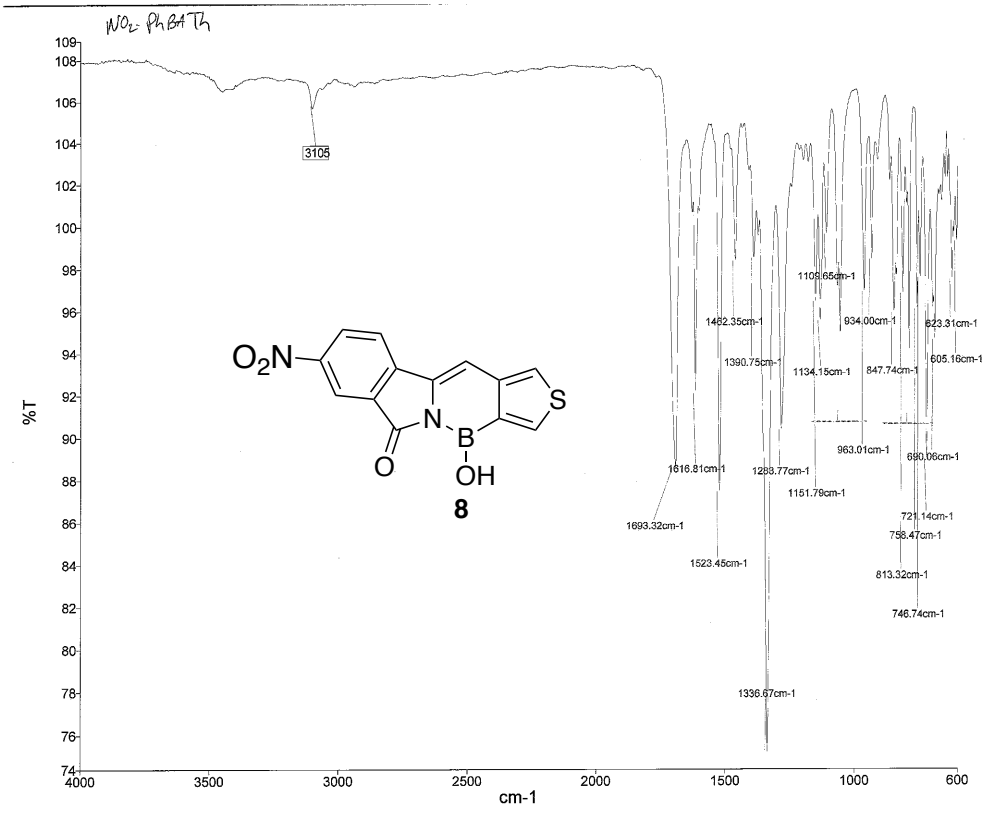
cm-1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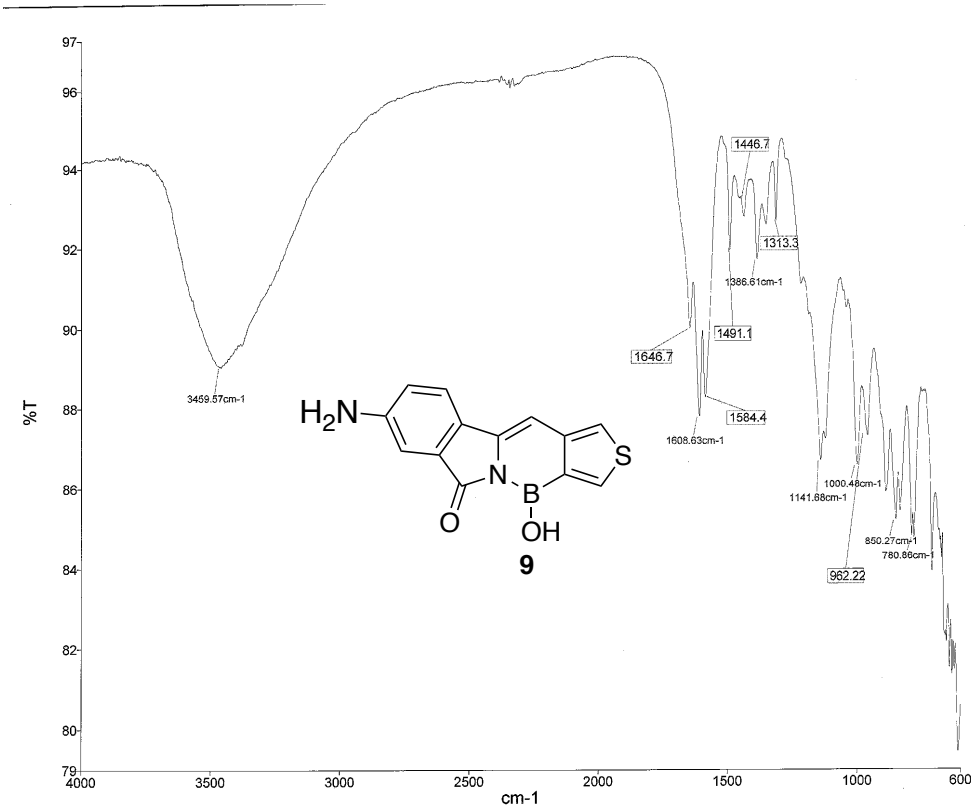
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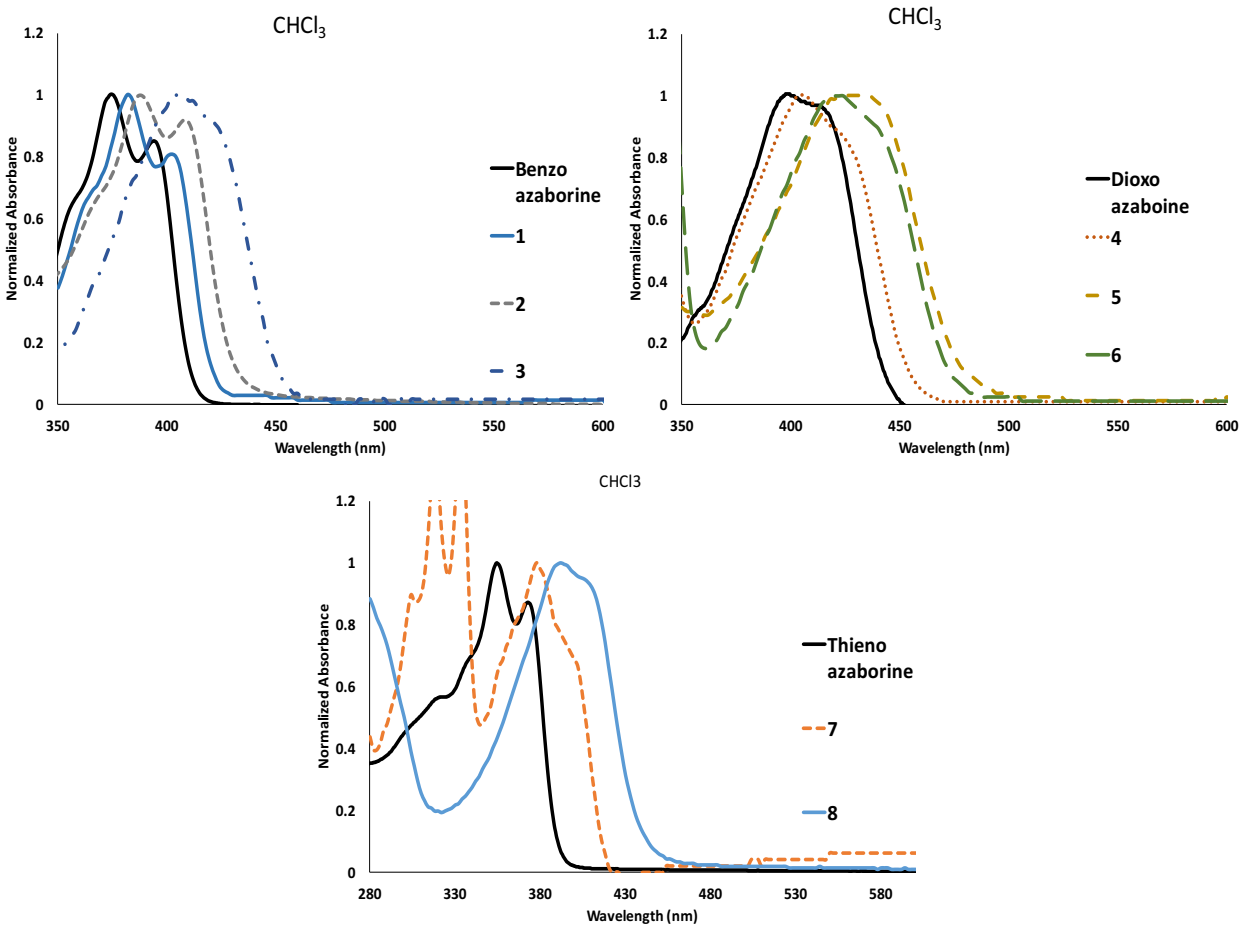
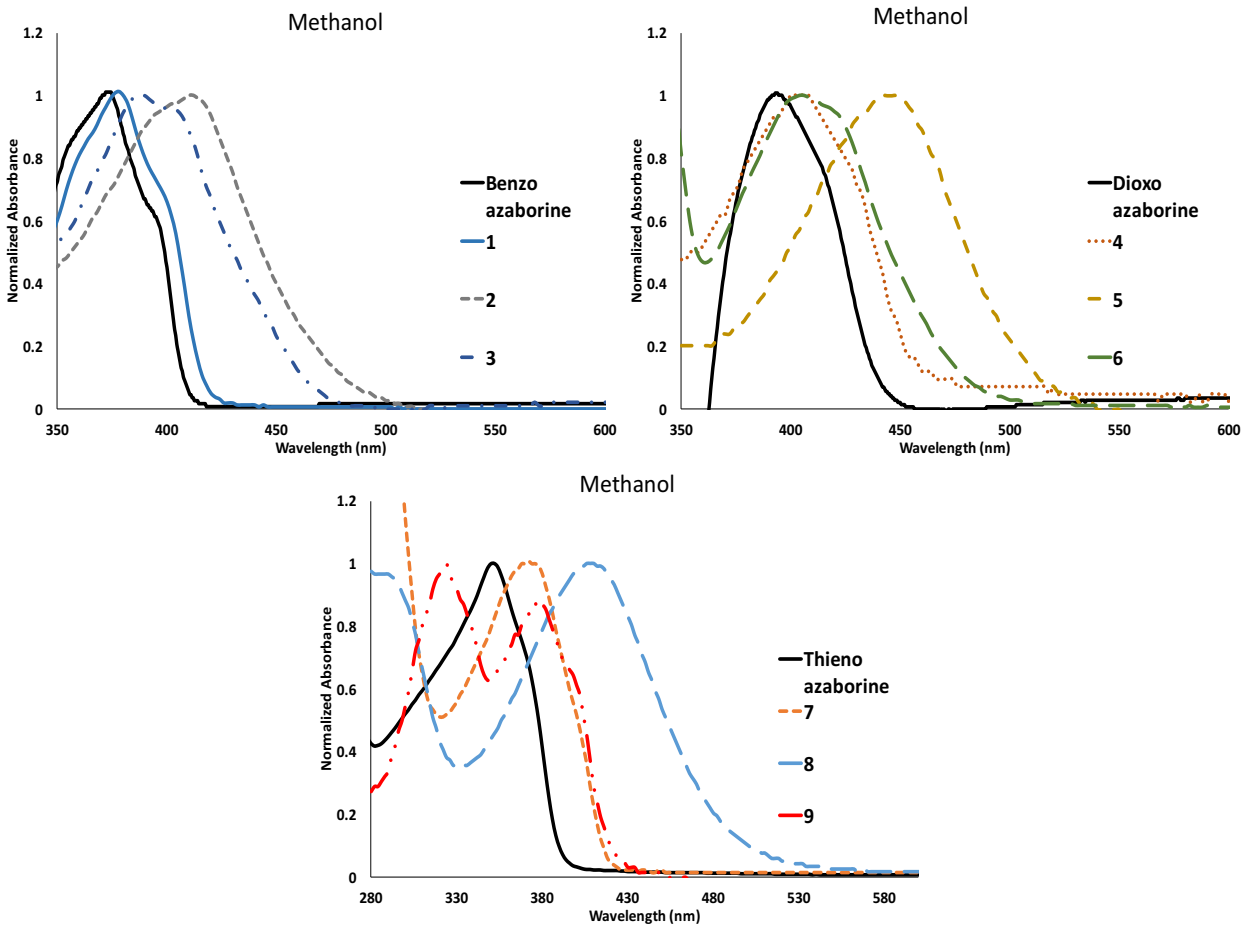
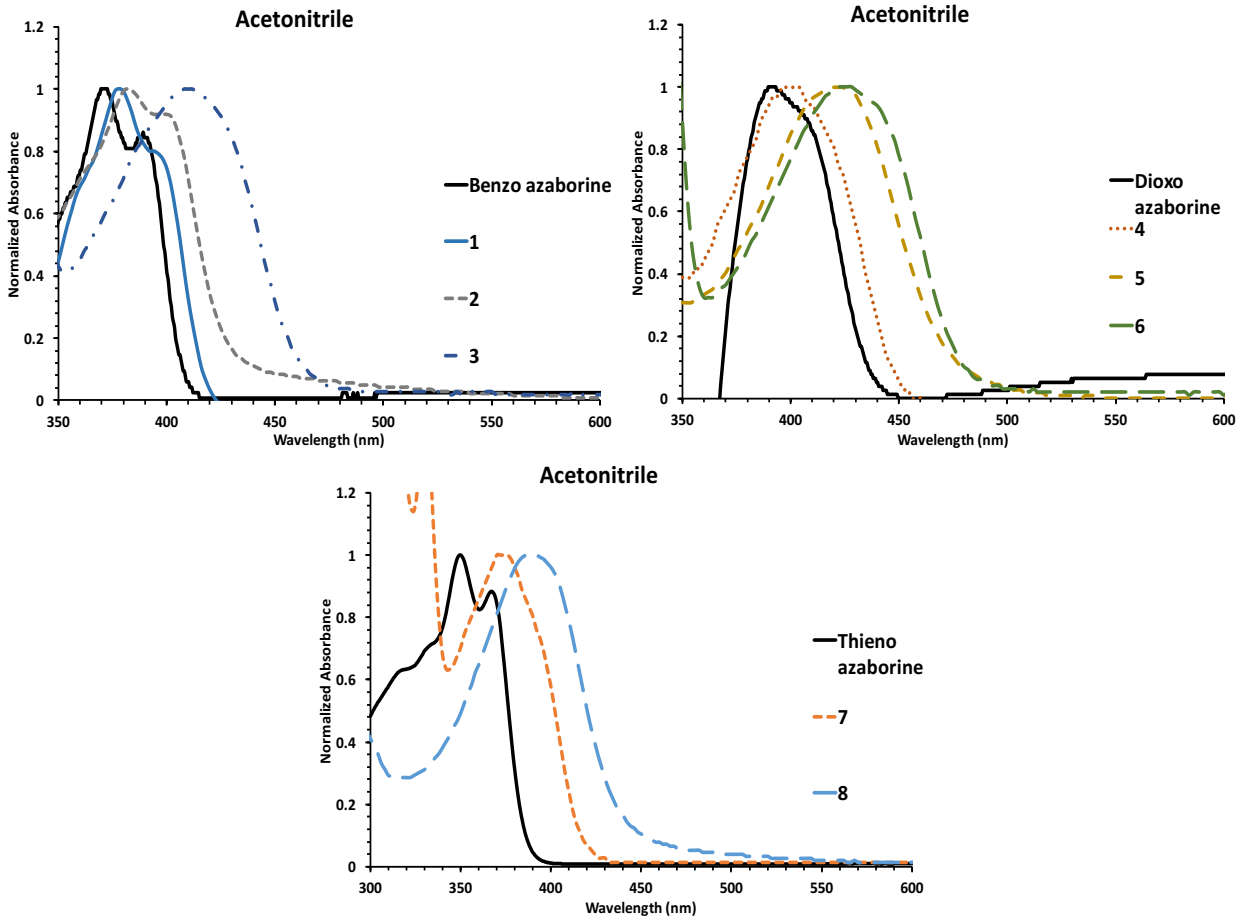
Normalized UV-visible spectra of compounds 1-8, benzo, dioxo, and thieno azaborines in chloroform.



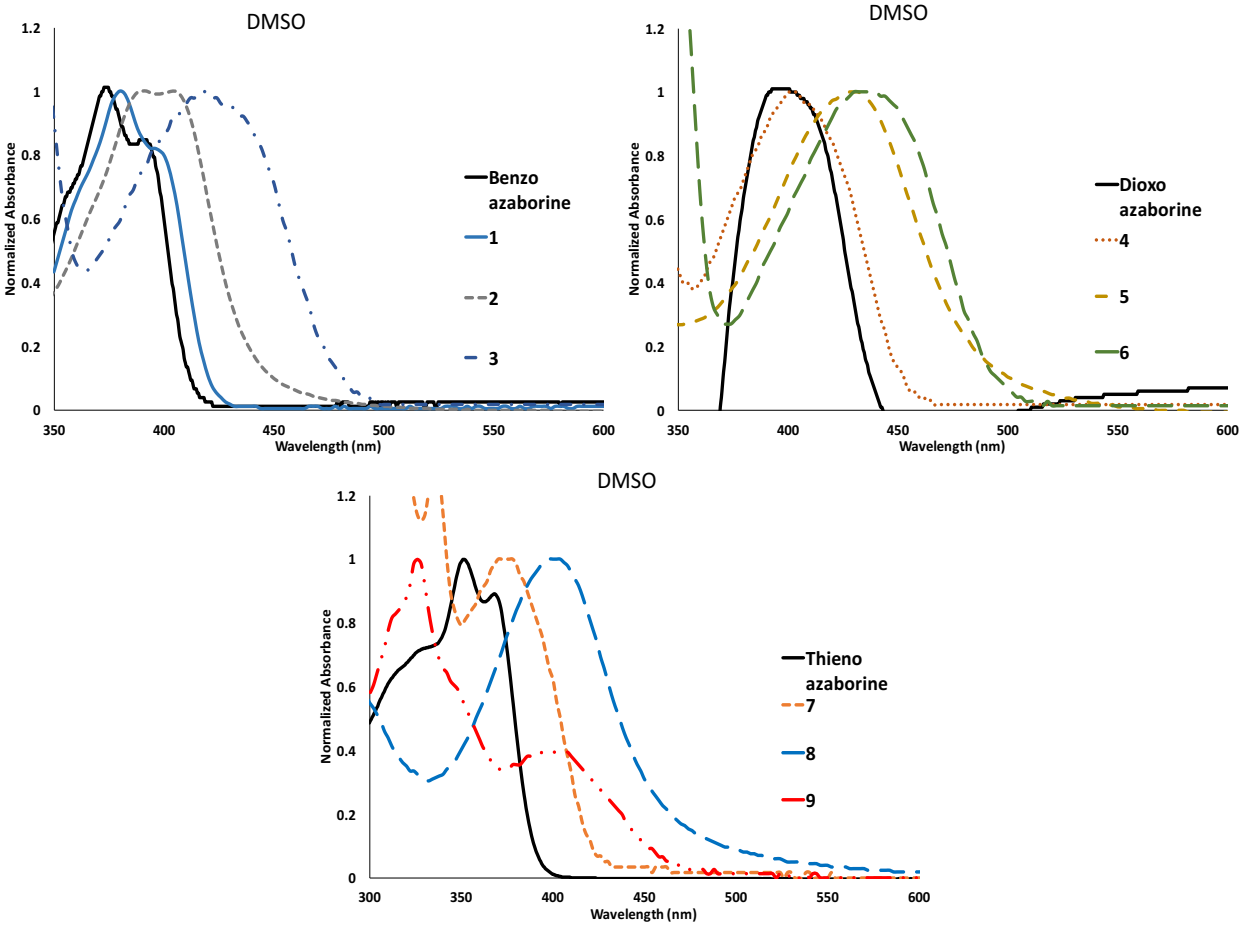
Normalized UV-visible spectra of compounds 1-9 benzo, dioxo, and thieno azaborines in methanol



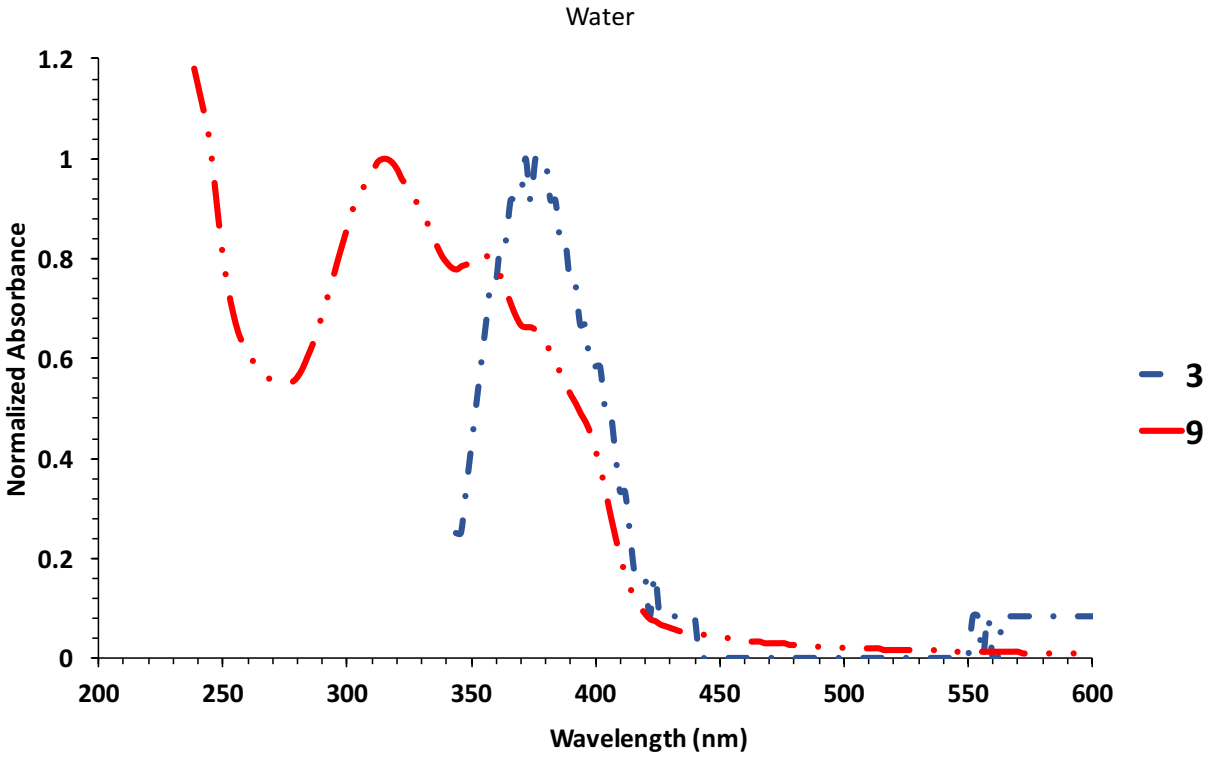
Normalized UV-visible spectra of compounds 1-8, benzo, dioxo, and thieno azaborines in acetonitrile



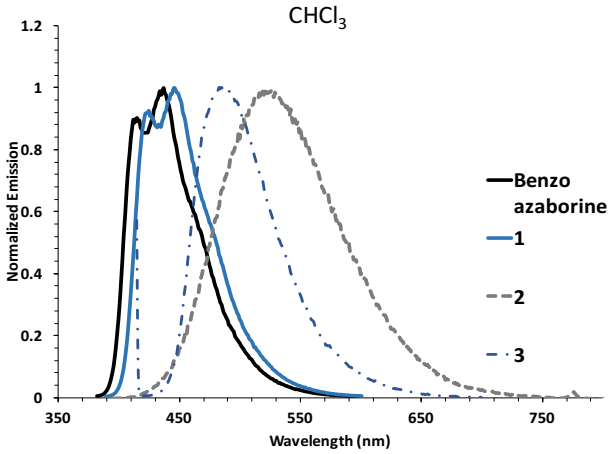
Normalized UV-visible spectra of compounds 1-9 in DMSO

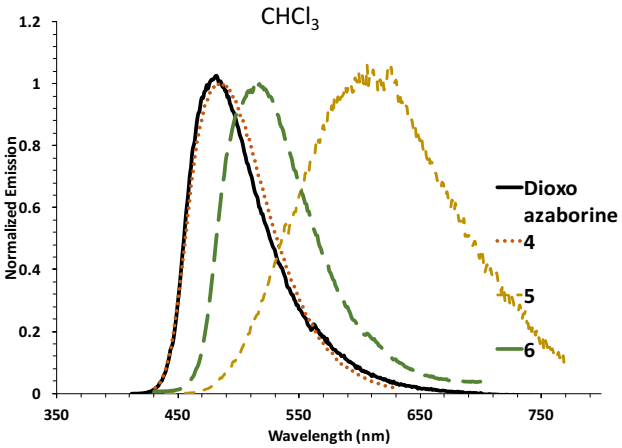


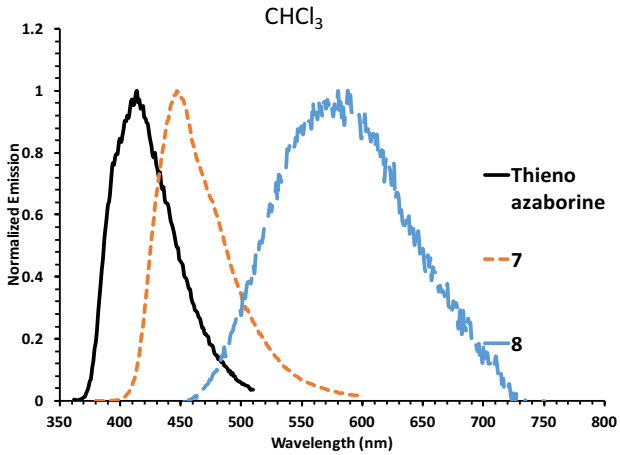
Normalized UV-visible spectra of compounds 3 and 9 in H_2O



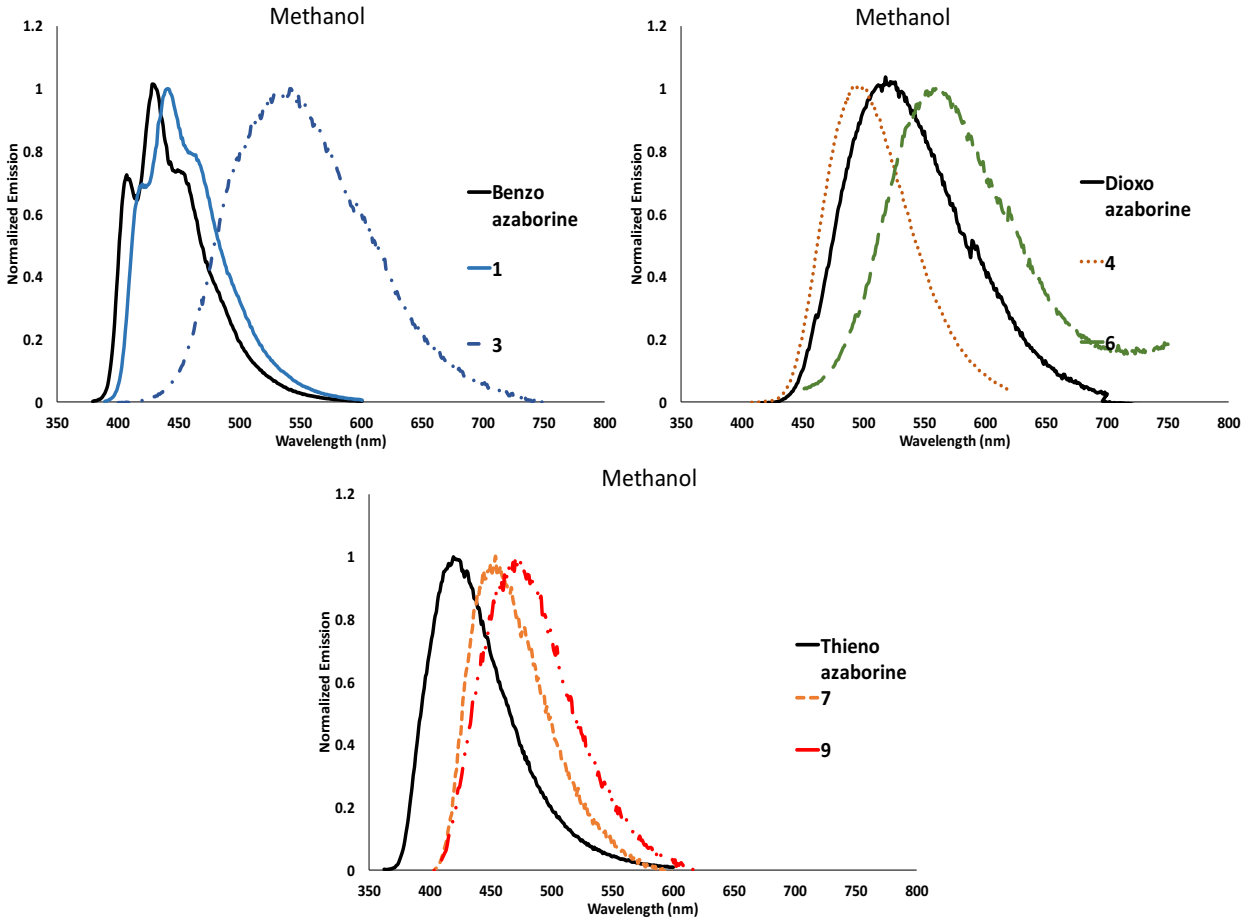
Normalized emission spectra of compounds 1-8, benzo, dioxo, and thieno azaborines in chloroform.



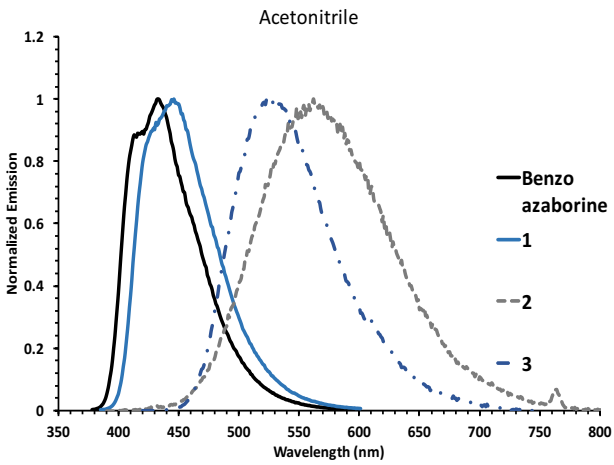


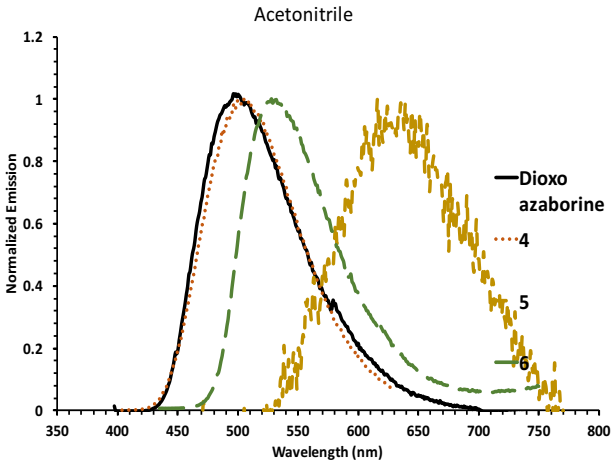


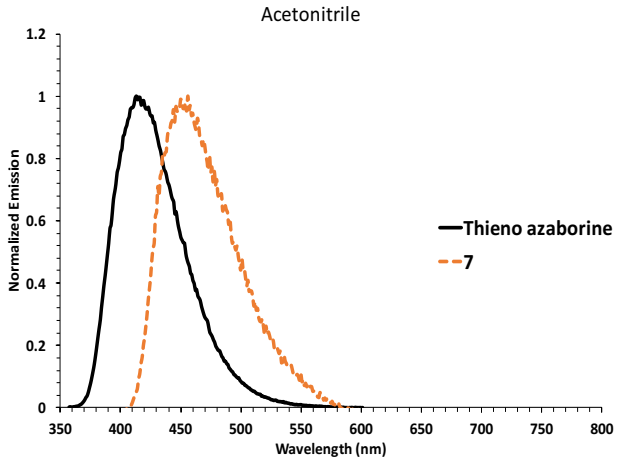
Normalized emission spectra of compounds 1, 3, 4, 6, 7, 9, benzo, dioxo, and thieno azaborines in methanol.



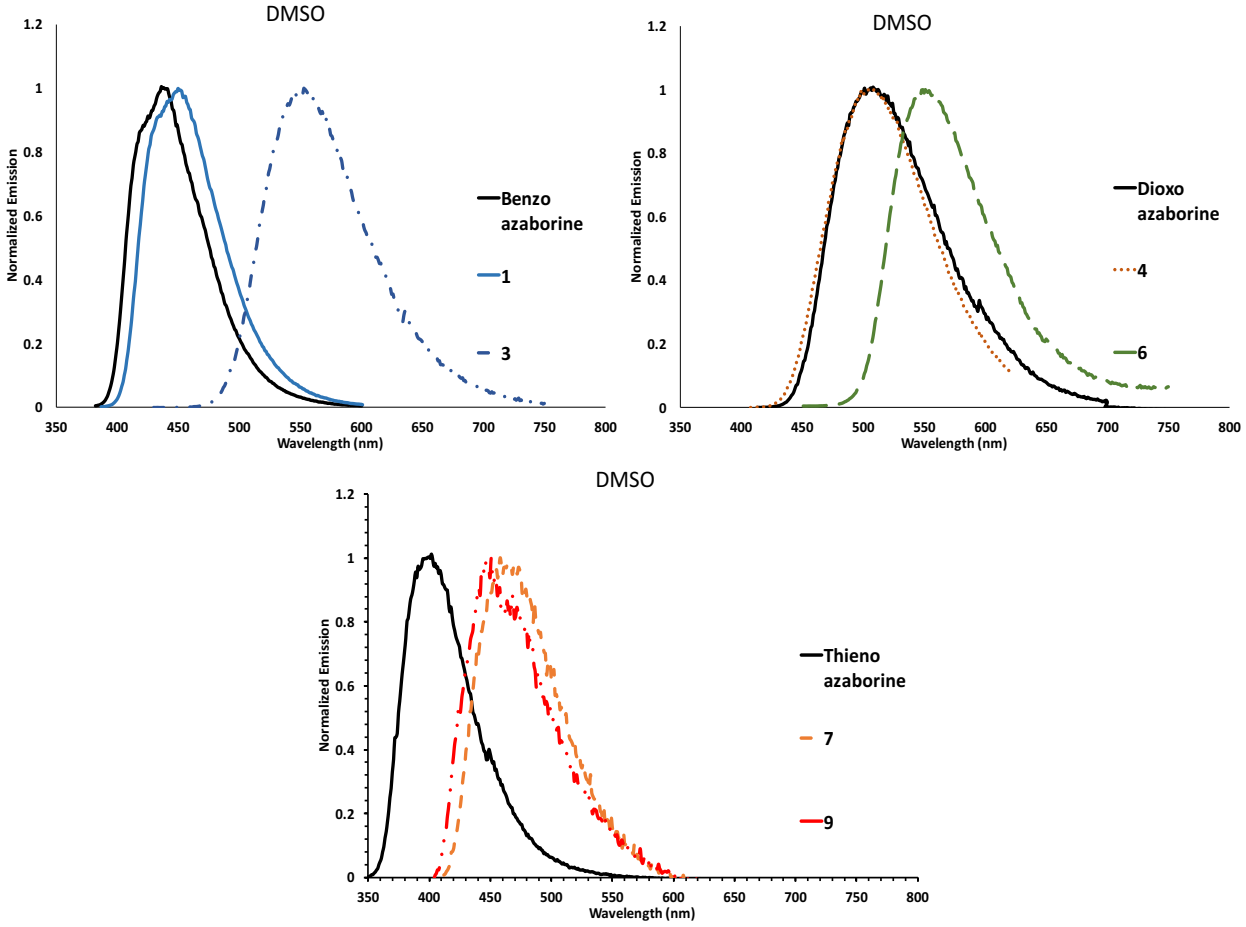
Normalized emission spectra of compounds 1-7, benzo, dioxo, and thieno azaborines in acetonitrile.



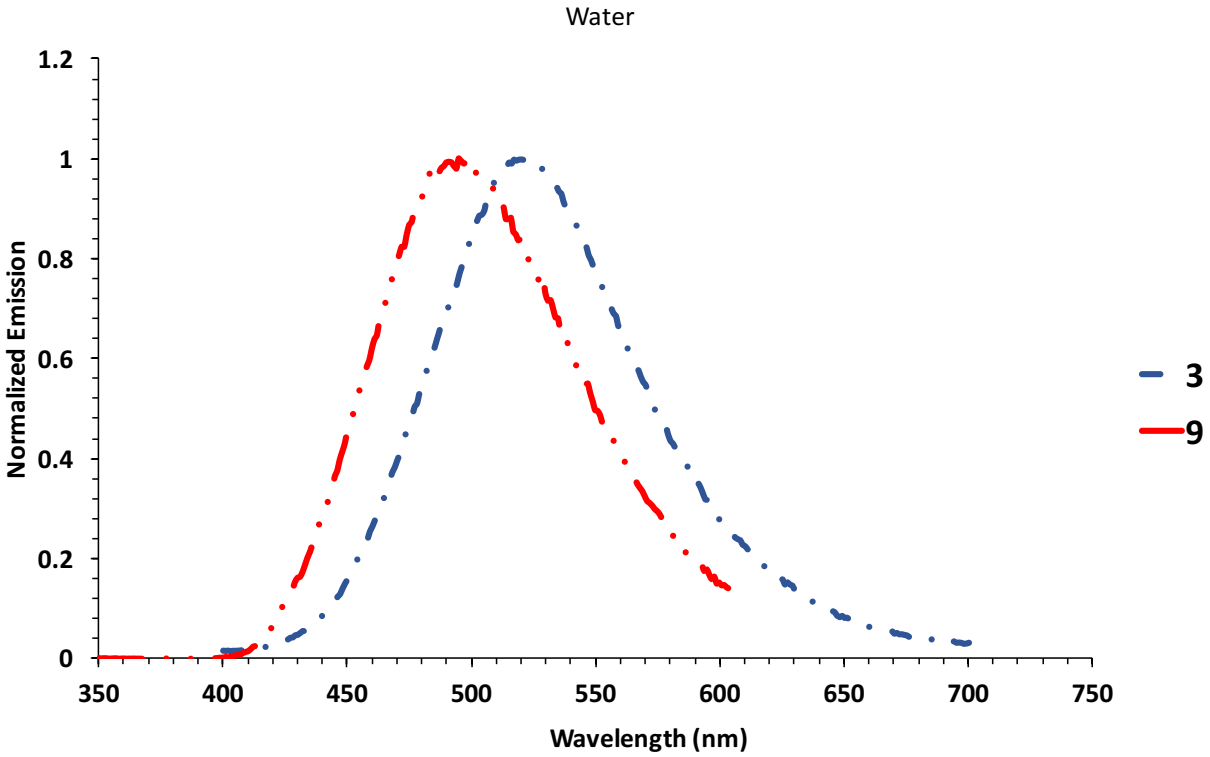




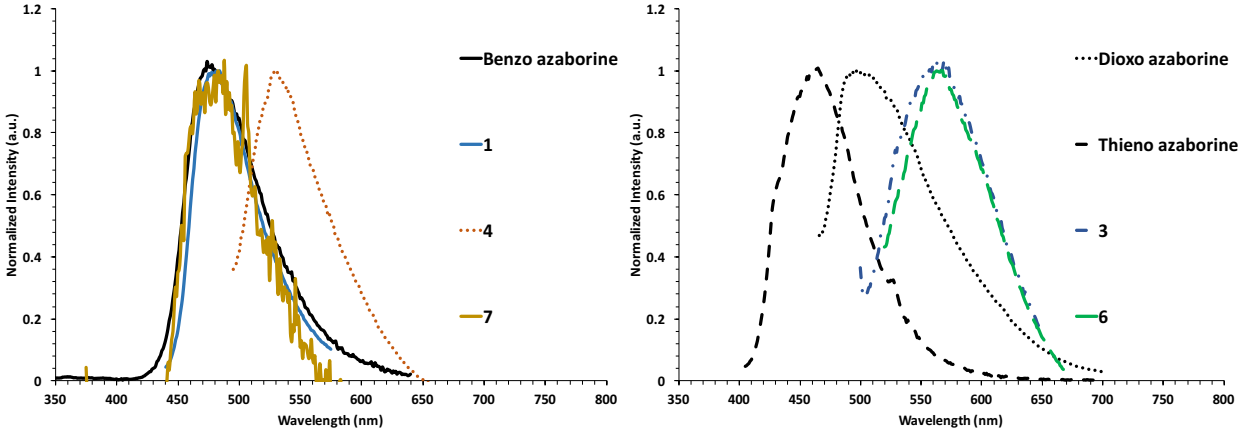
Normalized emission spectra of compounds 1, 3, 4, 6, 7, 9, benzo, dioxo, and thieno azaborines in DMSO.



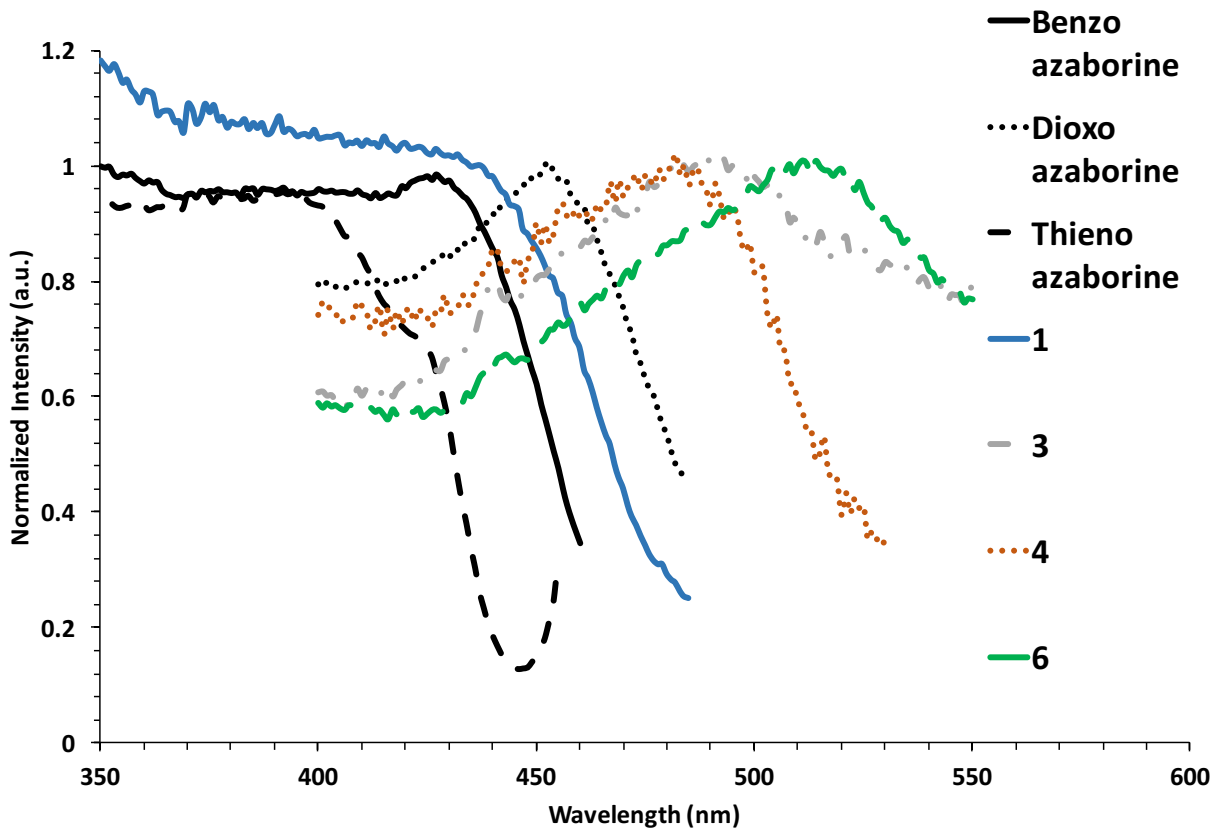
Normalized emission spectra of compounds 3 and 9 in H_2O.



Normalized emission spectra of compounds 1, 3, 4, 6, 7, benzo, dioxo and thieno azaborines in the solid state.



Normalized excitation spectra of compounds 1, 3, 4, 6, benzo, dioxo and thieno azaborines in the solid state.



Computational Methods

The calculations for simulated absorption and emission spectra were carried out using the Gaussian 09[1] implementation of the B3LYP[2,3] functional using the default pruned fine grid for energies (75, 302), default pruned coarse grids for Hessians (35, 110), and non-default SCF convergence for geometry optimizations (10^{-6}). Computations utilized the 6-31G(d')[4-6] basis sets for H, B, C, N, and O. The basis sets for Br and S, when present, were the Hay and Wadt basis set (BS) and effective core potential (ECP) [LANL2DZ][7,8] combination as modified by Gilbert and Sunderlin[9] [LANL2DZ(d,p)]. All geometries were fully optimized with corresponding analytical frequency calculations to ensure a zeroth-order saddle-point was achieved. Vertical transitions were computed from the DFT optimized geometries using time-dependent DFT (TDDFT)[10] to obtain the simulated absorption spectra. The first 50 vertical excitations were solved iteratively for TDDFT single points [TD(ROOT=1,NSTATES=50)] with default convergence criteria for the energy (10^{-6}) and non-default convergence for the wave function (10^{-6}). For TDDFT geometry optimizations, the first singlet excited states were optimized using analytical gradients,[11,12] and the first 30 singlet excitations were solved iteratively [TD(ROOT=1,NSTATES=30)] with default convergence criteria for the energy (10^{-6}) and non-default convergence for the wave function (10^{-6}). All solvent optimizations utilized the SMD solvation model [SCRF(SMD,SOLVENT=X)] where X is the solvent name. Computed excitations from SMD-TDDFT optimizations were corrected using non-linear-response solvation [SCRF(SMD,SOLVENT=X,EXTERNALITERATION)] single points on the optimized geometries and non-equilibrium ground state solvation at the excited state geometry with the difference in the energies corresponding to the emission wavelength. The computed absorption and emission spectra were simulated using an in-house Fortran program by convoluting[13] the computed excitation energies and oscillator strengths with a Gaussian line-shape and a broadening of 20 nm. Attachment and detachment density cube files were obtained using the Nancy_Ex[14-16] code and the images generated in Chemcraft with a contour value of 0.001.

Methodology Comparisons

Absorption

Overall, the deviations of the gas-phase λ_{max} are smaller than from incorporating the individual solvents via either solvation method (Table S1). Looking at the linear correlations (Figures S1 and S2), $CHCl_3$ and acetonitrile are somewhat worse using either solvation method while methanol and DMSO are a little better with either solvation method in comparison to the gas phase.

Table S1: Deviations of λ_{max} from experiment for various methods (in nm)

Method		$CHCl_3$	MeOH	DMSO	ACN
B3LYP	AAD	13	11	12	16
	MSD	11	10	5	15
	MAD	33	30	33	41
SMD-B3LYP//B3LYP	AAD	28	34	23	31
	MSD	28	34	23	31

	MAD	62	63	61	69
SMD-B3LYP	AAD	30	37	25	33
	MSD	30	37	25	33
	MAD	66	69	66	74

AAD is the absolute average deviation, MSD is the mean signed deviation, and MAD is the maximum absolute deviation

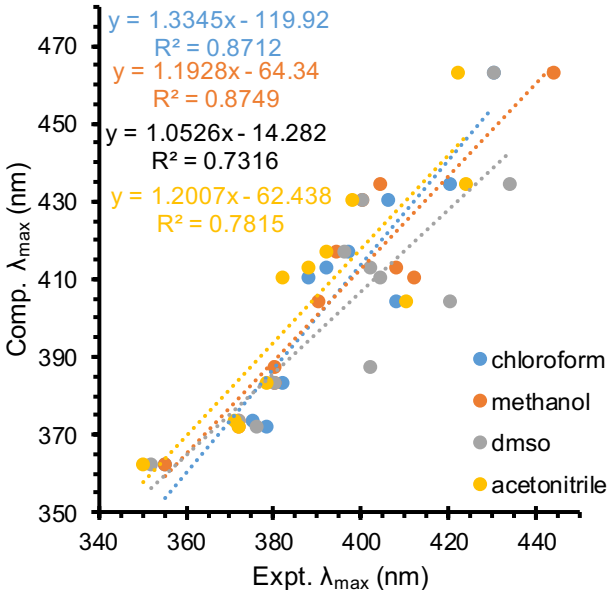


Figure S1: Computed gas-phase λ_{max} vs. experimental (various solvents)

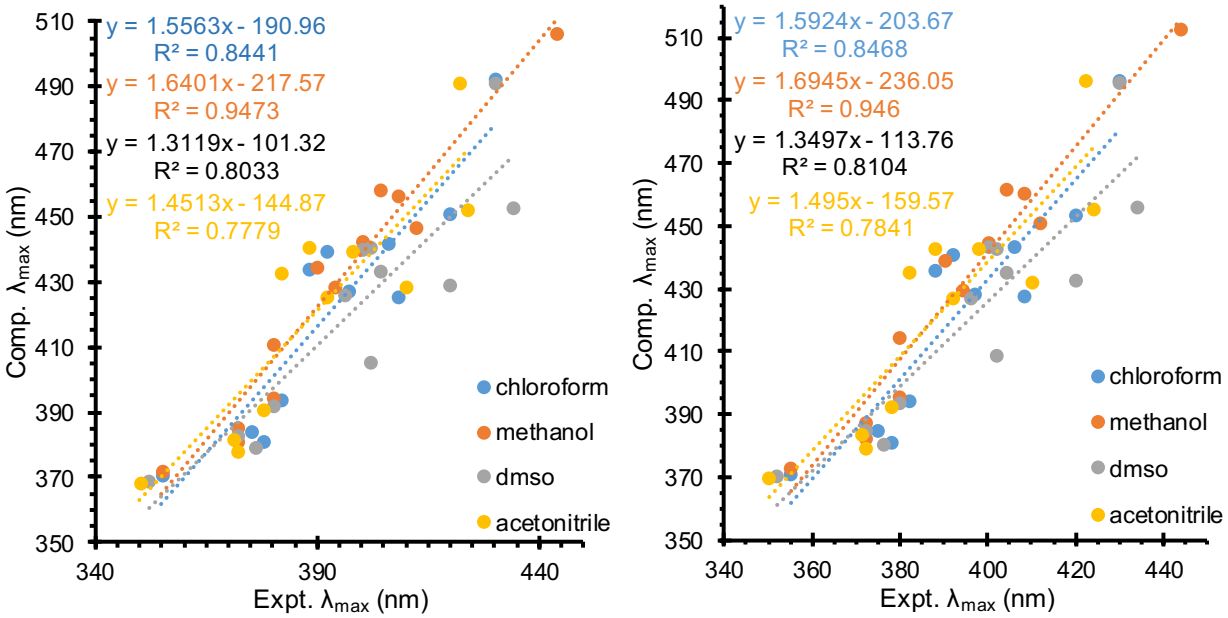


Figure S2: Computed vs. experimental λ_{max} using solvent single-points on gas-phase geometries (left) and solvent optimizations (right).

Emission

Emission maxima computed in the gas-phase do not correlate as well with the experimental values. Additionally, the large Stokes shifts observed for **2**, **5**, and **8** are not captured using the gas-phase model. Use of SMD-DFT to properly account for solvation effects in the excited state results in significantly larger deviations (Table S2) but a significantly improved linear correlation (Figure S3). The data suggest that although implicit solvation models greatly increase the scatter of the dataset, they are necessary in order to capture the overall trends in the emission maxima for these compounds, especially for those that having significant charge-transfer character.

Table S2: Deviations of λ_{em} from experiment for various methods (in nm)

Method		$CHCl_3$	MeOH	DMSO	ACN
B3LYP	AAD	33	25	27	43
	MSD	-31	-25	-27	-41
	MAD	103	74	86	137
SMD–B3LYP	AAD	80	145	88	104
	MSD	80	145	88	104
	MAD	145	303	188	207

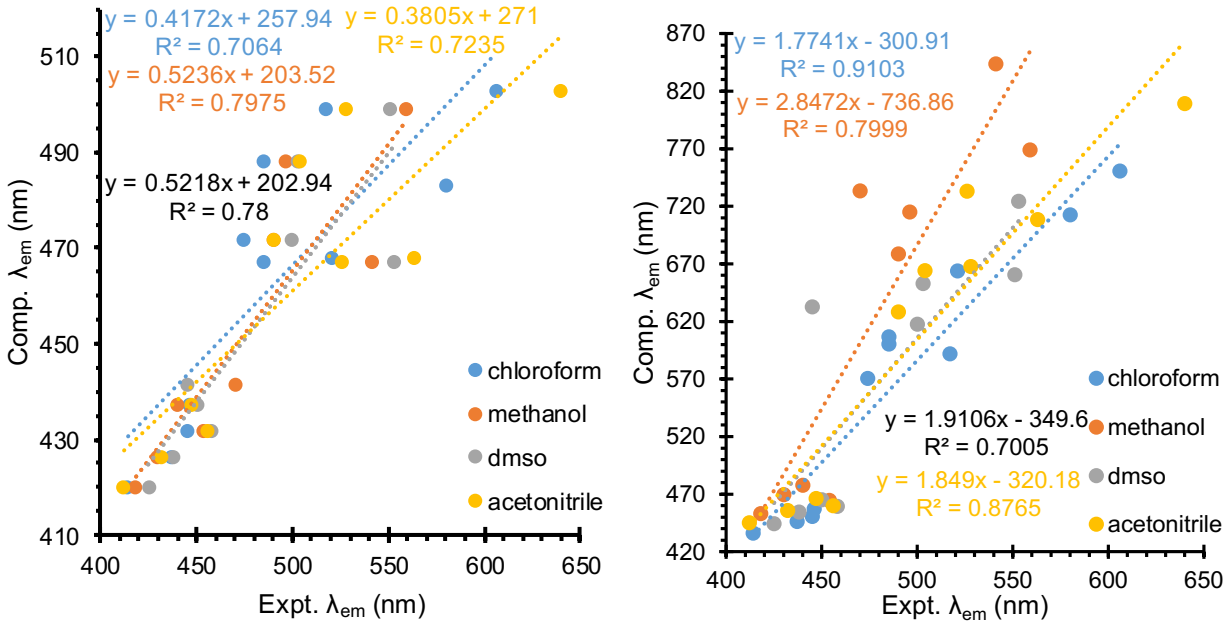
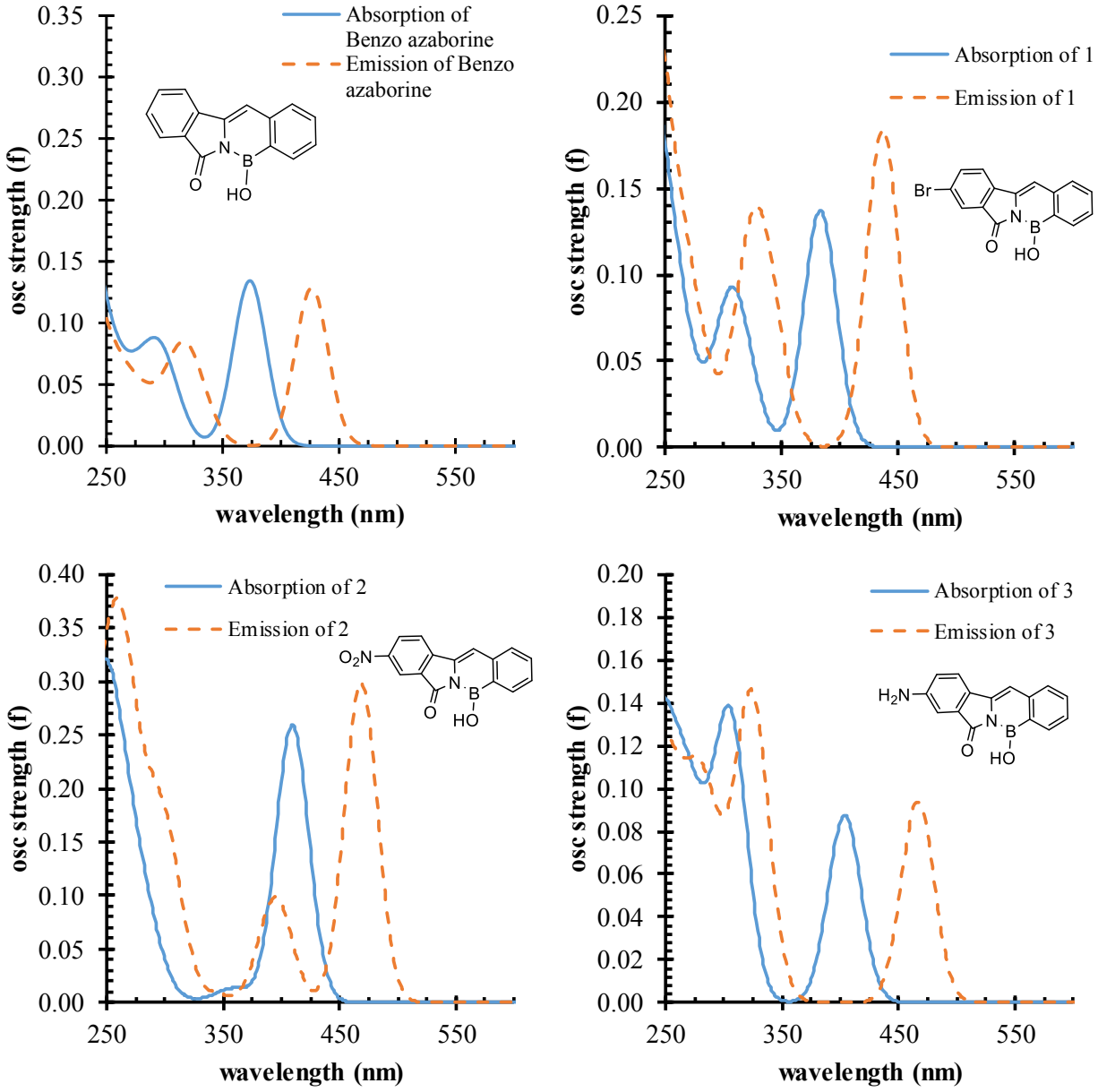
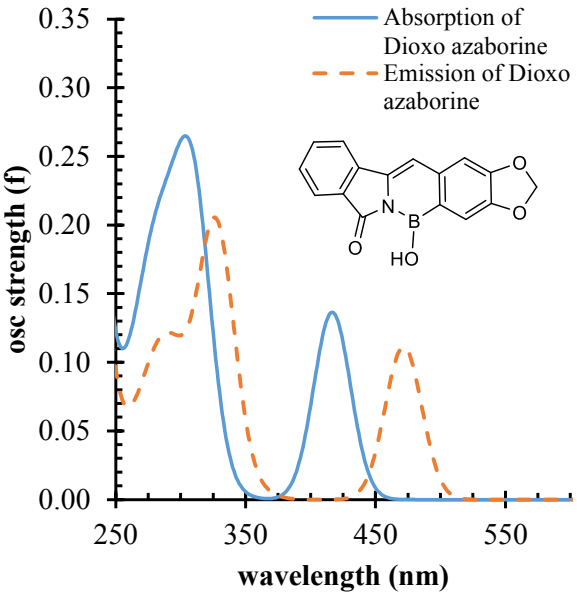
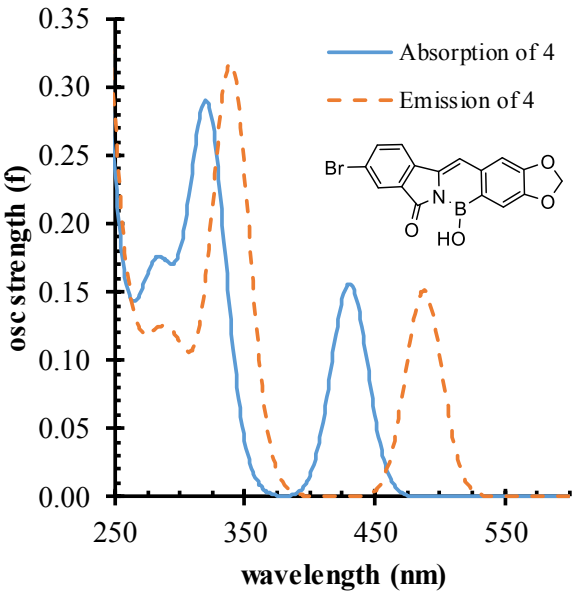


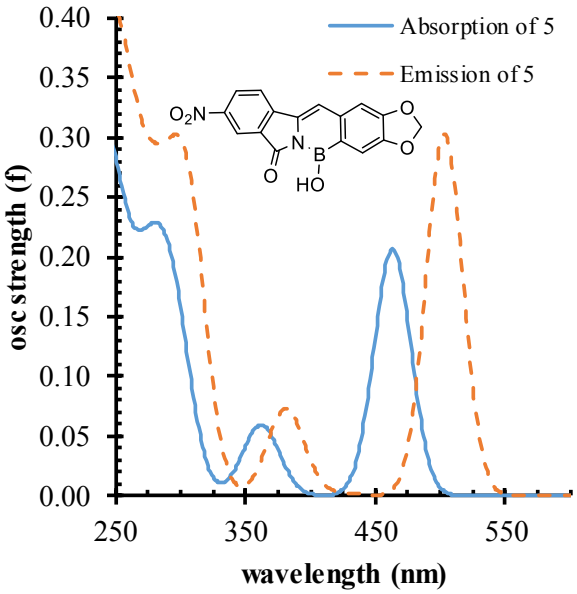
Figure S3: Computed gas-phase λ_{max} vs. experimental with various solvents (left) and solvent optimizations (right).

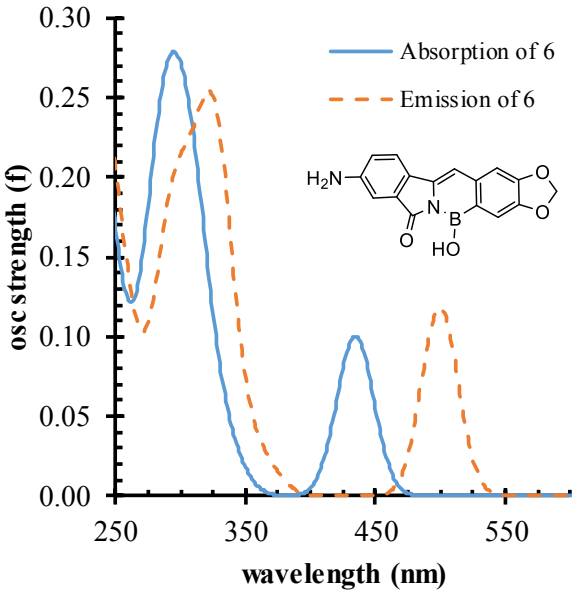
Simulated Gas-Phase Absorption and Emission Spectra

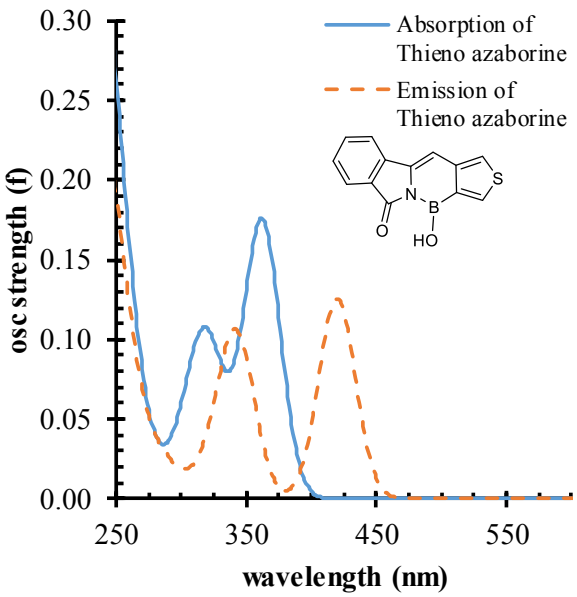


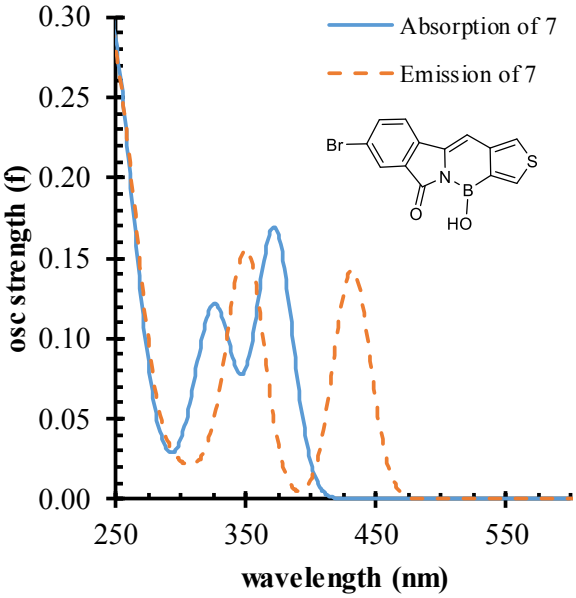

Absorption of Dioxo azaborine
Emission of Dioxo azaborine
osc strength (f)
wavelength (nm)


Absorption of 4
Emission of 4
Br
osc strength (f)
wavelength (nm)


Absorption of 5
Emission of 5
O2N
osc strength (f)
wavelength (nm)


Absorption of 6
Emission of 6
H2N
osc strength (f)
wavelength (nm)


Absorption of Thieno azaborine
Emission of Thieno azaborine
osc strength (f)
wavelength (nm)
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550


Absorption of 7
Emission of 7
Br
osc strength (f)
wavelength (nm)
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0.00
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350
450
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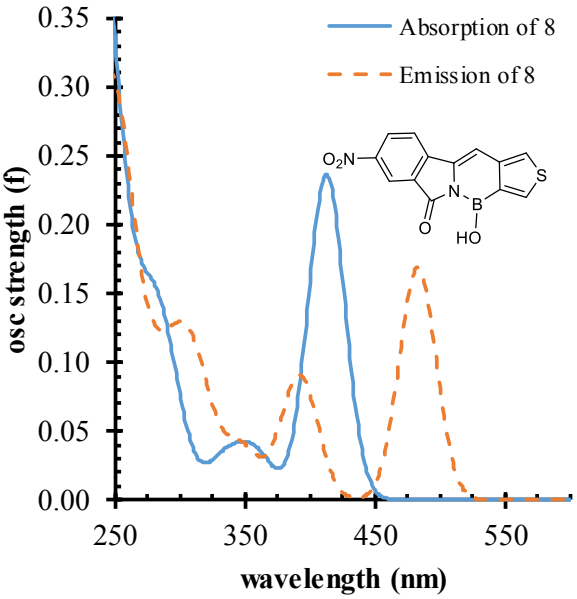
Absorption of 8
Emission of 8
O2N
osc strength (f)
wavelength (nm)
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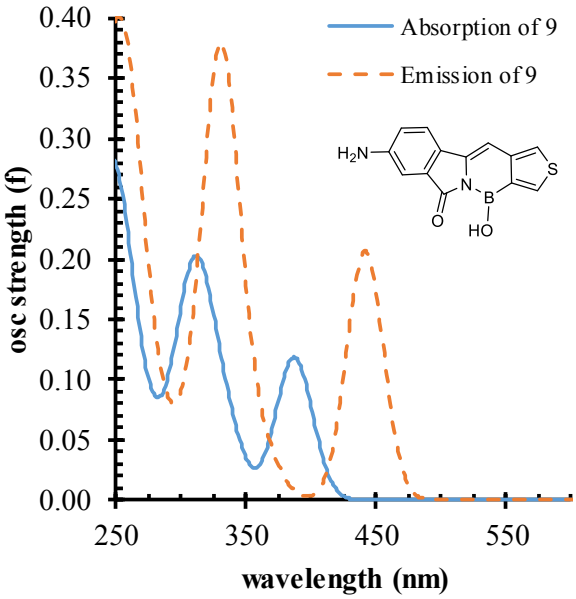
0.30
0.25
0.20
0.15
0.10
0.05
0.00
250
350
450
550


Absorption of 9
Emission of 9
H2N
osc strength (f)
wavelength (nm)
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0.30
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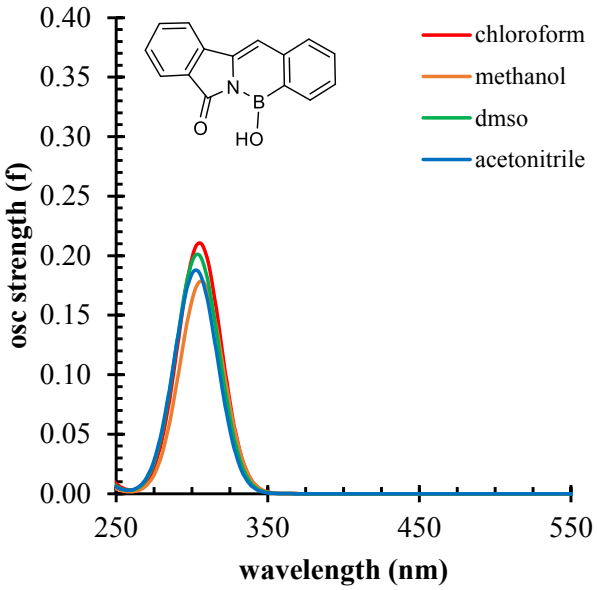
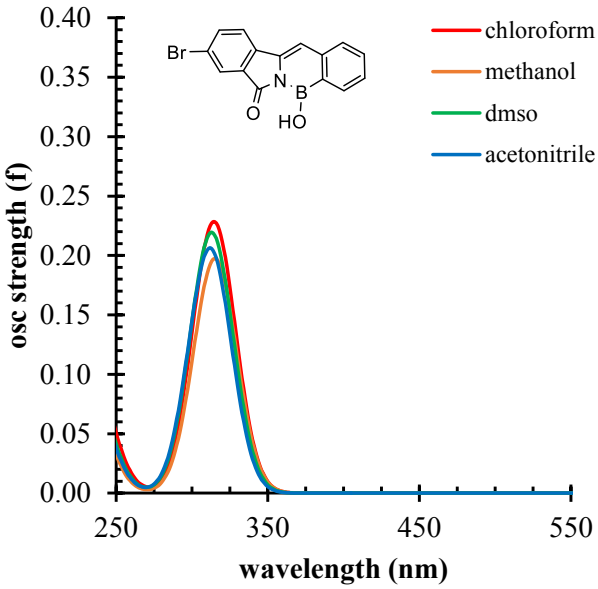
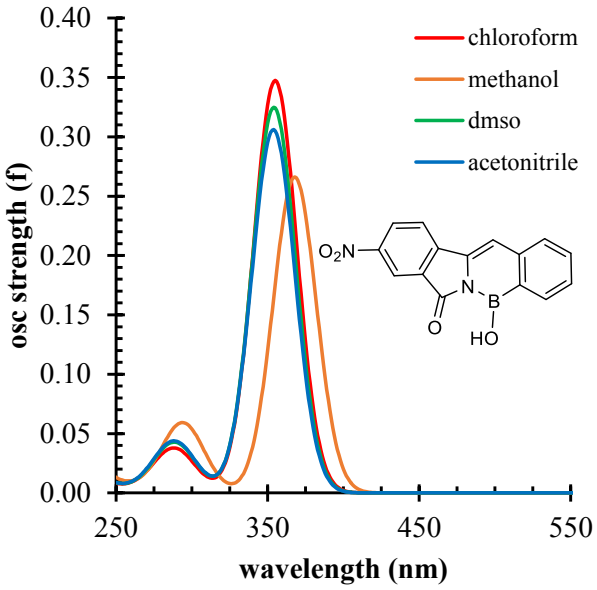
0.10
0.05
0.00
250
350
450
550

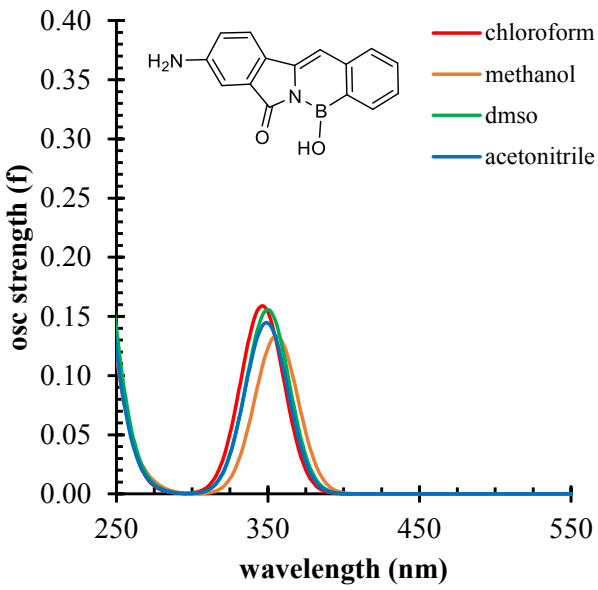
Simulated Solution-Phase Spectra

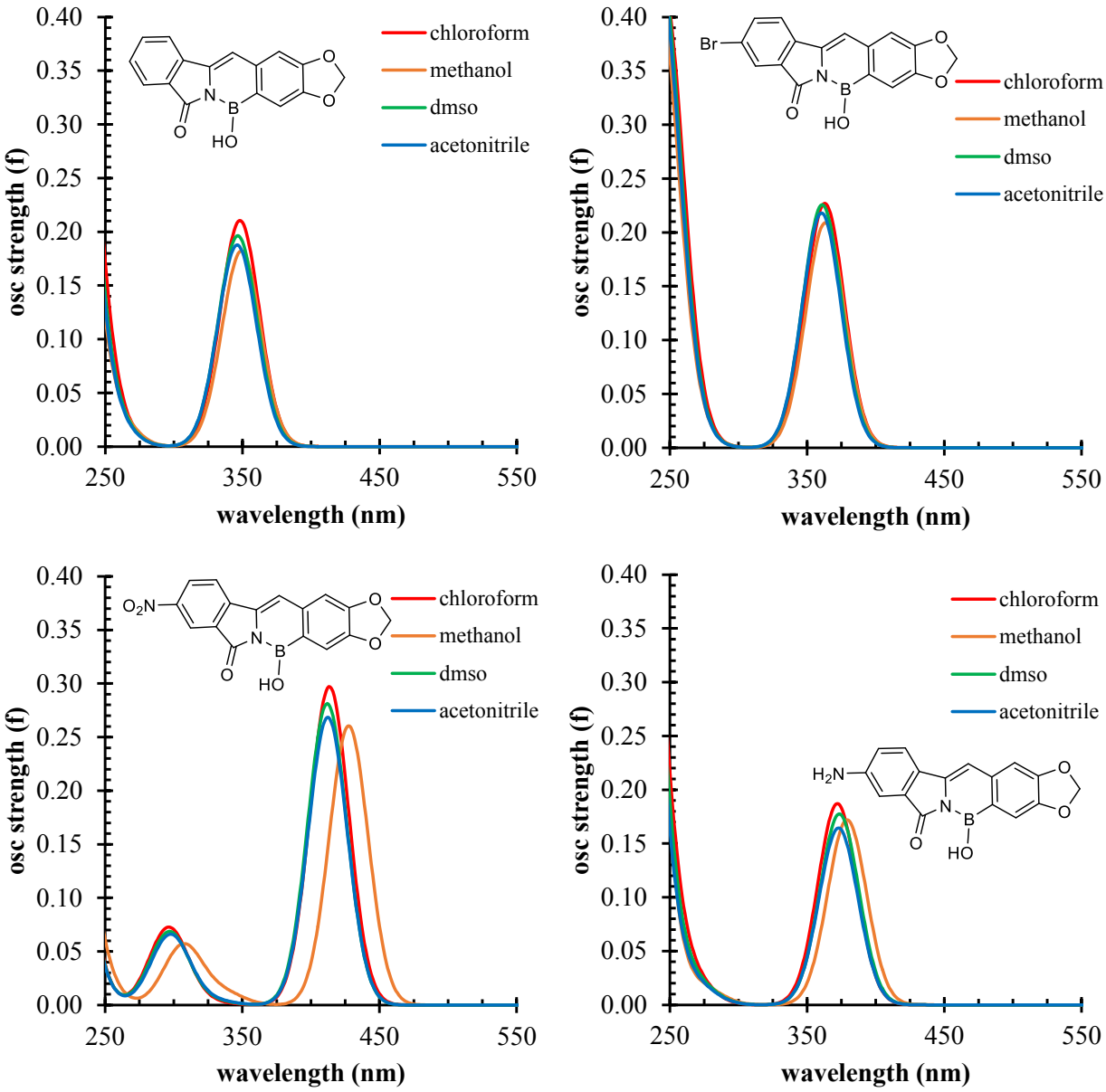
Solvent Single-Point Absorption







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methanol
dmso
acetonitrile
osc strength (f)
wavelength (nm)
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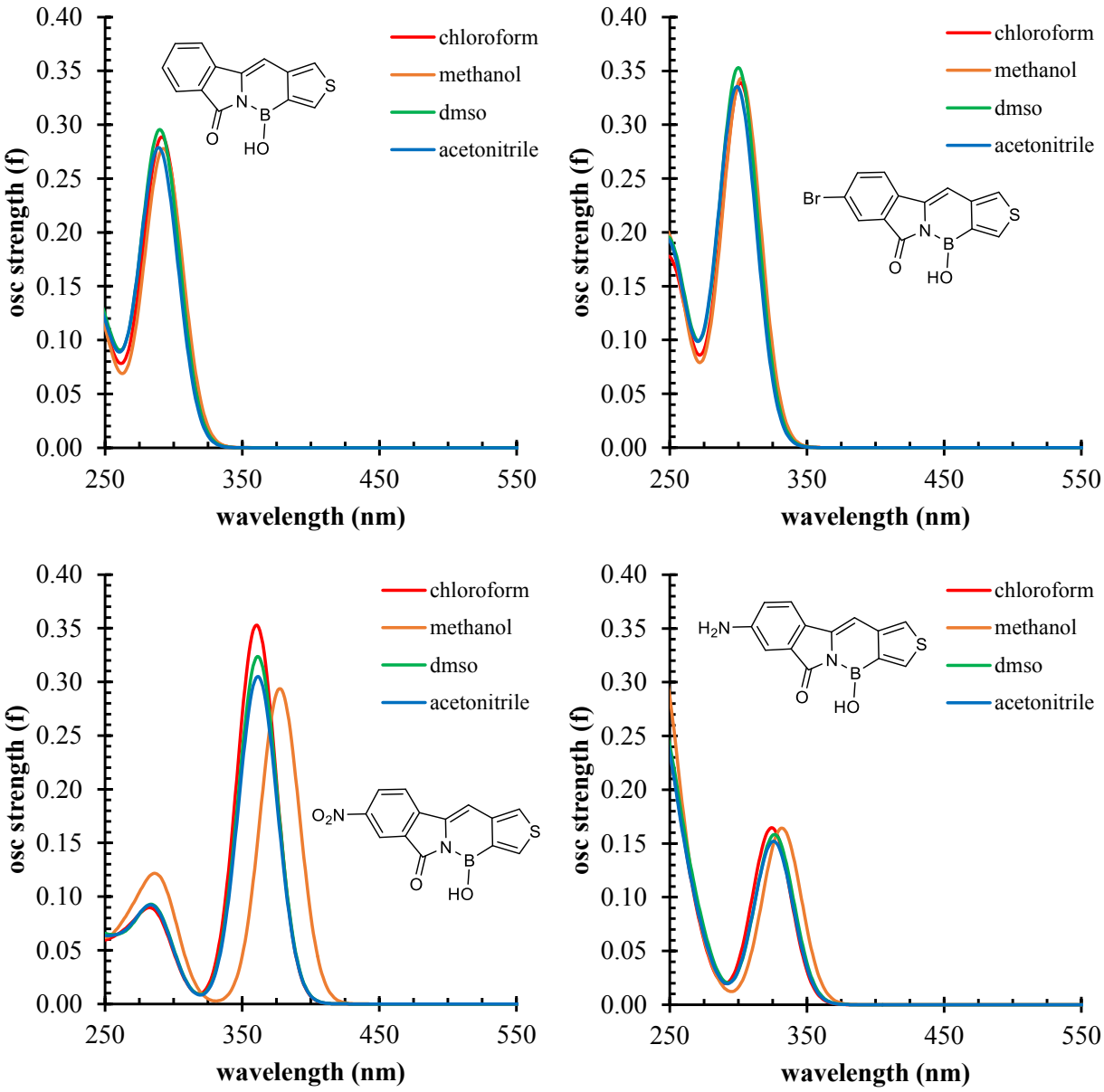
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
250
350
450
550
Br
O2N
H2N
N
B
HO
O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wavelength (nm)
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acetonitrile
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0.15
0.20
0.25
0.30
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Br
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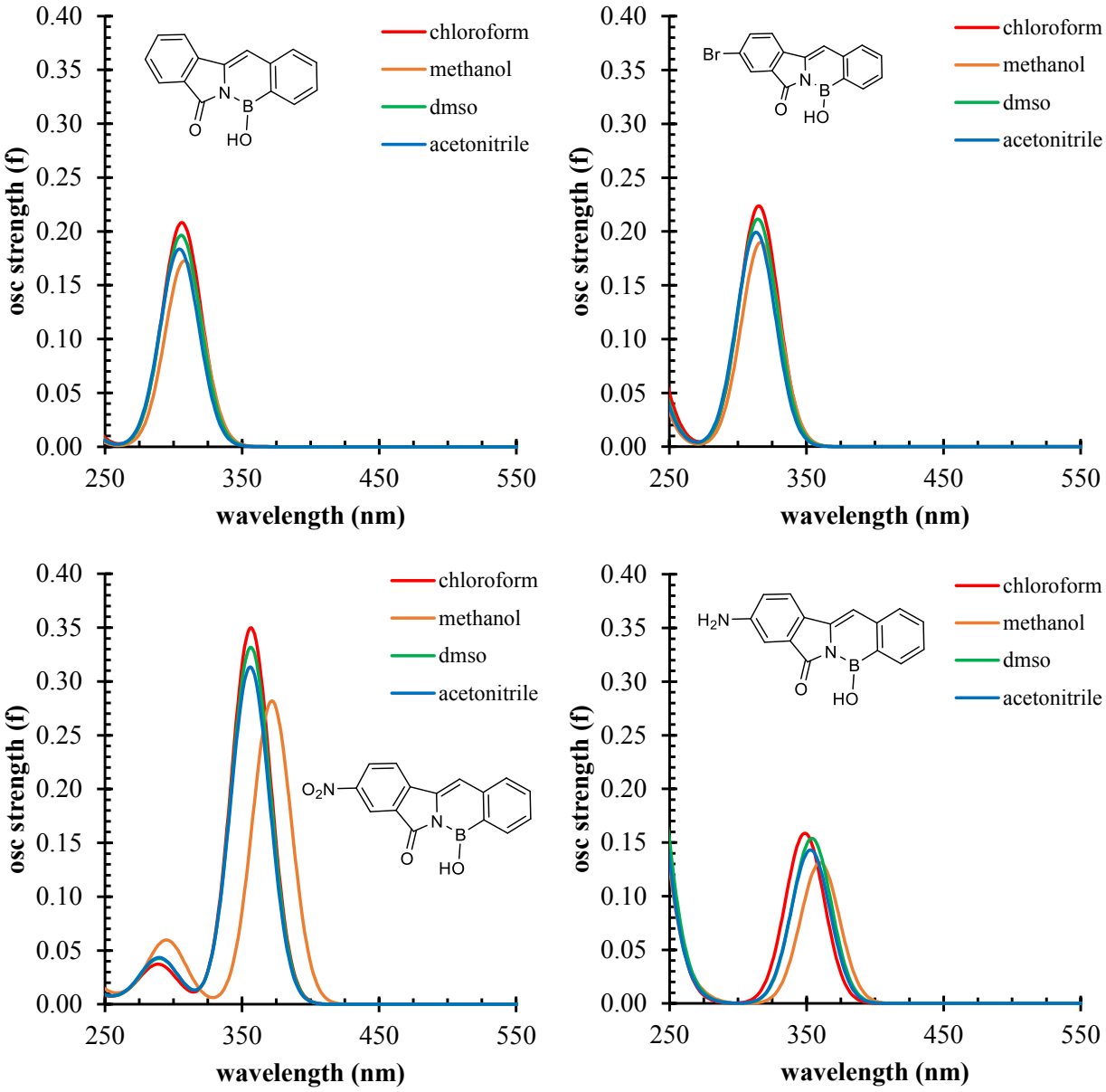
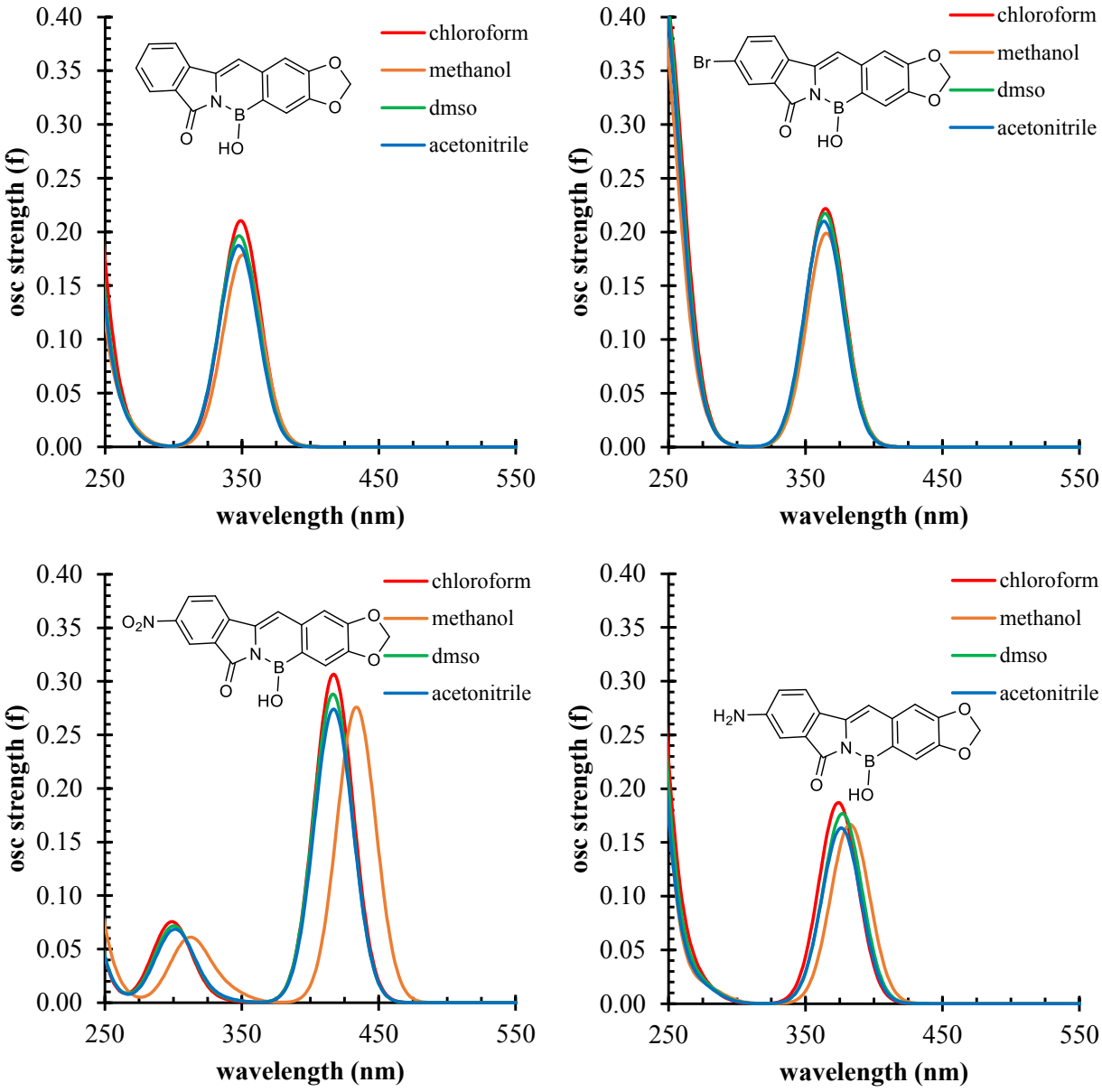
H2N
N
B
S
O
HO

Solvent-Optimized Absorption

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methanol
dmso
acetonitrile
osc strength (f)
wavelength (nm)
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0.05
0.10
0.15
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0.35
0.40
250
350
450
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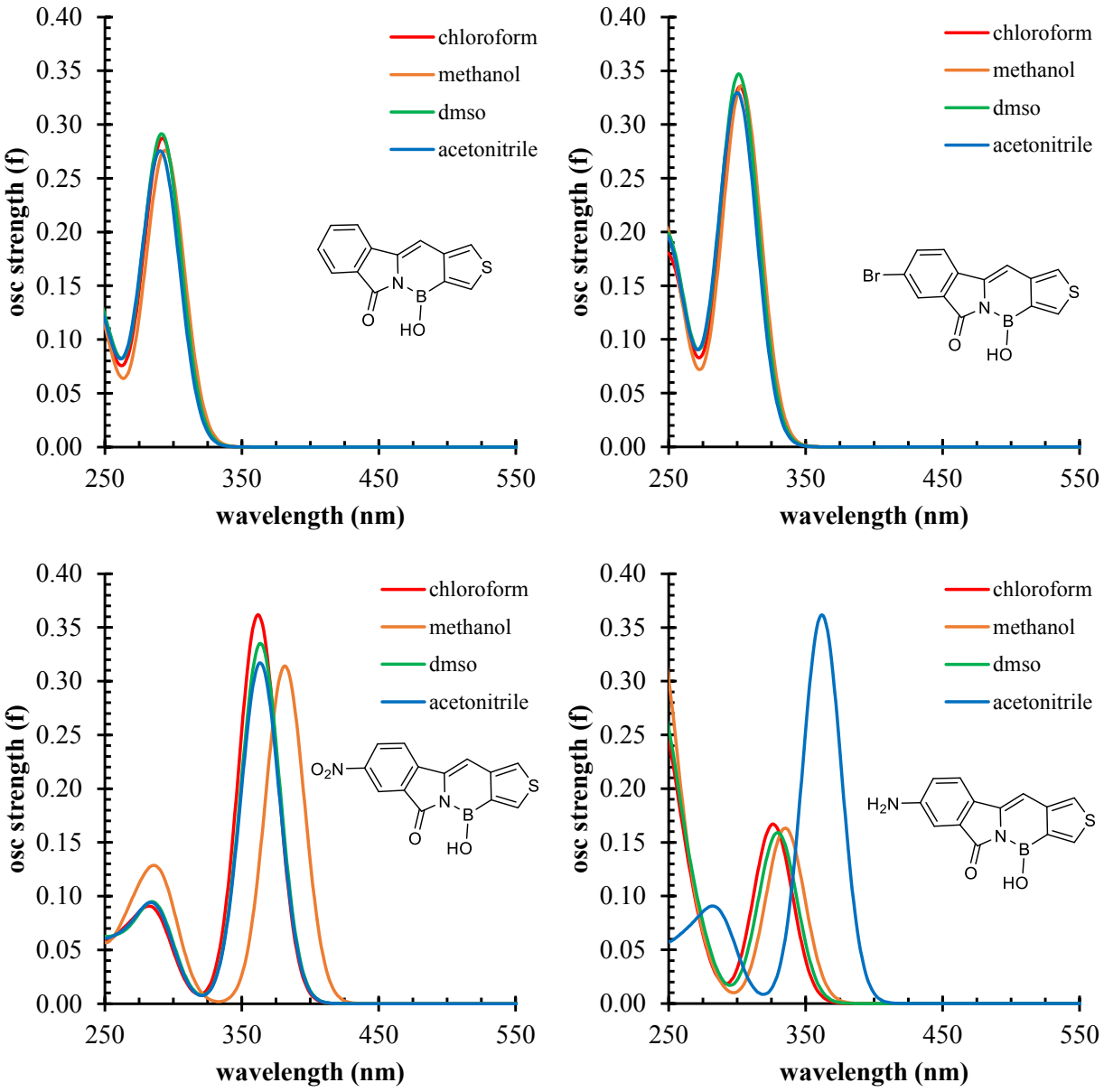
Br
O2N
H2N
HO
B
N
O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acetonitrile
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wavelength (nm)
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0.30
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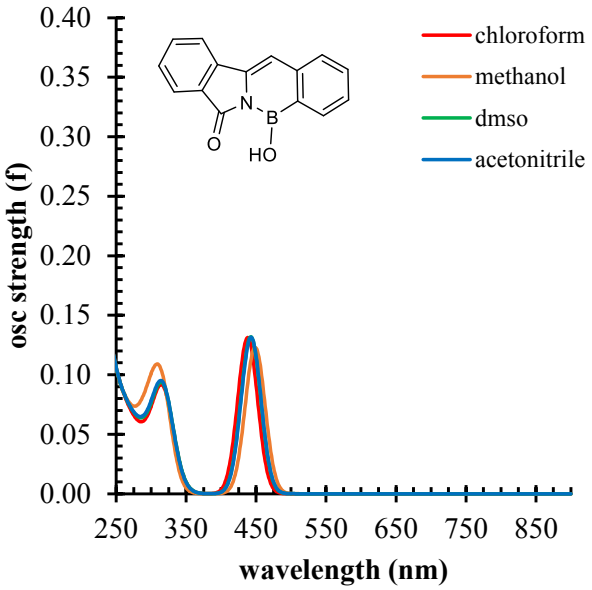
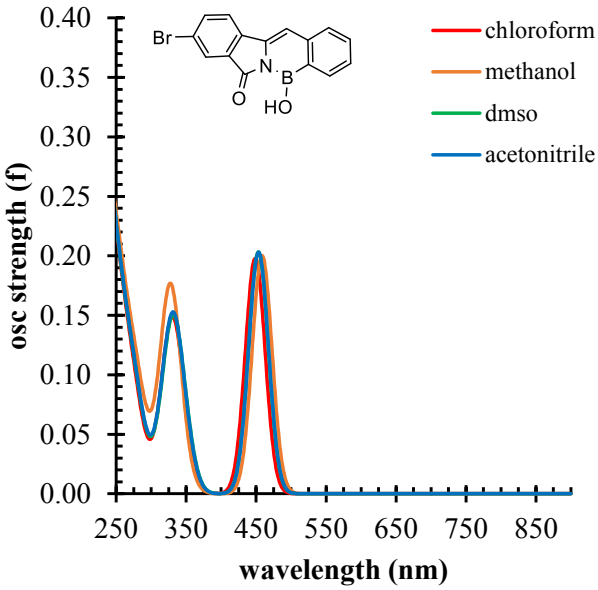
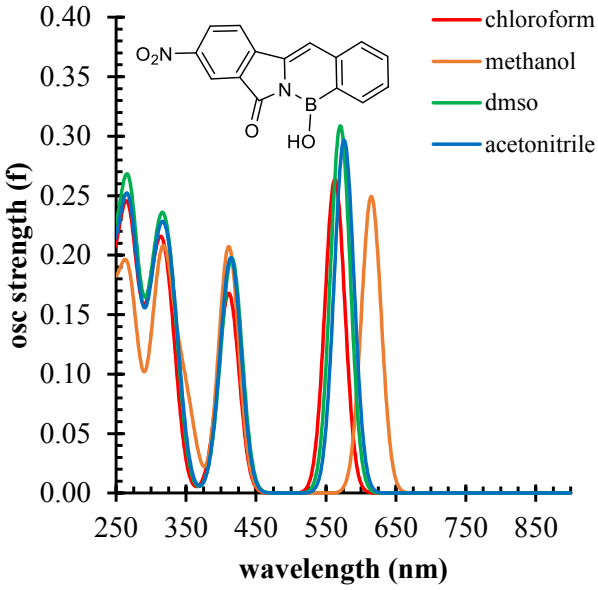
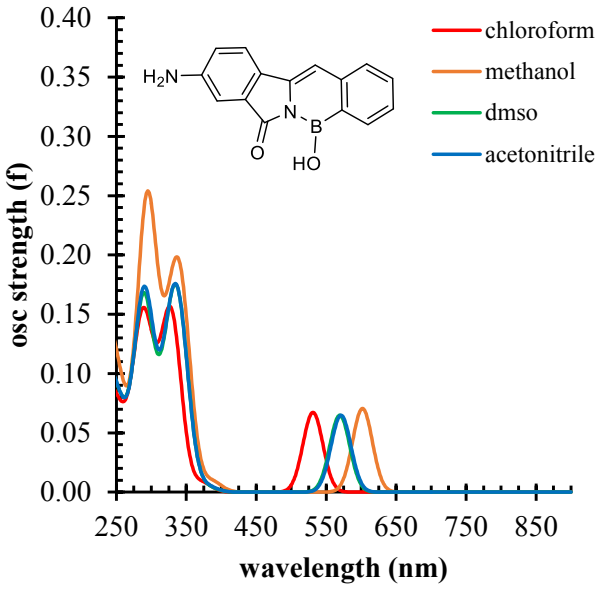
350
450
550
Br
O2N
H2N
N
B
O
HO
S

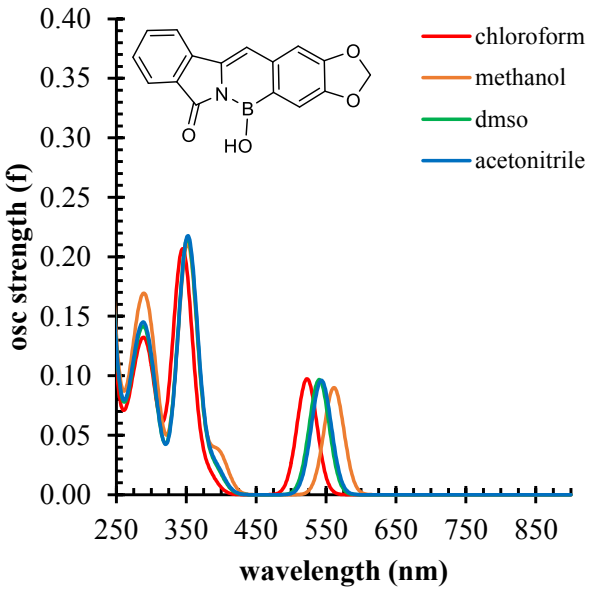
Solvent-Optimized Emission







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methanol
dmso
acetonitrile
osc strength (f)
wavelength (nm)
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0.05
0.10
0.15
0.20
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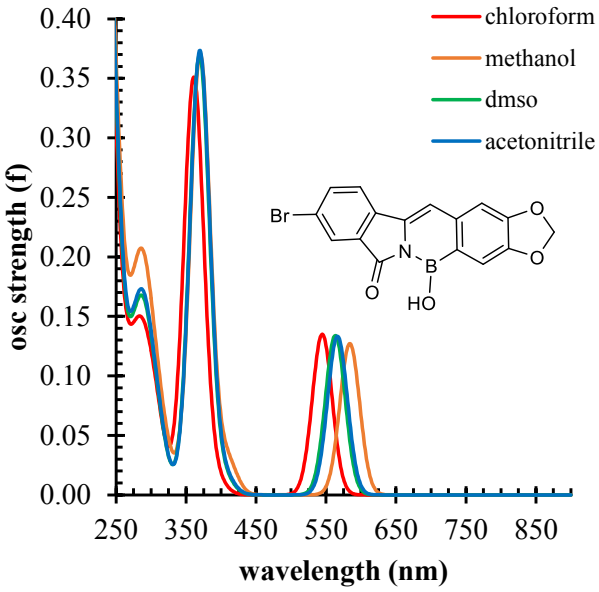
0.35
0.40
250
350
450
550
650
750
850
O
N
B
HO
O
O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wavelength (nm)
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750
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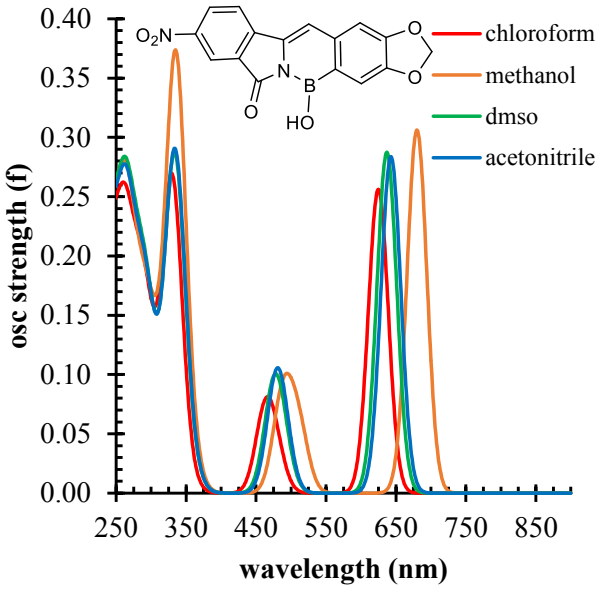
N
B
HO
O
O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acetonitrile
osc strength (f)
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0.05
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0.30
0.35
0.40
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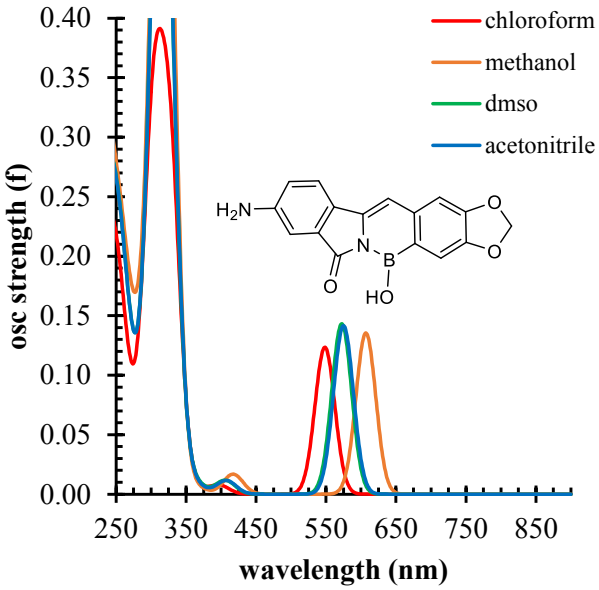
350
450
550
650
750
850
O2N
O
N
B
HO
O
O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methanol
dmso
acetonitrile
osc strength (f)
wavelength (nm)
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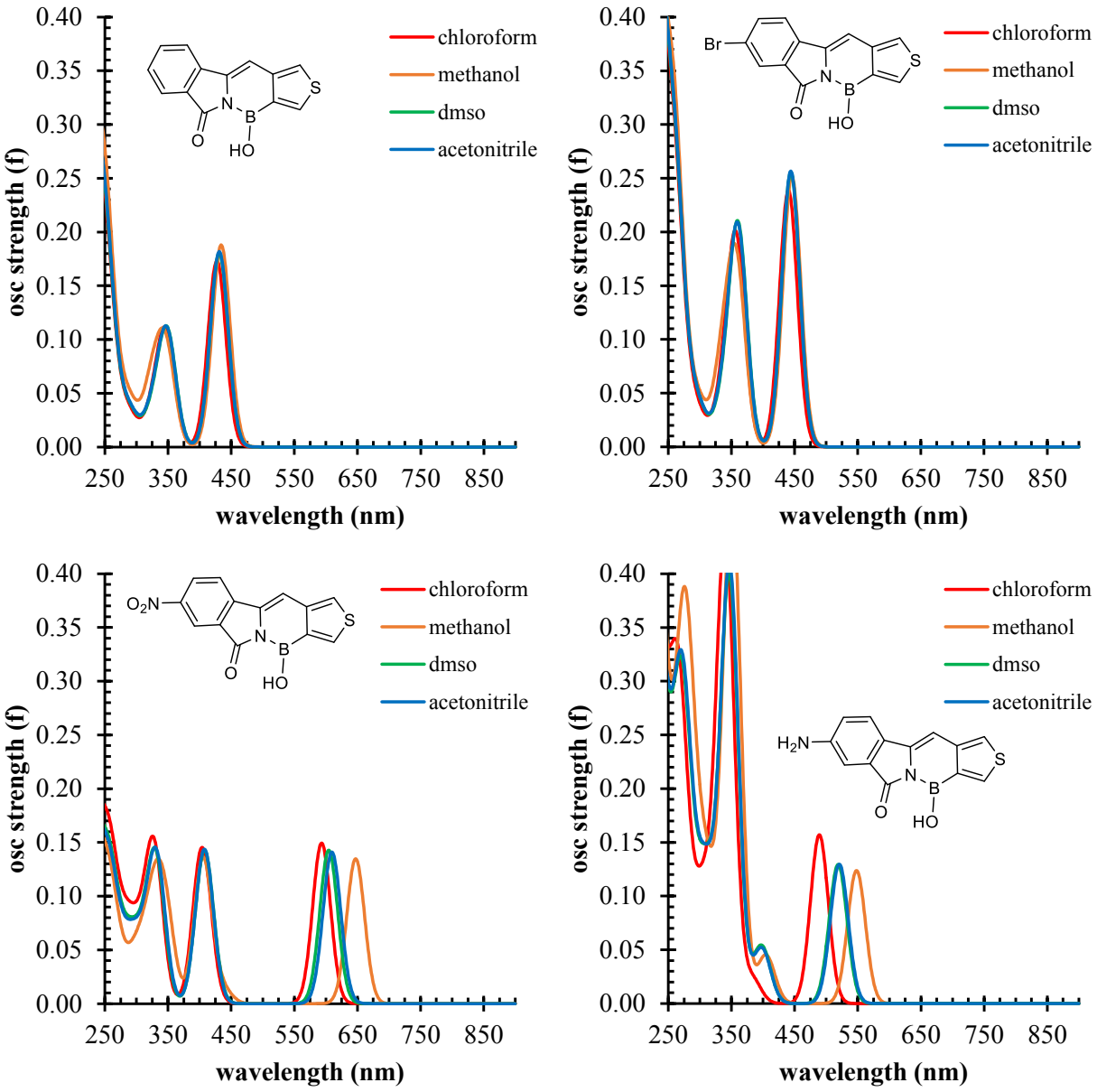
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
250
350
450
550
650
750
850
H2N
O
N
B
HO
O
O


osc strength (f)
wavelength (nm)
chloroform
methanol
dmso
acetonitrile
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
250
350
450
550
650
750
850
Br
O2N
H2N
N
B
S
O
HO

Attachment/Detachment Densities

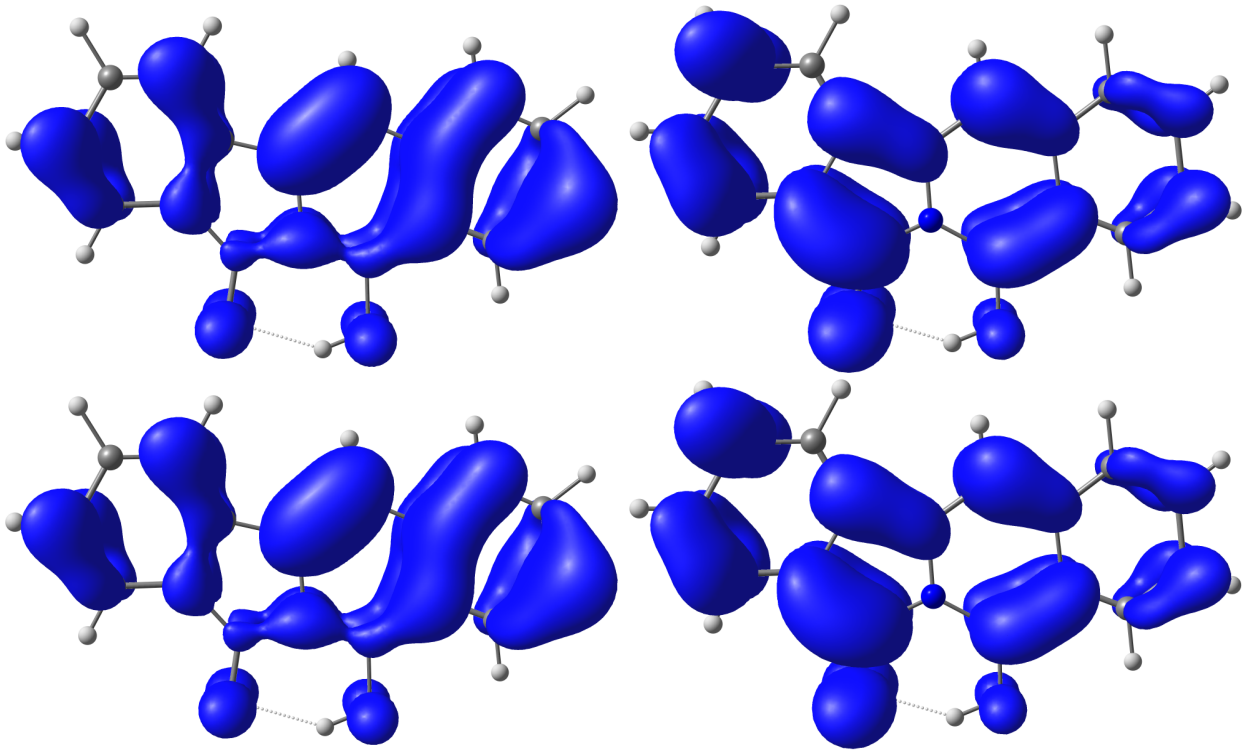


Figure S4: **Benzo** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

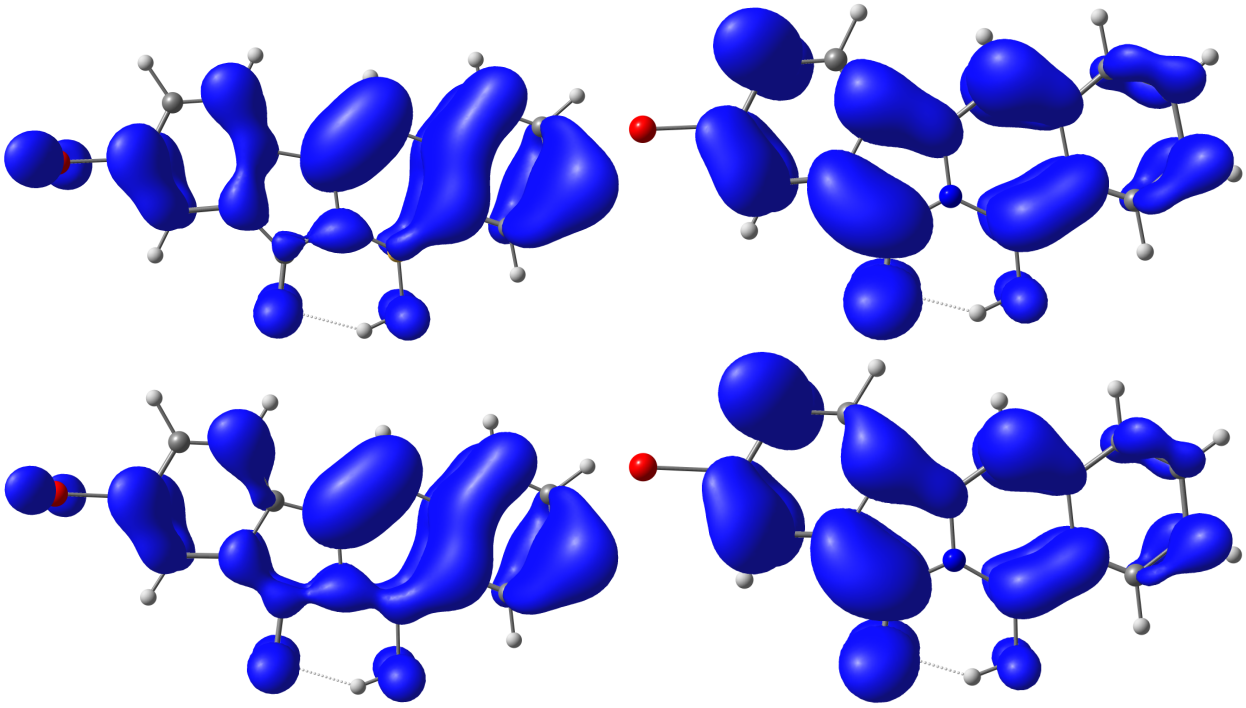


Figure S5: **1** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

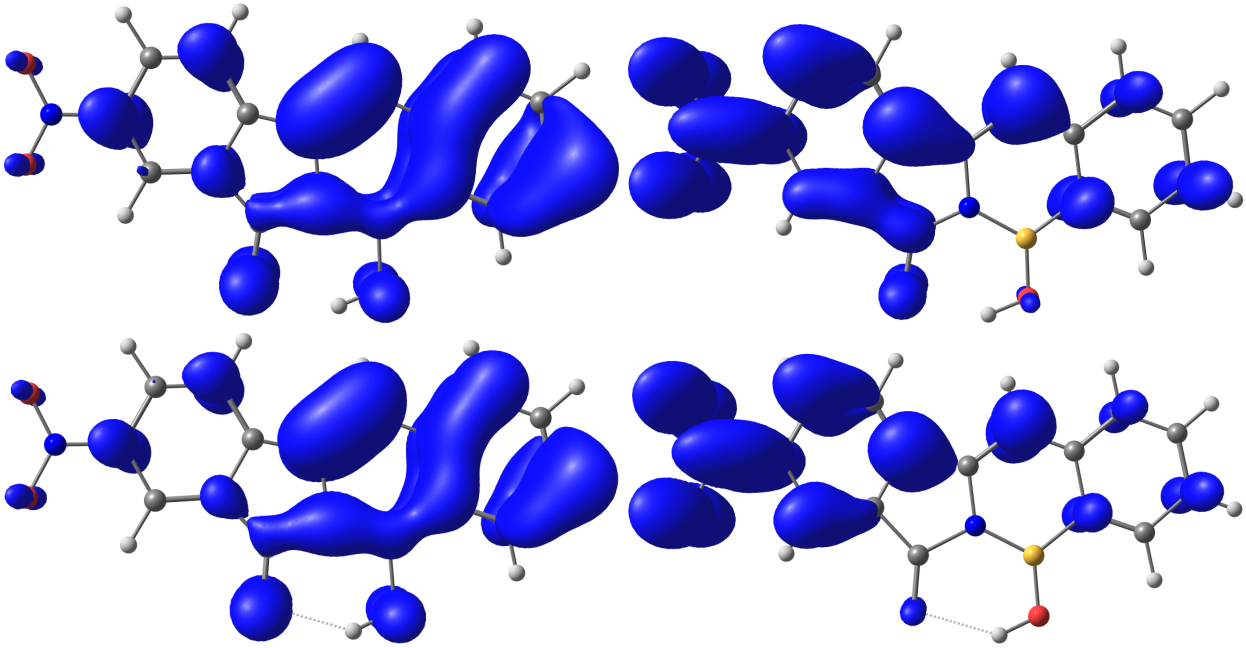


Figure S6: **2** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

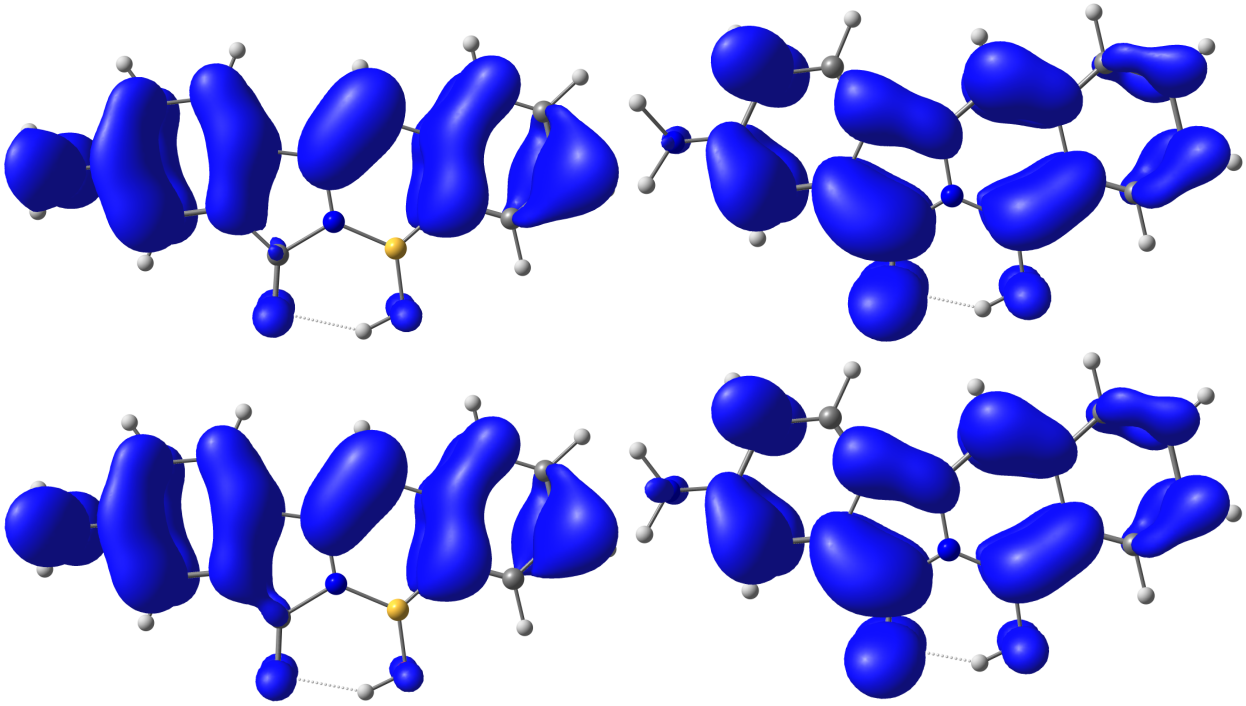


Figure S7: **3** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

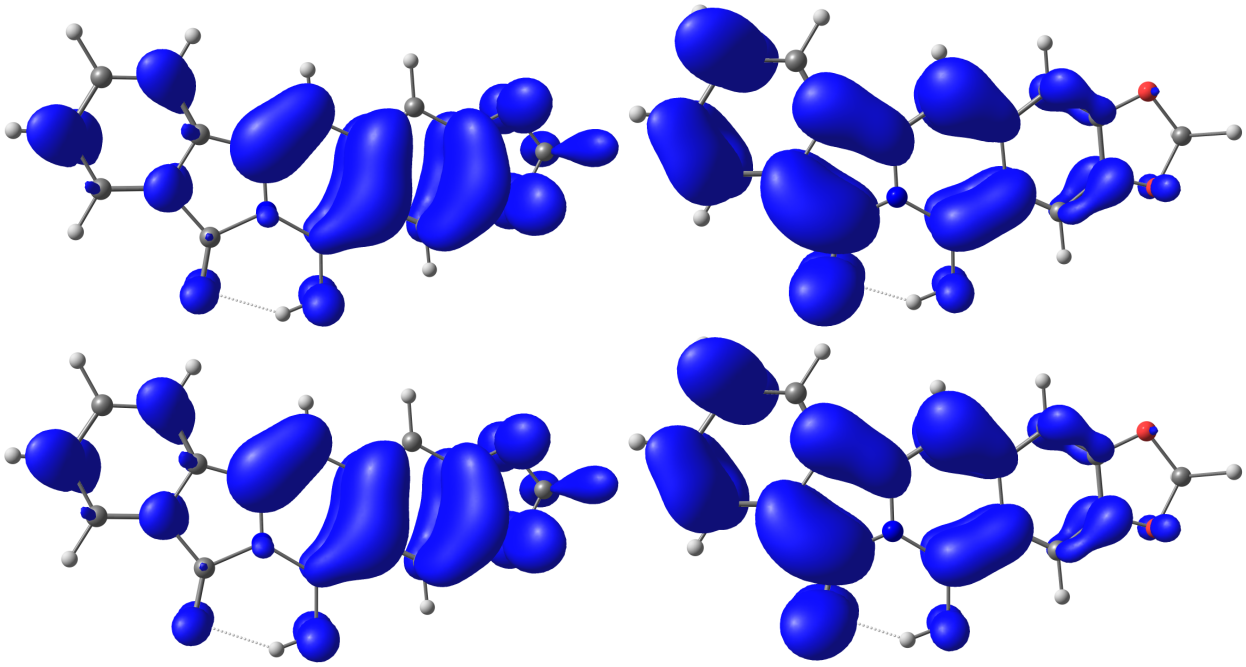


Figure S8: **Dioxo** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

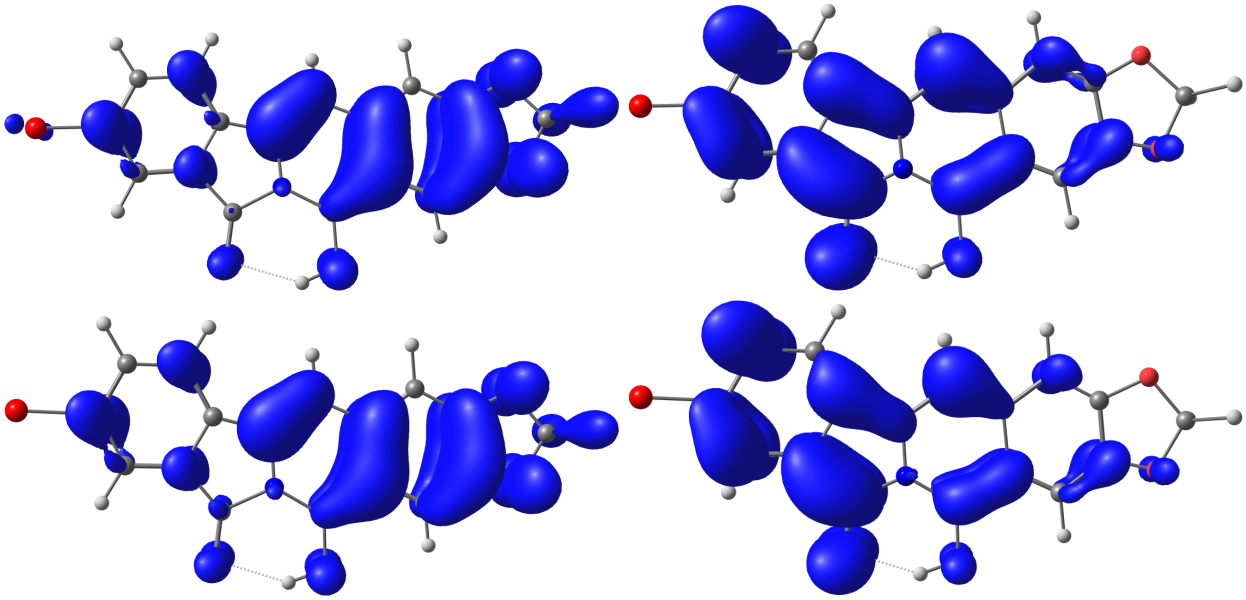


Figure S9: **4** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

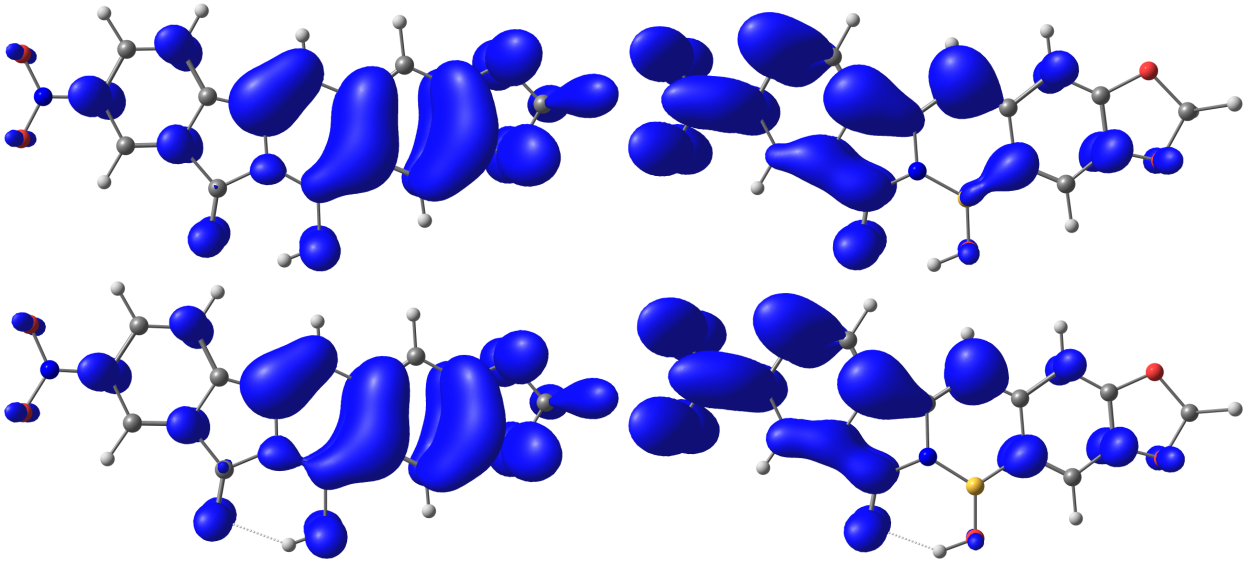


Figure S10: **5** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

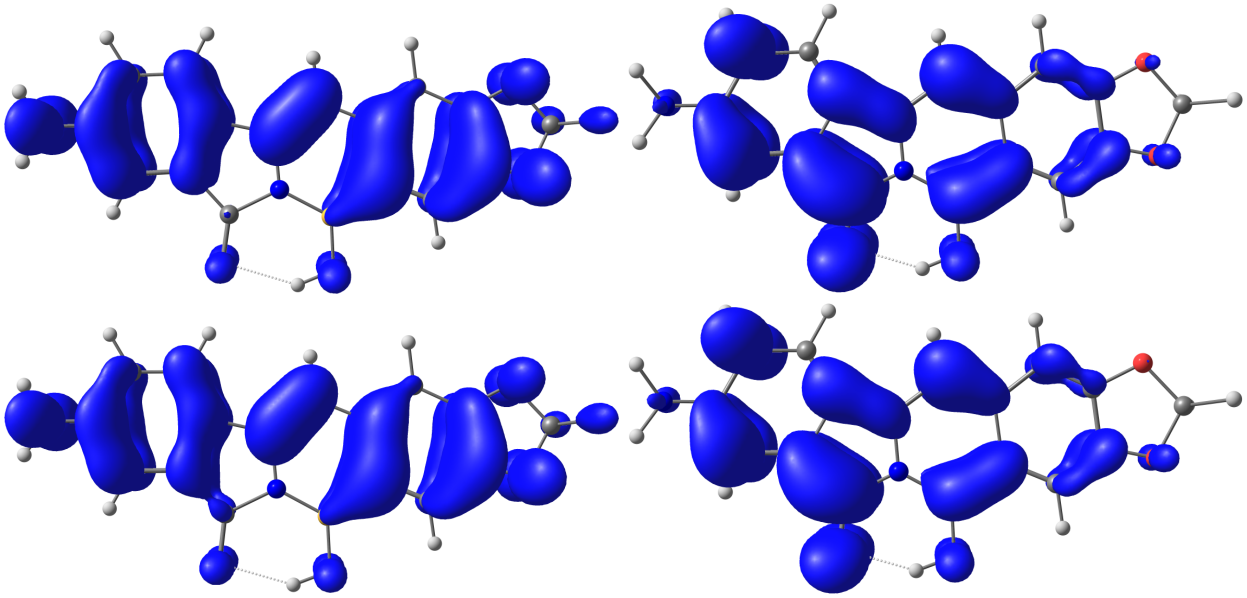


Figure S11: **6** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

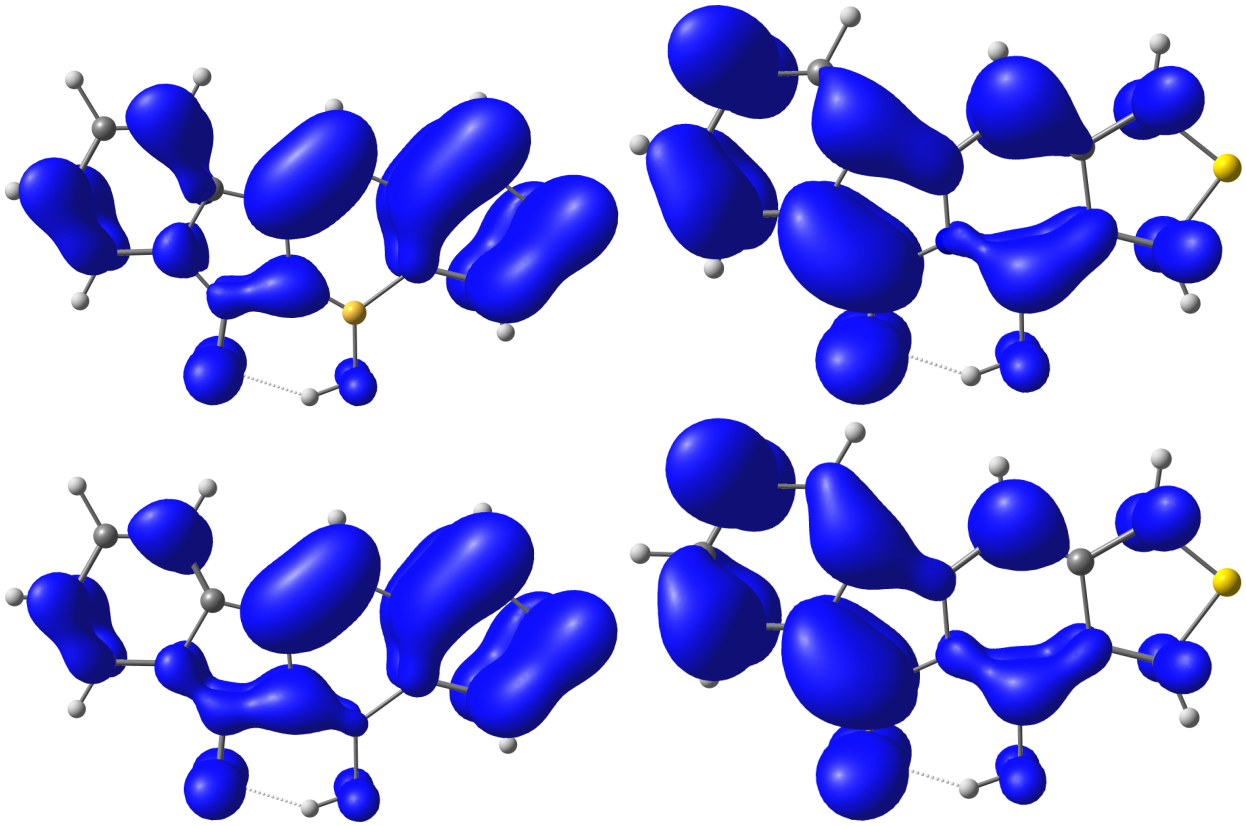


Figure S12: **Thieno azaborine** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

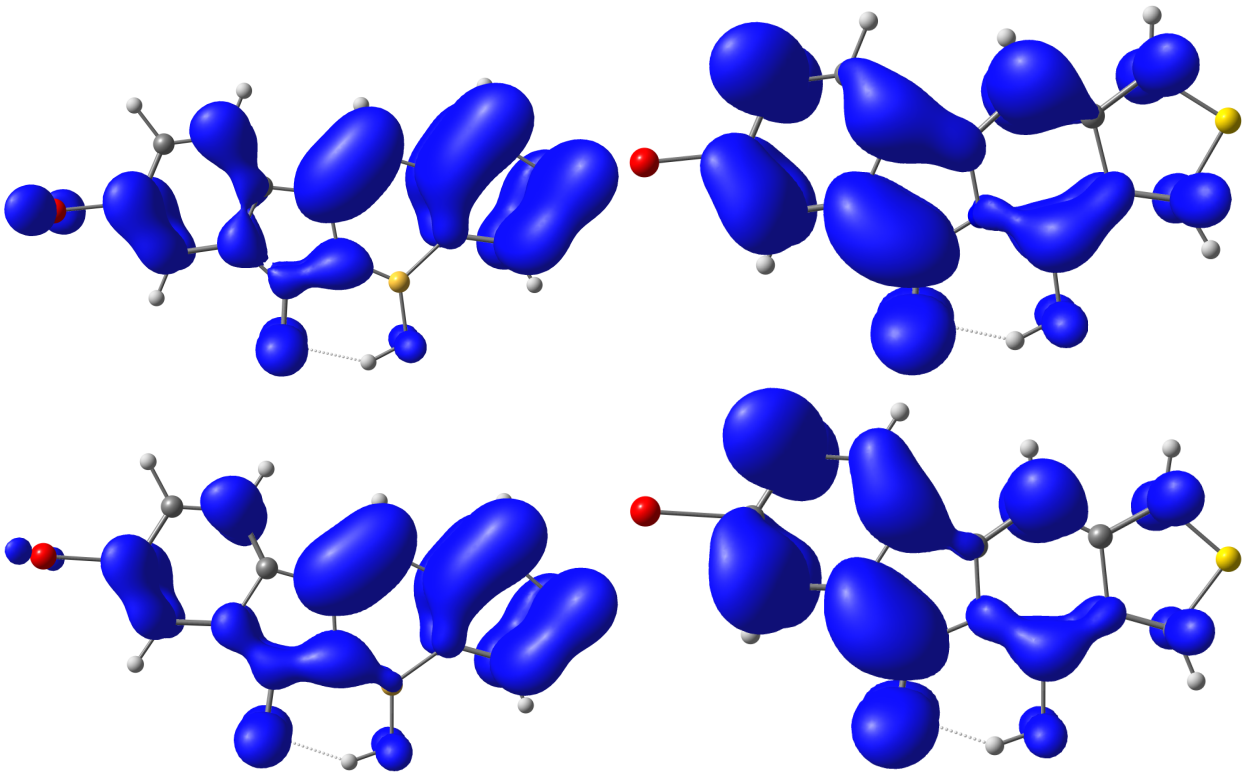


Figure S13: **7** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

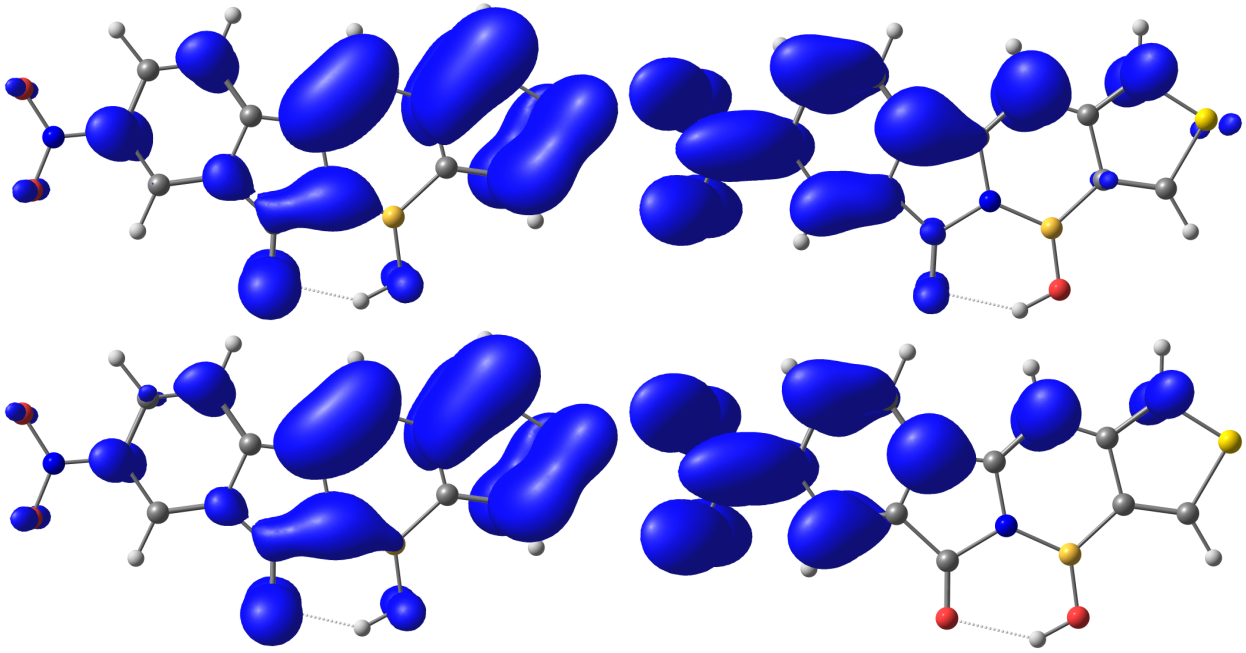


Figure S14: **8** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

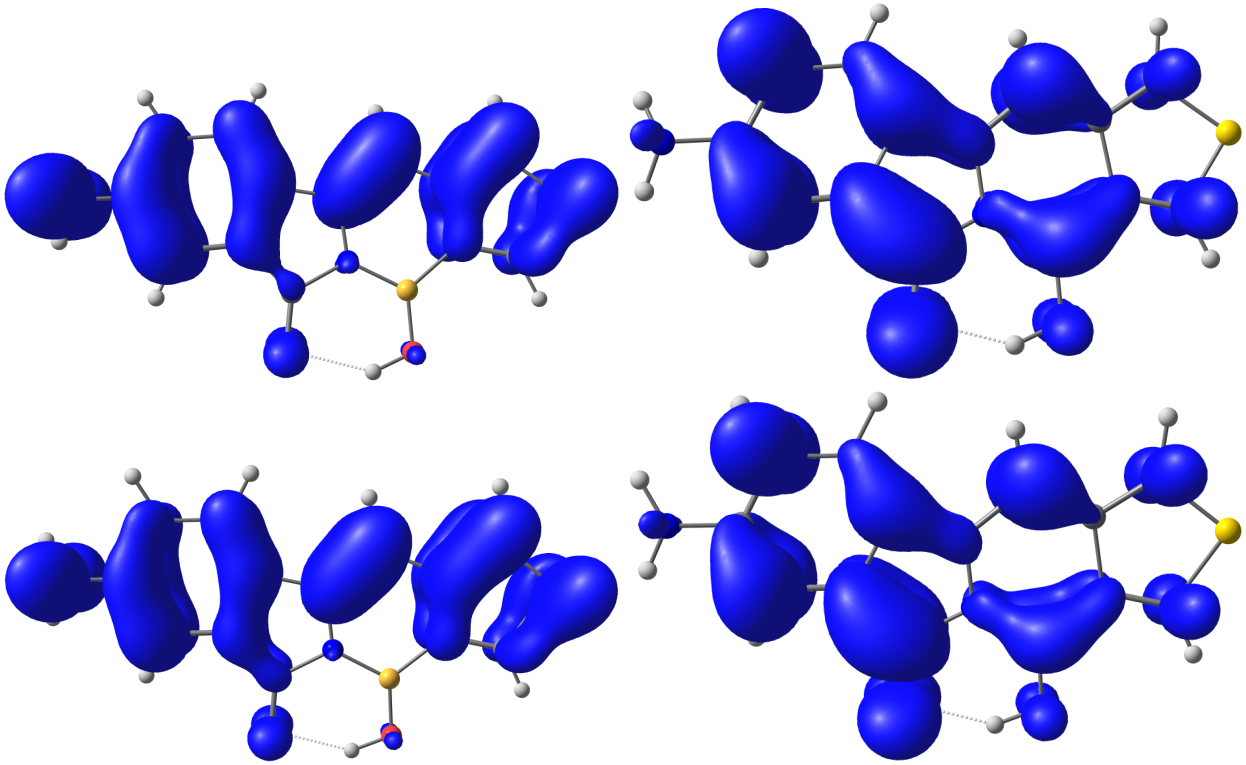


Figure S15: **9** detachment (Left) and attachment (Right) densities for GS (Top) and ES (Bottom)

Molecular Coordinates

GS-benzo

B 1.128122 1.395127 0.000000
O 1.275565 2.743826 0.000000
H 0.399249 3.173125 0.000000
N -0.202798 0.793268 0.000000
C -1.426827 1.484700 0.000001
O -1.527192 2.704847 0.000000
C -2.483851 0.448576 0.000001
C -3.869001 0.589902 0.000000
H -4.321258 1.578725 0.000001
C -4.643192 -0.572936 0.000001
C -4.029778 -1.837657 0.000001
H -4.652090 -2.730324 0.000001
C -2.638802 -1.974953 0.000001
H -2.181729 -2.961996 0.000001
C -1.862200 -0.813759 0.000001
C -0.412506 -0.597999 0.000000
C 0.630135 -1.465481 0.000000
H 0.431850 -2.534918 0.000000
C 2.010134 -1.009688 0.000000
C 3.068079 -1.941296 -0.000001
H 2.842891 -3.006944 0.000000
C 4.390205 -1.508456 -0.000001
C 4.685574 -0.137423 -0.000001
C 3.647291 0.793199 -0.000001
H 3.869663 1.858552 -0.000001
C 2.303585 0.385249 -0.000001
H 5.197460 -2.238634 -0.000001
H 5.721329 0.196098 -0.000001
H -5.728451 -0.503432 0.000001
el energy= -807.790998821
zpe= -807.570598
th energy= -807.557268
th enthalpy= -807.556324
free energy= -807.610463

ES-benzo

B -1.116634 1.407244 0.000000
O -1.263113 2.758842 -0.000001
H -0.372022 3.168679 -0.000003
N 0.203156 0.801040 -0.000001
C 1.473005 1.507085 -0.000002
O 1.520952 2.743503 0.000001
C 2.490165 0.480732 -0.000001
C 3.890620 0.561457 0.000001
H 4.386760 1.528717 0.000001
C 4.625301 -0.629700 0.000001
C 3.997540 -1.890222 0.000000
H 4.596692 -2.796594 0.000000
C 2.590824 -1.976309 -0.000001
H 2.100581 -2.948518 -0.000002
C 1.853668 -0.800026 -0.000001
C 0.414016 -0.559129 -0.000002
C -0.657840 -1.469573 -0.000001
H -0.437244 -2.533515 -0.000001
C -1.995487 -1.021751 0.000000
C -3.080603 -1.960825 0.000001
H -2.852769 -3.025352 0.000000
C -4.385500 -1.523827 0.000002
C -4.670816 -0.133844 0.000002
C -3.633065 0.799036 0.000002
H -3.860019 1.863200 0.000002
C -2.289794 0.400606 0.000001
H -5.202636 -2.241940 0.000002
H -5.705989 0.201388 0.000003
H 5.712814 -0.580566 0.000001
el energy= -807.783557970

GS-1

B 1.261336 -2.628728 0.000000
O 0.637296 -3.832553 0.000000
H -0.330319 -3.708549 0.000000
N 0.486794 -1.388852 0.000000
C -0.913855 -1.286819 0.000000
O -1.676971 -2.242751 0.000000
C -1.217124 0.163987 0.000000
C -2.452780 0.804333 0.000000
H -3.378118 0.236350 0.000000
C -2.439514 2.199463 0.000000
C -1.237241 2.926992 0.000000
H -1.269863 4.012450 0.000000
C -0.007398 2.265299 0.000000
H 0.916000 2.839702 0.000000
C 0.000000 0.868110 0.000000
C 1.085133 -0.114963 0.000000
C 2.434050 0.028288 0.000000
H 2.861965 1.028222 0.000000
C 3.329365 -1.116273 0.000000
C 4.726155 -0.927376 0.000000
H 5.129572 0.084257 0.000000
C 5.586031 -2.021108 0.000000
C 5.070899 -3.325426 0.000000
C 3.690692 -3.524265 0.000000
H 3.285100 -4.534095 0.000000
C 2.799260 -2.439417 0.000000
H 6.662679 -1.861646 0.000000
H 5.747610 -4.177445 0.000000
Br -4.106957 3.158395 0.000000
el energy= -820.360693950
zpe= -820.150685
th energy= -820.135766
th enthalpy= -820.134822
free energy= -820.193778

ES-1

B 1.188186 -2.664206 0.000000
O 0.545366 -3.861533 0.000000
H -0.421255 -3.700273 0.000000

N 0.447144 -1.416293 0.000000
C -0.996470 -1.277183 0.000000
O -1.741324 -2.263054 0.000000
C -1.250525 0.146178 0.000000
C -2.456125 0.862418 0.000000
H -3.413403 0.351133 0.000000
C -2.371331 2.257618 0.000000
C -1.149808 2.959132 0.000000
H -1.140968 4.043126 0.000000
C 0.054214 2.226683 0.000000
H 1.004851 2.756747 0.000000
C 0.000000 0.840892 0.000000
C 1.047564 -0.174603 0.000000
C 2.443826 -0.034188 0.000000
H 2.867600 0.966297 0.000000
C 3.291367 -1.164036 0.000000
C 4.717054 -1.006578 0.000000
H 5.134022 -0.001068 0.000000
C 5.542655 -2.107741 0.000000
C 4.988108 -3.413534 0.000000
C 3.604258 -3.592244 0.000000
H 3.186256 -4.596735 0.000000
C 2.726058 -2.500710 0.000000
H 6.623044 -1.981053 0.000000
H 5.649881 -4.277209 0.000000
Br -4.003954 3.272520 0.000000
el energy= -820.353513337

GS-2
B -2.503216 0.471917 0.000000
O -3.575755 -0.355945 0.000000
H -3.285476 -1.286955 0.000000
N -1.143783 -0.066782 0.000000
C -0.789851 -1.426134 0.000000
O -1.589711 -2.349813 0.000000
C 0.693069 -1.459272 0.000000
C 1.551406 -2.550586 0.000000
H 1.190550 -3.573681 0.000000
C 2.916884 -2.266494 0.000000
C 3.416897 -0.955132 0.000000
H 4.491808 -0.810295 0.000000
C 2.539820 0.127289 0.000000
H 2.927576 1.142770 0.000000
C 1.164252 -0.130722 0.000000
C 0.000000 0.752782 0.000000
C -0.101508 2.106712 0.000000
H 0.805624 2.706858 0.000000
C -1.387302 2.780360 0.000000
C -1.452063 4.188585 0.000000
H -0.529570 4.767321 0.000000
C -2.682669 4.837072 0.000000
C -3.872387 4.094422 0.000000
C -3.820287 2.700767 0.000000
H -4.740980 2.120754 0.000000
C -2.592913 2.019272 0.000000
H -2.720383 5.924652 0.000000
H -4.832366 4.606406 0.000000
N 3.876170 -3.386255 0.000000
O 3.418068 -4.521901 0.000000
O 5.070210 -3.109801 0.000000
el energy= -1012.28650798
zpe= -1012.063652
th energy= -1012.047703
th enthalpy= -1012.046759
free energy= -1012.107608

ES-2
B -2.496744 0.555659 0.000000
O -3.585592 -0.239097 0.000000
H -3.331311 -1.181881 0.000000
N -1.140341 -0.018496 0.000000
C -0.812212 -1.426256 0.000000
O -1.676617 -2.280369 0.000000
C 0.655248 -1.505582 0.000000
C 1.481563 -2.622624 0.000000
H 1.111089 -3.640918 0.000000
C 2.868993 -2.382691 0.000000
C 3.386219 -1.071511 0.000000
H 4.464688 -0.960624 0.000000
C 2.531789 0.036660 0.000000
H 2.945604 1.042740 0.000000
C 1.157078 -0.192132 0.000000
C 0.000000 0.738196 0.000000
C -0.061195 2.126792 0.000000
H 0.870215 2.686301 0.000000
C -1.303878 2.827294 0.000000
C -1.326993 4.253458 0.000000
H -0.384852 4.797948 0.000000
C -2.531686 4.937631 0.000000
C -3.745689 4.228605 0.000000
C -3.741042 2.823678 0.000000
H -4.683740 2.280607 0.000000
C -2.545490 2.104811 0.000000
H -2.538689 6.025077 0.000000
H -4.689552 4.768775 0.000000
N 3.777898 -3.494911 0.000000
O 3.273943 -4.648228 0.000000
O 5.010909 -3.239862 0.000000
el energy= -1012.27895213

GS-3
B -1.521476 1.387063 0.000732
O -1.691693 2.733989 0.002248
H -0.821811 3.176310 0.000953
N -0.180048 0.809353 -0.001544
C 1.029379 1.523257 -0.002716
O 1.108246 2.745747 -0.000413
C 2.108126 0.508348 -0.005999
C 3.483596 0.693711 -0.005238
H 3.904342 1.697384 -0.008418
C 4.309949 -0.445398 -0.004145
C 3.709196 -1.728427 -0.001431

H 4.353798 -2.606402 -0.004312
C 2.326684 -1.896779 -0.001773
H 1.905167 -2.899652 0.002181
C 1.508913 -0.763149 -0.004339
C 0.057627 -0.579531 -0.002319
C -0.971867 -1.463257 -0.001307
H -0.756412 -2.529399 -0.002293
C -2.359868 -1.031277 0.000379
C -3.402343 -1.980359 0.000787
H -3.158897 -3.042067 -0.000256
C -4.732078 -1.570882 0.002231
C -5.052441 -0.205551 0.003362
C -4.029897 0.742367 0.002998
H -4.270409 1.803891 0.003754
C -2.679250 0.357946 0.001518
H -5.526063 -2.315670 0.002380
H -6.093922 0.109782 0.004409
N 5.694841 -0.321940 -0.059889
H 6.073449 0.565063 0.241782
H 6.227798 -1.110460 0.279460
el energy= -863.144196317
zpe= -862.907226
th energy= -862.892367
th enthalpy= -862.891423
free energy= -862.948627

ES-3
B -1.509978 1.400244 0.000134
O -1.691105 2.753368 0.000988
H -0.809355 3.180490 0.000662
N -0.172228 0.837138 -0.001051
C 1.047645 1.568032 -0.001729
O 1.102585 2.813037 -0.000707
C 2.100303 0.563690 -0.002727
C 3.482229 0.694318 -0.002387
H 3.946932 1.678421 -0.003429
C 4.273065 -0.480164 -0.000837
C 3.665756 -1.774837 -0.001226
H 4.300610 -2.658085 -0.003677
C 2.285317 -1.898313 -0.001799
H 1.829485 -2.886315 -0.001067
C 1.489737 -0.739367 -0.002202
C 0.071927 -0.542478 -0.001556
C -0.973796 -1.469187 -0.001057
H -0.733802 -2.529741 -0.001745
C -2.325793 -1.051455 -0.000112
C -3.384895 -2.010462 0.000313
H -3.134549 -3.070604 -0.000282
C -4.701745 -1.604557 0.001464
C -5.020382 -0.222204 0.002248
C -4.007303 0.729329 0.001842
H -4.255812 1.788909 0.002396
C -2.648793 0.361829 0.000574
H -5.500819 -2.343343 0.001766
H -6.063528 0.088539 0.003095
N 5.637532 -0.384633 -0.015560
H 6.089171 0.511942 0.078362
H 6.212959 -1.205249 0.092412
el energy= -863.136721737

GS-dioxo
B 0.089882 1.573698 -0.002130
O 0.117908 2.931573 -0.000643
H -0.793417 3.280222 0.001067
N -1.181852 0.857306 -0.000546
C -2.462909 1.437224 0.002137
O -2.670781 2.643945 0.003615
C -3.422706 0.311038 0.002754
C -4.815024 0.327403 0.005187
H -5.353865 1.271905 0.006909
C -5.482282 -0.899790 0.005318
C -4.758004 -2.104465 0.003062
H -5.297852 -3.049291 0.003226
C -3.360239 -2.116813 0.000600
H -2.816799 -3.059113 -0.001137
C -2.689872 -0.890995 0.000448
C -1.266518 -0.545444 -0.001678
C -0.147149 -1.313072 -0.004475
H -0.247926 -2.395950 -0.005359
C 1.185727 -0.737427 -0.006861
C 2.315161 -1.598557 -0.009482
H 2.204673 -2.679635 -0.011816
C 3.559082 -1.008781 -0.009603
C 3.725917 0.381334 -0.008424
C 2.649222 1.241434 -0.007282
H 2.783385 2.319365 -0.008348
C 1.351321 0.678625 -0.005670
O 4.783464 -1.619711 -0.022878
O 5.064371 0.681441 -0.022255
H -6.569485 -0.927458 0.007178
C 5.754314 -0.567993 0.055795
H 6.287005 -0.635505 1.015721
H 6.451882 -0.654484 -0.786638
el energy= -996.317544570
zpe= -996.081596
th energy= -996.065825
th enthalpy= -996.064880
free energy= -996.125544

ES-dioxo
B 0.076087 1.570952 0.000056
O 0.116699 2.931336 0.000130
H -0.810977 3.256167 0.000230
N -1.172151 0.854068 0.000063
C -2.486756 1.450173 0.000032
O -2.638210 2.683974 -0.000153
C -3.415486 0.345399 -0.000018
C -4.820130 0.317597 -0.000119
H -5.386708 1.245469 -0.000178
C -5.459652 -0.922503 -0.000120
C -4.733651 -2.132300 -0.000030
H -5.261682 -3.082204 -0.000038

C -3.328009 -2.109918 0.000055
H -2.764381 -3.041723 0.000106
C -2.680921 -0.881186 0.000057
C -1.260374 -0.532368 0.000085
C -0.132734 -1.340122 0.000093
H -0.253364 -2.419092 0.000098
C 1.176976 -0.777246 0.000069
C 2.320272 -1.629040 0.000054
H 2.220180 -2.710137 0.000061
C 3.548921 -1.022967 0.000022
C 3.708477 0.391341 0.000003
C 2.626701 1.248378 0.000016
H 2.750761 2.327319 -0.000006
C 1.342034 0.677408 0.000040
O 4.776371 -1.605674 0.000076
O 5.033219 0.689974 0.000051
H -6.547858 -0.959410 -0.000188
C 5.738571 -0.550775 -0.000310
H 6.354700 -0.618902 0.905257
H 6.353878 -0.618832 -0.906459
el energy= -996.311509938

GS-4
B -1.571261 1.649333 -0.001273
O -1.689925 3.001498 -0.000353
H -0.806630 3.415100 0.000290
N -0.253935 1.017420 -0.000957
C 0.984246 1.680284 0.000202
O 1.117780 2.896336 0.001053
C 2.015646 0.615906 0.000066
C 3.402360 0.733984 0.000956
H 3.881904 1.708236 0.001850
C 4.136174 -0.452673 0.000678
C 3.508077 -1.709900 -0.000463
H 4.115305 -2.610409 -0.000636
C 2.115100 -1.807220 -0.001376
H 1.641502 -2.786178 -0.002260
C 1.362002 -0.629867 -0.001108
C -0.078894 -0.377581 -0.001795
C -1.146144 -1.216563 -0.003062
H -0.975156 -2.290577 -0.003744
C -2.513274 -0.729504 -0.003765
C -3.583699 -1.662896 -0.004938
H -3.402862 -2.734387 -0.006428
C -4.863462 -1.155627 -0.004432
C -5.120401 0.220881 -0.003358
C -4.102207 1.149809 -0.002982
H -4.306499 2.216606 -0.003171
C -2.770703 0.672852 -0.002794
O -6.044540 -1.844848 -0.010764
O -6.474273 0.433802 -0.009452
Br 6.058402 -0.373382 0.001909
C -7.084705 -0.858797 0.028458
H -7.735681 -0.982661 -0.846693
H -7.655154 -0.968798 0.961434
el energy= -1008.88738433

zpe= -1008.661944
th energy= -1008.644521
th enthalpy= -1008.643577
free energy= -1008.709887

ES-4
B -1.558770 1.649307 -0.000088
O -1.696835 3.002604 -0.000171
H -0.797844 3.397648 -0.000334
N -0.265265 1.018873 -0.000123
C 1.004939 1.703426 -0.000097
O 1.075155 2.942345 0.000159
C 2.006747 0.664177 -0.000073
C 3.409829 0.745700 0.000024
H 3.914462 1.706489 0.000096
C 4.117609 -0.453733 0.000008
C 3.497795 -1.720211 -0.000094
H 4.097965 -2.623152 -0.000097
C 2.092342 -1.787191 -0.000177
H 1.601556 -2.758902 -0.000235
C 1.359855 -0.610315 -0.000162
C -0.082534 -0.359832 -0.000168
C -1.148833 -1.241152 -0.000172
H -0.955957 -2.309505 -0.000194
C -2.497068 -0.768263 -0.000106
C -3.576712 -1.696345 -0.000075
H -3.402876 -2.767999 -0.000122
C -4.845260 -1.175910 0.000017
C -5.101612 0.224003 0.000072
C -4.081063 1.153174 0.000033
H -4.277823 2.221166 0.000065
C -2.760990 0.670154 -0.000046
O -6.028216 -1.841371 0.000045
O -6.442948 0.430654 0.000137
Br 6.044448 -0.386832 0.000125
C -7.061762 -0.855468 0.000273
H -7.670889 -0.966204 -0.905646
H -7.670483 -0.966200 0.906468
el energy= -1008.88140077

GS-5
B 0.247475 -1.973235 0.000000
O 1.060388 -3.059056 0.000000
H 1.995272 -2.781810 0.000000
N 0.804394 -0.622536 0.000000
C 2.168171 -0.285762 0.000000
O 3.081583 -1.097681 0.000000
C 2.219063 1.196308 0.000000
C 3.319985 2.041958 0.000000
H 4.338802 1.669323 0.000000
C 3.052371 3.411037 0.000000
C 1.746330 3.925956 0.000000
H 1.613814 5.002407 0.000000
C 0.653826 3.062015 0.000000
H -0.356979 3.461833 0.000000
C 0.895087 1.682780 0.000000

C 0.000000 0.530180 0.000000
C -1.356286 0.440534 0.000000
H -1.946163 1.354221 0.000000
C -2.046122 -0.833758 0.000000
C -3.466619 -0.854981 0.000000
H -4.048494 0.062681 0.000000
C -4.078393 -2.087647 0.000000
C -3.347367 -3.282980 0.000000
C -1.968506 -3.292829 0.000000
H -1.407739 -4.223016 0.000000
C -1.298111 -2.048247 0.000000
O -5.416027 -2.366161 0.000000
O -4.208812 -4.345786 0.000000
N 4.182478 4.356402 0.000000
O 5.313106 3.885570 0.000000
O 3.920718 5.553952 0.000000
C -5.529913 -3.795610 0.000000
H -6.061367 -4.118469 0.905089
H -6.061367 -4.118469 -0.905089
el energy= -1200.81359237
zpe= -1200.575207
th energy= -1200.556813
th enthalpy= -1200.555868
free energy= -1200.623178

ES-5
B 0.187370 -1.964531 0.000000
O 0.960623 -3.075203 0.000000
H 1.904733 -2.817567 0.000000
N 0.763977 -0.631485 0.000000
C 2.159939 -0.328282 0.000000
O 3.017543 -1.199973 0.000000
C 2.255149 1.136312 0.000000
C 3.381887 1.947576 0.000000
H 4.392284 1.553885 0.000000
C 3.169656 3.332403 0.000000
C 1.867093 3.886048 0.000000
H 1.773600 4.965401 0.000000
C 0.748183 3.048773 0.000000
H -0.250822 3.480196 0.000000
C 0.944339 1.669595 0.000000
C 0.000000 0.532330 0.000000
C -1.370068 0.493820 0.000000
H -1.926500 1.426067 0.000000
C -2.094288 -0.756023 0.000000
C -3.510176 -0.748991 0.000000
H -4.076442 0.177289 0.000000
C -4.140722 -1.973642 0.000000
C -3.430159 -3.199993 0.000000
C -2.046782 -3.239259 0.000000
H -1.501269 -4.178347 0.000000
C -1.365947 -2.011977 0.000000
O -5.470901 -2.230912 0.000000
O -4.313127 -4.229531 0.000000
N 4.311371 4.214739 0.000000
O 5.448593 3.697550 0.000000
O 4.087045 5.443879 0.000000
C -5.619496 -3.653319 0.000000
H -6.154870 -3.962870 0.906301
H -6.154870 -3.962870 -0.906301
el energy= -1200.80963088

GS-6
B 0.491600 1.601911 -0.003340
O 0.552626 2.959491 -0.002622
H -0.350470 3.328930 0.000787
N -0.798374 0.918339 0.000589
C -2.062068 1.531766 0.004997
O -2.239766 2.743953 0.004802
C -3.054022 0.431925 0.008577
C -4.440159 0.503412 0.010348
H -4.941984 1.469165 0.015602
C -5.170433 -0.699310 0.009007
C -4.466719 -1.928571 0.003556
H -5.037156 -2.856491 0.006271
C -3.074904 -1.983202 0.001275
H -2.572698 -2.948304 -0.004871
C -2.352387 -0.786527 0.004027
C -0.921649 -0.483646 -0.000368
C 0.179579 -1.277292 -0.004964
H 0.053222 -2.357508 -0.005391
C 1.527112 -0.734671 -0.009501
C 2.634887 -1.623320 -0.013155
H 2.497302 -2.701333 -0.015356
C 3.893659 -1.065230 -0.014201
C 4.096645 0.319577 -0.013606
C 3.042095 1.206250 -0.012058
H 3.202937 2.280583 -0.014252
C 1.730035 0.676487 -0.008787
O 5.102784 -1.707828 -0.032658
O 5.444465 0.584296 -0.034266
N -6.561451 -0.689439 0.067448
H -7.010057 0.163740 -0.236151
H -7.027325 -1.517862 -0.275827
C 6.096962 -0.681442 0.078566
H 6.589716 -0.757092 1.059886
H 6.824602 -0.792203 -0.734574
el energy= -1051.67048842
zpe= -1051.417952
th energy= -1051.400681
th enthalpy= -1051.399736
free energy= -1051.463109

ES-6
B 0.476588 1.609991 -0.000075
O 0.554213 2.972697 -0.001507
H -0.362435 3.323304 -0.000755
N -0.796176 0.934448 0.001546
C -2.081831 1.562815 0.002445
O -2.220674 2.801176 0.000338
C -3.044592 0.479328 0.005366
C -4.437594 0.499663 0.004856

H -4.977013 1.444943 0.007205
C -5.133585 -0.727961 0.003116
C -4.424883 -1.964750 0.001850
H -4.984611 -2.897512 0.007896
C -3.032559 -1.978081 0.002691
H -2.502148 -2.928870 0.000419
C -2.334028 -0.767209 0.003839
C -0.926969 -0.458511 0.002378
C 0.187294 -1.293143 0.001676
H 0.037655 -2.369170 0.003078
C 1.504735 -0.767289 0.000532
C 2.628900 -1.653213 0.000436
H 2.495509 -2.731100 0.001463
C 3.872674 -1.086056 -0.000835
C 4.070171 0.319987 -0.002106
C 3.015294 1.207047 -0.002059
H 3.172734 2.281740 -0.002835
C 1.708977 0.678577 -0.000552
O 5.087526 -1.706255 -0.001318
O 5.405709 0.584340 -0.003297
N -6.512566 -0.740259 0.041703
H -7.001572 0.113356 -0.184606
H -6.990677 -1.588584 -0.223849
C 6.076717 -0.676579 -0.000992
H 6.690847 -0.759433 0.905338
H 6.693445 -0.761366 -0.905303
el energy= -1051.66404738

GS-thieno
B -1.043360 1.443539 -0.000005
O -1.156710 2.792228 0.000002
H -0.266483 3.195412 0.000016
N 0.273155 0.802294 0.000009
C 1.505367 1.475976 0.000030
O 1.622717 2.696052 0.000036
C 2.549661 0.429248 0.000038
C 3.936812 0.555450 0.000057
H 4.399265 1.539561 0.000068
C 4.698202 -0.615031 0.000062
C 4.071349 -1.873680 0.000048
H 4.684108 -2.772900 0.000052
C 2.679487 -1.995957 0.000028
H 2.212260 -2.978225 0.000018
C 1.914525 -0.826279 0.000024
C 0.468028 -0.598329 0.000005
C -0.573438 -1.467916 -0.000014
H -0.379316 -2.537322 -0.000016
C -1.938879 -0.983903 -0.000030
C -3.083470 -1.754547 -0.000050
H -3.165747 -2.835042 -0.000058
S -4.514349 -0.769848 -0.000078
C -3.571417 0.691676 -0.000038
H -4.068392 1.654656 -0.000035
C -2.221836 0.441362 -0.000027
H 5.784206 -0.556998 0.000077
el energy= -740.481726729

zpe= -740.294994
th energy= -740.281985
th enthalpy= -740.281041
free energy= -740.334697

ES-thieno
B -1.031985 1.455212 -0.000005
O -1.149661 2.805214 0.000021
H -0.248038 3.192884 0.000052
N 0.264719 0.804803 0.000012
C 1.563982 1.495064 0.000037
O 1.614823 2.729519 0.000027
C 2.562915 0.462249 0.000046
C 3.970772 0.527083 0.000062
H 4.478971 1.487570 0.000071
C 4.688770 -0.674658 0.000070
C 4.050824 -1.925656 0.000061
H 4.637068 -2.839999 0.000067
C 2.631799 -1.992256 0.000043
H 2.129583 -2.958301 0.000035
C 1.916744 -0.812264 0.000035
C 0.465795 -0.557245 0.000013
C -0.598039 -1.465566 -0.000006
H -0.390045 -2.530836 -0.000001
C -1.927960 -0.978612 -0.000031
C -3.106565 -1.757895 -0.000032
H -3.180969 -2.838843 -0.000021
S -4.511557 -0.783806 -0.000143
C -3.563085 0.696823 -0.000011
H -4.071443 1.653756 0.000014
C -2.216233 0.453602 -0.000031
H 5.777071 -0.636880 0.000084
el energy= -740.472913995

GS-7
B -2.485581 1.436901 -0.000023
O -2.661063 2.778168 -0.000016
H -1.793158 3.226400 -0.000001
N -1.139714 0.855798 -0.000009
C 0.058379 1.585147 0.000012
O 0.125365 2.807902 0.000017
C 1.149293 0.583617 0.000020
C 2.526898 0.784346 0.000038
H 2.946736 1.785622 0.000049
C 3.329545 -0.356205 0.000042
C 2.777038 -1.648935 0.000029
H 3.436851 -2.511501 0.000033
C 1.392816 -1.828896 0.000010
H 0.978490 -2.834327 -0.000001
C 0.571068 -0.697943 0.000006
C -0.882606 -0.535218 -0.000013
C -1.884062 -1.451080 -0.000031
H -1.642112 -2.510717 -0.000033
C -3.269357 -1.029033 -0.000048
C -4.377911 -1.850975 -0.000067
H -4.411008 -2.934094 -0.000074

S -5.851206 -0.932222 -0.000096
C -4.975728 0.570557 -0.000056
H -5.516001 1.509930 -0.000053
C -3.616153 0.381731 -0.000045
Br 5.243305 -0.163488 0.000068
el energy= -753.051456390
zpe= -752.875144
th energy= -752.860544
th enthalpy= -752.859600
free energy= -752.918072

ES-7
B 2.486255 1.447998 0.000025
O 2.680586 2.788506 -0.000011
H 1.805971 3.231481 -0.000049
N 1.156656 0.868263 0.000007
C -0.100921 1.624790 -0.000019
O -0.091836 2.857812 0.000000
C -1.155147 0.645857 -0.000028
C -2.556233 0.801235 -0.000044
H -3.014273 1.784322 -0.000052
C -3.323980 -0.367340 -0.000053
C -2.776724 -1.658900 -0.000046
H -3.419602 -2.531147 -0.000053
C -1.360899 -1.796851 -0.000029
H -0.920280 -2.791828 -0.000022
C -0.580409 -0.661075 -0.000019
C 0.882208 -0.483162 0.000004
C 1.893674 -1.445596 0.000021
H 1.629721 -2.498414 0.000013
C 3.249086 -1.030675 0.000051
C 4.382526 -1.873333 0.000042
H 4.397461 -2.956756 0.000023
S 5.838194 -0.977730 0.000194
C 4.971790 0.552727 0.000017
H 5.531587 1.480519 -0.000018
C 3.614144 0.382864 0.000052
Br -5.242693 -0.191603 -0.000078
el energy= -753.042756115

GS-8
B 2.055122 1.439837 0.000036
O 2.229223 2.780289 -0.000001
H 1.363040 3.231180 -0.000102
N 0.710004 0.855139 -0.000011
C -0.490629 1.580508 0.000026
O -0.563296 2.801726 0.000129
C -1.577359 0.573143 -0.000037
C -2.953634 0.760301 -0.000041
H -3.405600 1.746459 0.000005
C -3.736884 -0.393037 -0.000039
C -3.183765 -1.683498 -0.000108
H -3.855171 -2.535277 -0.000084
C -1.801287 -1.851186 -0.000157
H -1.374354 -2.850805 -0.000199
C -0.991577 -0.708726 -0.000102
C 0.458362 -0.536264 -0.000082
C 1.462785 -1.450997 -0.000115
H 1.223194 -2.511137 -0.000159
C 2.844914 -1.025058 -0.000046
C 3.955779 -1.845493 -0.000036
H 3.990881 -2.928524 -0.000079
S 5.424907 -0.923921 0.000060
C 4.546749 0.577849 0.000094
H 5.085977 1.517779 0.000159
C 3.187696 0.386418 0.000035
N -5.205046 -0.255484 0.000050
O -5.665619 0.878994 -0.000401
O -5.870769 -1.284442 0.000608
el energy= -944.977288386
zpe= -944.788119
th energy= -944.772498
th enthalpy= -944.771554
free energy= -944.831923

ES-8
B -2.064868 1.441542 -0.000014
O -2.239970 2.775162 0.000069
H -1.380091 3.238652 0.000339
N -0.718842 0.839357 0.000284
C 0.523980 1.580746 0.000668
O 0.535873 2.795885 -0.000071
C 1.603834 0.585841 0.000301
C 2.983254 0.774942 -0.000016
H 3.454020 1.750361 -0.000128
C 3.777936 -0.388632 -0.000062
C 3.195093 -1.669683 0.000156
H 3.867868 -2.520266 0.000079
C 1.805282 -1.831226 0.000391
H 1.373044 -2.829373 0.000469
C 1.012505 -0.684434 0.000421
C -0.466040 -0.510860 0.000397
C -1.488092 -1.444602 0.000328
H -1.240660 -2.501536 0.000390
C -2.849962 -1.016443 0.000082
C -3.983974 -1.844624 -0.000044
H -4.008665 -2.928179 0.000035
S -5.446508 -0.938534 -0.000397
C -4.556421 0.576430 -0.000312
H -5.099500 1.514726 -0.000454
C -3.199146 0.388685 -0.000117
N 5.208338 -0.272689 -0.000317
O 5.685161 0.894696 -0.000545
O 5.884745 -1.338126 -0.000355
el energy= -944.968811290

GS-9
B 1.438087 1.436864 -0.000057
O 1.577924 2.783890 0.002112
H 0.694956 3.202777 0.000312
N 0.109026 0.822865 -0.001852
C -1.107325 1.521595 -0.002541

O -1.201110 2.744551 -0.000023
C -2.175546 0.497631 -0.005877
C -3.552985 0.670876 -0.004818
H -3.982042 1.670972 -0.007776
C -4.368943 -0.474907 -0.003877
C -3.757009 -1.753188 -0.001537
H -4.394119 -2.636610 -0.004699
C -2.373714 -1.909539 -0.002051
H -1.943770 -2.908866 0.001601
C -1.565092 -0.768462 -0.004535
C -0.116216 -0.575621 -0.002731
C 0.910244 -1.463369 -0.002025
H 0.696673 -2.529126 -0.003084
C 2.285855 -1.006310 -0.000023
C 3.415502 -1.798046 0.000942
H 3.477940 -2.879829 0.000103
S 4.866643 -0.840353 0.003118
C 3.950926 0.638439 0.003129
H 4.465521 1.592115 0.004205
C 2.596995 0.412793 0.001224
N -5.754826 -0.364403 -0.059633
H -6.141504 0.519283 0.241329
H -6.280428 -1.157501 0.280408
el energy= -795.834953925
zpe= -795.631653
th energy= -795.617104
th enthalpy= -795.616160
free energy= -795.672913

ES-9
B 1.426673 1.451737 0.000116
O 1.581982 2.803163 0.000900
H 0.688710 3.209192 0.000082
N 0.110602 0.848010 -0.001068
C -1.135715 1.565361 -0.001416
O -1.190345 2.808730 -0.000008
C -2.171656 0.554298 -0.003401
C -3.560244 0.668221 -0.003892
H -4.038178 1.645792 -0.006667
C -4.337103 -0.516607 -0.002207
C -3.721284 -1.802115 -0.001733
H -4.343603 -2.693624 -0.005905
C -2.329988 -1.905251 -0.002208
H -1.862804 -2.888295 -0.000778
C -1.553162 -0.743048 -0.002409
C -0.129162 -0.533018 -0.001505
C 0.911437 -1.462462 -0.001015
H 0.679334 -2.523441 -0.001950
C 2.255586 -1.012317 0.000030
C 3.406149 -1.818054 0.000689
H 3.458892 -2.900135 0.000301
S 4.836582 -0.872922 0.001985
C 3.933871 0.625976 0.001947
H 4.465922 1.569651 0.002562
C 2.578714 0.417654 0.000719
N -5.705628 -0.427206 -0.026614
H -6.152482 0.464388 0.124065
H -6.267035 -1.248047 0.141000
el energy= -795.827928729

chloroform-GS-benzo
B -1.126200 1.394183 0.000000
O -1.273389 2.746675 0.000000
H -0.395324 3.174237 -0.000001
N 0.203354 0.793669 -0.000001
C 1.427369 1.481682 -0.000003
O 1.525390 2.705203 0.000001
C 2.484352 0.449585 -0.000001
C 3.870780 0.590698 0.000001
H 4.328504 1.577297 0.000001
C 4.643449 -0.573326 0.000001
C 4.029405 -1.838243 0.000000
H 4.651381 -2.731082 0.000001
C 2.637852 -1.976004 -0.000001
H 2.179740 -2.962178 -0.000002
C 1.862553 -0.813712 -0.000002
C 0.412766 -0.598538 -0.000002
C -0.629973 -1.466003 -0.000001
H -0.432497 -2.535351 -0.000001
C -2.009534 -1.008163 0.000000
C -3.067380 -1.941114 0.000001
H -2.839979 -3.006095 0.000000
C -4.390469 -1.509661 0.000002
C -4.688017 -0.138434 0.000003
C -3.650002 0.793207 0.000002
H -3.880592 1.857336 0.000003
C -2.304442 0.387339 0.000001
H -5.196556 -2.241353 0.000002
H -5.724265 0.193850 0.000004
H 5.728850 -0.504148 0.000002
el energy= -807.810219010
zpe= -807.590072
th energy= -807.576693
th enthalpy= -807.575749
free energy= -807.630020

chloroform-ES-benzo
B -1.112918 1.406181 0.000000
O -1.244439 2.762690 0.000000
H -0.346265 3.159360 -0.000001
N 0.214381 0.803163 0.000000
C 1.465635 1.503349 -0.000001
O 1.525540 2.746813 0.000000
C 2.486957 0.477781 -0.000001
C 3.883836 0.559676 0.000000
H 4.382858 1.526488 0.000000
C 4.622236 -0.628687 0.000000
C 3.988279 -1.892393 -0.000001
H 4.591451 -2.796913 0.000000
C 2.593406 -1.986561 -0.000001
H 2.105557 -2.959376 -0.000001
C 1.841750 -0.803839 -0.000001

C 0.422282 -0.565172 -0.000001
C -0.666189 -1.471137 0.000000
H -0.449989 -2.536210 0.000000
C -1.994752 -1.019211 0.000000
C -3.084130 -1.958078 0.000001
H -2.855545 -3.022490 0.000000
C -4.388798 -1.519933 0.000001
C -4.672870 -0.130338 0.000001
C -3.631894 0.802582 0.000001
H -3.868683 1.865245 0.000001
C -2.289126 0.406274 0.000001
H -5.206259 -2.237908 0.000001
H -5.707240 0.207255 0.000002
H 5.709489 -0.580404 0.000000
el energy= -807.802239099

chloroform-GS-1
B 1.256576 -2.629978 0.000000
O 0.630480 -3.836715 0.000000
H -0.337585 -3.711332 0.000000
N 0.483190 -1.391103 0.000000
C -0.914855 -1.285364 0.000000
O -1.679868 -2.243495 0.000000
C -1.218286 0.163359 0.000000
C -2.453730 0.806365 0.000000
H -3.381580 0.241665 0.000000
C -2.432723 2.201007 0.000000
C -1.230368 2.928109 0.000000
H -1.253972 4.014083 0.000000
C -0.002336 2.263441 0.000000
H 0.921981 2.835562 0.000000
C 0.000000 0.866266 0.000000
C 1.084362 -0.117245 0.000000
C 2.433311 0.025786 0.000000
H 2.861631 1.025217 0.000000
C 3.325728 -1.121491 0.000000
C 4.723280 -0.932696 0.000000
H 5.126079 0.078903 0.000000
C 5.583253 -2.027126 0.000000
C 5.068217 -3.332070 0.000000
C 3.687496 -3.530459 0.000000
H 3.286911 -4.542680 0.000000
C 2.795074 -2.445147 0.000000
H 6.659897 -1.867502 0.000000
H 5.745038 -4.184115 0.000000
Br -4.102544 3.167516 0.000000
el energy= -820.381958308
zpe= -820.172166
th energy= -820.157224
th enthalpy= -820.156280
free energy= -820.215268

chloroform-ES-1
B 1.216975 -2.647855 0.000000
O 0.573918 -3.848632 0.000000
H -0.393246 -3.685034 0.000000
N 0.453622 -1.406467 0.000000
C -0.976102 -1.289917 0.000000
O -1.720883 -2.284196 0.000000
C -1.249408 0.131302 0.000000
C -2.461257 0.830437 0.000000
H -3.411364 0.303969 0.000000
C -2.395194 2.224931 0.000000
C -1.175578 2.940866 0.000000
H -1.176621 4.025770 0.000000
C 0.030621 2.234051 0.000000
H 0.972722 2.778142 0.000000
C 0.000000 0.836480 0.000000
C 1.046129 -0.154834 0.000000
C 2.451566 -0.008486 0.000000
H 2.866059 0.996011 0.000000
C 3.302237 -1.126922 0.000000
C 4.729321 -0.955146 0.000000
H 5.134510 0.055042 0.000000
C 5.566852 -2.047910 0.000000
C 5.026677 -3.358561 0.000000
C 3.642061 -3.551839 0.000000
H 3.243564 -4.564682 0.000000
C 2.751160 -2.472324 0.000000
H 6.645720 -1.909277 0.000000
H 5.696123 -4.216303 0.000000
Br -4.039899 3.227736 0.000000
el energy= -820.374329530

chloroform-GS-2
B -2.501030 0.471698 0.000000
O -3.576219 -0.358816 0.000000
H -3.283215 -1.289972 0.000000
N -1.144316 -0.069367 0.000000
C -0.789596 -1.424925 0.000000
O -1.592431 -2.350437 0.000000
C 0.691114 -1.460641 0.000000
C 1.548668 -2.552248 0.000000
H 1.185037 -3.574224 0.000000
C 2.914622 -2.265799 0.000000
C 3.414907 -0.953140 0.000000
H 4.488329 -0.798347 0.000000
C 2.538254 0.128666 0.000000
H 2.924212 1.144379 0.000000
C 1.163232 -0.132029 0.000000
C 0.000000 0.750795 0.000000
C -0.099049 2.104882 0.000000
H 0.809159 2.702688 0.000000
C -1.385197 2.778325 0.000000
C -1.446396 4.187314 0.000000
H -0.521895 4.762453 0.000000
C -2.675994 4.838869 0.000000
C -3.867920 4.098881 0.000000
C -3.819091 2.704600 0.000000
H -4.745353 2.132651 0.000000
C -2.593044 2.019058 0.000000
H -2.711388 5.926681 0.000000

H -4.827036 4.612765 0.000000
N 3.869479 -3.380848 0.000000
O 3.419075 -4.522302 0.000000
O 5.067587 -3.113660 0.000000
el energy= -1012.30749377
zpe= -1012.084770
th energy= -1012.068813
th enthalpy= -1012.067869
free energy= -1012.128805

chloroform-ES-2
B -2.497635 0.545910 0.000000
O -3.590820 -0.246975 0.000000
H -3.342139 -1.191299 0.000000
N -1.144834 -0.033817 0.000000
C -0.819301 -1.427184 0.000000
O -1.671690 -2.298970 0.000000
C 0.650926 -1.501548 0.000000
C 1.479200 -2.611149 0.000000
H 1.099255 -3.626404 0.000000
C 2.867779 -2.369635 0.000000
C 3.384459 -1.052836 0.000000
H 4.460623 -0.924784 0.000000
C 2.529177 0.049534 0.000000
H 2.938758 1.056824 0.000000
C 1.149216 -0.179532 0.000000
C 0.000000 0.728163 0.000000
C -0.064245 2.123944 0.000000
H 0.867031 2.683357 0.000000
C -1.301045 2.819233 0.000000
C -1.319101 4.247832 0.000000
H -0.374614 4.787728 0.000000
C -2.522084 4.933355 0.000000
C -3.736925 4.224590 0.000000
C -3.737867 2.818292 0.000000
H -4.686618 2.285802 0.000000
C -2.546217 2.095891 0.000000
H -2.528830 6.020836 0.000000
H -4.680140 4.766000 0.000000
N 3.771128 -3.477270 0.000000
O 3.286318 -4.641978 0.000000
O 5.009560 -3.237540 0.000000
el energy= -1012.30069077

chloroform-GS-3
B -1.519522 1.385572 -0.000250
O -1.690058 2.736306 0.002162
H -0.818243 3.176887 0.000678
N -0.179681 0.809704 -0.003508
C 1.029841 1.520663 -0.003607
O 1.104607 2.746519 -0.001354
C 2.109207 0.510141 -0.007178
C 3.485247 0.696283 -0.004522
H 3.914042 1.696441 -0.004179
C 4.312436 -0.444981 -0.002862
C 3.709488 -1.729343 -0.001046
H 4.356131 -2.605654 0.000556
C 2.327264 -1.897733 -0.003750
H 1.904468 -2.899936 0.000122
C 1.509710 -0.762614 -0.006924
C 0.058870 -0.580483 -0.005039
C -0.971655 -1.463872 -0.003884
H -0.757640 -2.530145 -0.005466
C -2.359163 -1.030041 -0.000644
C -3.401792 -1.980420 0.001040
H -3.156467 -3.041558 -0.000485
C -4.732429 -1.572285 0.004490
C -5.054973 -0.206769 0.006375
C -4.032608 0.741999 0.004706
H -4.280884 1.802203 0.006163
C -2.680328 0.359772 0.001254
H -5.525318 -2.318439 0.005699
H -6.096818 0.107594 0.009063
N 5.692404 -0.322190 -0.056399
H 6.072971 0.562830 0.254086
H 6.225217 -1.115188 0.277430
el energy= -863.167132682
zpe= -862.930478
th energy= -862.915605
th enthalpy= -862.914661
free energy= -862.971918

chloroform-ES-3
B -1.507624 1.394893 0.000007
O -1.671610 2.755610 0.000038
H -0.778315 3.162471 0.000052
N -0.166618 0.833526 -0.000034
C 1.043910 1.561949 -0.000089
O 1.095441 2.815085 -0.000067
C 2.100383 0.563207 -0.000034
C 3.480771 0.698481 0.000026
H 3.953902 1.678374 0.000053
C 4.276754 -0.476356 0.000049
C 3.664140 -1.776980 0.000006
H 4.305775 -2.655334 0.000038
C 2.292006 -1.905131 -0.000047
H 1.836873 -2.892993 -0.000059
C 1.487750 -0.741673 -0.000065
C 0.076779 -0.550904 -0.000065
C -0.977452 -1.472139 -0.000054
H -0.742773 -2.533957 -0.000063
C -2.326216 -1.049175 -0.000021
C -3.389126 -2.005960 -0.000008
H -3.140019 -3.066486 -0.000031
C -4.706725 -1.599022 0.000037
C -5.026597 -0.217370 0.000068
C -4.009976 0.731808 0.000051
H -4.265267 1.790636 0.000078
C -2.650310 0.364657 0.000008
H -5.505307 -2.338821 0.000049
H -6.069289 0.094996 0.000105
N 5.628635 -0.382340 0.000138

H 6.088887 0.517943 0.000097
H 6.212335 -1.207509 -0.000016
el energy= -863.158690107

chloroform-GS-dioxo
B 0.088506 1.572982 -0.005594
O 0.113749 2.934799 -0.003295
H -0.800140 3.279259 -0.002286
N -1.182540 0.858134 -0.005093
C -2.462771 1.434425 -0.000131
O -2.668982 2.644786 0.001106
C -3.422521 0.311634 0.003761
C -4.815969 0.327080 0.011505
H -5.360856 1.268333 0.014245
C -5.481427 -0.901216 0.015911
C -4.756184 -2.105809 0.012629
H -5.295593 -3.050859 0.016703
C -3.357923 -2.118215 0.004434
H -2.813740 -3.059858 0.002380
C -2.689316 -0.891304 0.000131
C -1.266159 -0.545759 -0.006539
C -0.146459 -1.313027 -0.012982
H -0.246668 -2.395644 -0.015068
C 1.185821 -0.734986 -0.016655
C 2.314812 -1.597724 -0.024835
H 2.200405 -2.678429 -0.034521
C 3.559685 -1.009146 -0.021196
C 3.728467 0.381852 -0.008875
C 2.652055 1.242700 -0.006238
H 2.793302 2.320223 -0.003009
C 1.352085 0.681676 -0.009527
O 4.781724 -1.619565 -0.049521
O 5.064855 0.680647 -0.025826
H -6.568692 -0.929386 0.022250
C 5.752631 -0.571381 0.103283
H 6.208332 -0.640094 1.101481
H 6.507171 -0.655530 -0.686324
el energy= -996.336907208
zpe= -996.101117
th energy= -996.085376
th enthalpy= -996.084431
free energy= -996.144841

chloroform-ES-dioxo
B 0.074545 1.573453 -0.000077
O 0.095117 2.938017 -0.000001
H -0.838075 3.248024 -0.000050
N -1.183702 0.859349 -0.000099
C -2.485904 1.448075 0.000202
O -2.650645 2.687143 0.000072
C -3.414956 0.341513 0.000023
C -4.817517 0.308923 -0.000022
H -5.391636 1.233141 0.000020
C -5.455646 -0.931984 -0.000047
C -4.719925 -2.140751 -0.000045
H -5.246993 -3.091829 -0.000082
C -3.321679 -2.119863 -0.000038
H -2.757261 -3.050828 -0.000089
C -2.668852 -0.883012 0.000012
C -1.266143 -0.530985 -0.000034
C -0.120524 -1.332768 -0.000059
H -0.239621 -2.412277 -0.000088
C 1.177530 -0.770728 -0.000003
C 2.325524 -1.627580 0.000087
H 2.218967 -2.708296 0.000120
C 3.552500 -1.026147 0.000131
C 3.710262 0.388938 0.000006
C 2.626760 1.250007 0.000000
H 2.767400 2.327270 -0.000025
C 1.341018 0.685862 -0.000015
O 4.779195 -1.605263 0.000360
O 5.024417 0.693174 0.000014
H -6.543499 -0.973272 -0.000043
C 5.745258 -0.549304 -0.000330
H 6.357082 -0.610144 0.907181
H 6.355935 -0.610244 -0.908631
el energy= -996.330329763

chloroform-GS-4
B -1.569944 1.650687 0.000101
O -1.685949 3.006777 -0.000184
H -0.800234 3.417240 -0.000174
N -0.252802 1.020152 0.000410
C 0.984166 1.679069 0.000346
O 1.117813 2.898220 0.000331
C 2.015207 0.617266 0.000178
C 3.402669 0.735177 -0.000024
H 3.883225 1.709182 -0.000118
C 4.131598 -0.453921 -0.000056
C 3.505047 -1.711783 0.000095
H 4.106817 -2.616149 0.000079
C 2.111879 -1.808099 0.000263
H 1.637475 -2.786179 0.000365
C 1.361390 -0.628937 0.000291
C -0.078831 -0.376251 0.000387
C -1.146339 -1.214596 0.000283
H -0.976081 -2.288481 0.000265
C -2.512803 -0.725214 0.000144
C -3.581681 -1.660879 0.000152
H -3.395399 -2.731569 0.000294
C -4.862792 -1.156299 -0.000003
C -5.123109 0.220389 -0.000211
C -4.105906 1.151155 -0.000229
H -4.318942 2.216853 -0.000371
C -2.771822 0.677564 -0.000019
O -6.039255 -1.847853 0.000079
O -6.474722 0.431662 -0.000253
Br 6.059795 -0.375234 -0.000265
C -7.088864 -0.865541 -0.000410
H -7.695777 -0.983681 -0.906969
H -7.696549 -0.983586 0.905631
el energy= -1008.90880642

zpe= -1008.683320
th energy= -1008.666012
th enthalpy= -1008.665068
free energy= -1008.729739

chloroform-ES-4

B	-1.558808	1.653190	-0.000082
O	-1.677731	3.012008	-0.000032
H	-0.772112	3.393000	-0.000020
N	-0.255098	1.026573	-0.000113
C	1.002724	1.704461	-0.000075
O	1.085348	2.949519	-0.000044
C	2.005617	0.664752	-0.000073
C	3.406481	0.744543	0.000001
H	3.911960	1.705825	0.000071
C	4.112711	-0.454695	-0.000001
C	3.487019	-1.722838	-0.000082
H	4.083418	-2.629216	-0.000080
C	2.089390	-1.792156	-0.000155
H	1.599423	-2.763777	-0.000209
C	1.349356	-0.609519	-0.000142
C	-0.077071	-0.356104	-0.000160
C	-1.160258	-1.232993	-0.000184
H	-0.969368	-2.302162	-0.000213
C	-2.497377	-0.760836	-0.000128
C	-3.579481	-1.695289	-0.000098
H	-3.397359	-2.765837	-0.000141
C	-4.846598	-1.181186	0.000008
C	-5.103731	0.219521	0.000076
C	-4.082918	1.154339	0.000035
H	-4.297658	2.219381	0.000093
C	-2.761677	0.679572	-0.000067
O	-6.027326	-1.845097	0.000069
O	-6.435487	0.429273	0.000184
Br	6.043942	-0.392777	0.000134
C	-7.066359	-0.860903	0.000215
H	-7.671086	-0.965786	-0.907917
H	-7.670880	-0.965840	0.908480

el energy= -1008.90261578

chloroform-GS-5

B	-1.117971	1.644014	-0.000190
O	-1.223688	2.999973	-0.000328
H	-0.336341	3.406384	-0.000320
N	0.193205	1.001330	-0.000126
C	1.436878	1.647035	-0.000045
O	1.585532	2.863423	-0.000057
C	2.454852	0.571800	-0.000021
C	3.839108	0.666058	0.000094
H	4.354354	1.620717	0.000187
C	4.543640	-0.539255	0.000053
C	3.903292	-1.790443	-0.000062
H	4.507446	-2.691260	-0.000093
C	2.513359	-1.865055	-0.000098
H	2.019527	-2.832884	-0.000132
C	1.783430	-0.669721	-0.000086
C	0.351650	-0.396700	-0.000123
C	-0.725106	-1.226377	-0.000116
H	-0.563063	-2.301466	-0.000124
C	-2.084376	-0.725278	-0.000094
C	-3.161900	-1.651762	0.000007
H	-2.985106	-2.723952	0.000019
C	-4.437430	-1.134874	0.000072
C	-4.683521	0.245288	0.000064
C	-3.657326	1.167149	-0.000077
H	-3.860737	2.234612	-0.000133
C	-2.328953	0.680882	-0.000133
O	-5.620487	-1.813295	0.000218
O	-6.030553	0.470494	0.000210
N	6.009293	-0.498356	0.000150
O	6.553202	0.602211	0.001086
O	6.616807	-1.565533	-0.000714
C	-6.659986	-0.820313	0.000186
H	-7.267918	-0.930909	-0.906365
H	-7.267960	-0.930916	0.906696

el energy= -1200.83465143
zpe= -1200.596422
th energy= -1200.578047
th enthalpy= -1200.577103
free energy= -1200.644332

chloroform-ES-5

B	0.245104	-1.971202	0.000000
O	1.051184	-3.059072	0.000000
H	1.989543	-2.784232	0.000000
N	0.796363	-0.621370	0.000000
C	2.172702	-0.279260	0.000000
O	3.066369	-1.115589	0.000000
C	2.226576	1.192488	0.000000
C	3.328725	2.033402	0.000000
H	4.346887	1.660719	0.000000
C	3.076129	3.416393	0.000000
C	1.753732	3.923382	0.000000
H	1.615935	4.998268	0.000000
C	0.660975	3.057202	0.000000
H	-0.350173	3.457779	0.000000
C	0.899386	1.679381	0.000000
C	0.000000	0.519790	0.000000
C	-1.375197	0.438329	0.000000
H	-1.953030	1.357839	0.000000
C	-2.064818	-0.818497	0.000000
C	-3.486684	-0.836796	0.000000
H	-4.063633	0.083052	0.000000
C	-4.093434	-2.068519	0.000000
C	-3.353493	-3.277944	0.000000
C	-1.963887	-3.292247	0.000000
H	-1.413811	-4.228745	0.000000
C	-1.307061	-2.056851	0.000000
O	-5.414866	-2.358864	0.000000
O	-4.198640	-4.323589	0.000000
N	4.178628	4.329525	0.000000
O	5.346609	3.858485	0.000000

O 3.928453 5.563770 0.000000
C -5.532493 -3.786669 0.000000
H -6.051000 -4.114195 0.908284
H -6.051000 -4.114195 -0.908284
el energy= -1200.82988977

chloroform-GS-6
B 0.490380 1.600980 -0.006244
O 0.548990 2.962557 -0.004539
H -0.356822 3.327813 -0.000673
N -0.798621 0.919151 -0.002198
C -2.062158 1.529407 0.004230
O -2.236385 2.745311 0.004908
C -3.054630 0.433334 0.009323
C -4.441705 0.505108 0.013862
H -4.951761 1.466437 0.018346
C -5.172700 -0.699783 0.014016
C -4.465760 -1.929728 0.006080
H -5.037062 -2.856768 0.005978
C -3.074199 -1.984092 0.001283
H -2.571531 -2.948793 -0.006896
C -2.352146 -0.786109 0.003279
C -0.921963 -0.483959 -0.003805
C 0.180231 -1.277103 -0.011221
H 0.054669 -2.357156 -0.012711
C 1.527242 -0.732384 -0.016979
C 2.634761 -1.622647 -0.023766
H 2.493202 -2.700257 -0.029998
C 3.894579 -1.066067 -0.022538
C 4.099718 0.319711 -0.016617
C 3.045593 1.207130 -0.014386
H 3.213647 2.280931 -0.014953
C 1.731246 0.679437 -0.013151
O 5.101307 -1.708343 -0.051131
O 5.445750 0.582648 -0.042515
N -6.559012 -0.691263 0.076461
H -7.010228 0.160480 -0.232943
H -7.024439 -1.522701 -0.265150
C 6.094693 -0.684550 0.121139
H 6.516602 -0.754695 1.134634
H 6.871147 -0.799030 -0.642516
el energy= -1051.69349997
zpe= -1051.441176
th energy= -1051.423949
th enthalpy= -1051.423005
free energy= -1051.486078

chloroform-ES-6
B -0.475418 1.610581 -0.000406
O -0.531930 2.980421 -0.000138
H 0.392836 3.311585 -0.000434
N 0.807197 0.939997 -0.000295
C 2.079761 1.563919 0.000203
O 2.227683 2.809891 0.000757
C 3.045911 0.481035 -0.001383
C 4.436294 0.500667 -0.001382
H 4.985964 1.440034 -0.001347
C 5.133649 -0.731854 -0.001360
C 4.413385 -1.972694 -0.001322
H 4.976610 -2.903211 -0.002028
C 3.031867 -1.986978 -0.001148
H 2.499424 -2.936083 0.000207
C 2.326503 -0.766088 -0.001216
C 0.934550 -0.458826 -0.000508
C -0.193424 -1.287339 -0.000308
H -0.046666 -2.364265 -0.000649
C -1.502871 -0.759317 -0.000041
C -2.631098 -1.648724 0.000336
H -2.492467 -2.726413 0.000446
C -3.875053 -1.086277 0.000608
C -4.073684 0.318090 0.000437
C -3.019055 1.206643 0.000115
H -3.190736 2.279829 0.000002
C -1.706855 0.685285 -0.000130
O -5.087972 -1.708961 0.001324
O -5.406129 0.584751 0.000845
N 6.495043 -0.753998 -0.018973
H 7.025120 0.100575 0.078116
H 6.997558 -1.623940 0.085705
C -6.084363 -0.680247 -0.000126
H -6.694973 -0.762812 -0.907730
H -6.697576 -0.762787 0.905672
el energy= -1051.68527524

chloroform-GS-thieno
B -1.041853 1.442137 -0.000007
O -1.156381 2.794462 0.000008
H -0.264820 3.196573 0.000028
N 0.273748 0.803177 0.000012
C 1.505313 1.473327 0.000037
O 1.620915 2.697068 0.000036
C 2.549764 0.430238 0.000043
C 3.938188 0.556522 0.000060
H 4.406286 1.538247 0.000069
C 4.698221 -0.615117 0.000065
C 4.070639 -1.874043 0.000054
H 4.683288 -2.773329 0.000058
C 2.678420 -1.997096 0.000036
H 2.210082 -2.978486 0.000026
C 1.914520 -0.826296 0.000031
C 0.468079 -0.598892 0.000008
C -0.573349 -1.468392 -0.000013
H -0.380559 -2.537931 -0.000012
C -1.938453 -0.982508 -0.000032
C -3.080901 -1.755604 -0.000039
H -3.162830 -2.836864 -0.000037
S -4.513922 -0.771463 -0.000111
C -3.573389 0.693862 -0.000024
H -4.079120 1.653427 -0.000008
C -2.223244 0.443033 -0.000030
H 5.784337 -0.557594 0.000079
el energy= -740.499324654

zpe= -740.312791
th energy= -740.299767
th enthalpy= -740.298822
free energy= -740.352496

chloroform-ES-thieno

B	-1.026461	1.449408	0.000004
O	-1.129212	2.803373	0.000021
H	-0.219632	3.176977	0.000050
N	0.278066	0.802359	0.000014
C	1.554014	1.492020	0.000030
O	1.614470	2.735468	0.000018
C	2.556879	0.461319	0.000038
C	3.960210	0.526795	0.000052
H	4.469399	1.488245	0.000056
C	4.684865	-0.667800	0.000060
C	4.039634	-1.925588	0.000056
H	4.631300	-2.837440	0.000062
C	2.638109	-2.001539	0.000041
H	2.140335	-2.969631	0.000035
C	1.902157	-0.816461	0.000032
C	0.474610	-0.568685	0.000010
C	-0.608040	-1.472969	-0.000011
H	-0.407285	-2.539929	-0.000013
C	-1.927455	-0.980488	-0.000032
C	-3.111508	-1.756308	-0.000052
H	-3.192313	-2.837670	-0.000057
S	-4.510170	-0.774125	-0.000099
C	-3.559180	0.704461	-0.000036
H	-4.072828	1.659715	-0.000028
C	-2.213506	0.455421	-0.000027
H	5.772778	-0.629629	0.000070

el energy= -740.491208391

chloroform-GS-7

B	2.484883	1.436035	0.000023
O	2.663669	2.780394	0.000008
H	1.795531	3.229612	-0.000014
N	1.139208	0.858328	0.000003
C	-0.057666	1.584537	-0.000024
O	-0.123576	2.810606	-0.000017
C	-1.148646	0.585877	-0.000027
C	-2.527140	0.786350	-0.000040
H	-2.948244	1.787321	-0.000048
C	-3.324926	-0.356921	-0.000044
C	-2.774160	-1.650344	-0.000035
H	-3.428931	-2.516953	-0.000038
C	-1.389825	-1.829385	-0.000020
H	-0.974091	-2.833741	-0.000011
C	-0.570738	-0.696277	-0.000016
C	0.882418	-0.534055	0.000005
C	1.882554	-1.450915	0.000026
H	1.641126	-2.510545	0.000025
C	3.267868	-1.028033	0.000047
C	4.373824	-1.852928	0.000057
H	4.405417	-2.936973	0.000054
S	5.849545	-0.935552	0.000132
C	4.977447	0.571306	0.000044
H	5.526433	1.506679	0.000030
C	3.617296	0.382636	0.000047
Br	-5.245126	-0.164118	-0.000066

el energy= -753.071132541
zpe= -752.895075
th energy= -752.880417
th enthalpy= -752.879473
free energy= -752.938120

chloroform-ES-7

B	-2.479899	1.442083	-0.000055
O	-2.660204	2.787302	-0.000134
H	-1.777067	3.217211	-0.000195
N	-1.142206	0.866094	-0.000055
C	0.093359	1.622178	-0.000057
O	0.092156	2.864443	0.000043
C	1.150871	0.645658	-0.000035
C	2.546953	0.800110	0.000017
H	3.001821	1.786286	0.000051
C	3.317667	-0.361526	0.000009
C	2.764171	-1.661618	-0.000047
H	3.408135	-2.534257	-0.000049
C	1.366739	-1.804709	-0.000089
H	0.929471	-2.801099	-0.000117
C	0.567876	-0.665803	-0.000078
C	-0.873134	-0.493798	-0.000083
C	-1.901323	-1.453987	-0.000114
H	-1.643765	-2.508681	-0.000166
C	-3.247213	-1.033040	-0.000074
C	-4.386528	-1.872180	-0.000189
H	-4.407370	-2.956633	-0.000273
S	-5.836059	-0.967836	0.000369
C	-4.966733	0.560324	-0.000201
H	-5.530771	1.486622	-0.000328
C	-3.609799	0.384039	-0.000033
Br	5.239953	-0.191000	0.000068

el energy= -753.063358795

chloroform-GS-8

B	-2.052750	1.439345	0.000005
O	-2.228693	2.783268	0.000062
H	-1.361472	3.233878	0.000184
N	-0.708208	0.857372	0.000106
C	0.490818	1.578766	0.000244
O	0.563920	2.803355	-0.000111
C	1.576992	0.573777	0.000086
C	2.952673	0.760528	-0.000031
H	3.401800	1.747964	-0.000076
C	3.734673	-0.394978	-0.000041
C	3.180157	-1.686453	0.000048
H	3.843217	-2.544731	0.000013
C	1.798384	-1.853296	0.000136
H	1.369604	-2.851605	0.000152
C	0.991056	-0.708822	0.000157

C -0.457307 -0.536092 0.000139
C -1.461225 -1.451094 0.000112
H -1.222951 -2.511400 0.000125
C -2.842649 -1.023349 0.000022
C -3.950874 -1.846622 -0.000030
H -3.984018 -2.930554 -0.000011
S -5.422080 -0.926147 -0.000130
C -4.547033 0.579837 -0.000102
H -5.094993 1.515725 -0.000141
C -3.187802 0.388553 -0.000042
N 5.196108 -0.256325 -0.000095
O 5.664925 0.877813 -0.000115
O 5.872769 -1.280626 -0.000143
el energy= -944.996614846
zpe= -944.807730
th energy= -944.792051
th enthalpy= -944.791107
free energy= -944.851744

chloroform-ES-8
B -2.062502 1.446985 0.000043
O -2.240742 2.782537 0.000038
H -1.384610 3.252880 0.000081
N -0.712344 0.850200 0.000055
C 0.517813 1.583499 0.000034
O 0.551752 2.801922 -0.000009
C 1.597087 0.583939 0.000049
C 2.972054 0.768300 0.000023
H 3.432054 1.749418 -0.000019
C 3.768655 -0.394671 0.000012
C 3.183468 -1.680163 0.000055
H 3.843541 -2.540134 0.000036
C 1.796357 -1.838710 0.000091
H 1.362206 -2.835430 0.000104
C 0.999337 -0.689989 0.000078
C -0.460665 -0.506562 0.000069
C -1.490103 -1.441606 0.000058
H -1.245450 -2.499447 0.000057
C -2.843336 -1.012596 0.000010
C -3.974151 -1.847997 -0.000047
H -3.992916 -2.932691 -0.000054
S -5.433891 -0.945515 -0.000058
C -4.551925 0.578747 -0.000090
H -5.108189 1.510025 -0.000132
C -3.197003 0.394735 -0.000008
N 5.191952 -0.272908 -0.000067
O 5.687112 0.891587 -0.000117
O 5.887545 -1.330284 -0.000072
el energy= -944.989014465

chloroform-GS-9
B 1.436128 1.435218 0.000368
O 1.576507 2.785935 0.003045
H 0.691660 3.203214 0.001241
N 0.108860 0.823111 -0.003149
C -1.107102 1.518644 -0.003914
O -1.197106 2.745194 -0.001119
C -2.176044 0.499084 -0.007374
C -3.554116 0.673310 -0.005112
H -3.990972 1.669942 -0.005372
C -4.371268 -0.474243 -0.003235
C -3.757303 -1.754091 -0.000405
H -4.396459 -2.635916 0.001649
C -2.374295 -1.910656 -0.002742
H -1.943169 -2.909320 0.001846
C -1.565492 -0.768285 -0.006476
C -0.117150 -0.577084 -0.004571
C 0.910234 -1.464078 -0.003660
H 0.698864 -2.530230 -0.005285
C 2.285533 -1.005040 -0.000751
C 3.413223 -1.798998 0.000410
H 3.475064 -2.881565 -0.000945
S 4.866656 -0.841895 0.004390
C 3.953131 0.640590 0.004498
H 4.476698 1.590450 0.006600
C 2.598831 0.414841 0.001612
N -5.752327 -0.363686 -0.057673
H -6.140434 0.518886 0.250426
H -6.278420 -1.160207 0.278426
el energy= -795.856228734
zpe= -795.653188
th energy= -795.638657
th enthalpy= -795.637713
free energy= -795.694398

chloroform-ES-9
B 1.421711 1.442001 -0.000083
O 1.559871 2.799977 -0.000171
H 0.653526 3.183809 -0.000210
N 0.101204 0.842335 0.000012
C -1.128019 1.560716 0.000180
O -1.181548 2.816016 0.000156
C -2.168443 0.556745 0.000054
C -3.555113 0.674233 0.000048
H -4.040723 1.648120 0.000130
C -4.337859 -0.508431 -0.000023
C -3.716436 -1.803807 -0.000051
H -4.348215 -2.689029 -0.000108
C -2.339528 -1.913798 -0.000021
H -1.873480 -2.896941 -0.000074
C -1.547611 -0.745823 0.000037
C -0.134372 -0.547590 0.000050
C 0.915068 -1.471565 0.000019
H 0.689081 -2.534223 0.000023
C 2.256745 -1.016683 -0.000014
C 3.410034 -1.815934 -0.000056
H 3.471563 -2.898414 -0.000056
S 4.839039 -0.860303 0.000112
C 3.933231 0.631583 -0.000177
H 4.467374 1.575338 -0.000299
C 2.576898 0.415461 -0.000050
N -5.692304 -0.423980 0.000035

H -6.159266 0.472677 -0.000422
H -6.269498 -1.253568 -0.000544
el energy= -795.848044998

methanol-GS-benzo
B -1.125453 1.393584 0.000000
O -1.279173 2.748460 0.000000
H -0.405936 3.184898 -0.000001
N 0.204500 0.796965 -0.000002
C 1.429070 1.478902 -0.000004
O 1.532512 2.705882 0.000000
C 2.483595 0.448961 -0.000001
C 3.870485 0.590537 0.000001
H 4.329615 1.576721 0.000001
C 4.641647 -0.574276 0.000001
C 4.026444 -1.839190 0.000000
H 4.648036 -2.732362 0.000001
C 2.634618 -1.977205 -0.000001
H 2.175247 -2.962775 -0.000002
C 1.861089 -0.813995 -0.000002
C 0.412803 -0.597155 -0.000002
C -0.628901 -1.465029 -0.000001
H -0.429502 -2.534008 -0.000001
C -2.008343 -1.007374 0.000000
C -3.064852 -1.941892 0.000001
H -2.836038 -3.006465 0.000000
C -4.388584 -1.511210 0.000002
C -4.687325 -0.140075 0.000003
C -3.650382 0.793181 0.000002
H -3.885856 1.856710 0.000003
C -2.303926 0.388112 0.000001
H -5.194451 -2.243189 0.000003
H -5.723870 0.191447 0.000004
H 5.727170 -0.506132 0.000003
el energy= -807.808227264
zpe= -807.588211
th energy= -807.574845
th enthalpy= -807.573901
free energy= -807.628087

methanol-ES-benzo
B -1.111832 1.405967 0.000000
O -1.249016 2.765916 0.000000
H -0.356134 3.171511 0.000000
N 0.218220 0.809406 0.000000
C 1.466358 1.500380 -0.000001
O 1.536665 2.750949 0.000000
C 2.485478 0.476443 -0.000001
C 3.882517 0.557298 -0.000001
H 4.384569 1.522808 -0.000001
C 4.618410 -0.632583 -0.000001
C 3.980867 -1.895852 -0.000001
H 4.583472 -2.800932 -0.000001
C 2.588085 -1.990321 -0.000001
H 2.097801 -2.961679 0.000000
C 1.836490 -0.803927 -0.000001
C 0.424052 -0.562905 0.000000
C -0.666923 -1.468530 0.000000
H -0.448731 -2.533310 0.000000
C -1.992954 -1.017645 0.000000
C -3.080480 -1.958943 0.000000
H -2.849845 -3.022797 0.000000
C -4.386138 -1.521871 0.000001
C -4.670931 -0.133202 0.000001
C -3.630858 0.802624 0.000001
H -3.873773 1.864304 0.000001
C -2.287968 0.407819 0.000001
H -5.203273 -2.240164 0.000001
H -5.705472 0.204053 0.000002
H 5.705779 -0.587107 -0.000001
el energy= -807.799717614

methanol-GS-1
B 1.254102 -2.631261 0.000000
O 0.633141 -3.844328 0.000000
H -0.335895 -3.729852 0.000000
N 0.477140 -1.395949 0.000000
C -0.917914 -1.283504 0.000000
O -1.689897 -2.240873 0.000000
C -1.219100 0.162918 0.000000
C -2.454148 0.807637 0.000000
H -3.382487 0.243471 0.000000
C -2.428387 2.201824 0.000000
C -1.225091 2.927454 0.000000
H -1.244305 4.013533 0.000000
C 0.002082 2.260805 0.000000
H 0.928106 2.830052 0.000000
C 0.000000 0.863857 0.000000
C 1.080986 -0.121167 0.000000
C 2.429090 0.022893 0.000000
H 2.855215 1.023246 0.000000
C 3.322144 -1.123438 0.000000
C 4.719319 -0.932225 0.000000
H 5.119816 0.080198 0.000000
C 5.580888 -2.025731 0.000000
C 5.067321 -3.331443 0.000000
C 3.686623 -3.531849 0.000000
H 3.291435 -4.546570 0.000000
C 2.792286 -2.447566 0.000000
H 6.657430 -1.864942 0.000000
H 5.745099 -4.182823 0.000000
Br -4.097356 3.172584 0.000000
el energy= -820.379827968
zpe= -820.170301
th energy= -820.155307
th enthalpy= -820.154362
free energy= -820.213499

methanol-ES-1
B 1.222357 -2.644766 0.000000
O 0.585814 -3.853416 0.000000
H -0.382536 -3.704026 0.000000

N 0.448716 -1.409372 0.000000
C -0.973781 -1.290923 0.000000
O -1.728533 -2.287098 0.000000
C -1.249796 0.127169 0.000000
C -2.462980 0.823493 0.000000
H -3.411895 0.294279 0.000000
C -2.397354 2.217662 0.000000
C -1.177480 2.934958 0.000000
H -1.178431 4.020137 0.000000
C 0.028873 2.233153 0.000000
H 0.970784 2.777226 0.000000
C 0.000000 0.832536 0.000000
C 1.041341 -0.154254 0.000000
C 2.448895 -0.005215 0.000000
H 2.858090 1.001555 0.000000
C 3.301283 -1.118314 0.000000
C 4.728015 -0.939632 0.000000
H 5.127826 0.072606 0.000000
C 5.570353 -2.029111 0.000000
C 5.035513 -3.341165 0.000000
C 3.650619 -3.541104 0.000000
H 3.261629 -4.558031 0.000000
C 2.754926 -2.466072 0.000000
H 6.648696 -1.886156 0.000000
H 5.708161 -4.196453 0.000000
Br -4.042970 3.219809 0.000000
el energy= -820.371684657

methanol-GS-2
B -2.500271 0.468600 0.000000
O -3.580107 -0.360942 0.000000
H -3.292611 -1.293699 0.000000
N -1.145004 -0.074063 0.000000
C -0.785810 -1.424826 0.000000
O -1.586670 -2.356757 0.000000
C 0.692077 -1.459369 0.000000
C 1.549006 -2.549830 0.000000
H 1.182765 -3.570933 0.000000
C 2.915328 -2.261434 0.000000
C 3.415179 -0.946980 0.000000
H 4.487735 -0.785998 0.000000
C 2.537901 0.133297 0.000000
H 2.921615 1.149694 0.000000
C 1.163152 -0.130042 0.000000
C 0.000000 0.749200 0.000000
C -0.099556 2.102886 0.000000
H 0.808664 2.700568 0.000000
C -1.385964 2.774898 0.000000
C -1.445756 4.184005 0.000000
H -0.520599 4.757890 0.000000
C -2.675236 4.836394 0.000000
C -3.867466 4.096836 0.000000
C -3.819670 2.702128 0.000000
H -4.748651 2.134057 0.000000
C -2.593929 2.015529 0.000000
H -2.710121 5.924267 0.000000
H -4.826295 4.611419 0.000000
N 3.864717 -3.371430 0.000000
O 3.420893 -4.518170 0.000000
O 5.066548 -3.112626 0.000000
el energy= -1012.30496901
zpe= -1012.082734
th energy= -1012.066695
th enthalpy= -1012.065751
free energy= -1012.127280

methanol-ES-2
B -2.498697 0.559673 0.000000
O -3.603693 -0.218243 0.000000
H -3.376311 -1.166985 0.000000
N -1.151467 -0.034863 0.000000
C -0.833149 -1.422842 0.000000
O -1.681695 -2.300406 0.000000
C 0.637949 -1.505205 0.000000
C 1.457667 -2.618725 0.000000
H 1.063203 -3.628627 0.000000
C 2.849531 -2.383669 0.000000
C 3.372765 -1.068445 0.000000
H 4.448456 -0.935516 0.000000
C 2.523823 0.037314 0.000000
H 2.936459 1.042969 0.000000
C 1.141874 -0.186278 0.000000
C 0.000000 0.721314 0.000000
C -0.050944 2.117961 0.000000
H 0.886681 2.666960 0.000000
C -1.279121 2.823291 0.000000
C -1.277829 4.251598 0.000000
H -0.325838 4.778023 0.000000
C -2.473039 4.951313 0.000000
C -3.694219 4.255037 0.000000
C -3.712896 2.847716 0.000000
H -4.669932 2.330123 0.000000
C -2.530934 2.111689 0.000000
H -2.468349 6.038758 0.000000
H -4.631635 4.806586 0.000000
N 3.740274 -3.489183 0.000000
O 3.259298 -4.664383 0.000000
O 4.991119 -3.273811 0.000000
el energy= -1012.29733864

methanol-GS-3
B -1.518994 1.384753 0.000812
O -1.696416 2.737879 0.001388
H -0.829434 3.187388 0.000727
N -0.178701 0.813310 -0.000128
C 1.031318 1.518664 -0.000732
O 1.109842 2.748150 0.000578
C 2.108925 0.510528 -0.003685
C 3.485488 0.697325 -0.003668
H 3.916954 1.696442 -0.002714
C 4.312076 -0.444923 -0.005481
C 3.707346 -1.729622 0.000013

H 4.353891 -2.605846 0.003071
C 2.325166 -1.898075 0.000698
H 1.901623 -2.899977 0.007279
C 1.508615 -0.762085 -0.002406
C 0.059399 -0.578986 -0.000684
C -0.970230 -1.462782 -0.000284
H -0.754222 -2.528650 -0.001036
C -2.357812 -1.029620 0.000520
C -3.398879 -1.981775 0.000471
H -3.151961 -3.042440 0.000033
C -4.730266 -1.574712 0.000824
C -5.054349 -0.209391 0.001259
C -4.033317 0.741263 0.001373
H -4.286661 1.800719 0.001638
C -2.680078 0.360192 0.001037
H -5.522726 -2.321340 0.000688
H -6.096563 0.103919 0.001446
N 5.690691 -0.324120 -0.068508
H 6.071884 0.558497 0.250592
H 6.220444 -1.121038 0.263411
el energy= -863.167665608
zpe= -862.931157
th energy= -862.916313
th enthalpy= -862.915369
free energy= -862.972515

methanol-ES-3
B -1.506880 1.391495 -0.000212
O -1.675611 2.757623 -0.000433
H -0.786227 3.171748 -0.000633
N -0.164661 0.837158 -0.000023
C 1.045411 1.557425 0.000324
O 1.101923 2.818828 0.000491
C 2.100442 0.563038 0.000096
C 3.480537 0.701131 0.000040
H 3.957115 1.679503 0.000120
C 4.276230 -0.475889 -0.000076
C 3.660596 -1.778076 -0.000132
H 4.303755 -2.655024 -0.000213
C 2.290805 -1.907078 -0.000076
H 1.834348 -2.894232 -0.000141
C 1.486401 -0.741395 0.000039
C 0.078808 -0.550715 0.000060
C -0.976199 -1.470736 0.000043
H -0.739612 -2.532155 0.000089
C -2.324590 -1.048074 0.000029
C -3.386181 -2.006249 0.000116
H -3.135633 -3.066323 0.000200
C -4.704778 -1.600337 0.000114
C -5.026707 -0.219505 0.000002
C -4.011154 0.731421 -0.000098
H -4.272485 1.789345 -0.000192
C -2.650404 0.365245 -0.000077
H -5.502678 -2.340909 0.000194
H -6.069683 0.091888 -0.000008
N 5.623239 -0.385149 -0.000052
H 6.085301 0.515623 -0.000255
H 6.204343 -1.213856 -0.000468
el energy= -863.158712114

methanol-GS-dioxo
B 0.087446 1.572811 -0.001381
O 0.117232 2.938037 -0.001144
H -0.793737 3.289583 -0.002164
N -1.184287 0.861375 -0.001808
C -2.464270 1.430944 -0.001149
O -2.675824 2.644563 -0.002605
C -3.422314 0.310924 0.001816
C -4.816361 0.325921 0.005043
H -5.363718 1.265951 0.004225
C -5.479753 -0.903416 0.009651
C -4.752807 -2.107528 0.010965
H -5.291743 -3.052884 0.015308
C -3.354250 -2.119500 0.007057
H -2.807763 -3.059766 0.008415
C -2.688109 -0.891535 0.002283
C -1.266278 -0.544752 -0.001707
C -0.147233 -1.311678 -0.006464
H -0.247806 -2.394266 -0.007789
C 1.184873 -0.733107 -0.010632
C 2.312384 -1.597242 -0.021226
H 2.195880 -2.677724 -0.031658
C 3.557212 -1.008718 -0.020712
C 3.726946 0.381216 -0.007746
C 2.652272 1.243698 -0.002267
H 2.799429 2.320656 0.000458
C 1.351358 0.683632 -0.003771
O 4.781135 -1.620626 -0.056707
O 5.066024 0.680134 -0.029924
H -6.567034 -0.933104 0.012522
C 5.756956 -0.573770 0.096417
H 6.210056 -0.643645 1.094287
H 6.506904 -0.655886 -0.696343
el energy= -996.335494444
zpe= -996.100067
th energy= -996.084309
th enthalpy= -996.083365
free energy= -996.143541

methanol-ES-dioxo
B 0.073797 1.574977 -0.000080
O 0.095037 2.944101 0.000069
H -0.834395 3.261182 0.000104
N -1.189593 0.865999 -0.000197
C -2.487994 1.443515 -0.000136
O -2.666349 2.689204 -0.000175
C -3.414602 0.338662 -0.000021
C -4.817051 0.303469 0.000156
H -5.395618 1.225291 0.000182
C -5.451284 -0.939441 0.000300
C -4.710305 -2.146515 0.000271
H -5.236385 -3.098316 0.000391

C -3.314306 -2.125054 0.000091
H -2.746730 -3.053865 0.000067
C -2.662563 -0.883670 -0.000052
C -1.268523 -0.527742 -0.000205
C -0.116253 -1.327013 -0.000294
H -0.235949 -2.406752 -0.000355
C 1.176520 -0.766467 -0.000238
C 2.325452 -1.626781 -0.000286
H 2.214716 -2.707190 -0.000440
C 3.551460 -1.027906 -0.000097
C 3.709251 0.386621 0.000103
C 2.626214 1.250923 0.000118
H 2.776576 2.327095 0.000297
C 1.339871 0.690393 -0.000083
O 4.780532 -1.606259 -0.000154
O 5.020405 0.692535 0.000260
H -6.538897 -0.984760 0.000440
C 5.748464 -0.549940 0.000360
H 6.355512 -0.607402 0.910014
H 6.356226 -0.607125 -0.908831
el energy= -996.328038878

methanol-GS-4
B -1.568390 1.650744 0.000140
O -1.689527 3.009655 0.000229
H -0.807380 3.427214 0.000366
N -0.250889 1.023493 0.000169
C 0.986348 1.675832 -0.000053
O 1.126088 2.898124 -0.000253
C 2.014831 0.615983 0.000009
C 3.402470 0.734677 -0.000064
H 3.881392 1.709694 -0.000182
C 4.129299 -0.455074 0.000008
C 3.502894 -1.713340 0.000159
H 4.102473 -2.619320 0.000220
C 2.109558 -1.809641 0.000227
H 1.633990 -2.787089 0.000341
C 1.360582 -0.629632 0.000140
C -0.078493 -0.375132 0.000155
C -1.145503 -1.212985 0.000114
H -0.974400 -2.286733 0.000095
C -2.511705 -0.722871 0.000048
C -3.578920 -1.659945 -0.000012
H -3.390728 -2.730298 -0.000013
C -4.860007 -1.155453 -0.000053
C -5.121371 0.220042 -0.000024
C -4.106035 1.152570 0.000010
H -4.324760 2.217446 0.000020
C -2.771002 0.679850 0.000047
O -6.037898 -1.849122 -0.000012
O -6.475995 0.430630 0.000063
Br 6.058386 -0.375591 -0.000105
C -7.092232 -0.868871 -0.000371
H -7.695372 -0.986756 -0.908139
H -7.696192 -0.987000 0.906806
el energy= -1008.90739637

zpe= -1008.682173
th energy= -1008.664897
th enthalpy= -1008.663952
free energy= -1008.728396

methanol-ES-4
B -1.558761 1.656691 -0.000079
O -1.679413 3.019534 -0.000009
H -0.778090 3.407669 0.000005
N -0.249358 1.036738 -0.000121
C 1.005035 1.704771 -0.000106
O 1.100115 2.957070 -0.000071
C 2.005605 0.666412 -0.000085
C 3.406186 0.744272 -0.000008
H 3.912978 1.705253 0.000054
C 4.109328 -0.456427 0.000005
C 3.479246 -1.723986 -0.000068
H 4.072823 -2.632601 -0.000052
C 2.084288 -1.793021 -0.000147
H 1.592061 -2.763311 -0.000192
C 1.344140 -0.606250 -0.000150
C -0.073788 -0.348894 -0.000177
C -1.163313 -1.225228 -0.000206
H -0.969406 -2.294143 -0.000237
C -2.494825 -0.755950 -0.000150
C -3.576734 -1.695417 -0.000128
H -3.389303 -2.765139 -0.000182
C -4.843048 -1.185223 -0.000005
C -5.101816 0.214666 0.000088
C -4.082595 1.154203 0.000049
H -4.308207 2.217262 0.000128
C -2.760553 0.684705 -0.000070
O -6.025329 -1.850165 0.000063
O -6.431032 0.424578 0.000218
Br 6.040226 -0.398651 0.000144
C -7.067140 -0.867481 0.000233
H -7.668251 -0.968895 -0.909445
H -7.668031 -0.968979 0.910050
el energy= -1008.90040352

methanol-GS-5
B -1.116455 1.646982 0.000194
O -1.228384 3.005453 0.000163
H -0.345087 3.419900 0.000165
N 0.195909 1.008522 0.000322
C 1.439480 1.647560 0.000142
O 1.595070 2.866677 0.000140
C 2.455015 0.573452 0.000091
C 3.838421 0.666978 -0.000081
H 4.351595 1.622941 -0.000237
C 4.540033 -0.541103 -0.000045
C 3.897085 -1.792713 0.000170
H 4.495640 -2.697266 0.000208
C 2.508103 -1.865053 0.000288
H 2.010889 -2.831000 0.000406
C 1.781804 -0.667345 0.000232

C 0.352887 -0.391750 0.000311
C -0.722896 -1.221966 0.000219
H -0.558863 -2.296751 0.000184
C -2.081613 -0.721425 0.000126
C -3.156189 -1.650771 -0.000011
H -2.975717 -2.722336 -0.000063
C -4.432138 -1.135563 -0.000136
C -4.680757 0.243150 -0.000091
C -3.657384 1.168225 0.000036
H -3.868171 2.234538 0.000014
C -2.327610 0.684652 0.000124
O -5.615898 -1.817355 -0.000374
O -6.030729 0.466130 -0.000251
N 5.998070 -0.503492 -0.000279
O 6.553508 0.594056 -0.001150
O 6.611998 -1.569344 0.000383
C -6.660966 -0.827613 -0.000204
H -7.265138 -0.938651 -0.907908
H -7.264900 -0.938727 0.907643
el energy= -1200.83290254
zpe= -1200.595001
th energy= -1200.576716
th enthalpy= -1200.575772
free energy= -1200.642076

methanol-ES-5
B 0.277648 -1.975085 0.000000
O 1.094895 -3.055529 0.000000
H 2.032050 -2.781033 0.000000
N 0.815071 -0.617205 0.000000
C 2.178818 -0.250944 0.000000
O 3.096410 -1.063267 0.000000
C 2.208453 1.222606 0.000000
C 3.296882 2.078350 0.000000
H 4.317609 1.712706 0.000000
C 3.021548 3.459842 0.000000
C 1.689235 3.942479 0.000000
H 1.522125 5.013465 0.000000
C 0.611771 3.059199 0.000000
H -0.405883 3.441863 0.000000
C 0.874302 1.684290 0.000000
C 0.000000 0.512194 0.000000
C -1.375321 0.410863 0.000000
H -1.962906 1.324548 0.000000
C -2.047655 -0.850049 0.000000
C -3.471081 -0.881326 0.000000
H -4.054969 0.034150 0.000000
C -4.064877 -2.117440 0.000000
C -3.310220 -3.316984 0.000000
C -1.917959 -3.318009 0.000000
H -1.364486 -4.252579 0.000000
C -1.274674 -2.078388 0.000000
O -5.383278 -2.426029 0.000000
O -4.137410 -4.371842 0.000000
N 4.101264 4.383418 0.000000
O 5.290184 3.939904 0.000000
O 3.849549 5.626690 0.000000
C -5.483340 -3.856456 0.000000
H -5.992101 -4.190977 0.909986
H -5.992101 -4.190977 -0.909986
el energy= -1200.82679563

methanol-GS-6
B -0.489200 1.600758 -0.002423
O -0.552835 2.965661 0.001801
H 0.349440 3.339160 0.003012
N 0.800020 0.922047 -0.003225
C 2.063747 1.525595 -0.000499
O 2.243014 2.744768 0.003157
C 3.054511 0.432669 -0.002813
C 4.441956 0.505779 0.002428
H 4.953876 1.466315 0.006444
C 5.172264 -0.699951 0.003095
C 4.464114 -1.930216 0.003079
H 5.036354 -2.856696 0.006735
C 3.072539 -1.985203 -0.001769
H 2.568600 -2.949280 0.001437
C 2.351314 -0.786483 -0.005306
C 0.922369 -0.483471 -0.006442
C -0.179643 -1.276025 -0.010359
H -0.054226 -2.356088 -0.013370
C -1.526345 -0.730458 -0.012684
C -2.632397 -1.622180 -0.019405
H -2.488860 -2.699529 -0.026673
C -3.892166 -1.065732 -0.018827
C -4.098260 0.318992 -0.013529
C -3.046045 1.208241 -0.009597
H -3.220482 2.281270 -0.010519
C -1.730685 0.681532 -0.007923
O -5.100776 -1.709755 -0.051586
O -5.447073 0.581845 -0.044172
N 6.557437 -0.692580 -0.052120
H 7.005504 0.155655 0.273532
H 7.016171 -1.529031 0.288687
C -6.099184 -0.687137 0.119186
H -6.871280 -0.801235 -0.647500
H -6.518478 -0.756461 1.132327
el energy= -1051.69463194
zpe= -1051.442809
th energy= -1051.425529
th enthalpy= -1051.424585
free energy= -1051.487987

methanol-ES-6
B -0.474957 1.610744 0.000014
O -0.532712 2.986897 0.000017
H 0.389168 3.323704 0.000019
N 0.811840 0.946865 -0.000071
C 2.081834 1.561380 -0.000083
O 2.238338 2.815553 -0.000036
C 3.047258 0.481981 -0.000039
C 4.437280 0.500980 0.000043

H 4.994697 1.435906 0.000072
C 5.131033 -0.735943 0.000050
C 4.405840 -1.977519 0.000008
H 4.970700 -2.907084 0.000024
C 3.027776 -1.990348 -0.000042
H 2.491084 -2.936850 -0.000067
C 2.324044 -0.764261 -0.000069
C 0.937666 -0.455747 -0.000060
C -0.193240 -1.281715 -0.000023
H -0.046339 -2.358809 -0.000054
C -1.500521 -0.753512 0.000029
C -2.627584 -1.646047 0.000029
H -2.485107 -2.723368 0.000004
C -3.871993 -1.086201 0.000042
C -4.073247 0.316047 0.000054
C -3.021206 1.207479 0.000065
H -3.202756 2.279421 0.000062
C -1.705849 0.689715 0.000045
O -5.085777 -1.712846 0.000048
O -5.407817 0.581382 0.000065
N 6.485143 -0.764555 0.000051
H 7.026554 0.089649 0.000091
H 6.987771 -1.642041 0.000116
C -6.088103 -0.686291 -0.000123
H -6.695835 -0.769105 -0.908265
H -6.696211 -0.769172 0.907755
el energy= -1051.68545069

methanol-GS-thieno
B -1.041450 1.440666 -0.000007
O -1.164707 2.795206 0.000009
H -0.279056 3.208712 0.000028
N 0.274862 0.806128 0.000011
C 1.506294 1.470283 0.000035
O 1.627242 2.697728 0.000035
C 2.548663 0.429867 0.000042
C 3.937536 0.557265 0.000060
H 4.406479 1.538866 0.000070
C 4.696685 -0.614688 0.000066
C 4.068411 -1.873953 0.000054
H 4.681054 -2.773319 0.000059
C 2.676035 -1.997962 0.000035
H 2.206766 -2.978895 0.000024
C 1.913188 -0.826623 0.000029
C 0.468259 -0.598251 0.000007
C -0.572183 -1.468312 -0.000013
H -0.378269 -2.537703 -0.000012
C -1.937003 -0.982322 -0.000031
C -3.078399 -1.756362 -0.000039
H -3.159399 -2.837934 -0.000037
S -4.511871 -0.772518 -0.000109
C -3.572901 0.694159 -0.000024
H -4.081096 1.652853 -0.000010
C -2.222335 0.442860 -0.000029
H 5.782890 -0.557735 0.000081
el energy= -740.498301649

zpe= -740.312063
th energy= -740.299003
th enthalpy= -740.298059
free energy= -740.351811

methanol-ES-thieno
B -1.025594 1.448020 -0.000009
O -1.134601 2.805442 -0.000201
H -0.229731 3.187946 -0.000301
N 0.282551 0.808052 -0.000012
C 1.552020 1.488759 -0.000030
O 1.624146 2.740335 0.000094
C 2.554456 0.460471 -0.000037
C 3.957278 0.525447 -0.000014
H 4.469184 1.485835 0.000018
C 4.680686 -0.669852 -0.000066
C 4.032200 -1.927823 -0.000131
H 4.624376 -2.839619 -0.000170
C 2.634304 -2.005547 -0.000134
H 2.134767 -2.972517 -0.000169
C 1.896117 -0.816727 -0.000083
C 0.477286 -0.567912 -0.000052
C -0.609169 -1.472449 -0.000098
H -0.407674 -2.539486 -0.000197
C -1.924816 -0.980020 -0.000053
C -3.108692 -1.757139 -0.000313
H -3.188025 -2.838977 -0.000462
S -4.506300 -0.775058 0.000733
C -3.557247 0.705075 -0.000431
H -4.074279 1.658933 -0.000741
C -2.211542 0.456036 -0.000002
H 5.768638 -0.633776 -0.000065
el energy= -740.489847347

methanol-GS-7
B 2.483969 1.435237 0.000013
O 2.669438 2.781788 0.000024
H 1.805720 3.238891 0.000022
N 1.137780 0.861974 0.000011
C -0.058696 1.582540 0.000009
O -0.128628 2.812442 -0.000025
C -1.147766 0.586147 -0.000009
C -2.526706 0.787034 -0.000032
H -2.947223 1.788371 -0.000043
C -3.322252 -0.357018 -0.000033
C -2.771886 -1.650859 -0.000014
H -3.424693 -2.519023 -0.000016
C -1.387418 -1.829799 0.000005
H -0.970535 -2.833662 0.000016
C -0.569806 -0.695898 0.000007
C 0.881757 -0.532816 0.000018
C 1.880624 -1.450265 0.000034
H 1.636751 -2.509325 0.000046
C 3.265882 -1.027779 0.000046
C 4.370036 -1.854448 0.000093
H 4.399924 -2.938738 0.000121

S 5.846640 -0.937590 0.000003
C 4.976568 0.571161 0.000100
H 5.528535 1.505098 0.000134
C 3.616289 0.382761 0.000036
Br -5.243579 -0.164531 -0.000057
el energy= -753.070128441
zpe= -752.894223
th energy= -752.879563
th enthalpy= -752.878619
free energy= -752.937243

methanol-ES-7
B -2.477862 1.440645 0.000014
O -2.662192 2.789130 -0.000139
H -1.783304 3.226024 -0.000207
N -1.136950 0.870928 0.000016
C 0.092668 1.618915 0.000006
O 0.102420 2.869226 0.000104
C 1.148940 0.644560 -0.000008
C 2.543771 0.800455 -0.000001
H 2.996411 1.788139 0.000020
C 3.313994 -0.360814 -0.000047
C 2.758368 -1.662031 -0.000093
H 3.401704 -2.535606 -0.000131
C 1.365314 -1.808096 -0.000087
H 0.928117 -2.804341 -0.000114
C 0.562772 -0.666638 -0.000042
C -0.869568 -0.493362 -0.000015
C -1.901926 -1.454340 -0.000056
H -1.642743 -2.508774 -0.000142
C -3.243866 -1.033172 -0.000028
C -4.383521 -1.873265 -0.000277
H -4.403375 -2.958124 -0.000411
S -5.831954 -0.968119 0.000659
C -4.963631 0.560839 -0.000405
H -5.529896 1.486125 -0.000701
C -3.606809 0.384280 0.000009
Br 5.236327 -0.191831 -0.000072
el energy= -753.062105394

methanol-GS-8
B -2.051687 1.439615 0.005087
O -2.234802 2.785411 0.008167
H -1.372135 3.243968 0.009511
N -0.706111 0.862392 0.004718
C 0.492190 1.578281 0.004762
O 0.570709 2.806271 0.006167
C 1.576330 0.574675 0.002920
C 2.951012 0.761947 -0.000299
H 3.396420 1.751061 -0.002094
C 3.731979 -0.395112 0.000355
C 3.175798 -1.687766 0.004173
H 3.834256 -2.549601 0.004792
C 1.794974 -1.853820 0.004701
H 1.364472 -2.851256 0.005583
C 0.989553 -0.707926 0.003815
C -0.455841 -0.533494 0.003427
C -1.458442 -1.449719 0.000625
H -1.216827 -2.509260 -0.000829
C -2.839265 -1.022757 -0.001335
C -3.945531 -1.848302 -0.005955
H -3.976023 -2.932551 -0.008738
S -5.417957 -0.929543 -0.007433
C -4.545537 0.578834 -0.001577
H -5.096850 1.513104 -0.000835
C -3.186006 0.388781 0.001182
N 5.186028 -0.258471 -0.005048
O 5.665094 0.873468 -0.040085
O 5.869714 -1.280154 0.024207
el energy= -944.995296098
zpe= -944.806748
th energy= -944.791040
th enthalpy= -944.790096
free energy= -944.850930

methanol-ES-8
B -2.063561 1.452267 0.000127
O -2.248741 2.788238 0.000124
H -1.397638 3.266181 0.000182
N -0.710288 0.861112 0.000167
C 0.515274 1.588057 0.000052
O 0.564691 2.808083 -0.000055
C 1.593201 0.585317 0.000083
C 2.966503 0.768042 -0.000067
H 3.417371 1.753495 -0.000185
C 3.761514 -0.397255 -0.000131
C 3.173686 -1.683364 0.000017
H 3.822820 -2.551697 -0.000036
C 1.787285 -1.838591 0.000171
H 1.349607 -2.833427 0.000243
C 0.992987 -0.687467 0.000182
C -0.459620 -0.498659 0.000198
C -1.486965 -1.437383 0.000188
H -1.237872 -2.494317 0.000205
C -2.837427 -1.010672 0.000075
C -3.964080 -1.852151 -0.000051
H -3.976094 -2.937277 -0.000055
S -5.424686 -0.954839 -0.000198
C -4.549251 0.575271 -0.000154
H -5.111527 1.503090 -0.000248
C -3.194848 0.396181 0.000026
N 5.177214 -0.278422 -0.000368
O 5.693838 0.884824 -0.000105
O 5.888721 -1.332737 0.000076
el energy= -944.987241885

methanol-GS-9
B 1.435968 1.433847 0.000707
O 1.584842 2.786767 0.001623
H 0.705355 3.214255 0.000885
N 0.107843 0.826778 -0.000365
C -1.108205 1.516517 -0.000851

O -1.202389 2.747035 0.000425
C -2.175589 0.499635 -0.003998
C -3.554293 0.674660 -0.003826
H -3.993730 1.670299 -0.002812
C -4.370871 -0.473710 -0.005347
C -3.755250 -1.753983 0.000217
H -4.394614 -2.635511 0.003482
C -2.372408 -1.910902 0.000723
H -1.940496 -2.909239 0.007404
C -1.564420 -0.767714 -0.002662
C -0.117716 -0.575946 -0.001016
C 0.908759 -1.463474 -0.000800
H 0.695780 -2.529347 -0.001738
C 2.284075 -1.004992 0.000215
C 3.410469 -1.800300 0.000257
H 3.471209 -2.883177 -0.000392
S 4.864624 -0.843873 0.001193
C 3.953132 0.640208 0.001871
H 4.479566 1.588909 0.002559
C 2.598341 0.414558 0.001081
N -5.750753 -0.365298 -0.068231
H -6.139175 0.514406 0.250214
H -6.273110 -1.165978 0.266374
el energy= -795.857696429
zpe= -795.654927
th energy= -795.640381
th enthalpy= -795.639437
free energy= -795.696190

methanol-ES-9
B 1.420965 1.437814 0.000077
O 1.564328 2.800742 0.000167
H 0.662034 3.192431 0.000116
N 0.098742 0.845245 -0.000237
C -1.128565 1.555583 -0.000582
O -1.188011 2.820136 -0.000264
C -2.167962 0.556354 -0.000186
C -3.554466 0.677123 0.000209
H -4.042651 1.649913 0.000343
C -4.337386 -0.506738 0.000285
C -3.712930 -1.804044 0.000041
H -4.346980 -2.687438 0.000160
C -2.339162 -1.916209 -0.000286
H -1.872582 -2.898988 -0.000393
C -1.545713 -0.746072 -0.000383
C -0.136279 -0.548919 -0.000418
C 0.914418 -1.471748 -0.000327
H 0.687415 -2.534332 -0.000383
C 2.255592 -1.016752 -0.000105
C 3.408027 -1.816036 0.000047
H 3.469429 -2.898827 -0.000015
S 4.837828 -0.859846 0.000210
C 3.933309 0.631855 0.000374
H 4.469571 1.574879 0.000603
C 2.576163 0.414834 0.000097
N -5.687199 -0.425811 0.000885
H -6.156131 0.471214 -0.000119
H -6.261806 -1.258835 -0.000408
el energy= -795.849003833

dmso-GS-benzo
B -1.125490 1.395564 0.000000
O -1.264062 2.750415 0.000002
H -0.376837 3.159767 0.000004
N 0.203096 0.794771 0.000003
C 1.426857 1.483021 0.000007
O 1.520552 2.707876 -0.000002
C 2.484434 0.451466 0.000001
C 3.871950 0.588006 -0.000004
H 4.337823 1.570616 -0.000005
C 4.641264 -0.578275 -0.000005
C 4.025035 -1.842182 -0.000003
H 4.645177 -2.736194 -0.000004
C 2.633085 -1.976537 0.000001
H 2.170741 -2.960699 0.000002
C 1.861734 -0.811918 0.000003
C 0.412597 -0.597151 0.000003
C -0.629452 -1.465097 0.000003
H -0.431055 -2.534211 0.000003
C -2.008606 -1.006056 0.000001
C -3.064901 -1.941187 0.000000
H -2.834913 -3.005461 0.000001
C -4.388867 -1.511723 -0.000001
C -4.688160 -0.140701 -0.000003
C -3.651676 0.793007 -0.000002
H -3.887041 1.856039 -0.000003
C -2.304920 0.389858 0.000000
H -5.194297 -2.243976 -0.000002
H -5.724724 0.190426 -0.000004
H 5.726742 -0.511043 -0.000008
el energy= -807.806664916
zpe= -807.586430
th energy= -807.573079
th enthalpy= -807.572135
free energy= -807.626367

dmso-ES-benzo
B -1.112094 1.408143 0.000000
O -1.231733 2.766539 0.000000
H -0.324775 3.144491 0.000000
N 0.216710 0.804609 0.000000
C 1.464749 1.504685 -0.000001
O 1.524719 2.749449 0.000000
C 2.486393 0.478281 -0.000001
C 3.883302 0.556249 -0.000001
H 4.388719 1.519910 -0.000001
C 4.619815 -0.633783 -0.000001
C 3.981957 -1.896825 -0.000001
H 4.583903 -2.802254 -0.000001
C 2.589000 -1.989746 -0.000001
H 2.097519 -2.960550 -0.000001
C 1.837452 -0.803148 0.000000

C 0.424232 -0.564705 0.000000
C -0.668787 -1.470199 0.000000
H -0.452312 -2.535290 0.000000
C -1.993997 -1.016733 0.000000
C -3.082997 -1.957317 0.000001
H -2.852579 -3.021206 0.000000
C -4.388510 -1.520185 0.000001
C -4.673598 -0.131485 0.000001
C -3.632573 0.803444 0.000001
H -3.874650 1.864944 0.000001
C -2.289721 0.409684 0.000001
H -5.205616 -2.238448 0.000001
H -5.707937 0.206011 0.000001
H 5.707049 -0.587789 -0.000001
el energy= -807.798139907

dmso-GS-1
B 1.251103 -2.632108 0.000000
O 0.614259 -3.834937 0.000000
H -0.351158 -3.686991 0.000000
N 0.480523 -1.392622 0.000000
C -0.916785 -1.285693 0.000000
O -1.680203 -2.246494 0.000000
C -1.219355 0.162830 0.000000
C -2.453311 0.809427 0.000000
H -3.383950 0.249401 0.000000
C -2.426295 2.203893 0.000000
C -1.223258 2.929203 0.000000
H -1.242164 4.015137 0.000000
C 0.003154 2.261202 0.000000
H 0.930072 2.828909 0.000000
C 0.000000 0.864345 0.000000
C 1.082979 -0.119712 0.000000
C 2.431706 0.022125 0.000000
H 2.860869 1.021092 0.000000
C 3.321470 -1.127289 0.000000
C 4.719271 -0.938629 0.000000
H 5.120940 0.073263 0.000000
C 5.579384 -2.033158 0.000000
C 5.064076 -3.338278 0.000000
C 3.683130 -3.536505 0.000000
H 3.285677 -4.550054 0.000000
C 2.789946 -2.451388 0.000000
H 6.656055 -1.873828 0.000000
H 5.740601 -4.190552 0.000000
Br -4.095007 3.175421 0.000000
el energy= -820.378052926
zpe= -820.168223
th energy= -820.153289
th enthalpy= -820.152345
free energy= -820.211352

dmso-ES-1
B 1.218801 -2.647826 0.000000
O 0.566147 -3.844383 0.000000
H -0.398259 -3.661187 0.000000
N 0.451913 -1.406241 0.000000
C -0.975214 -1.294339 0.000000
O -1.718631 -2.291632 0.000000
C -1.251032 0.127332 0.000000
C -2.461890 0.827146 0.000000
H -3.413787 0.303687 0.000000
C -2.394873 2.221646 0.000000
C -1.174468 2.937766 0.000000
H -1.174050 4.022816 0.000000
C 0.030475 2.233185 0.000000
H 0.973703 2.775026 0.000000
C 0.000000 0.832616 0.000000
C 1.042823 -0.153375 0.000000
C 2.451990 -0.007730 0.000000
H 2.864929 0.997424 0.000000
C 3.300545 -1.123926 0.000000
C 4.728208 -0.948471 0.000000
H 5.129462 0.063171 0.000000
C 5.569009 -2.039069 0.000000
C 5.032750 -3.350587 0.000000
C 3.647281 -3.547651 0.000000
H 3.256438 -4.563622 0.000000
C 2.752674 -2.472064 0.000000
H 6.647477 -1.897286 0.000000
H 5.703971 -4.206882 0.000000
Br -4.040488 3.225226 0.000000
el energy= -820.369871169

dmso-GS-2
B -2.500463 0.471865 0.000000
O -3.573997 -0.363763 0.000000
H -3.264119 -1.289374 0.000000
N -1.145021 -0.069531 0.000000
C -0.790932 -1.424842 0.000000
O -1.595768 -2.350196 0.000000
C 0.689163 -1.461564 0.000000
C 1.547625 -2.552059 0.000000
H 1.184712 -3.574088 0.000000
C 2.913656 -2.264871 0.000000
C 3.413269 -0.951632 0.000000
H 4.485820 -0.792081 0.000000
C 2.536092 0.129565 0.000000
H 2.919324 1.146123 0.000000
C 1.161791 -0.133135 0.000000
C 0.000000 0.750106 0.000000
C -0.097297 2.104012 0.000000
H 0.811240 2.701073 0.000000
C -1.383862 2.776882 0.000000
C -1.442894 4.186263 0.000000
H -0.517244 4.759233 0.000000
C -2.671607 4.839912 0.000000
C -3.864877 4.101755 0.000000
C -3.818003 2.707174 0.000000
H -4.746697 2.139071 0.000000
C -2.593012 2.019078 0.000000
H -2.705231 5.927743 0.000000

H -4.822936 4.617546 0.000000
N 3.866961 -3.379498 0.000000
O 3.416753 -4.522743 0.000000
O 5.066662 -3.114703 0.000000
el energy= -1012.30560478
zpe= -1012.083092
th energy= -1012.067084
th enthalpy= -1012.066140
free energy= -1012.127321

dmso-ES-2
B -2.498266 0.538767 0.000000
O -3.587209 -0.263886 0.000000
H -3.315725 -1.201659 0.000000
N -1.146281 -0.041274 0.000000
C -0.820780 -1.429614 0.000000
O -1.670079 -2.308391 0.000000
C 0.649674 -1.500452 0.000000
C 1.482419 -2.604039 0.000000
H 1.106735 -3.620947 0.000000
C 2.871019 -2.358845 0.000000
C 3.385092 -1.038366 0.000000
H 4.460435 -0.903630 0.000000
C 2.527337 0.059577 0.000000
H 2.930515 1.069309 0.000000
C 1.145079 -0.172950 0.000000
C 0.000000 0.723535 0.000000
C -0.068670 2.123379 0.000000
H 0.862527 2.683234 0.000000
C -1.303609 2.813021 0.000000
C -1.320936 4.242876 0.000000
H -0.375185 4.780442 0.000000
C -2.523519 4.928231 0.000000
C -3.738267 4.218709 0.000000
C -3.740303 2.811945 0.000000
H -4.691740 2.284300 0.000000
C -2.550293 2.088180 0.000000
H -2.530968 6.015639 0.000000
H -4.681483 4.760090 0.000000
N 3.773306 -3.465032 0.000000
O 3.292158 -4.631139 0.000000
O 5.011578 -3.227532 0.000000
el energy= -1012.29882884

dmso-GS-3
B -1.519371 1.386925 0.000787
O -1.682039 2.739735 0.002064
H -0.801478 3.163465 0.001645
N -0.180376 0.810710 -0.000779
C 1.029127 1.522524 -0.001599
O 1.099555 2.749320 -0.000518
C 2.109315 0.512852 -0.004320
C 3.486230 0.696493 -0.003690
H 3.922406 1.693318 -0.002367
C 4.311974 -0.447126 -0.004902
C 3.706630 -1.731399 0.000160
H 4.352423 -2.608023 0.004111
C 2.324169 -1.897201 -0.000017
H 1.898440 -2.898159 0.006483
C 1.509098 -0.760217 -0.003327
C 0.059013 -0.578950 -0.001631
C -0.970723 -1.463330 -0.001089
H -0.755591 -2.529315 -0.001926
C -2.357917 -1.028665 0.000188
C -3.399205 -1.981141 0.000412
H -3.151542 -3.041574 -0.000273
C -4.730710 -1.575050 0.001421
C -5.055394 -0.209754 0.002255
C -4.034588 0.741091 0.002096
H -4.287419 1.800271 0.002738
C -2.680928 0.361561 0.001087
H -5.522728 -2.321984 0.001537
H -6.097639 0.103126 0.003003
N 5.690370 -0.326371 -0.066273
H 6.072342 0.555440 0.253888
H 6.220994 -1.124138 0.261963
el energy= -863.165661161
zpe= -862.928945
th energy= -862.914115
th enthalpy= -862.913171
free energy= -862.970350

dmso-ES-3
B -1.507716 1.395625 -0.000167
O -1.663609 2.758275 -0.000309
H -0.762129 3.149009 -0.000492
N -0.166013 0.834882 0.000038
C 1.043387 1.565246 0.000366
O 1.088696 2.819551 0.000377
C 2.101256 0.567406 0.000121
C 3.482295 0.700039 -0.000014
H 3.965797 1.674848 -0.000003
C 4.276792 -0.478481 -0.000122
C 3.660060 -1.780016 -0.000097
H 4.301999 -2.657715 -0.000181
C 2.290040 -1.905160 0.000017
H 1.830842 -2.891101 -0.000003
C 1.487280 -0.738014 0.000126
C 0.079284 -0.549686 0.000149
C -0.976122 -1.471903 0.000118
H -0.739504 -2.533296 0.000170
C -2.323928 -1.048411 0.000052
C -3.386689 -2.006648 0.000082
H -3.135909 -3.066695 0.000169
C -4.705307 -1.601476 0.000012
C -5.028191 -0.220471 -0.000105
C -4.011955 0.730059 -0.000143
H -4.271471 1.788159 -0.000245
C -2.651046 0.365778 -0.000063
H -5.502754 -2.342488 0.000040
H -6.071214 0.090562 -0.000171
N 5.624172 -0.388562 -0.000153

H 6.087269 0.511620 -0.000500
H 6.204908 -1.217458 -0.000673
el energy= -863.156826671

dmso-GS-dioxo
B -0.088251 1.574163 -0.006470
O -0.105375 2.937415 -0.003319
H 0.815330 3.263954 0.000391
N 1.181845 0.858616 -0.003854
C 2.461949 1.434670 0.002586
O 2.666074 2.646318 0.005226
C 3.422000 0.312493 0.005798
C 4.815961 0.324821 0.013830
H 5.366419 1.262825 0.017780
C 5.478682 -0.905241 0.016837
C 4.751514 -2.108901 0.011862
H 5.289703 -3.054542 0.014672
C 3.353050 -2.118941 0.003566
H 2.804753 -3.058099 0.000051
C 2.688018 -0.890332 0.000587
C 1.265261 -0.545193 -0.006424
C 0.145851 -1.312388 -0.014336
H 0.245253 -2.395056 -0.016780
C -1.185624 -0.732072 -0.019519
C -2.313468 -1.596133 -0.027804
H -2.193184 -2.676227 -0.036652
C -3.559666 -1.009707 -0.024923
C -3.730119 0.382127 -0.015569
C -2.654067 1.243790 -0.012953
H -2.798148 2.321145 -0.011803
C -1.352615 0.684817 -0.013523
O -4.779853 -1.620362 -0.057410
O -5.065155 0.679431 -0.040850
H 6.565838 -0.935264 0.023198
C -5.747020 -0.572886 0.131511
H -6.536499 -0.664927 -0.620653
H -6.154885 -0.632898 1.150792
el energy= -996.335883521
zpe= -996.099722
th energy= -996.084128
th enthalpy= -996.083184
free energy= -996.142693

dmso-ES-dioxo
B 0.074079 1.575907 -0.000125
O 0.082449 2.941284 -0.000449
H -0.857176 3.232892 -0.000538
N -1.186759 0.860953 0.000236
C -2.486212 1.448853 0.000209
O -2.653182 2.688783 0.000125
C -3.415126 0.341147 0.000066
C -4.817309 0.304276 -0.000160
H -5.397268 1.225098 -0.000243
C -5.452888 -0.938516 -0.000213
C -4.712811 -2.146016 -0.000059
H -5.238667 -3.097821 -0.000075
C -3.316296 -2.123451 0.000113
H -2.748046 -3.051885 0.000234
C -2.664509 -0.882690 0.000144
C -1.267878 -0.529760 0.000239
C -0.115952 -1.329836 0.000157
H -0.233573 -2.409712 0.000232
C 1.177189 -0.766563 -0.000022
C 2.326092 -1.625454 -0.000169
H 2.213143 -2.705659 -0.000240
C 3.553339 -1.026814 -0.000153
C 3.711293 0.388233 0.000147
C 2.627569 1.251329 0.000058
H 2.773250 2.328144 0.000154
C 1.340990 0.690532 -0.000036
O 4.778778 -1.606252 -0.000187
O 5.022244 0.694091 0.000568
H -6.540493 -0.982774 -0.000349
C 5.747053 -0.550079 -0.000241
H 6.358518 -0.609781 0.907011
H 6.357655 -0.609102 -0.908147
el energy= -996.328800476

dmso-GS-4
B -1.569538 1.652109 0.000174
O -1.677815 3.010359 0.000105
H -0.783680 3.402756 0.000341
N -0.252994 1.021721 0.000564
C 0.983134 1.681484 0.000548
O 1.112639 2.902279 0.000590
C 2.015132 0.620520 0.000413
C 3.403386 0.735043 0.000185
H 3.889719 1.706006 0.000177
C 4.128622 -0.455896 -0.000068
C 3.502059 -1.713469 -0.000105
H 4.100882 -2.619739 -0.000350
C 2.108705 -1.806969 0.000147
H 1.630727 -2.783192 0.000087
C 1.361289 -0.625991 0.000413
C -0.078671 -0.374359 0.000549
C -1.145417 -1.213411 0.000578
H -0.974275 -2.287106 0.000642
C -2.511547 -0.722757 0.000345
C -3.579119 -1.660052 0.000461
H -3.388206 -2.729920 0.000840
C -4.861574 -1.157850 -0.000030
C -5.123661 0.219153 -0.000830
C -4.107146 1.151049 -0.000772
H -4.323516 2.216104 -0.001294
C -2.771685 0.680075 -0.000120
O -6.035019 -1.850850 -0.000362
O -6.473427 0.430391 -0.001993
Br 6.058083 -0.377379 -0.000394
C -7.087880 -0.868691 0.001035
H -7.697502 -0.988059 -0.902946
H -7.693191 -0.985883 0.908289
el energy= -1008.90750300

zpe= -1008.681954
th energy= -1008.664606
th enthalpy= -1008.663662
free energy= -1008.729069

dmso-ES-4

B	-1.559164	1.657018	-0.000072
O	-1.665932	3.017699	-0.000037
H	-0.752178	3.380246	-0.000040
N	-0.252222	1.030795	-0.000092
C	1.002306	1.708884	-0.000055
O	1.085598	2.955238	-0.000020
C	2.005743	0.668362	-0.000058
C	3.406397	0.744107	0.000001
H	3.916727	1.703022	0.000062
C	4.109933	-0.456724	-0.000003
C	3.481309	-1.724530	-0.000072
H	4.075081	-2.632794	-0.000071
C	2.085474	-1.792077	-0.000131
H	1.592293	-2.761927	-0.000177
C	1.345876	-0.605951	-0.000118
C	-0.074812	-0.351853	-0.000132
C	-1.163546	-1.228846	-0.000155
H	-0.971432	-2.297965	-0.000179
C	-2.495913	-0.756865	-0.000110
C	-3.578185	-1.694649	-0.000084
H	-3.389836	-2.764167	-0.000119
C	-4.845545	-1.184256	0.000005
C	-5.103829	0.216197	0.000059
C	-4.083627	1.154007	0.000025
H	-4.304265	2.217841	0.000075
C	-2.761597	0.684053	-0.000059
O	-6.024804	-1.849523	0.000057
O	-6.432552	0.427580	0.000146
Br	6.041653	-0.397314	0.000112
C	-7.066370	-0.865016	0.000196
H	-7.671627	-0.967945	-0.907281
H	-7.671413	-0.967974	0.907814

el energy= -1008.90093228

dmso-GS-5

B	-1.117541	1.645976	-0.000565
O	-1.215012	3.004252	-0.001883
H	-0.318971	3.391676	-0.001539
N	0.193096	1.003568	0.001060
C	1.435860	1.649595	0.001043
O	1.581075	2.867784	0.000416
C	2.454739	0.575138	0.001603
C	3.839307	0.665773	0.001191
H	4.358731	1.617983	0.001005
C	4.541287	-0.541309	0.000313
C	3.898930	-1.791767	0.000334
H	4.498255	-2.695649	-0.000524
C	2.509186	-1.863572	0.001538
H	2.011020	-2.829065	0.001859
C	1.782878	-0.666428	0.001905
C	0.351755	-0.394318	0.001874
C	-0.724175	-1.224511	0.002228
H	-0.561502	-2.299455	0.003021
C	-2.082998	-0.722022	0.001256
C	-3.158779	-1.650382	0.001908
H	-2.976609	-2.721666	0.003382
C	-4.435777	-1.136239	0.000418
C	-4.684160	0.243999	-0.001980
C	-3.658905	1.167375	-0.002392
H	-3.866094	2.234167	-0.004145
C	-2.328981	0.684140	-0.000609
O	-5.615679	-1.816784	0.000044
O	-6.029825	0.468526	-0.004410
N	6.005536	-0.502386	-0.001400
O	6.553131	0.597972	0.006659
O	6.613523	-1.570463	-0.010954
C	-6.658752	-0.824598	0.001708
H	-7.270557	-0.938302	-0.901287
H	-7.263179	-0.933380	0.910418

el energy= -1200.83545312
zpe= -1200.597129
th energy= -1200.578716
th enthalpy= -1200.577772
free energy= -1200.645994

dmso-ES-5

B	0.265449	-1.971272	0.000000
O	1.089230	-3.047559	0.000000
H	2.018918	-2.745938	0.000000
N	0.807125	-0.616584	0.000000
C	2.177333	-0.263016	0.000000
O	3.083260	-1.089002	0.000000
C	2.216358	1.209272	0.000000
C	3.306980	2.062732	0.000000
H	4.329363	1.701743	0.000000
C	3.040256	3.444031	0.000000
C	1.710350	3.936382	0.000000
H	1.557735	5.009325	0.000000
C	0.628248	3.059214	0.000000
H	-0.388013	3.446276	0.000000
C	0.881360	1.681649	0.000000
C	0.000000	0.517841	0.000000
C	-1.378535	0.420901	0.000000
H	-1.963982	1.335809	0.000000
C	-2.053246	-0.837930	0.000000
C	-3.476992	-0.866275	0.000000
H	-4.056317	0.052071	0.000000
C	-4.075068	-2.100630	0.000000
C	-3.325172	-3.304034	0.000000
C	-1.933965	-3.309148	0.000000
H	-1.380924	-4.243932	0.000000
C	-1.285176	-2.071138	0.000000
O	-5.393672	-2.401183	0.000000
O	-4.157588	-4.355984	0.000000
N	4.132587	4.365710	0.000000
O	5.306936	3.906782	0.000000

O 3.873429 5.599129 0.000000
C -5.500311 -3.831562 0.000000
H -6.014643 -4.165033 0.908092
H -6.014643 -4.165033 -0.908092
el energy= -1200.83038967

dmso-GS-6
B -0.490355 1.602644 -0.007468
O -0.542087 2.965721 -0.000869
H 0.370501 3.314416 0.002354
N 0.797956 0.920561 -0.008243
C 2.061503 1.531348 -0.001585
O 2.231882 2.748602 0.004261
C 3.054946 0.436105 -0.002932
C 4.442729 0.504555 0.007470
H 4.961142 1.461310 0.015263
C 5.171292 -0.702792 0.009130
C 4.462122 -1.932278 0.004915
H 5.033453 -2.859201 0.009885
C 3.070554 -1.983598 -0.005076
H 2.563492 -2.946026 -0.004724
C 2.351678 -0.783480 -0.009466
C 0.921890 -0.482353 -0.013562
C -0.180030 -1.275959 -0.020468
H -0.054882 -2.356037 -0.025012
C -1.526494 -0.729561 -0.021952
C -2.632856 -1.621369 -0.028220
H -2.486135 -2.698287 -0.037591
C -3.894002 -1.067134 -0.022463
C -4.101335 0.319244 -0.013370
C -3.047652 1.207699 -0.011593
H -3.218847 2.281178 -0.009786
C -1.731690 0.682428 -0.014251
O -5.098044 -1.710321 -0.052075
O -5.445620 0.580892 -0.039292
N 6.556636 -0.696504 -0.040366
H 7.004548 0.150508 0.288554
H 7.013557 -1.533791 0.300684
C -6.091300 -0.688283 0.140715
H -6.883668 -0.804819 -0.605031
H -6.490708 -0.757451 1.163061
el energy= -1051.69455572
zpe= -1051.442086
th energy= -1051.424947
th enthalpy= -1051.424003
free energy= -1051.486655

dmso-ES-6
B -0.475305 1.612855 -0.000118
O -0.521100 2.984482 -0.000090
H 0.410692 3.297468 -0.000137
N 0.809392 0.942180 -0.000213
C 2.079990 1.566901 -0.000161
O 2.226562 2.814254 -0.000174
C 3.047226 0.484188 -0.000107
C 4.437485 0.501143 0.000019
H 4.996696 1.434981 0.000055
C 5.132284 -0.735669 0.000158
C 4.407791 -1.977652 0.000142
H 4.972923 -2.906986 0.000262
C 3.029249 -1.989116 0.000002
H 2.491863 -2.935325 0.000017
C 2.325267 -0.763457 -0.000124
C 0.937294 -0.457450 -0.000207
C -0.194141 -1.284821 -0.000267
H -0.048597 -2.362064 -0.000328
C -1.501169 -0.754507 -0.000189
C -2.629596 -1.645479 -0.000244
H -2.485524 -2.722606 -0.000412
C -3.875088 -1.086326 -0.000015
C -4.076058 0.317359 0.000326
C -3.021853 1.206852 0.000281
H -3.197905 2.279604 0.000485
C -1.706588 0.689373 -0.000018
O -5.084944 -1.712175 0.000176
O -5.407934 0.583522 0.000854
N 6.486976 -0.762936 0.000225
H 7.027713 0.091528 0.000746
H 6.990837 -1.639566 0.000947
C -6.085804 -0.684636 -0.000428
H -6.696630 -0.768037 -0.907277
H -6.698526 -0.768857 0.905025
el energy= -1051.68565979

dmso-GS-thieno
B -1.041127 1.443742 -0.000002
O -1.146330 2.798106 -0.000014
H -0.245843 3.181219 -0.000008
N 0.273473 0.804363 0.000007
C 1.504616 1.474639 0.000016
O 1.616453 2.699857 0.000042
C 2.549645 0.431984 0.000029
C 3.939136 0.553489 0.000051
H 4.415359 1.531139 0.000064
C 4.695826 -0.620313 0.000052
C 4.065970 -1.878224 0.000032
H 4.676703 -2.778714 0.000034
C 2.673444 -1.997755 0.000013
H 2.200646 -2.976976 0.000000
C 1.913460 -0.824610 0.000012
C 0.467762 -0.597730 -0.000001
C -0.573180 -1.467334 -0.000019
H -0.380727 -2.536906 -0.000030
C -1.937705 -0.979668 -0.000032
C -3.077933 -1.755464 -0.000072
H -3.157037 -2.837034 -0.000095
S -4.512499 -0.773797 -0.000006
C -3.575383 0.694547 -0.000075
H -4.087740 1.650676 -0.000100
C -2.224496 0.446306 -0.000023
H 5.781997 -0.564806 0.000067
el energy= -740.496674480

zpe= -740.310089
th energy= -740.297077
th enthalpy= -740.296133
free energy= -740.349833

dmso-ES-thieno

B	-1.025174	1.450034	0.000003
O	-1.115968	2.805302	0.000081
H	-0.197780	3.159717	0.000159
N	0.281298	0.802696	0.000019
C	1.551765	1.492961	0.000034
O	1.613392	2.738250	-0.000037
C	2.555576	0.461903	0.000056
C	3.958463	0.524303	0.000068
H	4.472759	1.483354	0.000064
C	4.682480	-0.670807	0.000096
C	4.033244	-1.928912	0.000107
H	4.624713	-2.841083	0.000127
C	2.635231	-2.005200	0.000086
H	2.134937	-2.971840	0.000086
C	1.896857	-0.816344	0.000059
C	0.477268	-0.569953	0.000022
C	-0.611705	-1.473706	0.000006
H	-0.412679	-2.541139	0.000026
C	-1.926778	-0.978814	-0.000029
C	-3.111250	-1.755336	0.000003
H	-3.191029	-2.837055	0.000027
S	-4.509668	-0.772746	-0.000280
C	-3.559309	0.706691	0.000065
H	-4.077526	1.659684	0.000155
C	-2.213781	0.458106	-0.000035
H	5.770318	-0.634526	0.000112

el energy= -740.488150770

dmso-GS-7

B	2.483689	1.436769	0.000017
O	2.652503	2.783914	0.000032
H	1.773805	3.213485	0.000029
N	1.139426	0.858656	0.000010
C	-0.056372	1.585085	0.000006
O	-0.118900	2.812500	-0.000029
C	-1.147775	0.587824	-0.000012
C	-2.526826	0.787026	-0.000036
H	-2.951033	1.786602	-0.000050
C	-3.321946	-0.357679	-0.000035
C	-2.771917	-1.651225	-0.000014
H	-3.424432	-2.519459	-0.000013
C	-1.387283	-1.828967	0.000006
H	-0.969272	-2.832305	0.000020
C	-0.570269	-0.694779	0.000006
C	0.882290	-0.533723	0.000018
C	1.881652	-1.450914	0.000035
H	1.639235	-2.510219	0.000046
C	3.266703	-1.026261	0.000047
C	4.370683	-1.853297	0.000087
H	4.399847	-2.937504	0.000111
S	5.847848	-0.937539	0.000016
C	4.978395	0.571838	0.000092
H	5.532058	1.504591	0.000120
C	3.617948	0.384893	0.000037
Br	-5.243449	-0.165407	-0.000061

el energy= -753.068224128
zpe= -752.892108
th energy= -752.877468
th enthalpy= -752.876523
free energy= -752.935169

dmso-ES-7

B	-2.478635	1.442138	-0.000020
O	-2.647203	2.789523	0.000000
H	-1.754086	3.200331	0.000029
N	-1.138598	0.866939	-0.000004
C	0.090875	1.624563	0.000014
O	0.089090	2.868964	0.000004
C	1.149745	0.648312	0.000025
C	2.545140	0.800339	0.000040
H	3.003853	1.785020	0.000047
C	3.314882	-0.361361	0.000048
C	2.758836	-1.662616	0.000041
H	3.401344	-2.536652	0.000047
C	1.365344	-1.806073	0.000024
H	0.926498	-2.801617	0.000016
C	0.563589	-0.664295	0.000015
C	-0.869683	-0.494099	-0.000007
C	-1.903422	-1.455111	-0.000026
H	-1.645682	-2.509819	-0.000023
C	-3.245323	-1.032502	-0.000048
C	-4.384968	-1.872729	-0.000058
H	-4.404468	-2.957491	-0.000057
S	-5.834643	-0.968009	-0.000143
C	-4.966105	0.561036	-0.000035
H	-5.533631	1.485406	-0.000014
C	-3.609355	0.385429	-0.000047
Br	5.238040	-0.192844	0.000069

el energy= -753.060113732

dmso-GS-8

B	-2.051848	1.440421	-0.000021
O	-2.217708	2.787529	-0.000040
H	-1.339139	3.216923	-0.000119
N	-0.708491	0.858541	-0.000100
C	0.489500	1.579953	-0.000164
O	0.559087	2.806358	-0.000011
C	1.576228	0.576441	-0.000103
C	2.952230	0.761153	-0.000017
H	3.403665	1.747221	0.000041
C	3.732477	-0.395724	0.000012
C	3.176497	-1.686864	-0.000060
H	3.835523	-2.548043	-0.000021
C	1.794778	-1.852262	-0.000135
H	1.362806	-2.849042	-0.000147
C	0.990176	-0.706422	-0.000145

C -0.457143 -0.534692 -0.000128
C -1.459793 -1.450598 -0.000099
H -1.219589 -2.510322 -0.000111
C -2.840949 -1.021350 -0.000020
C -3.946898 -1.847093 0.000041
H -3.976962 -2.931284 0.000033
S -5.420304 -0.929206 0.000132
C -4.548325 0.579562 0.000104
H -5.101544 1.512555 0.000150
C -3.188477 0.390762 0.000028
N 5.192220 -0.259264 0.000192
O 5.665337 0.874928 0.000241
O 5.869713 -1.284434 0.000014
el energy= -944.995831084
zpe= -944.807024
th energy= -944.791328
th enthalpy= -944.790384
free energy= -944.851218

dmso-ES-8
B -2.060287 1.448935 0.000029
O -2.224911 2.788160 0.000029
H -1.355736 3.234330 0.000059
N -0.710119 0.853122 0.000031
C 0.514631 1.584693 0.000010
O 0.552433 2.805792 -0.000018
C 1.593999 0.584564 0.000024
C 2.967575 0.764742 0.000013
H 3.430715 1.744408 -0.000008
C 3.764477 -0.398664 0.000007
C 3.177011 -1.685749 0.000028
H 3.833032 -2.548820 0.000018
C 1.790954 -1.841981 0.000046
H 1.352734 -2.836842 0.000051
C 0.993052 -0.691537 0.000038
C -0.458033 -0.505671 0.000030
C -1.491695 -1.441014 0.000022
H -1.247000 -2.498879 0.000016
C -2.840506 -1.009749 -0.000003
C -3.969826 -1.848047 -0.000048
H -3.984674 -2.933008 -0.000060
S -5.429231 -0.947297 -0.000005
C -4.550742 0.580509 -0.000070
H -5.112733 1.508380 -0.000099
C -3.196526 0.398939 -0.000007
N 5.185522 -0.274094 -0.000035
O 5.682371 0.890839 -0.000051
O 5.884951 -1.329404 -0.000030
el energy= -944.988447914

dmso-GS-9
B 1.436041 1.436643 0.000835
O 1.568296 2.789226 0.002105
H 0.674838 3.188942 0.001400
N 0.109544 0.824373 -0.000744
C -1.106289 1.520704 -0.001339
O -1.192154 2.748463 -0.000094
C -2.176108 0.502018 -0.004403
C -3.555216 0.673376 -0.003879
H -4.000056 1.666359 -0.002543
C -4.370626 -0.476588 -0.005076
C -3.754067 -1.756244 0.000472
H -4.392500 -2.638299 0.004553
C -2.370924 -1.910074 0.000510
H -1.936525 -2.907313 0.007327
C -1.564802 -0.765659 -0.003175
C -0.117209 -0.575477 -0.001526
C 0.909394 -1.463342 -0.001223
H 0.697631 -2.529366 -0.002212
C 2.284447 -1.003137 0.000027
C 3.410223 -1.799560 0.000175
H 3.469475 -2.882444 -0.000567
S 4.865426 -0.845024 0.001492
C 3.955296 0.640224 0.002253
H 4.484467 1.587190 0.003222
C 2.600103 0.417034 0.001167
N -5.750328 -0.368642 -0.067148
H -6.139820 0.510580 0.251131
H -6.273512 -1.169758 0.264907
el energy= -795.855615833
zpe= -795.652571
th energy= -795.638053
th enthalpy= -795.637109
free energy= -795.693851

dmso-ES-9
B 1.420919 1.441604 -0.000033
O 1.550868 2.800962 0.000051
H 0.636596 3.168975 0.000038
N 0.099879 0.842329 -0.000107
C -1.127443 1.563313 -0.000117
O -1.174827 2.820277 -0.000081
C -2.168942 0.560729 -0.000062
C -3.556629 0.676032 0.000034
H -4.051239 1.645470 0.000081
C -4.338326 -0.509152 0.000065
C -3.712647 -1.806009 0.000018
H -4.345554 -2.690075 0.000069
C -2.338657 -1.914310 -0.000066
H -1.869404 -2.895896 -0.000092
C -1.546629 -0.742901 -0.000102
C -0.136708 -0.548126 -0.000114
C 0.914805 -1.472726 -0.000077
H 0.688078 -2.535311 -0.000062
C 2.255840 -1.016902 -0.000011
C 3.408945 -1.816323 0.000114
H 3.470433 -2.899035 0.000149
S 4.839802 -0.860290 -0.000053
C 3.934358 0.631449 0.000278
H 4.471548 1.573782 0.000461
C 2.577476 0.415595 0.000018
N -5.688640 -0.429380 0.000254

H -6.158912 0.466887 -0.000101
H -6.262634 -1.262753 -0.000177
el energy= -795.847002923

acetonitrile-GS-benzo
B -1.125399 1.394497 0.000000
O -1.267879 2.748694 0.000000
H -0.384114 3.165015 -0.000001
N 0.203190 0.794090 -0.000001
C 1.427084 1.482192 -0.000004
O 1.522207 2.706997 0.000001
C 2.484512 0.450739 -0.000001
C 3.871786 0.589756 0.000001
H 4.334420 1.574035 0.000001
C 4.642684 -0.575814 0.000001
C 4.027194 -1.840411 0.000000
H 4.648196 -2.733815 0.000001
C 2.635113 -1.976613 -0.000001
H 2.174088 -2.961358 -0.000002
C 1.862191 -0.812764 -0.000002
C 0.412680 -0.598089 -0.000002
C -0.629483 -1.466187 -0.000001
H -0.431081 -2.535300 -0.000001
C -2.008911 -1.007153 0.000000
C -3.066253 -1.941357 0.000001
H -2.837098 -3.005801 0.000000
C -4.390042 -1.510609 0.000002
C -4.688810 -0.139137 0.000003
C -3.651183 0.793574 0.000002
H -3.884630 1.857228 0.000003
C -2.304691 0.388787 0.000001
H -5.195804 -2.242550 0.000002
H -5.725274 0.192309 0.000004
H 5.728114 -0.507893 0.000002
el energy= -807.810384629
zpe= -807.590317
th energy= -807.576953
th enthalpy= -807.576008
free energy= -807.630232

acetonitrile-ES-benzo
B -1.111854 1.406747 0.000000
O -1.234252 2.764886 0.000000
H -0.329639 3.148117 0.000000
N 0.216801 0.803830 0.000000
C 1.464487 1.503752 0.000000
O 1.524363 2.749035 0.000000
C 2.486363 0.478051 -0.000001
C 3.883254 0.557920 -0.000001
H 4.386648 1.522665 -0.000001
C 4.620910 -0.631509 -0.000001
C 3.983977 -1.895262 -0.000001
H 4.586892 -2.800033 -0.000001
C 2.590938 -1.989689 -0.000001
H 2.100644 -2.961078 -0.000001
C 1.838079 -0.803781 0.000000
C 0.424442 -0.565730 0.000000
C -0.668834 -1.471117 0.000000
H -0.452623 -2.536264 0.000000
C -1.994308 -1.017676 0.000000
C -3.084133 -1.957489 0.000001
H -2.854226 -3.021491 0.000000
C -4.389460 -1.519286 0.000001
C -4.673893 -0.130127 0.000001
C -3.631976 0.803942 0.000001
H -3.872251 1.866008 0.000001
C -2.289475 0.408702 0.000001
H -5.206921 -2.237156 0.000001
H -5.708088 0.207811 0.000001
H 5.708114 -0.584702 -0.000001
el energy= -807.801848082

acetonitrile-GS-1
B 1.253602 -2.630682 0.000000
O 0.622043 -3.836121 0.000000
H -0.344669 -3.698035 0.000000
N 0.481799 -1.391978 0.000000
C -0.915817 -1.285258 0.000000
O -1.680314 -2.245059 0.000000
C -1.218775 0.163066 0.000000
C -2.453832 0.807439 0.000000
H -3.382741 0.244368 0.000000
C -2.429042 2.202059 0.000000
C -1.226383 2.928721 0.000000
H -1.246811 4.014715 0.000000
C 0.001107 2.262459 0.000000
H 0.927026 2.831670 0.000000
C 0.000000 0.865354 0.000000
C 1.083703 -0.118406 0.000000
C 2.432481 0.024656 0.000000
H 2.860793 1.023977 0.000000
C 3.323322 -1.124216 0.000000
C 4.721302 -0.935354 0.000000
H 5.122947 0.076530 0.000000
C 5.581602 -2.030033 0.000000
C 5.066660 -3.335542 0.000000
C 3.685536 -3.533846 0.000000
H 3.287219 -4.547136 0.000000
C 2.792378 -2.448410 0.000000
H 6.658220 -1.870349 0.000000
H 5.743548 -4.187516 0.000000
Br -4.099012 3.171495 0.000000
el energy= -820.381797819
zpe= -820.172106
th energy= -820.157158
th enthalpy= -820.156214
free energy= -820.215228

acetonitrile-ES-1
B 1.220555 -2.645960 0.000000
O 0.571303 -3.844375 0.000000
H -0.394303 -3.668235 0.000000

N 0.453072 -1.405249 0.000000
C -0.973726 -1.293728 0.000000
O -1.717130 -2.291493 0.000000
C -1.250479 0.127439 0.000000
C -2.462428 0.825705 0.000000
H -3.413226 0.300138 0.000000
C -2.396940 2.220279 0.000000
C -1.176975 2.937723 0.000000
H -1.178210 4.022784 0.000000
C 0.028968 2.234463 0.000000
H 0.971576 2.777327 0.000000
C 0.000000 0.833753 0.000000
C 1.043724 -0.151912 0.000000
C 2.452904 -0.005775 0.000000
H 2.865560 0.999503 0.000000
C 3.302194 -1.121861 0.000000
C 4.730032 -0.946856 0.000000
H 5.131675 0.064632 0.000000
C 5.570479 -2.038010 0.000000
C 5.033718 -3.349618 0.000000
C 3.648103 -3.546130 0.000000
H 3.255546 -4.561500 0.000000
C 2.754250 -2.469766 0.000000
H 6.648985 -1.896679 0.000000
H 5.704687 -4.206096 0.000000
Br -4.043511 3.222497 0.000000
el energy= -820.373620185

acetonitrile-GS-2
B -2.500319 0.469786 0.000000
O -3.573961 -0.365369 0.000000
H -3.269150 -1.292899 0.000000
N -1.144274 -0.070119 0.000000
C -0.789215 -1.424955 0.000000
O -1.594163 -2.350263 0.000000
C 0.691027 -1.460806 0.000000
C 1.550115 -2.551033 0.000000
H 1.188402 -3.573519 0.000000
C 2.916045 -2.262784 0.000000
C 3.415169 -0.949173 0.000000
H 4.487715 -0.788932 0.000000
C 2.537173 0.131598 0.000000
H 2.919779 1.148390 0.000000
C 1.162778 -0.131856 0.000000
C 0.000000 0.750632 0.000000
C -0.098914 2.104593 0.000000
H 0.808949 2.702652 0.000000
C -1.386378 2.776241 0.000000
C -1.447384 4.185641 0.000000
H -0.522453 4.759767 0.000000
C -2.677203 4.837626 0.000000
C -3.869726 4.097809 0.000000
C -3.820856 2.703167 0.000000
H -4.748408 2.133068 0.000000
C -2.594667 2.016904 0.000000
H -2.712348 5.925412 0.000000
H -4.828614 4.612083 0.000000
N 3.869636 -3.376947 0.000000
O 3.420588 -4.520310 0.000000
O 5.069087 -3.112447 0.000000
el energy= -1012.30911961
zpe= -1012.086583
th energy= -1012.070618
th enthalpy= -1012.069674
free energy= -1012.130595

acetonitrile-ES-2
B -2.498229 0.538452 0.000000
O -3.588517 -0.261374 0.000000
H -3.326090 -1.201923 0.000000
N -1.145933 -0.040992 0.000000
C -0.820412 -1.429202 0.000000
O -1.669741 -2.307341 0.000000
C 0.650549 -1.500246 0.000000
C 1.482648 -2.604513 0.000000
H 1.105894 -3.621128 0.000000
C 2.871654 -2.359328 0.000000
C 3.385824 -1.038917 0.000000
H 4.461161 -0.903817 0.000000
C 2.528078 0.059339 0.000000
H 2.931525 1.068938 0.000000
C 1.145838 -0.173136 0.000000
C 0.000000 0.723881 0.000000
C -0.068602 2.123525 0.000000
H 0.862490 2.683479 0.000000
C -1.303974 2.813487 0.000000
C -1.321650 4.243281 0.000000
H -0.376006 4.781031 0.000000
C -2.524750 4.928254 0.000000
C -3.739360 4.218263 0.000000
C -3.740892 2.811317 0.000000
H -4.691676 2.282397 0.000000
C -2.550244 2.088267 0.000000
H -2.532635 6.015659 0.000000
H -4.682788 4.759283 0.000000
N 3.773468 -3.464983 0.000000
O 3.292916 -4.631892 0.000000
O 5.012627 -3.229390 0.000000
el energy= -1012.30225914

acetonitrile-GS-3
B -1.519061 1.385899 0.000373
O -1.685046 2.738222 0.001880
H -0.807757 3.168682 0.001301
N -0.180112 0.810243 -0.001656
C 1.029198 1.521884 -0.002268
O 1.100016 2.748824 -0.000912
C 2.109515 0.512511 -0.005033
C 3.486347 0.697214 -0.003559
H 3.921162 1.694717 -0.001777
C 4.312658 -0.446139 -0.004156
C 3.707880 -1.730797 -0.000242

H 4.354363 -2.606916 0.003598
C 2.325360 -1.897465 -0.001352
H 1.899830 -2.898490 0.004394
C 1.509602 -0.760746 -0.004547
C 0.059233 -0.579765 -0.002813
C -0.970774 -1.464071 -0.002116
H -0.755883 -2.530113 -0.003175
C -2.358199 -1.029435 -0.000139
C -3.400258 -1.981234 0.000633
H -3.153072 -3.041795 -0.000295
C -4.731649 -1.574130 0.002529
C -5.055737 -0.208437 0.003712
C -4.033977 0.741580 0.002985
H -4.285259 1.801244 0.003925
C -2.680640 0.360807 0.001090
H -5.524004 -2.320743 0.003090
H -6.097840 0.104922 0.005180
N 5.691279 -0.324907 -0.063516
H 6.072657 0.557119 0.256781
H 6.221823 -1.122514 0.265235
el energy= -863.169426578
zpe= -862.932915
th energy= -862.918056
th enthalpy= -862.917111
free energy= -862.974353

acetonitrile-ES-3
B -1.507197 1.394468 -0.000162
O -1.664248 2.757270 -0.000341
H -0.764428 3.151752 -0.000507
N -0.165869 0.833763 0.000077
C 1.043366 1.563336 0.000427
O 1.089283 2.818281 0.000414
C 2.101160 0.566231 0.000154
C 3.482003 0.700848 -0.000022
H 3.963017 1.676937 -0.000025
C 4.277521 -0.477011 -0.000157
C 3.661623 -1.779090 -0.000109
H 4.304570 -2.656071 -0.000215
C 2.291512 -1.905886 0.000047
H 1.833306 -2.892267 0.000032
C 1.487535 -0.739433 0.000175
C 0.079227 -0.551202 0.000203
C -0.976874 -1.472720 0.000166
H -0.741056 -2.534289 0.000226
C -2.324705 -1.048689 0.000072
C -3.388261 -2.006175 0.000089
H -3.137934 -3.066329 0.000194
C -4.706710 -1.599955 -0.000019
C -5.028775 -0.218521 -0.000162
C -4.011635 0.731176 -0.000187
H -4.270180 1.789564 -0.000310
C -2.651003 0.365610 -0.000071
H -5.504575 -2.340527 -0.000001
H -6.071602 0.093144 -0.000257
N 5.625101 -0.386428 -0.000233
H 6.087850 0.513930 -0.000626
H 6.206215 -1.215057 -0.000822
el energy= -863.160580113

acetonitrile-GS-dioxo
B -0.087940 1.573649 -0.006982
O -0.108771 2.936896 -0.003964
H 0.809020 3.271716 -0.001130
N 1.182340 0.858716 -0.005202
C 2.462502 1.434453 0.001610
O 2.667110 2.646052 0.004199
C 3.422437 0.312308 0.005356
C 4.816458 0.325751 0.014383
H 5.365292 1.264757 0.018578
C 5.480018 -0.903987 0.018148
C 4.753228 -2.108148 0.012980
H 5.291752 -3.053608 0.016495
C 3.354596 -2.118982 0.003634
H 2.807059 -3.058573 0.000076
C 2.688650 -0.890650 -0.000033
C 1.265730 -0.545432 -0.007606
C 0.146302 -1.312907 -0.015482
H 0.246131 -2.395528 -0.017975
C -1.185514 -0.733057 -0.020020
C -2.313861 -1.596864 -0.028160
H -2.195384 -2.677220 -0.037568
C -3.559801 -1.009634 -0.024071
C -3.729889 0.382110 -0.013032
C -2.653539 1.243582 -0.010820
H -2.797319 2.320978 -0.008378
C -1.352255 0.683939 -0.013079
O -4.780481 -1.620139 -0.054110
O -5.065199 0.679807 -0.034262
H 6.567188 -0.933542 0.025404
C -5.750300 -0.572767 0.123782
H -6.527831 -0.661617 -0.641200
H -6.172423 -0.635831 1.136575
el energy= -996.338488975
zpe= -996.102564
th energy= -996.086937
th enthalpy= -996.085993
free energy= -996.145655

acetonitrile-ES-dioxo
B 0.073903 1.575776 0.000498
O 0.084363 2.941371 0.000520
H -0.853439 3.238417 0.000829
N -1.187087 0.861280 0.000677
C -2.486561 1.448431 -0.000135
O -2.653953 2.688862 -0.000245
C -3.415300 0.340895 -0.000063
C -4.817734 0.304590 -0.000455
H -5.397021 1.225852 -0.000670
C -5.453632 -0.938064 -0.000652
C -4.713548 -2.145900 -0.000442
H -5.239364 -3.097737 -0.000626

C -3.316927 -2.123647 0.000009
H -2.748986 -3.052250 0.000208
C -2.664696 -0.882939 0.000173
C -1.268058 -0.529787 0.000477
C -0.116120 -1.329884 0.000639
H -0.233873 -2.409724 0.000845
C 1.177233 -0.766948 0.000483
C 2.326340 -1.625846 0.000542
H 2.215413 -2.706279 0.000882
C 3.553298 -1.026645 0.000112
C 3.711661 0.388579 -0.000406
C 2.627558 1.251664 -0.000272
H 2.773240 2.328464 -0.000521
C 1.341034 0.690372 0.000208
O 4.778824 -1.606031 0.000104
O 5.022800 0.693723 -0.000846
H -6.541247 -0.982180 -0.001015
C 5.747674 -0.550694 -0.000558
H 6.358114 -0.610108 0.907337
H 6.357651 -0.610755 -0.908719
el energy= -996.331369523

acetonitrile-GS-4
B -1.569181 1.651257 -0.000078
O -1.679702 3.009303 -0.000180
H -0.788348 3.408194 -0.000160
N -0.252783 1.020566 0.000374
C 0.983379 1.679421 0.000360
O 1.114649 2.900029 0.000454
C 2.015007 0.618639 0.000208
C 3.402982 0.735299 0.000032
H 3.886233 1.707924 -0.000015
C 4.129550 -0.455124 -0.000045
C 3.503568 -1.713319 0.000047
H 4.103614 -2.618805 0.000008
C 2.110093 -1.808379 0.000194
H 1.633299 -2.785184 0.000263
C 1.361447 -0.627985 0.000260
C -0.078722 -0.376076 0.000360
C -1.146051 -1.214521 0.000194
H -0.975671 -2.288354 0.000164
C -2.512215 -0.723454 0.000058
C -3.580432 -1.660264 0.000099
H -3.390297 -2.730324 0.000251
C -4.862522 -1.157040 -0.000042
C -5.124048 0.220054 -0.000291
C -4.107113 1.151534 -0.000343
H -4.322899 2.216810 -0.000548
C -2.771784 0.679588 -0.000131
O -6.037068 -1.849030 0.000008
O -6.474168 0.431452 -0.000428
Br 6.059239 -0.375997 -0.000227
C -7.089960 -0.867349 0.000093
H -7.696578 -0.985635 -0.905932
H -7.696083 -0.985174 0.906525
el energy= -1008.91007107

zpe= -1008.684656
th energy= -1008.667348
th enthalpy= -1008.666403
free energy= -1008.731113

acetonitrile-ES-4
B -1.558919 1.655896 -0.000072
O -1.666973 3.016604 -0.000035
H -0.754889 3.383226 -0.000035
N -0.252074 1.029851 -0.000096
C 1.002233 1.707365 -0.000061
O 1.085806 2.954312 -0.000027
C 2.005685 0.667359 -0.000061
C 3.406409 0.744495 0.000001
H 3.915284 1.704229 0.000064
C 4.110709 -0.455952 -0.000003
C 3.482474 -1.724233 -0.000075
H 4.077085 -2.631970 -0.000074
C 2.086635 -1.792924 -0.000136
H 1.594316 -2.763204 -0.000183
C 1.346019 -0.607162 -0.000123
C -0.074794 -0.353179 -0.000136
C -1.163965 -1.229772 -0.000157
H -0.972240 -2.298973 -0.000181
C -2.496517 -0.757716 -0.000110
C -3.579376 -1.695179 -0.000083
H -3.391969 -2.764933 -0.000118
C -4.846503 -1.183999 0.000008
C -5.104194 0.216744 0.000064
C -4.083611 1.154218 0.000028
H -4.304606 2.218035 0.000079
C -2.761759 0.683464 -0.000057
O -6.026624 -1.847880 0.000062
O -6.432585 0.428365 0.000157
Br 6.042701 -0.396383 0.000115
C -7.068012 -0.863590 0.000186
H -7.672085 -0.966121 -0.907958
H -7.671907 -0.966164 0.908445
el energy= -1008.90343589

acetonitrile-GS-5
B -1.116984 1.645030 -0.000357
O -1.217170 3.003157 -0.001252
H -0.324157 3.397721 -0.001202
N 0.193384 1.002278 0.000593
C 1.436355 1.647538 0.000444
O 1.583010 2.865444 -0.000089
C 2.454736 0.573142 0.000987
C 3.839040 0.665800 0.000712
H 4.355991 1.619364 0.000408
C 4.542144 -0.540649 0.000374
C 3.900744 -1.791762 0.000767
H 4.501830 -2.694472 0.000638
C 2.510873 -1.865206 0.001535
H 2.014040 -2.831379 0.002085
C 1.783129 -0.668571 0.001373

C 0.351799 -0.396027 0.001210
C -0.724631 -1.225876 0.001302
H -0.562436 -2.300899 0.001831
C -2.083493 -0.723018 0.000647
C -3.160099 -1.650853 0.000897
H -2.979021 -2.722381 0.001629
C -4.436687 -1.135568 0.000146
C -4.684249 0.244848 -0.000883
C -3.658498 1.167645 -0.001118
H -3.865048 2.234620 -0.001928
C -2.328781 0.683364 -0.000305
O -5.617785 -1.814884 0.000101
O -6.030125 0.469813 -0.001654
N 6.006138 -0.500289 -0.000973
O 6.552841 0.600303 0.004359
O 6.615783 -1.567184 -0.007581
C -6.660675 -0.822764 0.000021
H -7.268517 -0.934380 -0.905809
H -7.267104 -0.932730 0.907041
el energy= -1200.83772285
zpe= -1200.599594
th energy= -1200.581209
th enthalpy= -1200.580265
free energy= -1200.647736

acetonitrile-ES-5
B 0.265398 -1.971516 0.000000
O 1.086586 -3.049400 0.000000
H 2.018925 -2.755609 0.000000
N 0.807093 -0.616626 0.000000
C 2.177030 -0.263129 0.000000
O 3.082348 -1.089388 0.000000
C 2.216461 1.209700 0.000000
C 3.307626 2.062655 0.000000
H 4.329964 1.701308 0.000000
C 3.040842 3.444354 0.000000
C 1.710968 3.936904 0.000000
H 1.558059 5.009885 0.000000
C 0.628626 3.059837 0.000000
H -0.387546 3.447068 0.000000
C 0.881705 1.682107 0.000000
C 0.000000 0.517890 0.000000
C -1.378297 0.421167 0.000000
H -1.963619 1.336128 0.000000
C -2.053555 -0.837780 0.000000
C -3.477258 -0.865925 0.000000
H -4.057435 0.051910 0.000000
C -4.075121 -2.100398 0.000000
C -3.325418 -3.304187 0.000000
C -1.934018 -3.309438 0.000000
H -1.380595 -4.244052 0.000000
C -1.285542 -2.071112 0.000000
O -5.393606 -2.401027 0.000000
O -4.158471 -4.355436 0.000000
N 4.132862 4.365244 0.000000
O 5.307738 3.906655 0.000000
O 3.876207 5.599581 0.000000
C -5.500928 -3.830989 0.000000
H -6.014787 -4.163605 0.908254
H -6.014787 -4.163605 -0.908254
el energy= -1200.83263733

acetonitrile-GS-6
B -0.489940 1.601668 -0.008519
O -0.544434 2.964768 -0.001508
H 0.365453 3.320697 0.001808
N 0.798205 0.919600 -0.009715
C 2.061797 1.529840 -0.002180
O 2.233209 2.746920 0.004267
C 3.054950 0.434813 -0.003364
C 4.442568 0.505471 0.008435
H 4.958007 1.463894 0.017126
C 5.172693 -0.700971 0.010377
C 4.464408 -1.931187 0.004894
H 5.036698 -2.857512 0.009949
C 3.072679 -1.984337 -0.006427
H 2.567296 -2.947638 -0.006987
C 2.352127 -0.784971 -0.010854
C 0.922036 -0.483733 -0.015491
C -0.180195 -1.277151 -0.022619
H -0.055278 -2.357244 -0.027532
C -1.526833 -0.730633 -0.023367
C -2.633890 -1.621988 -0.028847
H -2.488648 -2.699164 -0.038279
C -3.894719 -1.066799 -0.021735
C -4.101223 0.319654 -0.012267
C -3.047184 1.207677 -0.011324
H -3.217807 2.281271 -0.008804
C -1.731446 0.681476 -0.015215
O -5.099652 -1.709361 -0.048312
O -5.445817 0.581992 -0.035035
N 6.558296 -0.693267 -0.037330
H 7.004941 0.154360 0.291799
H 7.015915 -1.529983 0.304240
C -6.094138 -0.686803 0.138328
H -6.880303 -0.801293 -0.614316
H -6.500305 -0.756757 1.157548
el energy= -1051.69719743
zpe= -1051.444921
th energy= -1051.427753
th enthalpy= -1051.426809
free energy= -1051.489597

acetonitrile-ES-6
B -0.475105 1.611576 0.000013
O -0.522340 2.983486 0.000015
H 0.408067 3.300558 -0.000008
N 0.809449 0.941375 -0.000067
C 2.079904 1.565679 -0.000097
O 2.226126 2.813790 -0.000046
C 3.047224 0.483612 -0.000078
C 4.437661 0.501783 -0.000025

H 4.995610 1.436383 0.000002
C 5.133470 -0.734322 0.000042
C 4.409527 -1.976704 0.000080
H 4.975231 -2.905667 0.000149
C 3.030757 -1.989366 0.000030
H 2.494379 -2.936122 0.000059
C 2.325590 -0.764299 -0.000063
C 0.937381 -0.458461 -0.000116
C -0.194314 -1.285783 -0.000136
H -0.048650 -2.363002 -0.000162
C -1.501526 -0.755687 -0.000101
C -2.630565 -1.646367 -0.000112
H -2.487867 -2.723733 -0.000174
C -3.875700 -1.086298 -0.000020
C -4.076040 0.317627 0.000084
C -3.021477 1.206836 0.000083
H -3.197275 2.279658 0.000169
C -1.706615 0.688455 -0.000010
O -5.086541 -1.711038 0.000036
O -5.407711 0.584211 0.000215
N 6.488494 -0.760638 -0.000074
H 7.028518 0.094287 0.000823
H 6.993032 -1.636866 0.001201
C -6.087152 -0.683252 -0.000007
H -6.697951 -0.766325 -0.906766
H -6.698208 -0.766504 0.906557
el energy= -1051.68824567

acetonitrile-GS-thieno
B -1.040947 1.442648 -0.000004
O -1.149421 2.796785 -0.000016
H -0.251895 3.186735 -0.000011
N 0.273521 0.803577 0.000004
C 1.504518 1.473427 0.000013
O 1.617316 2.698601 0.000041
C 2.549474 0.431336 0.000027
C 3.938638 0.555444 0.000051
H 4.411387 1.534891 0.000064
C 4.697044 -0.617513 0.000052
C 4.068290 -1.876264 0.000032
H 4.680213 -2.775945 0.000033
C 2.675678 -1.997837 0.000011
H 2.204319 -2.977744 -0.000003
C 1.913970 -0.825574 0.000009
C 0.467873 -0.598880 -0.000004
C -0.573338 -1.468393 -0.000023
H -0.380612 -2.537921 -0.000035
C -1.938178 -0.980825 -0.000034
C -3.079219 -1.755926 -0.000075
H -3.159249 -2.837406 -0.000100
S -4.513088 -0.772588 0.000009
C -3.574845 0.695070 -0.000078
H -4.085288 1.652233 -0.000105
C -2.224189 0.445297 -0.000024
H 5.783166 -0.560978 0.000068
el energy= -740.499914132

zpe= -740.313465
th energy= -740.300443
th enthalpy= -740.299499
free energy= -740.353176

acetonitrile-ES-thieno
B -1.025047 1.449130 0.000005
O -1.118036 2.804369 0.000052
H -0.201820 3.163642 0.000107
N 0.281349 0.802306 0.000021
C 1.551525 1.492194 0.000041
O 1.613137 2.738031 -0.000004
C 2.555573 0.461726 0.000050
C 3.958483 0.525574 0.000057
H 4.471306 1.485424 0.000056
C 4.683302 -0.669178 0.000073
C 4.034796 -1.927821 0.000080
H 4.627013 -2.839491 0.000090
C 2.636651 -2.005210 0.000066
H 2.137210 -2.972275 0.000063
C 1.897361 -0.816805 0.000050
C 0.477402 -0.570559 0.000022
C -0.611642 -1.474293 0.000004
H -0.412219 -2.541654 0.000014
C -1.927037 -0.979625 -0.000028
C -3.112059 -1.755848 -0.000022
H -3.192309 -2.837505 -0.000011
S -4.509974 -0.772160 -0.000203
C -3.559051 0.706959 0.000010
H -4.075994 1.660667 0.000056
C -2.213594 0.457389 -0.000032
H 5.771121 -0.632258 0.000082
el energy= -740.491376144

acetonitrile-GS-7
B 2.483636 1.436092 0.000020
O 2.655710 2.782691 0.000034
H 1.780483 3.219234 0.000033
N 1.139301 0.858503 0.000015
C -0.056428 1.584739 0.000010
O -0.119295 2.812263 -0.000026
C -1.147960 0.587549 -0.000009
C -2.527012 0.787293 -0.000035
H -2.950343 1.787305 -0.000049
C -3.322470 -0.357400 -0.000035
C -2.772676 -1.651186 -0.000013
H -3.425786 -2.518970 -0.000014
C -1.387934 -1.829344 0.000009
H -0.969771 -2.832601 0.000023
C -0.570555 -0.695157 0.000010
C 0.882247 -0.534157 0.000023
C 1.881784 -1.451378 0.000041
H 1.639212 -2.510657 0.000052
C 3.267122 -1.027042 0.000050
C 4.371720 -1.853692 0.000090
H 4.401546 -2.937867 0.000115

S 5.848425 -0.936746 0.000004
C 4.978229 0.572175 0.000093
H 5.530739 1.505572 0.000120
C 3.617807 0.384203 0.000039
Br -5.244249 -0.164952 -0.000065
el energy= -753.071453362
zpe= -752.895441
th energy= -752.880802
th enthalpy= -752.879858
free energy= -752.938448

acetonitrile-ES-7
B -2.478358 1.441414 -0.000011
O -2.649113 2.788584 0.000010
H -1.758566 3.204728 0.000045
N -1.138536 0.866236 0.000006
C 0.090958 1.623118 0.000026
O 0.089847 2.867924 0.000003
C 1.149754 0.647245 0.000031
C 2.545094 0.800641 0.000037
H 3.002022 1.786218 0.000039
C 3.315373 -0.360856 0.000044
C 2.759817 -1.662480 0.000044
H 3.403208 -2.535861 0.000048
C 1.366239 -1.806927 0.000034
H 0.927758 -2.802617 0.000029
C 0.563822 -0.665424 0.000027
C -0.869826 -0.495099 0.000005
C -1.903952 -1.455813 -0.000017
H -1.646430 -2.510577 -0.000017
C -3.246006 -1.033008 -0.000044
C -4.386451 -1.872634 -0.000063
H -4.406783 -2.957362 -0.000064
S -5.835438 -0.966587 -0.000136
C -4.965976 0.561924 -0.000047
H -5.532174 1.487063 -0.000034
C -3.609256 0.385102 -0.000043
Br 5.238746 -0.192106 0.000053
el energy= -753.063346150

acetonitrile-GS-8
B -2.051421 1.439627 -0.000031
O -2.220453 2.785909 0.000019
H -1.345715 3.222906 0.000069
N -0.708103 0.857860 -0.000003
C 0.489825 1.579113 0.000077
O 0.560261 2.805385 -0.000140
C 1.576391 0.575321 -0.000042
C 2.952162 0.760720 -0.000090
H 3.402998 1.747198 -0.000063
C 3.733105 -0.395881 -0.000085
C 3.177548 -1.687439 -0.000084
H 3.837520 -2.547949 -0.000082
C 1.795795 -1.853374 -0.000056
H 1.364093 -2.850296 -0.000054
C 0.990474 -0.707713 -0.000022
C -0.457072 -0.535806 -0.000002
C -1.460268 -1.451354 0.000006
H -1.220314 -2.511175 0.000008
C -2.841579 -1.022179 0.000009
C -3.948473 -1.847130 0.000028
H -3.979570 -2.931244 0.000045
S -5.420939 -0.927431 0.000040
C -4.547768 0.580543 0.000013
H -5.099161 1.514556 0.000020
C -3.188096 0.390172 -0.000015
N 5.192730 -0.257904 0.000053
O 5.664543 0.876363 0.000232
O 5.871601 -1.281768 -0.000010
el energy= -944.998769807
zpe= -944.810002
th energy= -944.794326
th enthalpy= -944.793382
free energy= -944.854073

acetonitrile-ES-8
B -2.060658 1.448912 0.000023
O -2.230482 2.787081 0.000025
H -1.366471 3.243080 0.000045
N -0.710174 0.853790 0.000020
C 0.514759 1.585320 0.000000
O 0.553680 2.806009 -0.000018
C 1.594274 0.584865 0.000011
C 2.967777 0.766036 0.000002
H 3.428664 1.746851 -0.000010
C 3.764803 -0.397695 -0.000001
C 3.177496 -1.684872 0.000013
H 3.833699 -2.547734 0.000008
C 1.791401 -1.841528 0.000024
H 1.353197 -2.836352 0.000030
C 0.993550 -0.690994 0.000020
C -0.458046 -0.505055 0.000016
C -1.491062 -1.441055 0.000011
H -1.245606 -2.498751 0.000005
C -2.840373 -1.010660 -0.000004
C -3.969908 -1.849093 -0.000040
H -3.984882 -2.934040 -0.000050
S -5.429166 -0.947839 0.000008
C -4.550467 0.579940 -0.000051
H -5.111458 1.508363 -0.000071
C -3.196233 0.397927 -0.000003
N 5.185512 -0.274322 -0.000023
O 5.684911 0.889785 -0.000023
O 5.885344 -1.329831 -0.000004
el energy= -944.991286940

acetonitrile-GS-9
B 1.435813 1.435709 0.000585
O 1.571210 2.787991 0.002070
H 0.680702 3.194151 0.001249
N 0.109319 0.823987 -0.001398
C -1.106405 1.519975 -0.001920

O -1.192860 2.747861 -0.000503
C -2.176248 0.501561 -0.005039
C -3.555239 0.674084 -0.003859
H -3.998525 1.667830 -0.002221
C -4.371277 -0.475577 -0.004495
C -3.755284 -1.755634 0.000031
H -4.394442 -2.637171 0.003946
C -2.372073 -1.910400 -0.000684
H -1.937963 -2.907748 0.005449
C -1.565207 -0.766276 -0.004188
C -0.117344 -0.576221 -0.002427
C 0.909474 -1.464051 -0.001956
H 0.697399 -2.530023 -0.003124
C 2.284821 -1.004108 -0.000183
C 3.411306 -1.799973 0.000377
H 3.471446 -2.882784 -0.000416
S 4.865889 -0.843904 0.002423
C 3.954796 0.640716 0.002879
H 4.482503 1.588491 0.004162
C 2.599748 0.416192 0.001209
N -5.751193 -0.367086 -0.064767
H -6.140088 0.512346 0.253699
H -6.274389 -1.168029 0.267698
el energy= -795.858908060
zpe= -795.655978
th energy= -795.641458
th enthalpy= -795.640514
free energy= -795.697203

acetonitrile-ES-9
B 1.420604 1.440488 -0.000004
O 1.551575 2.800048 0.000052
H 0.638771 3.171516 0.000031
N 0.099793 0.841441 -0.000085
C -1.127321 1.561597 -0.000154
O -1.175274 2.819295 -0.000079
C -2.168848 0.559698 -0.000066
C -3.556349 0.676806 0.000038
H -4.048899 1.647322 0.000082
C -4.338975 -0.507818 0.000064
C -3.714059 -1.805148 0.000006
H -4.347891 -2.688570 0.000055
C -2.339951 -1.914957 -0.000078
H -1.871652 -2.896978 -0.000098
C -1.546845 -0.744144 -0.000112
C -0.136639 -0.549387 -0.000111
C 0.915397 -1.473449 -0.000063
H 0.688914 -2.536088 -0.000049
C 2.256510 -1.017371 0.000003
C 3.410331 -1.816259 0.000113
H 3.472581 -2.898901 0.000142
S 4.840399 -0.858820 -0.000052
C 3.934188 0.632383 0.000244
H 4.470273 1.575325 0.000399
C 2.577386 0.415299 0.000032
N -5.689458 -0.427401 0.000259
H -6.159378 0.469051 -0.000061
H -6.263834 -1.260514 -0.000157
el energy= -795.850277500

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