Highly twisted carbazole-borane derivatives. B-N Stereodynamic analysis and consequences on their emission properties.

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Supporting information

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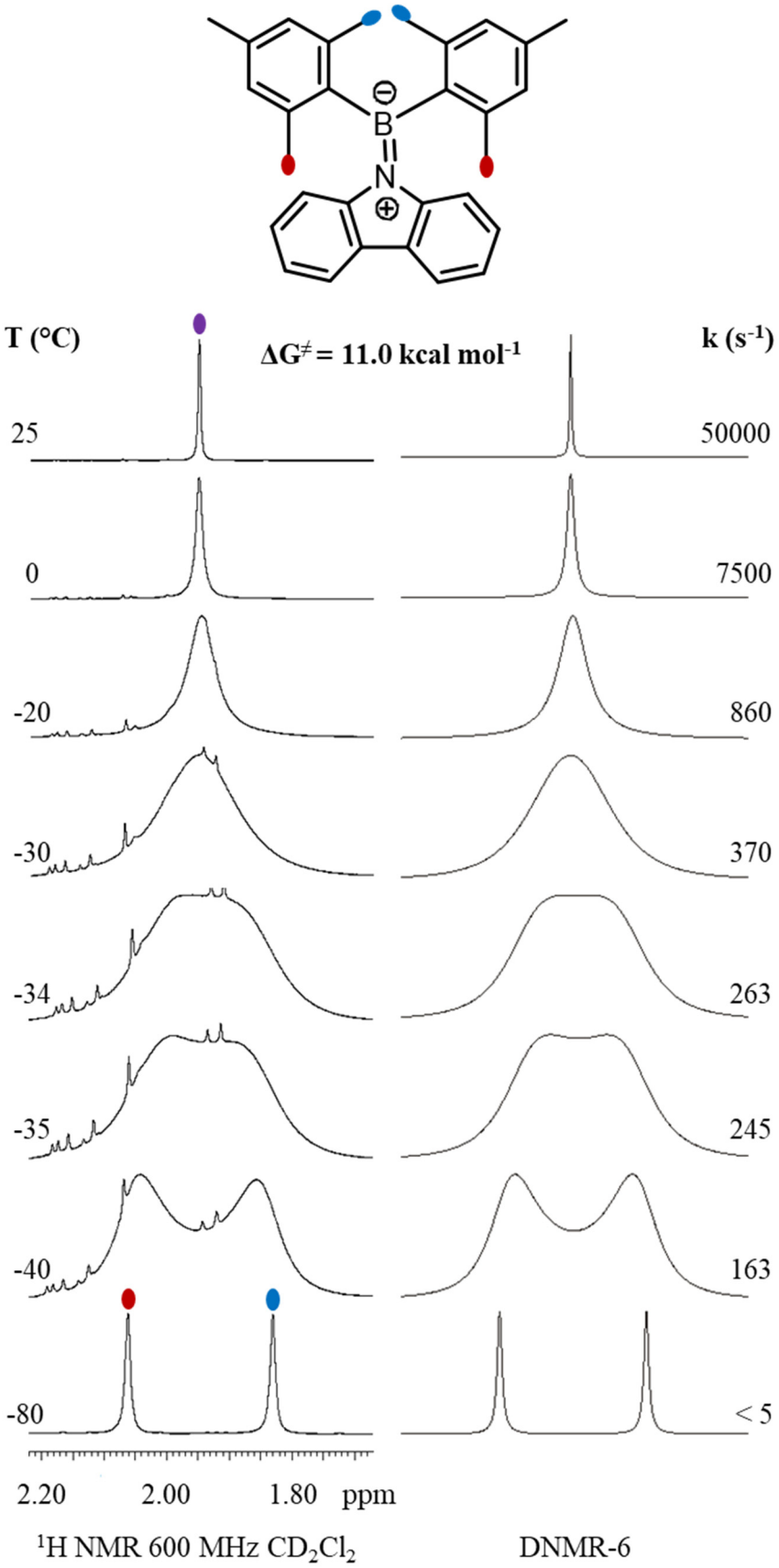


Figure S1. Left: ^{1}H-NMR variable temperature spectra of the *ortho* methyls of compound **1** (600 MHz in CD_2Cl_2). Right: line shape simulation with the corresponding rate constants.

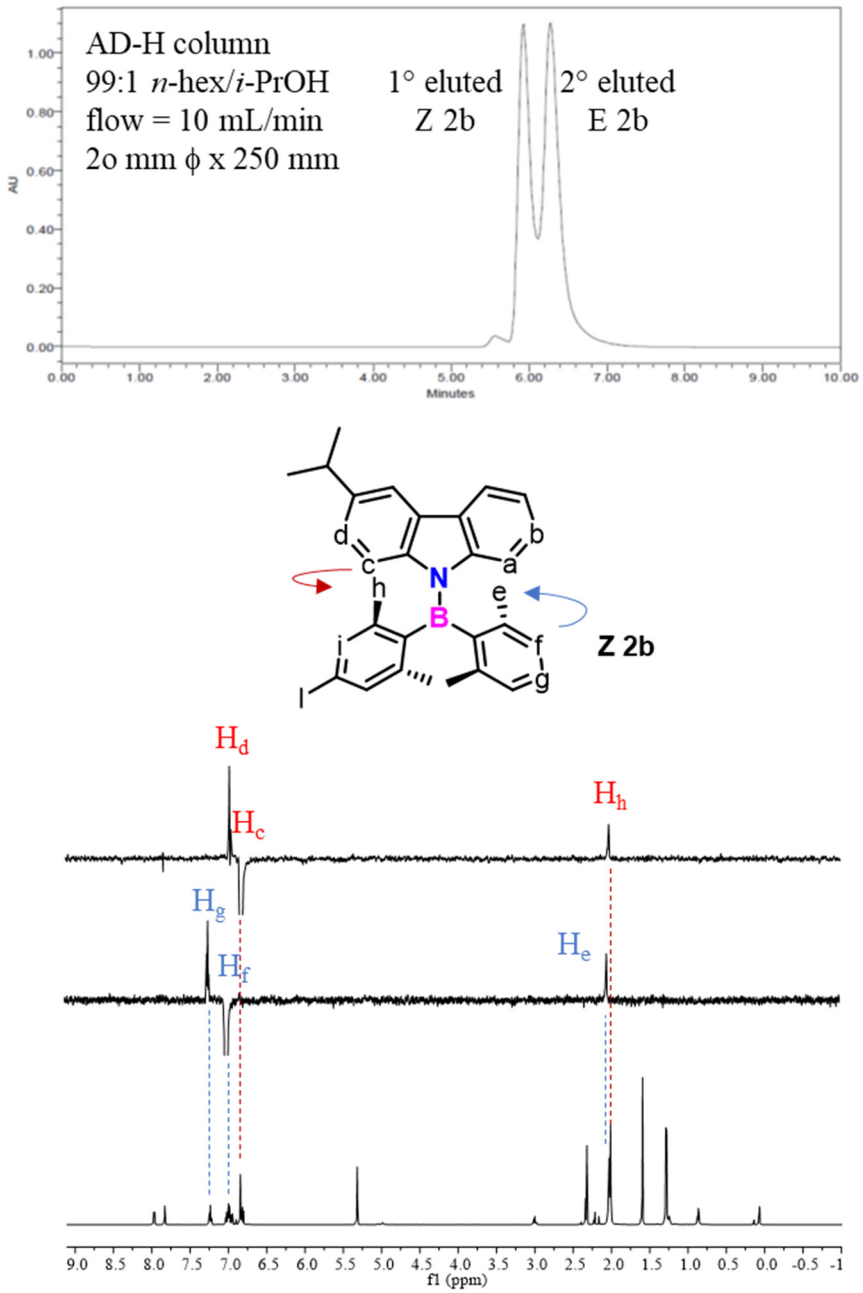


Figure S2. Top: CSP-HPLC separations of two stereoisomer **2b**. Bottom: Characterization of first eluted HPLC by NOESY experiments gives Z configuration (**Z 2b**).

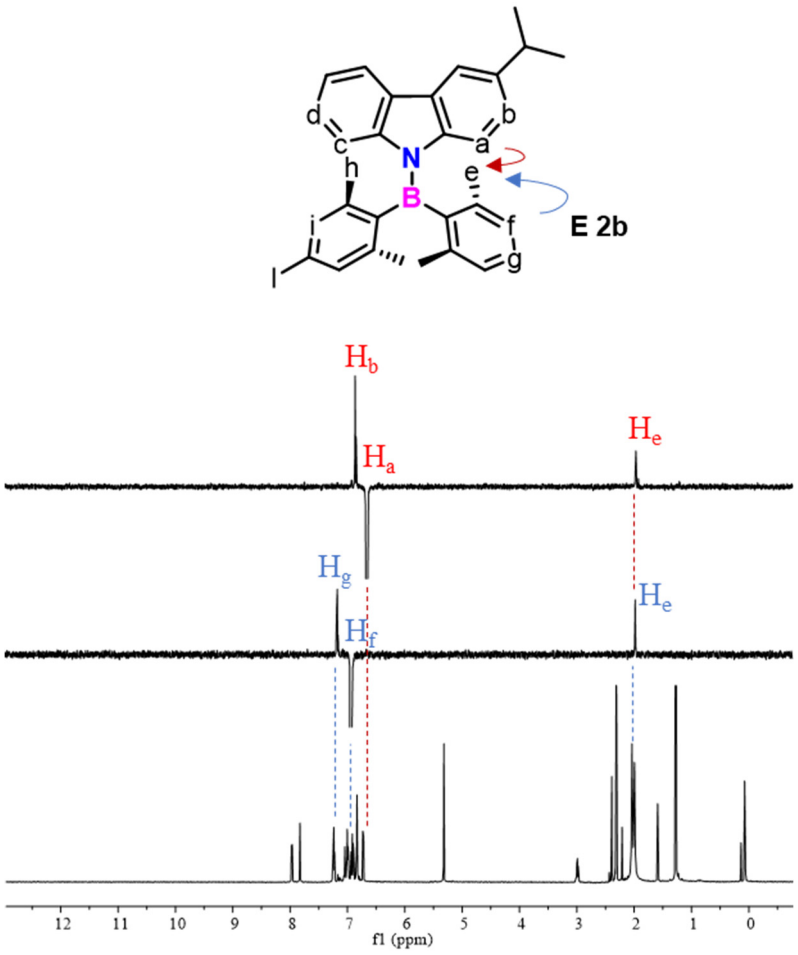
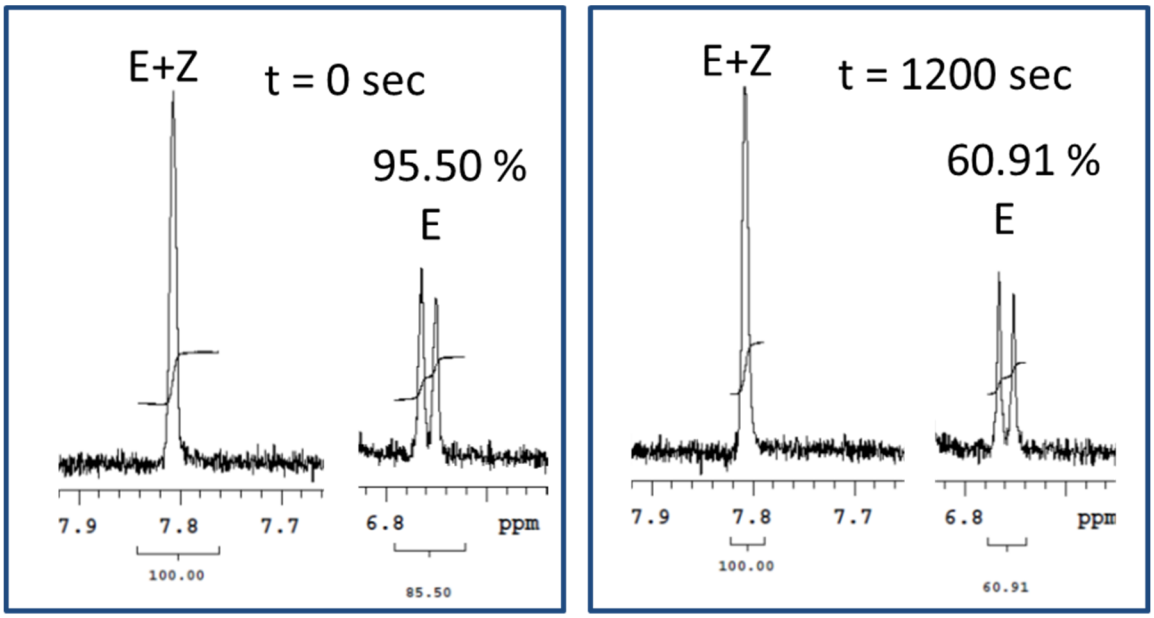
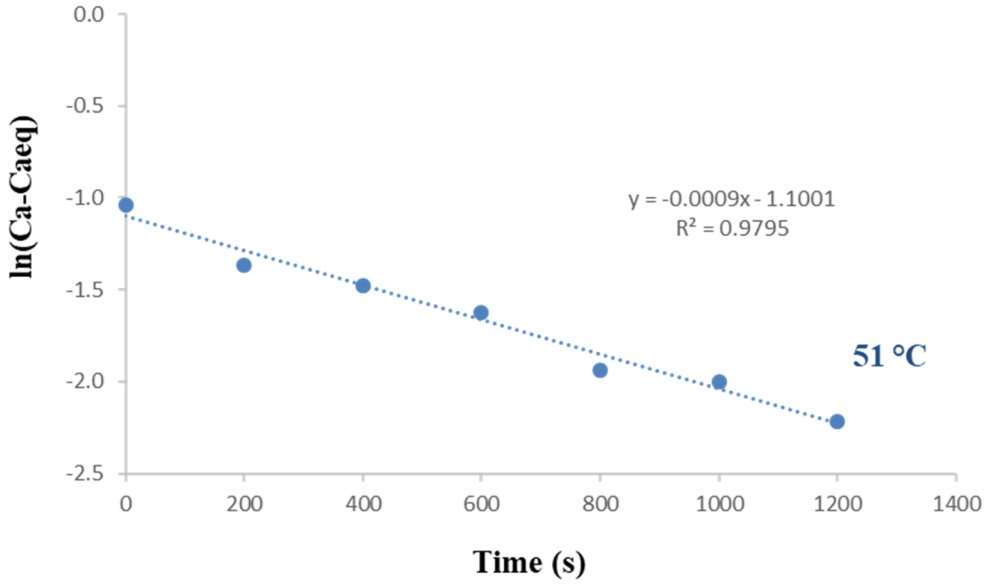


Figure S3. Characterization of second eluted HPLC by NOESY experiments gives E configuration (**E 2b**).





t (s)	T (°C)	
	51	
	% E	ln (Ca - Caeq)
0	85.5	-1.0356
200	75.56	-1.3641
400	72.82	-1.4775
600	69.73	-1.6230
800	64.41	-1.9372
1000	63.55	-1.9988
1200	60.91	-2.2155
$\Delta G^{\neq}$ (kcal/mol)	24.0	

Figure S4. Kinetic analysis starting from the **E-2b** isomer.

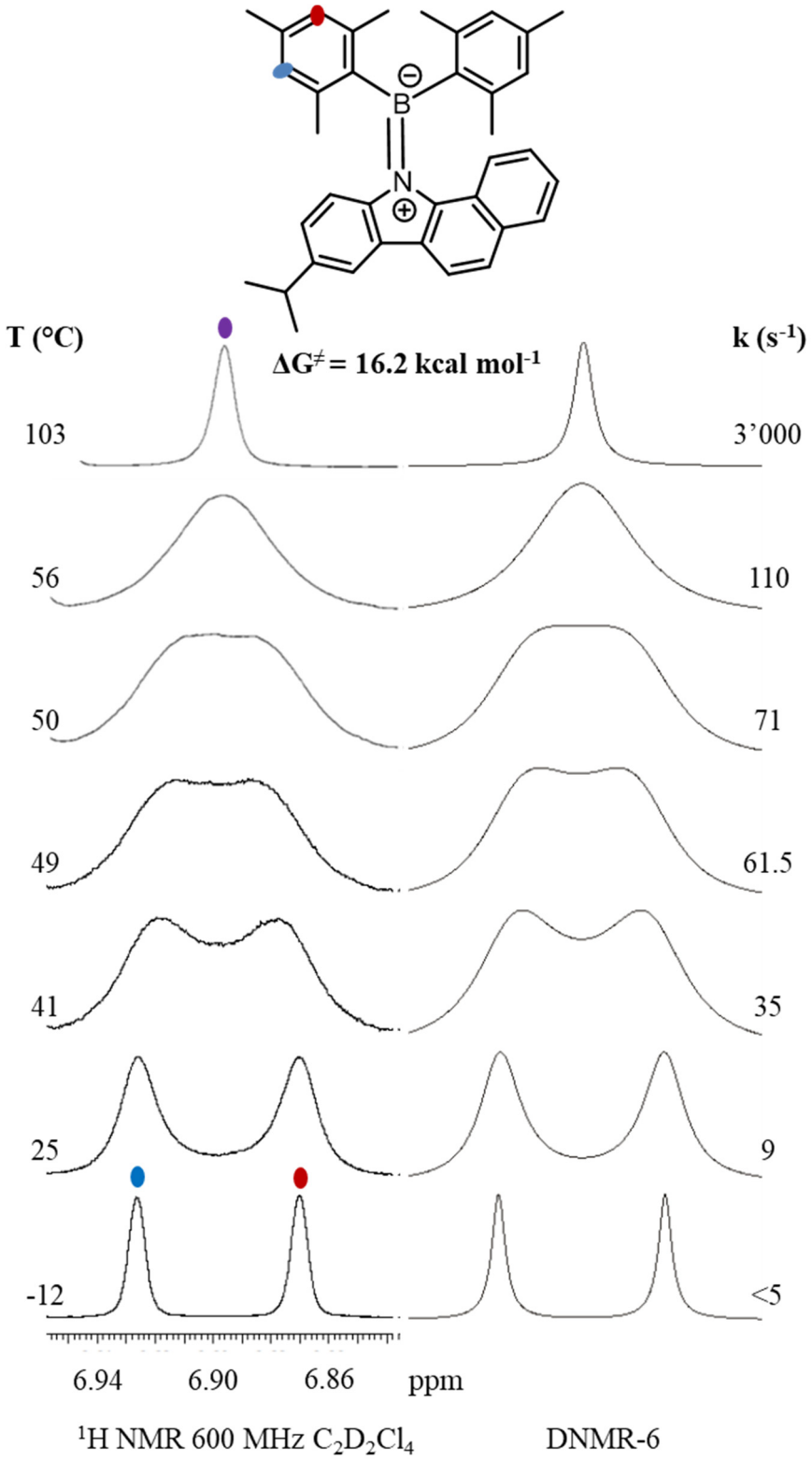
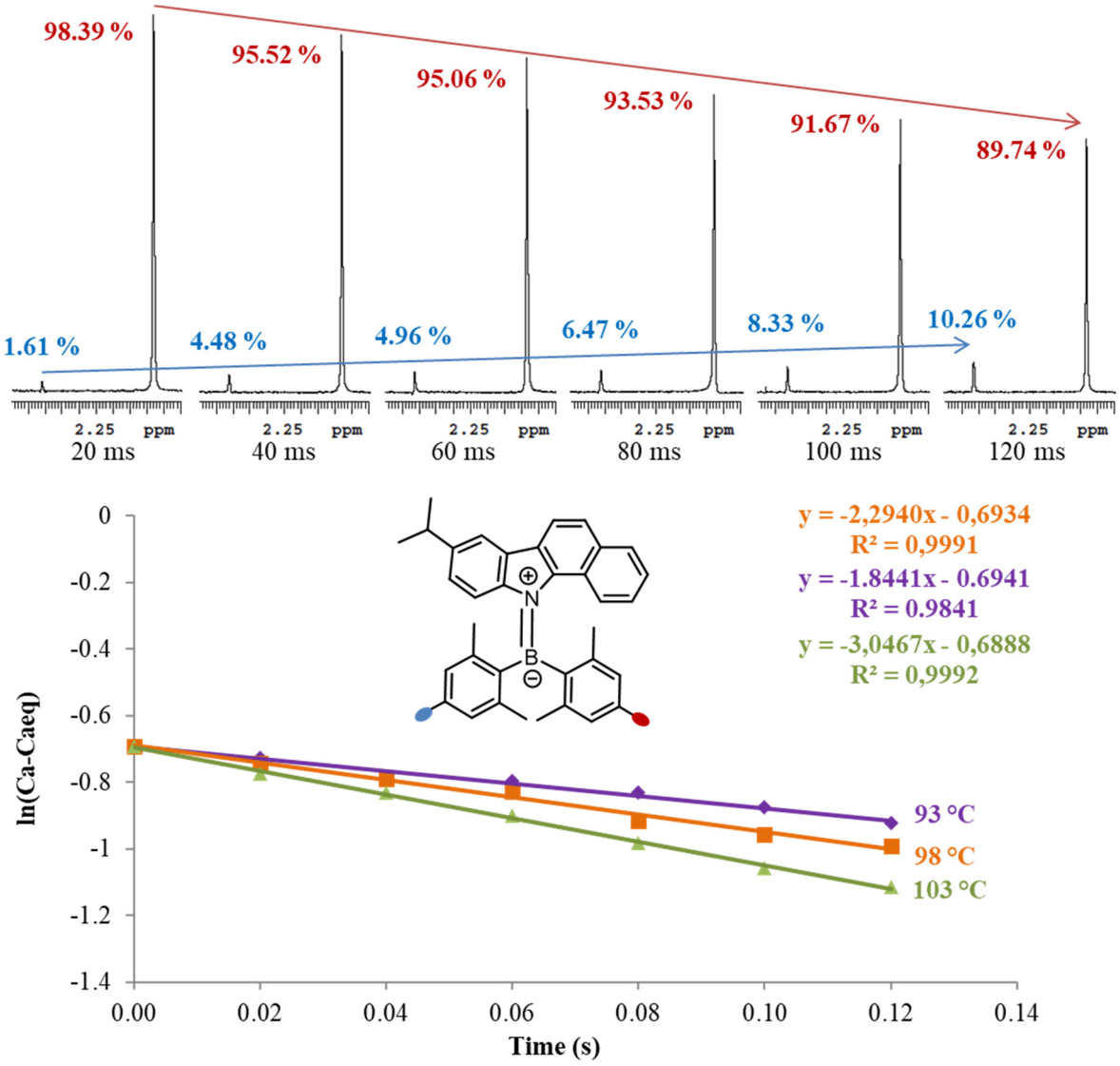


Figure S5. Left: ^{1}H-NMR variable temperature spectra of the *ortho* methyls of compound **6** (600 MHz in $C_2D_2Cl_4$). Right: line shape simulation with the corresponding rate constants.



t (s)	T (°C)		
	93	98	103
	ln (Ca - Caeq)		
0	-0.693	-0.693	-0.693
0.02	-0.733	-0.743	-0.780
0.04	-0.779	-0.789	-0.844
0.06	-0.809	-0.828	-0.909
0.08	-0.839	-0.915	-1.002
0.1	-0.876	-0.957	-1.061
0.12	-0.924	-0.991	-1.141
$\Delta G^{\neq}$ (kcal/mol)	21.63	21.69	21.73
	21.7		

Figure S6. 1D-EXSY spectra were acquired at three different temperatures (+93, +98 and +103 °C) to derive three rate constants useful for the determination of the energy barrier of compound **6**.

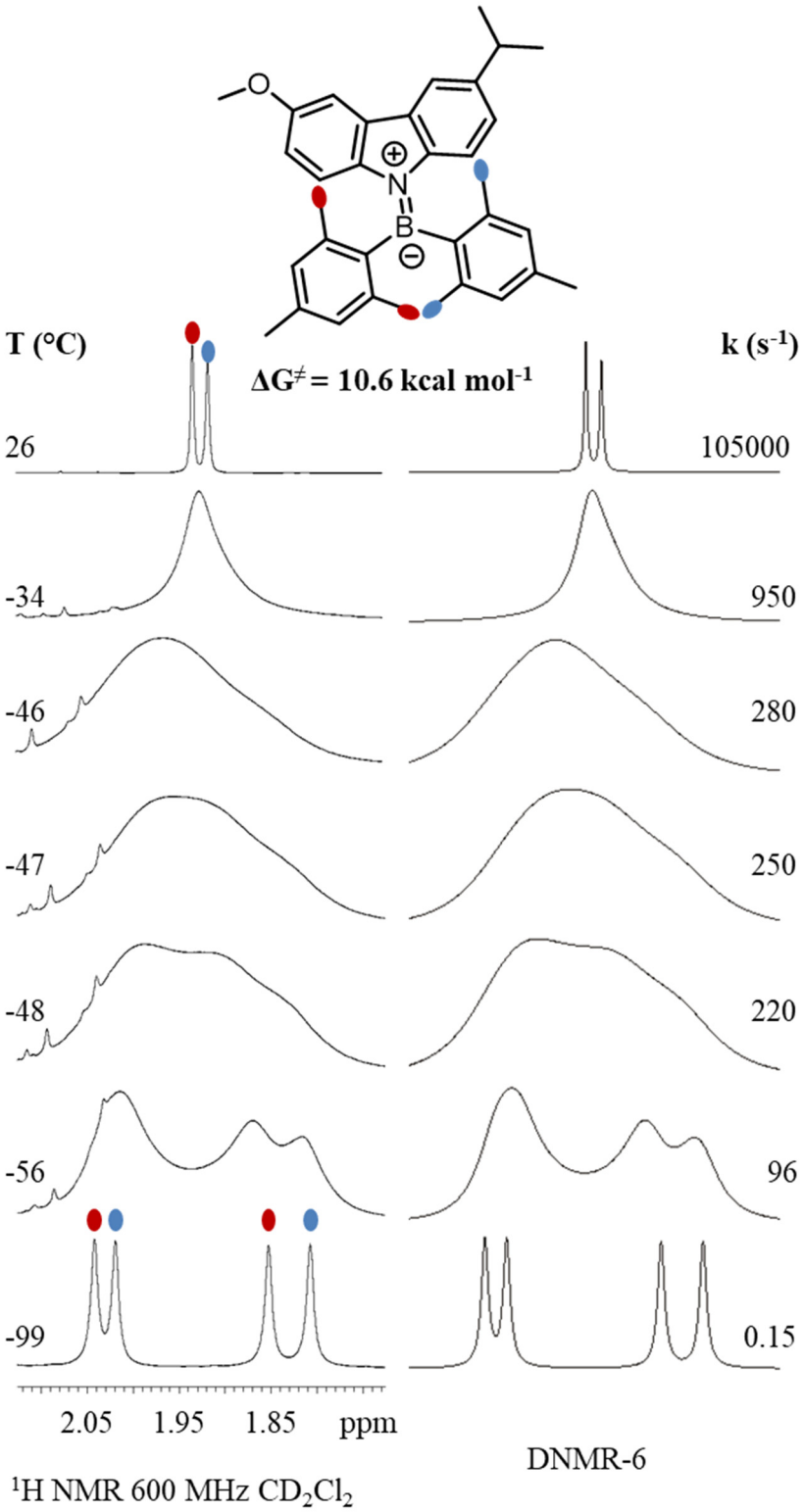


Figure S7. Left: ^{1}H-NMR variable temperature spectra of the *ortho* methyls of compound **3** (600 MHz in CD_2Cl_2). Right: line shape simulation with the corresponding rate constants.

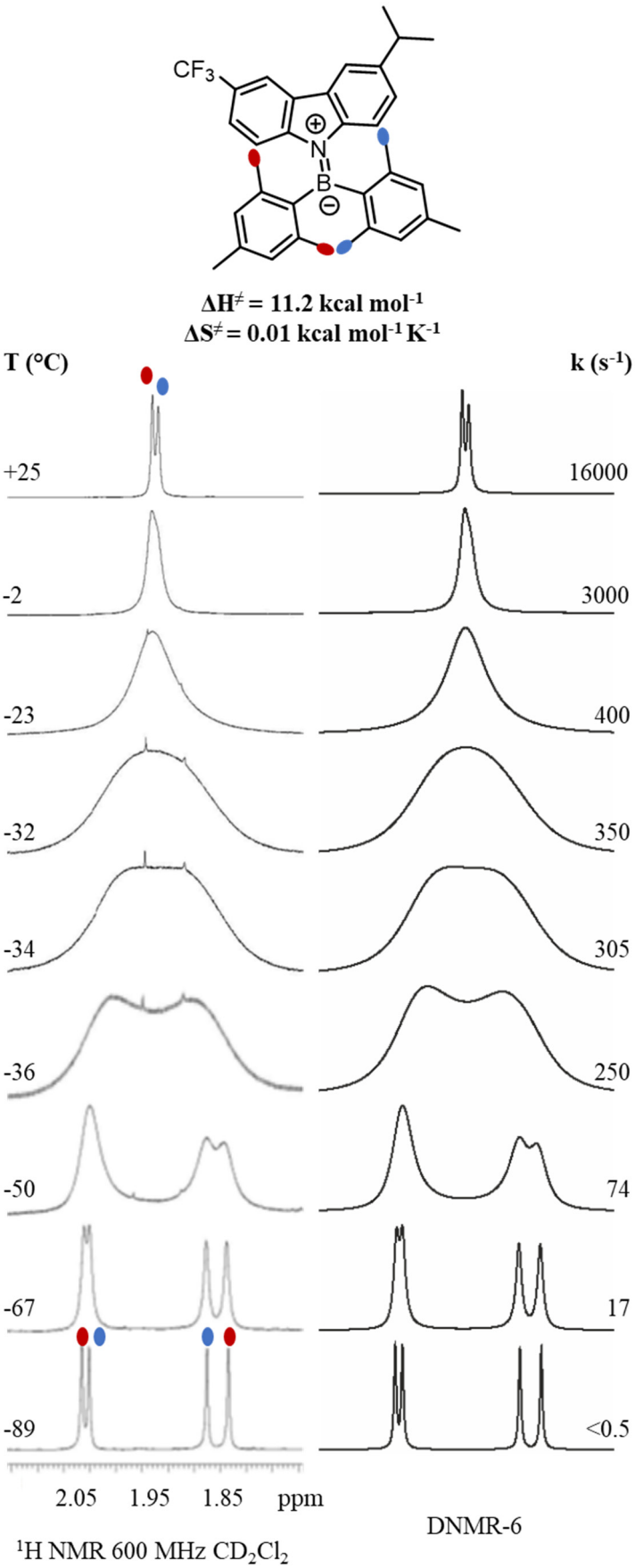


Figure S8. Left: ^{1}H-NMR variable temperature spectra of the *ortho* methyls of compound **4** (600 MHz in CD_2Cl_2). Right: line shape simulation with the corresponding rate constants.

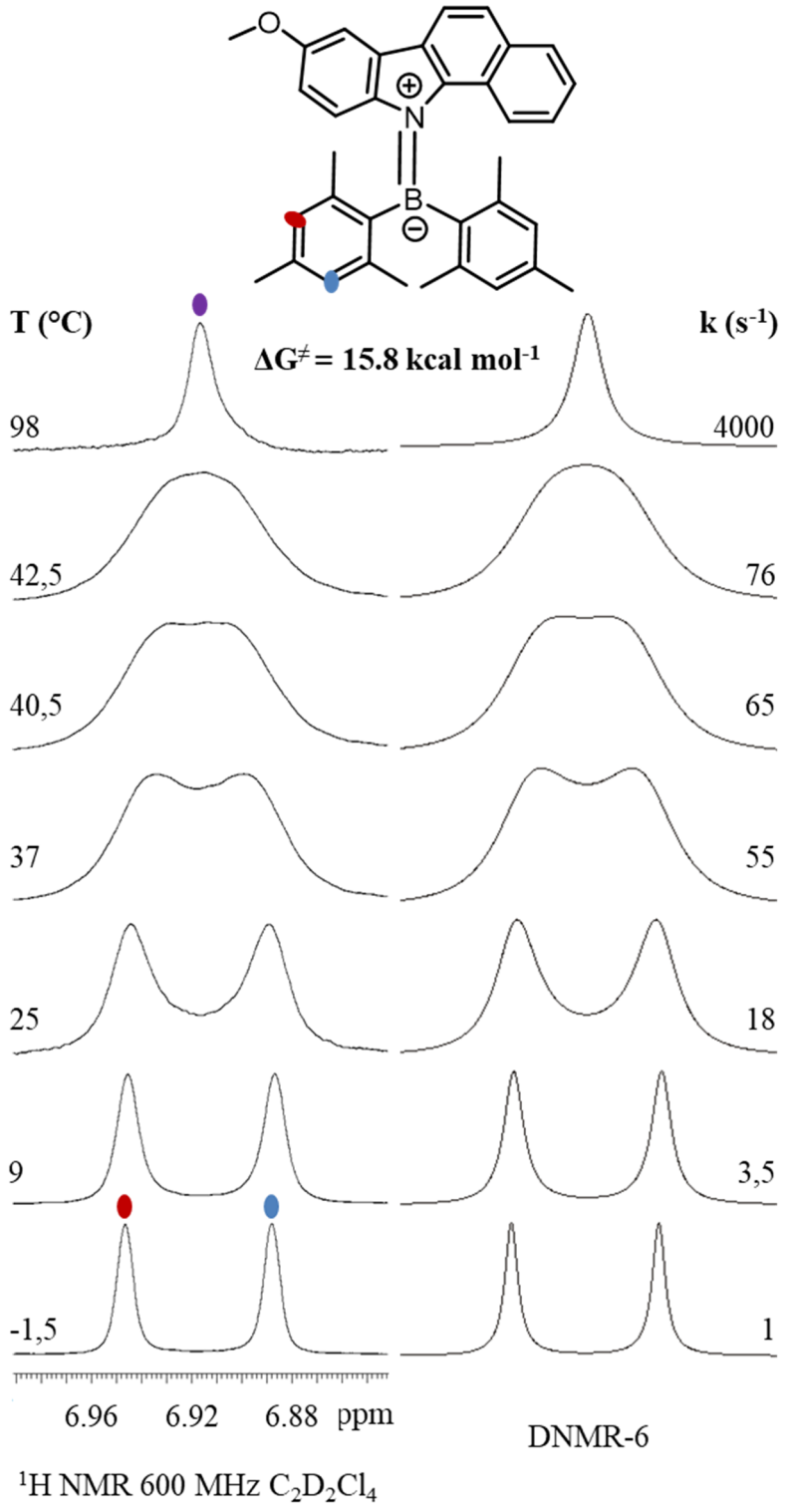


Figure S9. Left: ^{1}H-NMR variable temperature spectra of the *ortho* methyls of compound **7** (600 MHz in $C_2D_2Cl_4$). Right: line shape simulation with the corresponding rate constants.

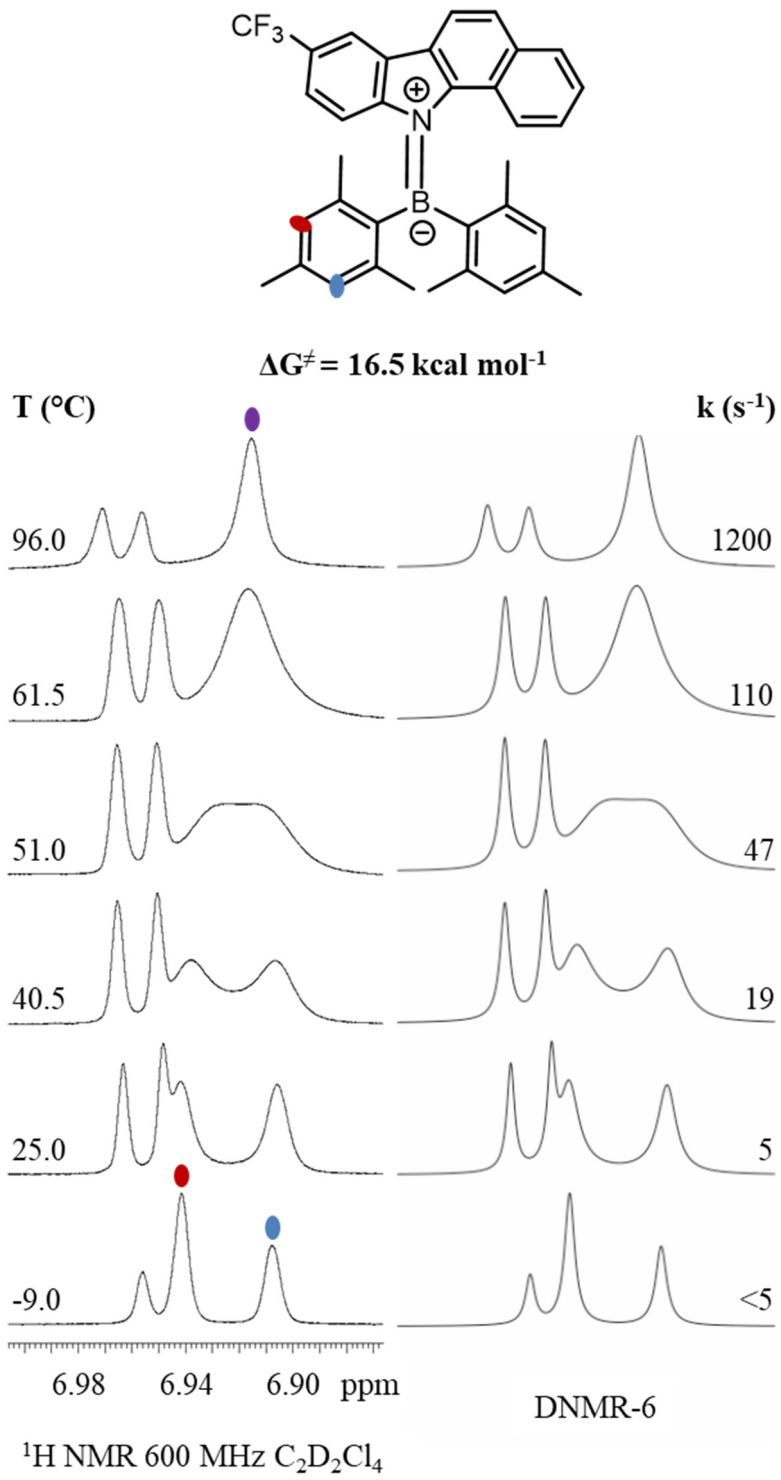
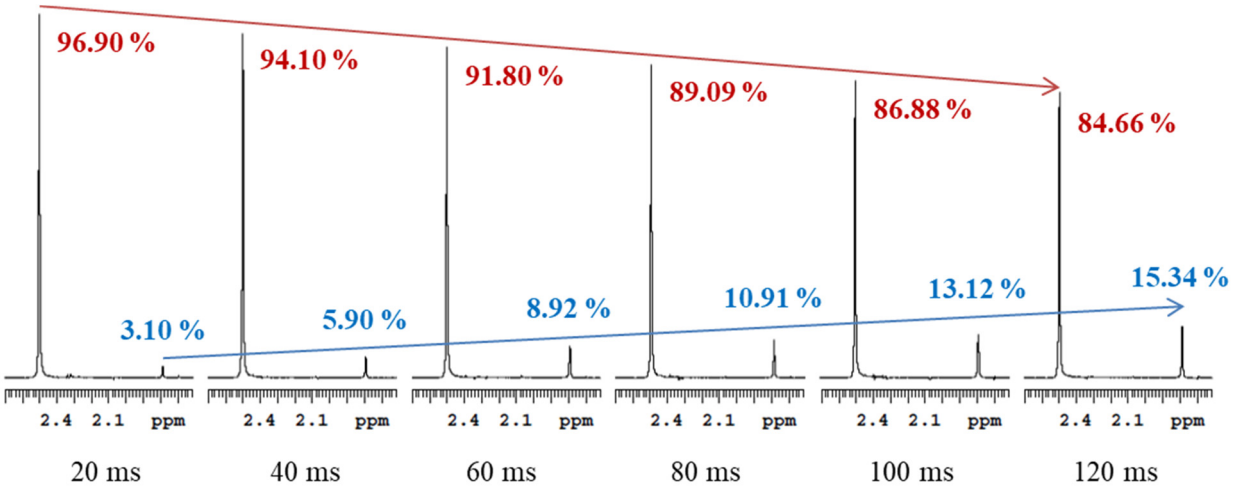
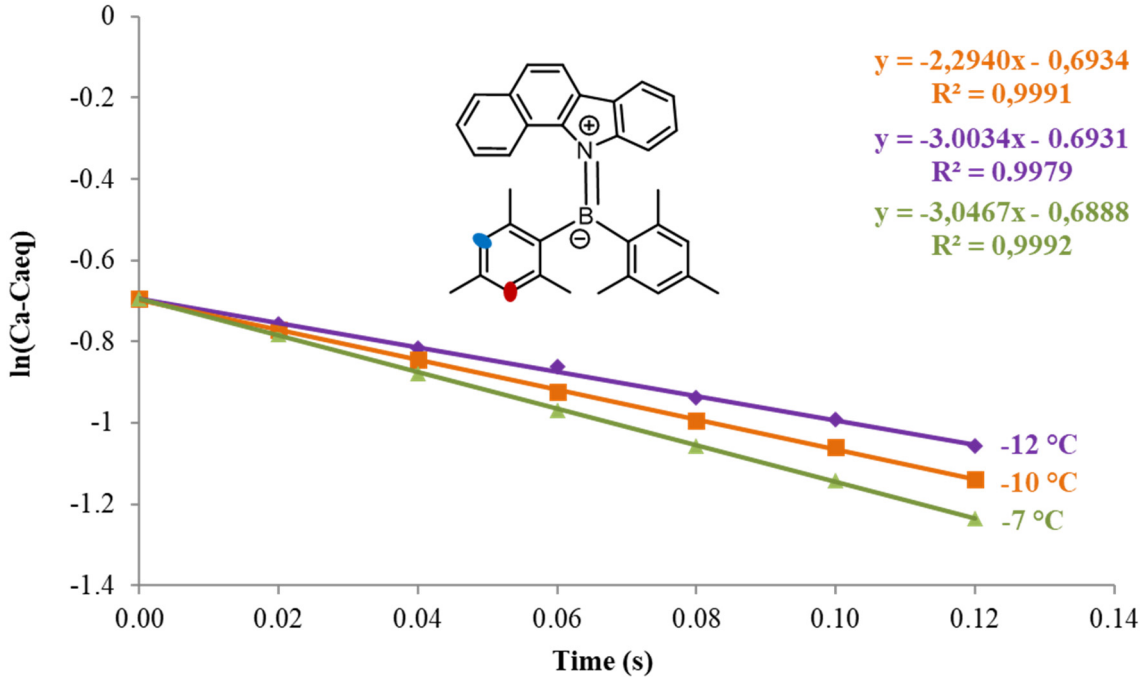


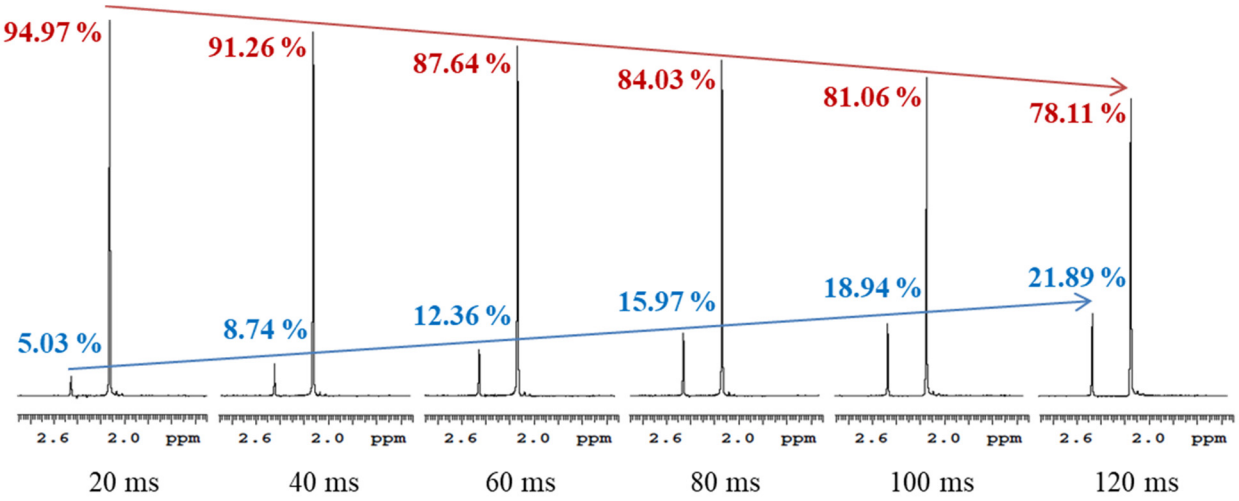
Figure S10. Left: ^{1}H-NMR variable temperature spectra of the *ortho* methyls of compound **8** (600 MHz in $C_2D_2Cl_4$). Right: line shape simulation with the corresponding rate constants.

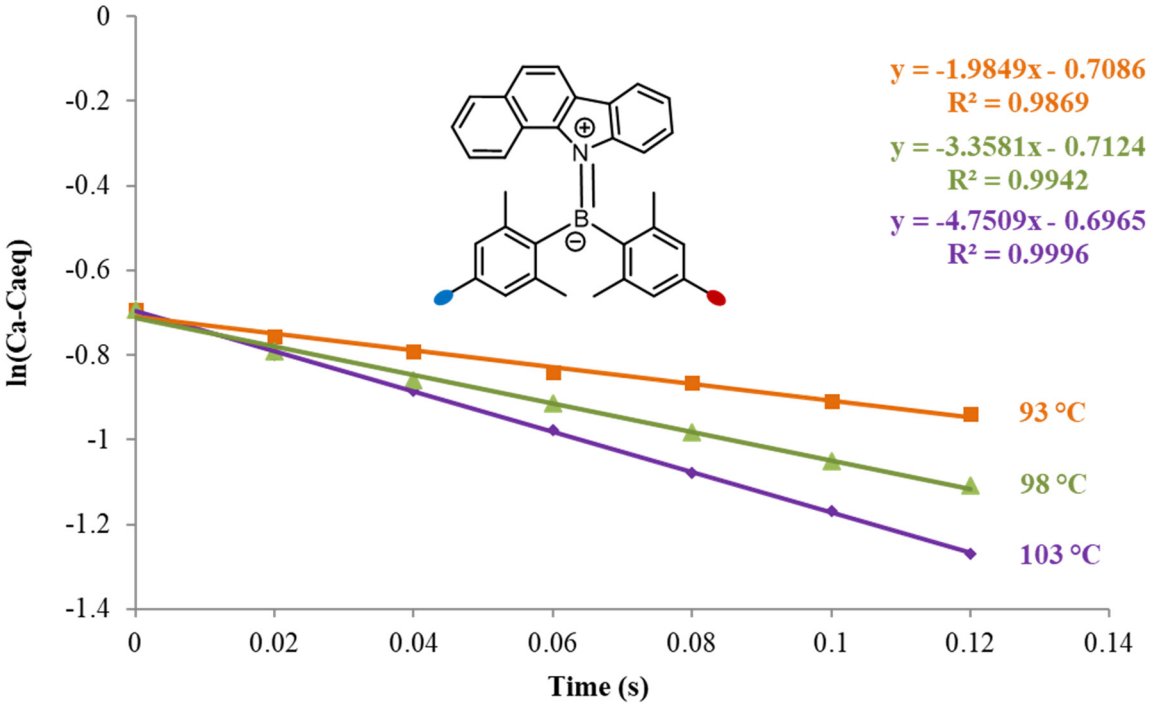




t (s)	T (°C)		
	-12	-10	-7
	ln (Ca - Caeq)		
0.0	-0.693147181	-0.693147181	-0.693147181
0.02	-0.757152511	-0.772190388	-0.783071888
0.04	-0.818710404	-0.84304027	-0.87803202
0.06	-0.872273846	-0.922560345	-0.968110481
0.08	-0.939303506	-0.99479296	-1.056127677
0.10	-0.997500787	-1.060161102	-1.141624179
0.12	-1.059583902	-1.140059479	-1.233744963
$\Delta G^{\neq}$ (kcal/mol)	15.00	15.01	15.08
	15.0		

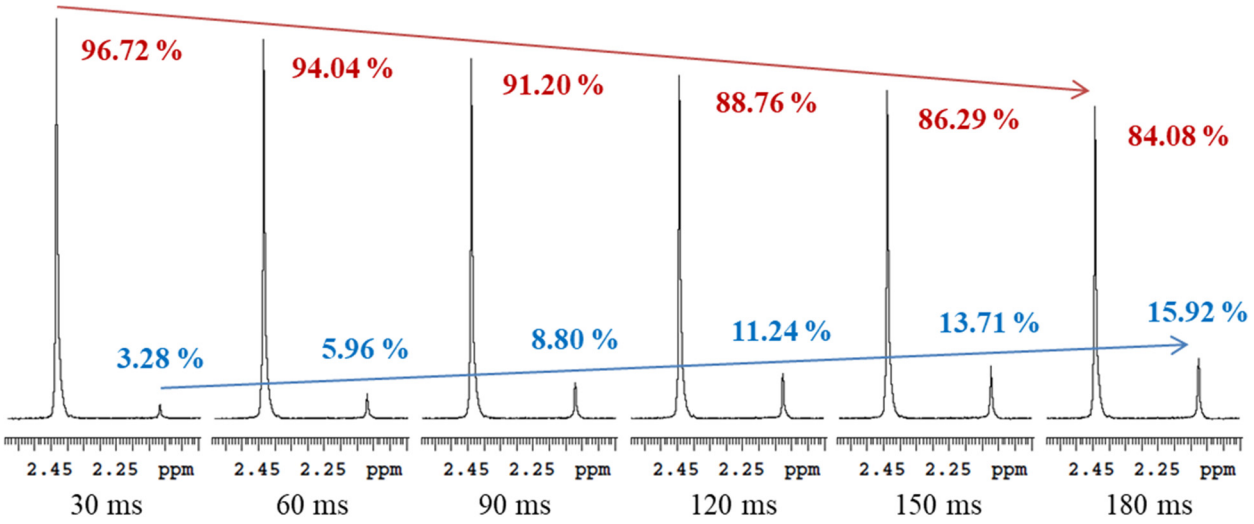
Figure S11. 1D-EXSY spectra were acquired at three different temperatures (-12, -10 and -7 °C) to derive three rate constants useful for the determination of the energy barrier of compound **5**.

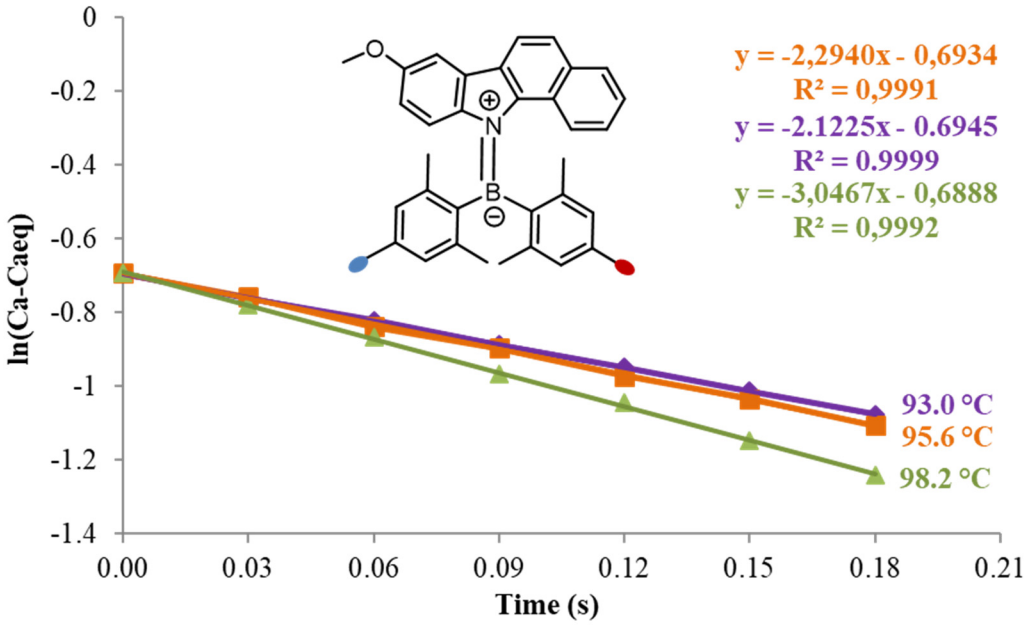




t (s)	T (°C)		
	93	98	103
	ln (Ca - Caeq)		
0	-0.693147181	-0.693147181	-0.693147181
0.02	-0.756299996	-0.792083928	-0.799174585
0.04	-0.792304752	-0.858257701	-0.885276678
0.06	-0.841183259	-0.915041512	-0.977102871
0.08	-0.86441011	-0.981896489	-1.077927697
0.1	-0.908322562	-1.049536451	-1.169249368
0.12	-0.93828075	-1.10714862	-1.269044801
$\Delta G^{\neq}$ (kcal/mol)	21.58	21.50	21.54
	21.5		

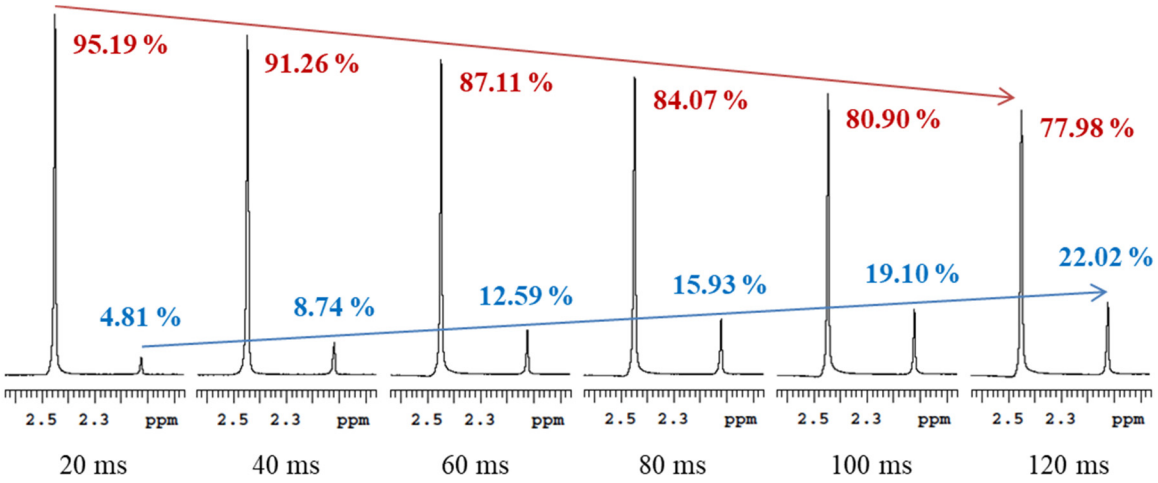
Figure S12. 1D-EXSY spectra were acquired at three different temperatures (93, 98 and 103 °C) to derive three rate constants useful for the determination of the energy barrier of compound **5**.

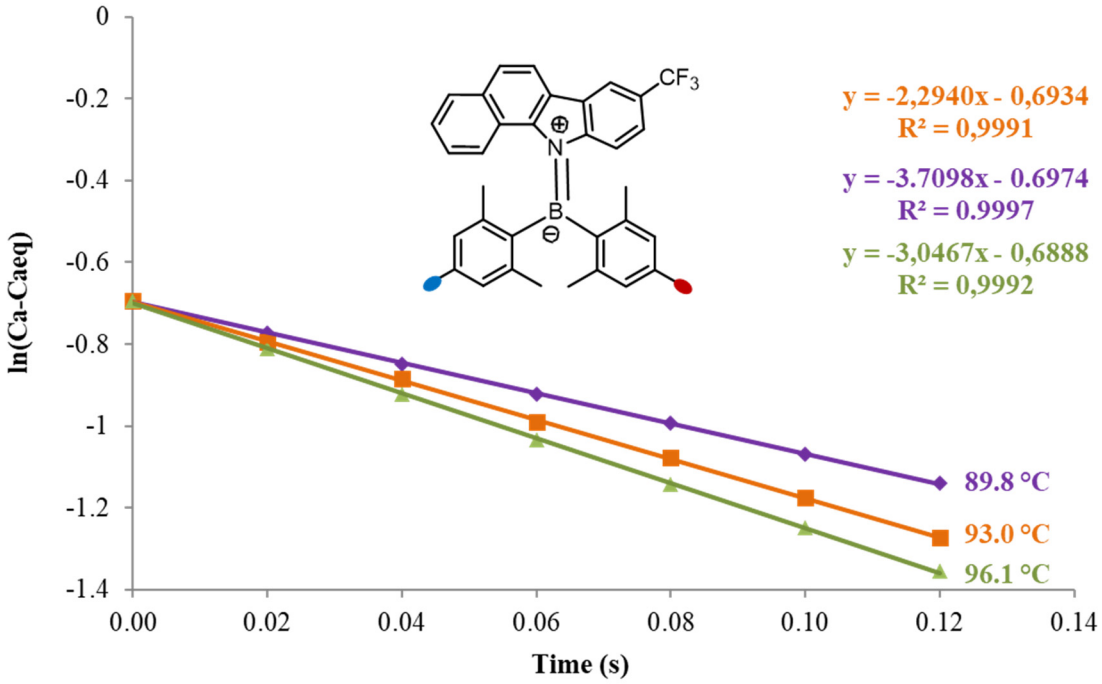




t (s)	T (°C)		
	93	95.6	98.2
	ln (Ca - Caeq)		
0	-0.693147181	-0.693147181	-0.693147181
0.03	-0.760997847	-0.757152511	-0.780013114
0.06	-0.820071874	-0.838635487	-0.867500568
0.09	-0.88673193	-0.897468978	-0.966531948
0.12	-0.947781399	-0.972067747	-1.044124103
0.15	-1.013627965	-1.033386504	-1.14696255
0.18	-1.076459484	-1.106846094	-1.242713633
$\Delta G^{\neq}$ (kcal/mol)	21.53	21.63	21.58
	21.6		

Figure S13. 1D-EXSY spectra were acquired at three different temperatures (93, 95.6 and 98.2 °C) to derive three rate constants useful for the determination of the energy barrier of compound **7**.





t (s)	T (°C)		
	89.8	93	96.1
	ln (Ca - Caeq)		
0	-0.693147181	-0.693147181	-0.693147181
0.02	-0.773489933	-0.794294363	-0.809680997
0.04	-0.849333264	-0.885276678	-0.923063616
0.06	-0.921303274	-0.991283711	-1.033105486
0.08	-0.993711879	-1.076752954	-1.141937413
0.1	-1.068277089	-1.174414002	-1.248621556
0.12	-1.140998005	-1.273680217	-1.355183366
$\Delta G^{\neq}$ (kcal/mol)	20.93	20.94	21.02
	21.0		

Figure S14. 1D-EXSY spectra were acquired at three different temperatures (89.9, 93.0 and 96.1 °C) to derive three rate constants useful for the determination of the energy barrier of compound **8**.

Table S1. Photophysical data summary for compounds **2 –8**

Compd	Solvent	$\Delta\theta$ $s1^{q\text{-}GSeq}$ calc. (°)	Stokes Shift calc. (eV)	Stokes Shift sper. (eV)	ΔE-abs E_4-E_3	ΔE-emi E_6-E_7	ΔE-S^1 E_4-E_6 (eV)	ΔE-S^0 E_7-E_3 (eV)
2a	HEX	33.3	1.39	1.07	4.27	2.88	0.89	0.50
	THF	32.4	1.66	1.23	4.30	2.64	1.11	0.55
	ACN	31.9	1.77	1.32	4.32	2.54	1.20	0.58
2a-E	HEX	32.9	1.44	/	4.28	2.83	0.92	0.52
	THF	31.9	1.71	/	4.29	2.58	1.15	0.57
	ACN	31.8	1.84	/	4.31	2.47	1.24	0.60
2a-Z	HEX	33.2	1.44	/	4.26	2.83	0.91	0.52
	THF	32.4	1.72	/	4.29	2.57	1.15	0.57
	ACN	31.9	1.83	/	4.31	2.47	1.24	0.60
3	HEX	34.8	1.52	1.11	4.16	2.64	0.94	0.58
	THF	33.7	1.86	1.31	4.19	2.33	1.22	0.65
	ACN	33.4	2.00	1.41	4.22	2.21	1.32	0.68
4	HEX	29.1	1.21	0.95	4.25	3.04	0.74	0.47
	THF	28.1	1.47	1.12	4.26	2.79	0.96	0.51
	ACN	28.1	1.60	1.22	4.29	2.69	1.07	0.54
5	HEX	27.0	1.10	0.96	3.89	2.80	0.68	0.40
	THF	25.6	1.38	1.01	3.91	2.52	0.92	0.46
	ACN	24.2	1.52	1.17	3.92	2.40	1.02	0.50
6	HEX	27.3	1.09	0.96	3.89	2.79	0.69	0.40
	THF	25.4	1.36	1.02	3.90	2.53	0.91	0.46
	ACN	24.9	1.50	1.23	3.91	2.41	1.01	0.49
7	HEX	27.6	1.13	1.01	3.87	2.76	0.71	0.41
	THF	26.4	1.42	1.04	3.89	2.46	0.95	0.47
	ACN	25.8	1.55	1.24	3.90	2.34	1.05	0.51
8	HEX	24.9	1.02	0.78	3.91	2.90	0.62	0.40
	THF	23.3	1.34	0.97	3.94	2.59	0.88	0.46
	ACN	22.5	1.49	1.05	3.95	2.46	0.99	0.50

Table S2. Photophysical data summary for compound **2 –8**

Compd	Solvent	ΔE-abs E_4-E_3	ΔE-emi E_6-E_7	ΔE-S^1 E_4-E_6 (eV)	ΔE-S^0 E_7-E_3 (eV)
2a	HEX	4.27	2.88	0.89	0.50
	THF	4.30	2.64	1.11	0.55
	ACN	4.32	2.54	1.20	0.58
2b-E	HEX	4.28	2.83	0.92	0.52
	THF	4.29	2.58	1.15	0.57
	ACN	4.31	2.47	1.24	0.60
2b-Z	HEX	4.26	2.83	0.91	0.52
	THF	4.29	2.57	1.15	0.57
	ACN	4.31	2.47	1.24	0.60
3	HEX	4.16	2.64	0.94	0.58
	THF	4.19	2.33	1.22	0.65
	ACN	4.22	2.21	1.32	0.68
4	HEX	4.25	3.04	0.74	0.47
	THF	4.26	2.79	0.96	0.51
	ACN	4.29	2.69	1.07	0.54
5	HEX	3.89	2.80	0.68	0.40
	THF	3.91	2.52	0.92	0.46
	ACN	3.92	2.40	1.02	0.50
6	HEX	3.89	2.79	0.69	0.40
	THF	3.90	2.53	0.91	0.46
	ACN	3.91	2.41	1.01	0.49
7	HEX	3.87	2.76	0.71	0.41
	THF	3.89	2.46	0.95	0.47
	ACN	3.90	2.34	1.05	0.51
8	HEX	3.91	2.90	0.62	0.40
	THF	3.94	2.59	0.88	0.46
	ACN	3.95	2.46	0.99	0.50

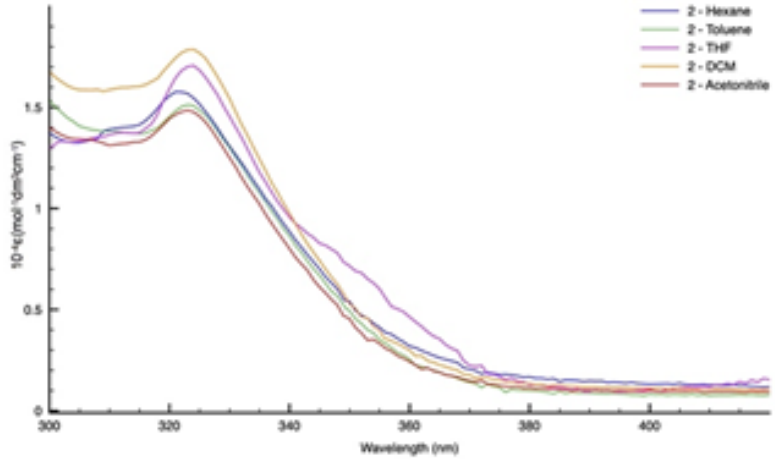


Figure S15: Absorption Profiles of compound **2a**, 298K, 10^{-5} M.

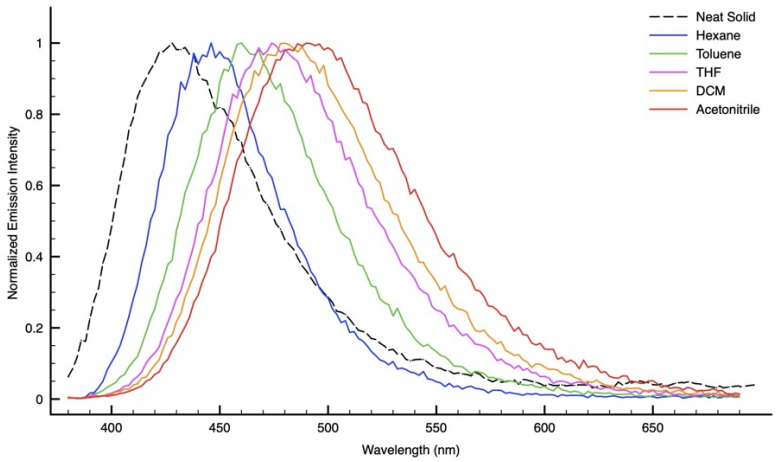


Figure S16: Normalized Emission Profiles of compound **2a**, 298K.

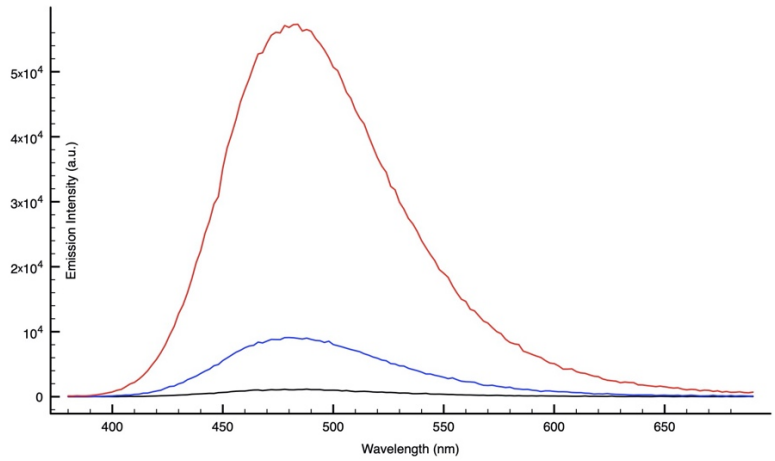


Figure S17: Emission Profiles of compound **2a**, 10^{-6} M (black line), 10^{-5} M (blue line) and 10^{-4}M (red line), CH_2Cl_2, λ_{exc} = 350 nm, 298K.

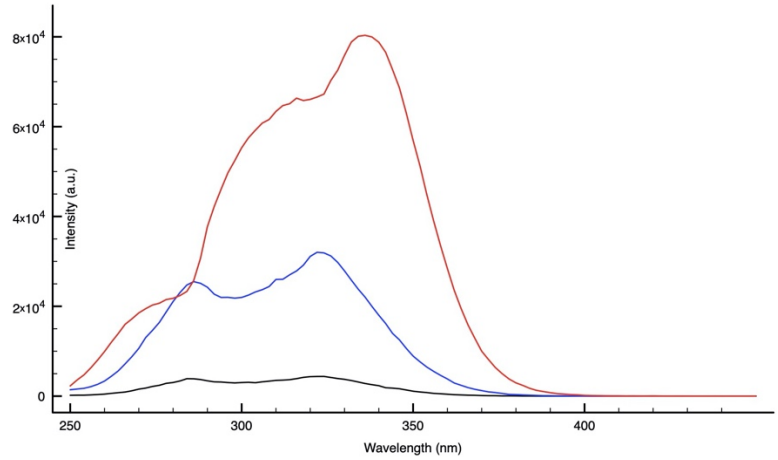


Figure S18: Excitation profiles of compound **2a**, 10^{-6} M (black line), 10^{-5} M (blue line) and 10^{-4}M (red line), CH_2Cl_2, λ_{emi} = 482 nm, 298K.

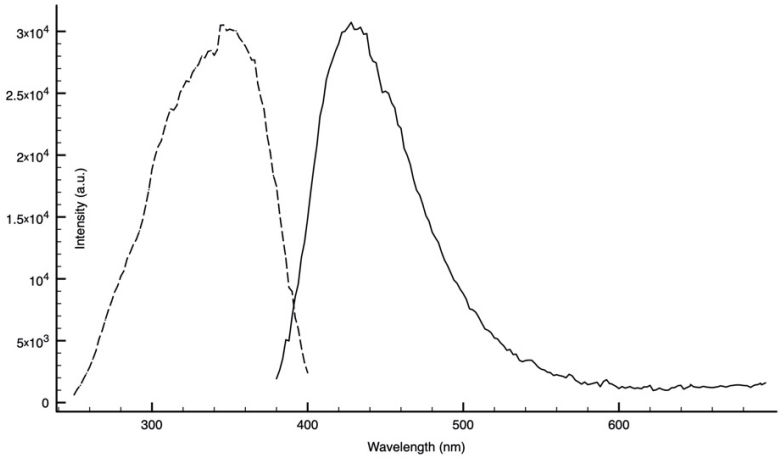


Figure S19: Emission (solid line) and Excitation (dashed line) profiles of compound **2a**, Neat solid Matrix, 298K.

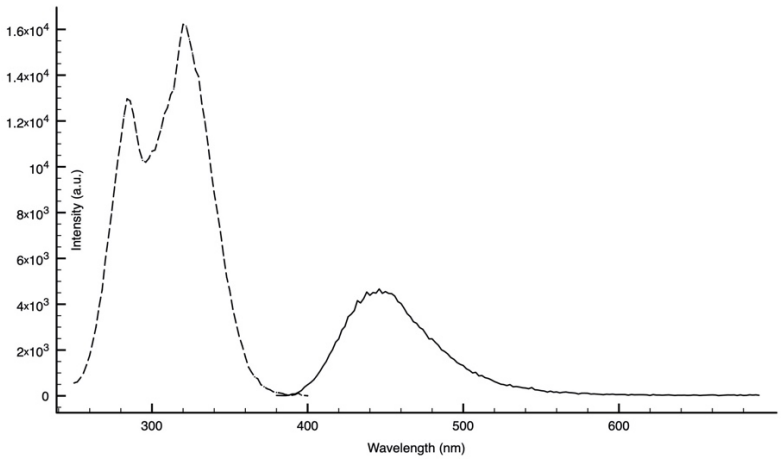


Figure S20: Emission (solid line) and Excitation (dashed line) profiles of compound **2a**, 10^{-5} M Hexane, 298K.

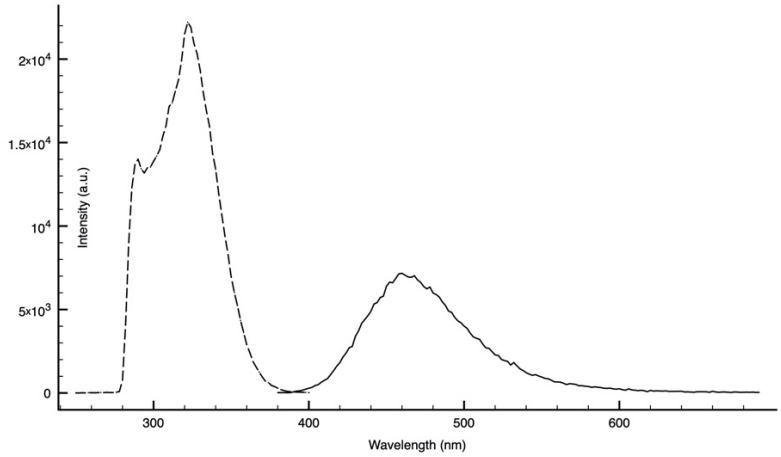


Figure S21: Emission (solid line) and Excitation (dashed line) profiles of compound **2a**, 10^{-5} M Toluene, 298K.

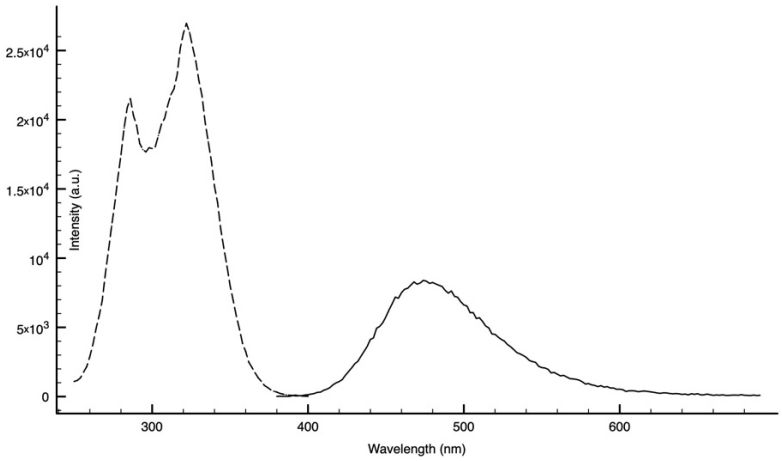


Figure S22: Emission (solid line) and Excitation (dashed line) profiles of compound **2a**, 10^{-5} M THF, 298K.

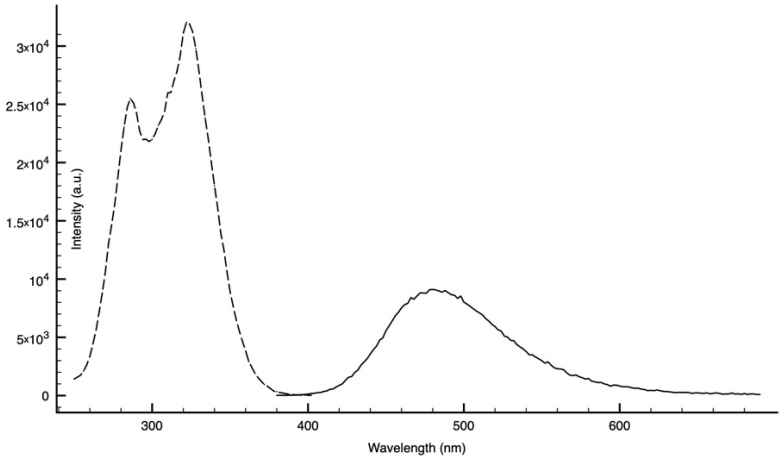


Figure S23: Emission (solid line) and Excitation (dashed line) profiles of compound **2a**, 10^{-5} M DCM, 298K.

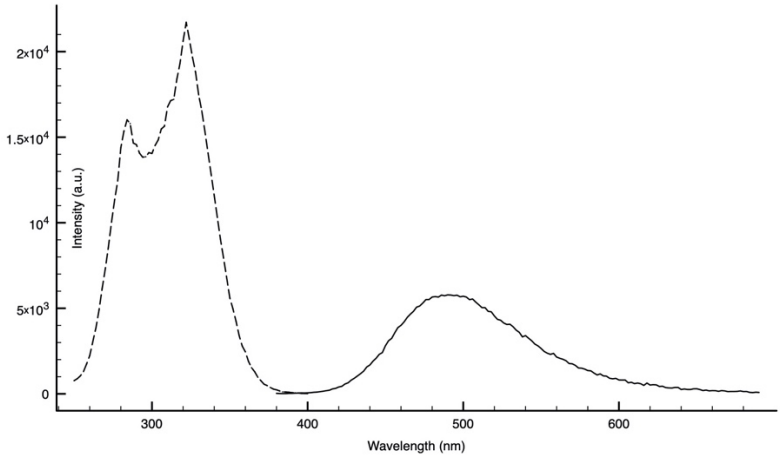


Figure S24: Emission (solid line) and Excitation (dashed line) profiles of compound **2a**, 10^{-5} M Acetonitrile, 298K.

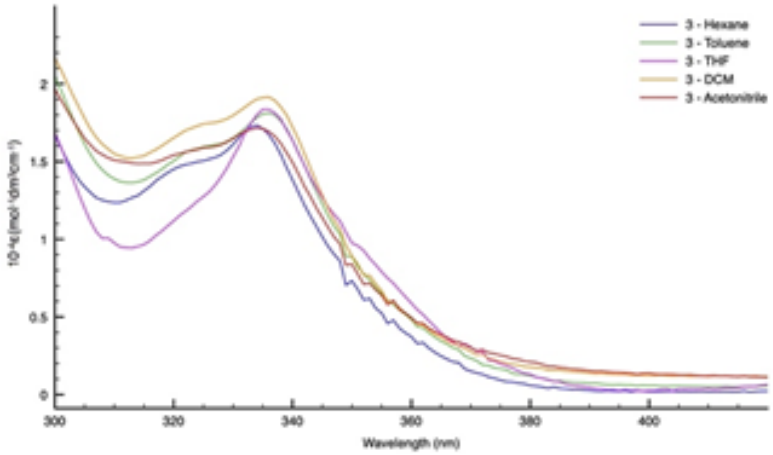


Figure S25: Absorption Profiles of compound **3**, 298 K, 10^{-5} M .

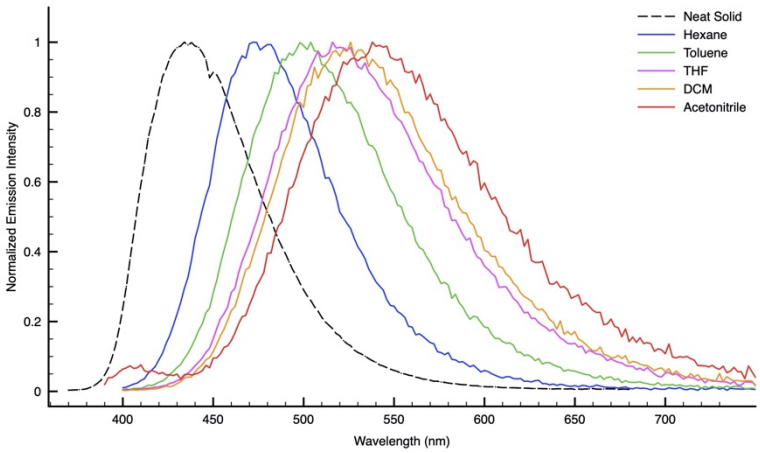


Figure S26: Normalized Emission Profiles of compound **3**, 298K.

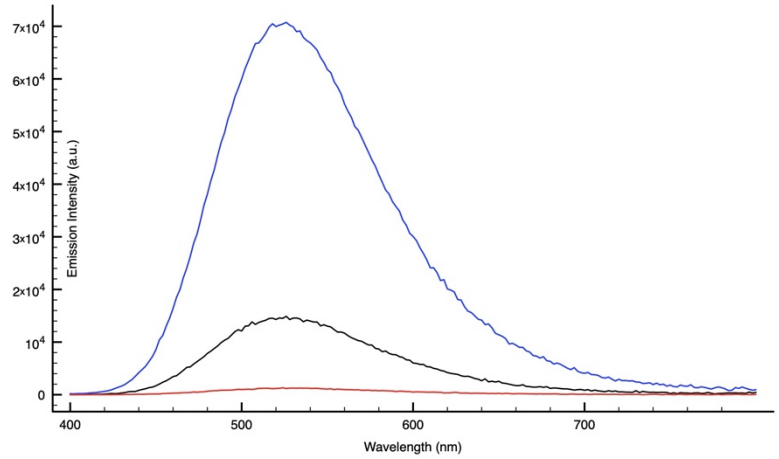


Figure S27: Emission Profiles of compound **3**, $1.29*10^{-5}$ M (black line), $1.29*10^{-4}$ M (blue line) and $12.9*10^{-4}$M (red line), CH_2Cl_2, λ_{exc} = 350 nm, 298K.

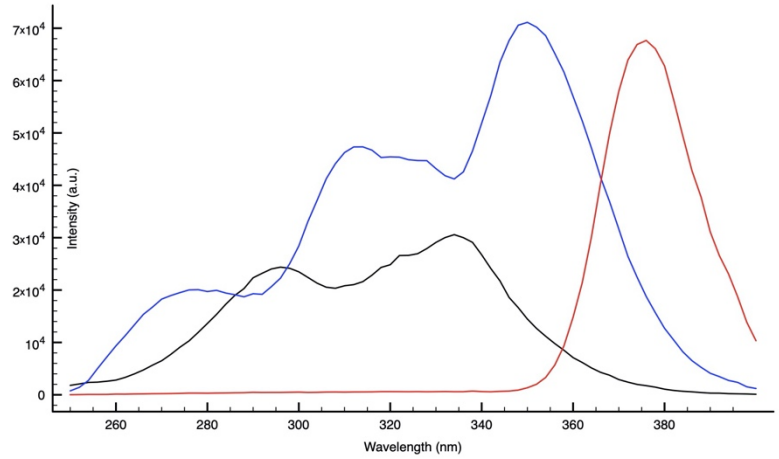


Figure S28: Excitation profiles of compound **3**, $1.29*10^{-5}$ M (black line), $1.29*10^{-4}$ M (blue line) and $12.9*10^{-4}$M (red line), CH_2Cl_2, λ_{emi} = 524 nm, 298K.

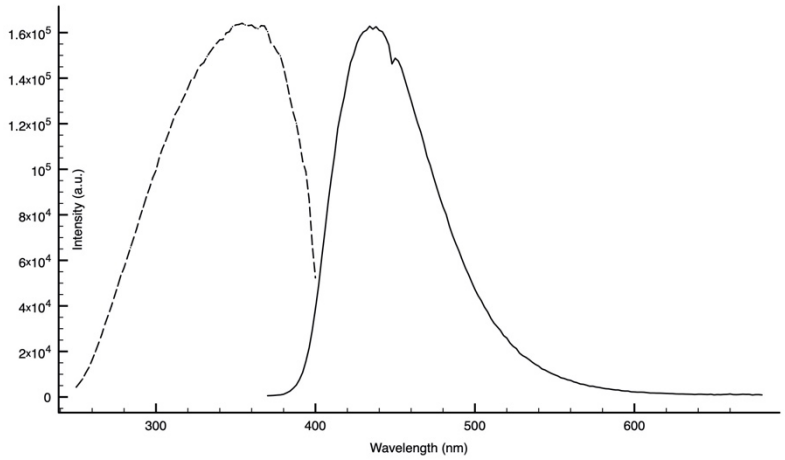


Figure S29: Emission (solid line) and Excitation (dashed line) profiles of compound **3**, Neat solid Matrix, 298K.

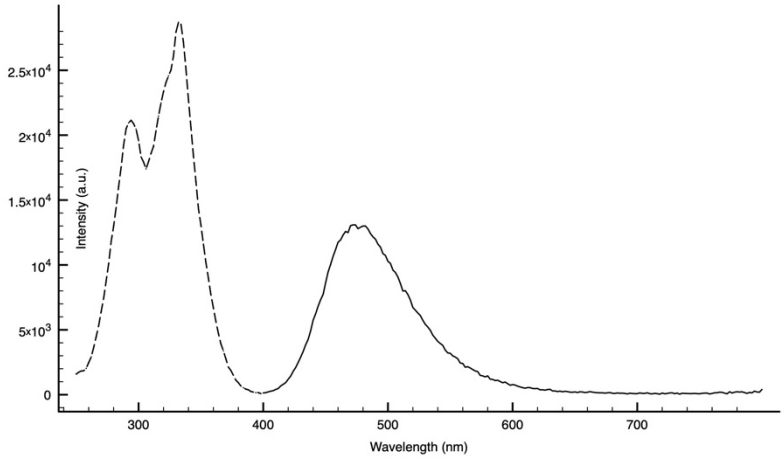


Figure S30: Emission (solid line) and Excitation (dashed line) profiles of compound **3** 10^{-5}M, Hexane, 298K.

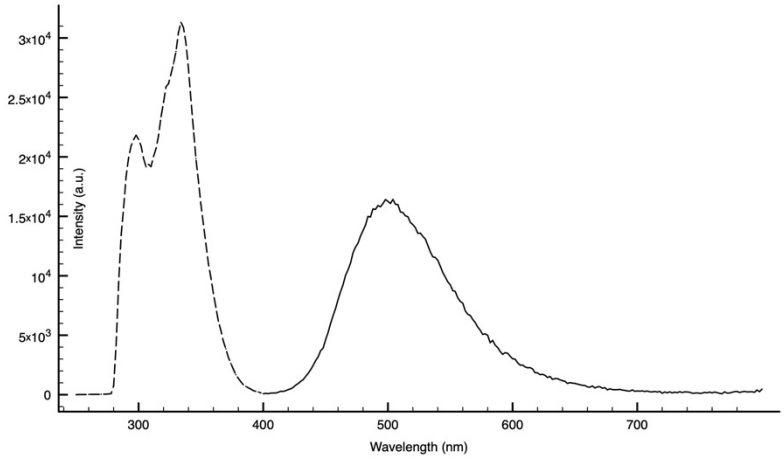


Figure S31: Emission (solid line) and Excitation (dashed line) profiles of compound **3** 10^{-5}M, Toluene, 298K.

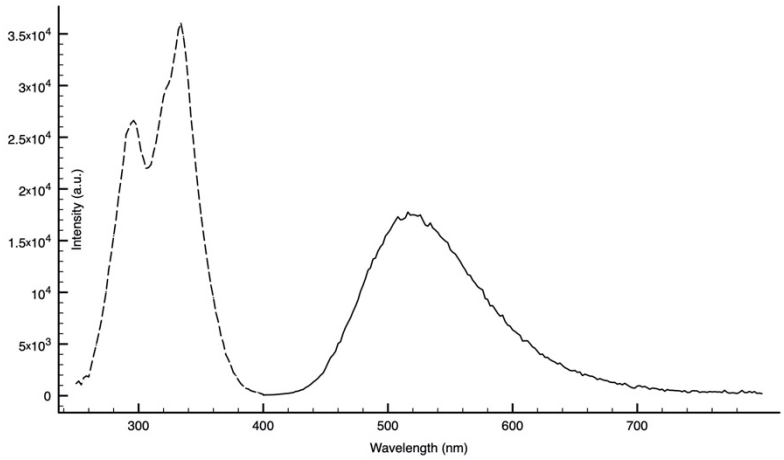


Figure S32: Emission (solid line) and Excitation (dashed line) profiles of compound **3** 10^{-5}M, THF, 298K.

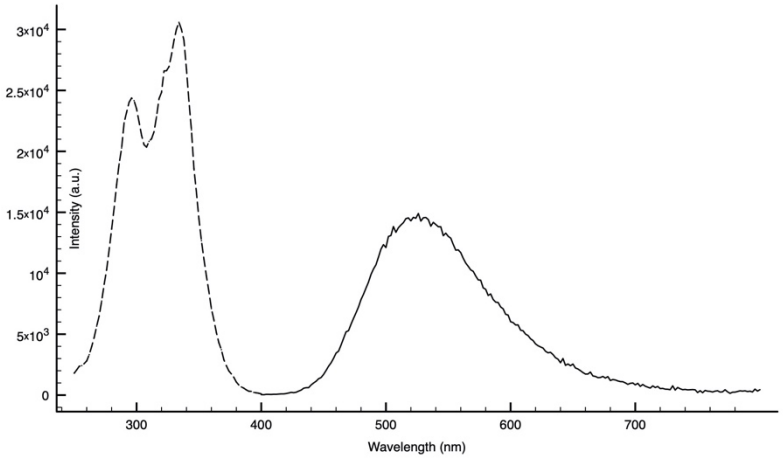


Figure S33: Emission (solid line) and Excitation (dashed line) profiles of compound **3** $1.29*10^{-4}$M, DCM, 298K.

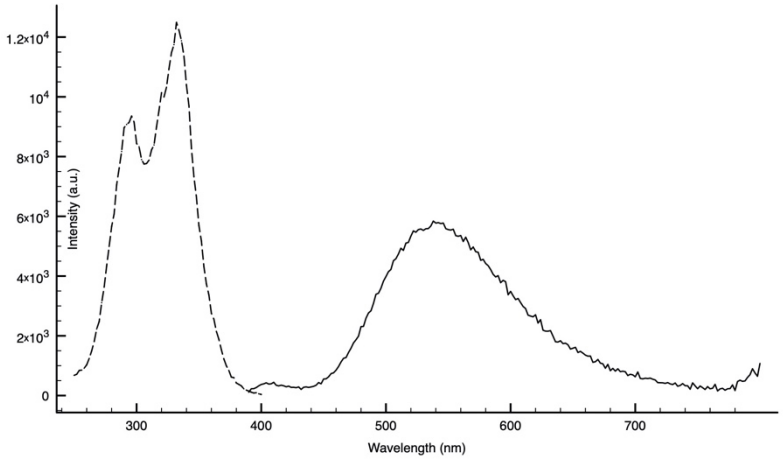


Figure S34: Emission (solid line) and Excitation (dashed line) profiles of compound **3** 10^{-5}M, CH_3CN, 298K.

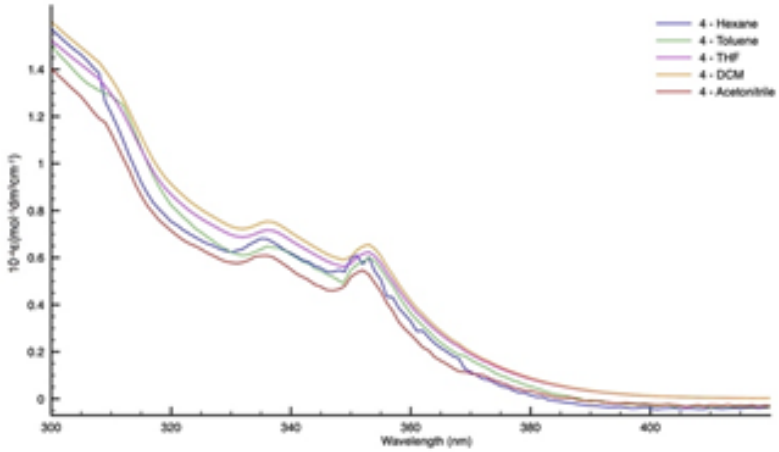


Figure S35: Absorption Profiles of compound **4**, 298 K, 10^{-5} M.

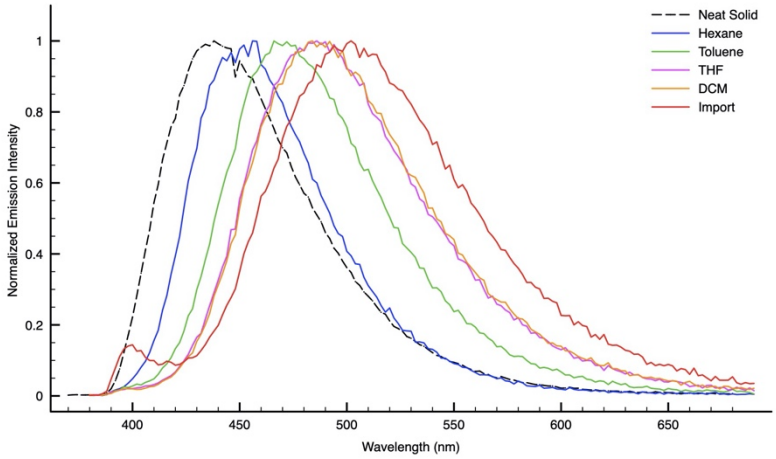


Figure S36: Normalized Emission Profiles of compound **4**, 298K.

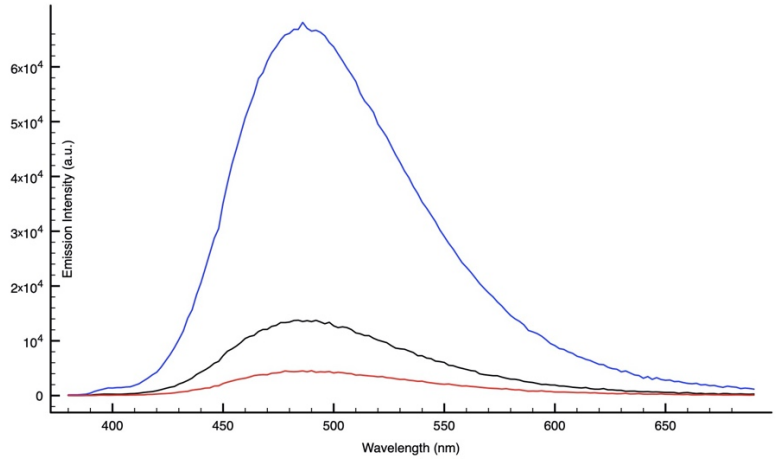


Figure S37: Emission Profiles of compound **4**, 10^{-6} M (black line), 10^{-5} M (blue line) and 10^{-4}M (red line), CH_2Cl_2, λ_{exc} = 350 nm, 298K.

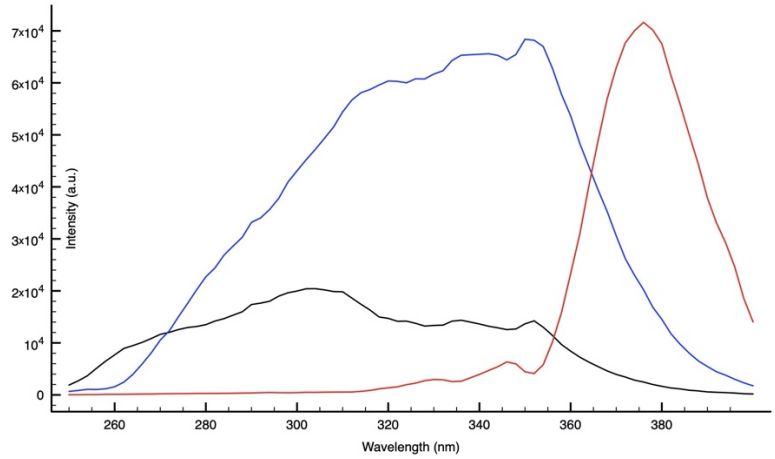


Figure S38: Excitation profiles of compound **4**, 10^{-6} M (black line), 10^{-5} M (blue line) and 10^{-4}M (red line), CH_2Cl_2, λ_{emi} = 438 nm, 298K.

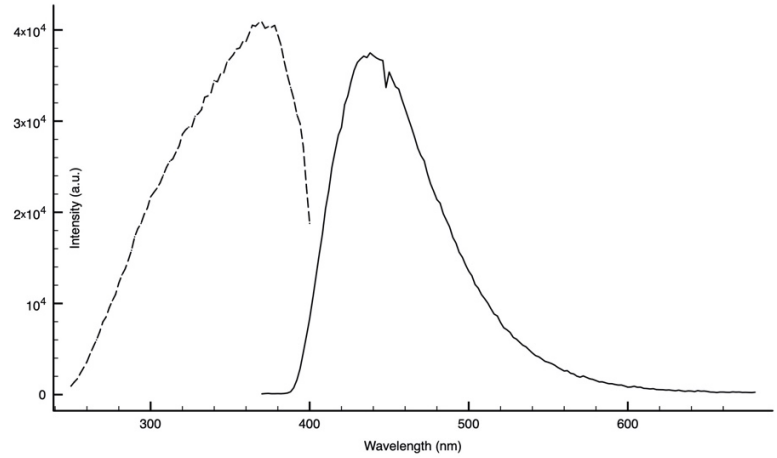


Figure S39: Emission (solid line) and Excitation (dashed line) profiles of compound **4**, Neat solid Matrix, 298K.

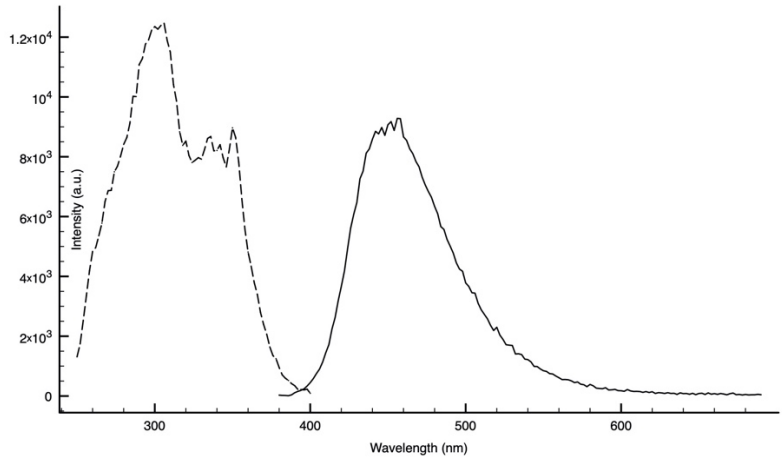


Figure S40: Emission (solid line) and Excitation (dashed line) profiles of compound **4**, 10^{-5} M Hexane, 298K.

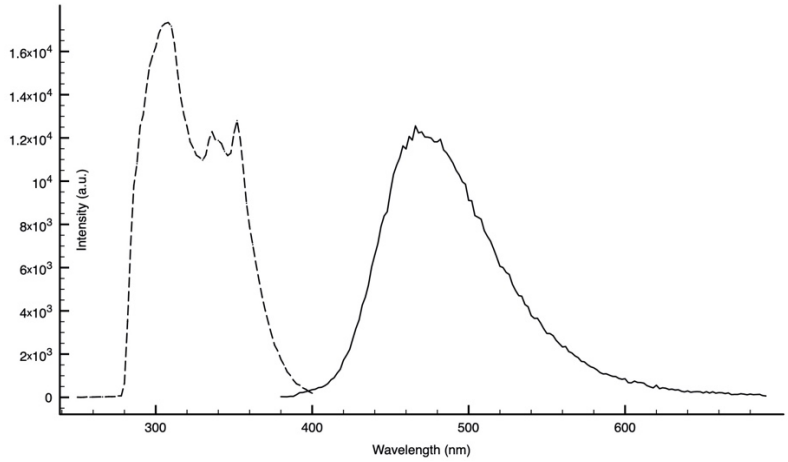


Figure 41: Emission (solid line) and Excitation (dashed line) profiles of compound **4**, 10^{-5} M Toluene, 298K.

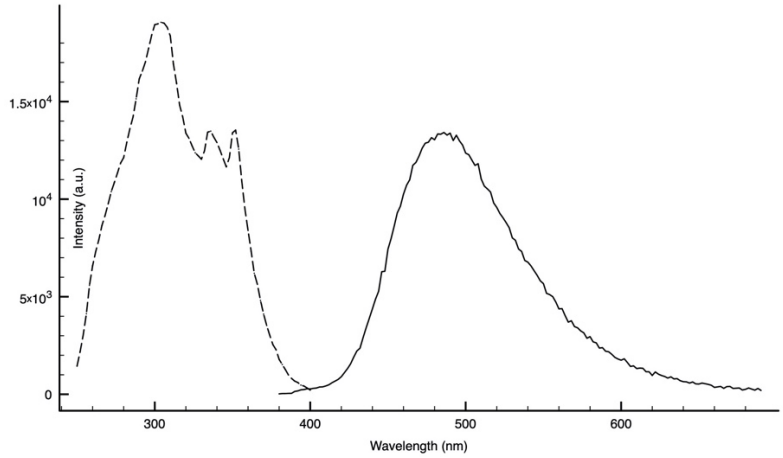


Figure S42: Emission (solid line) and Excitation (dashed line) profiles of compound **4**, 10^{-5} M THF, 298K.

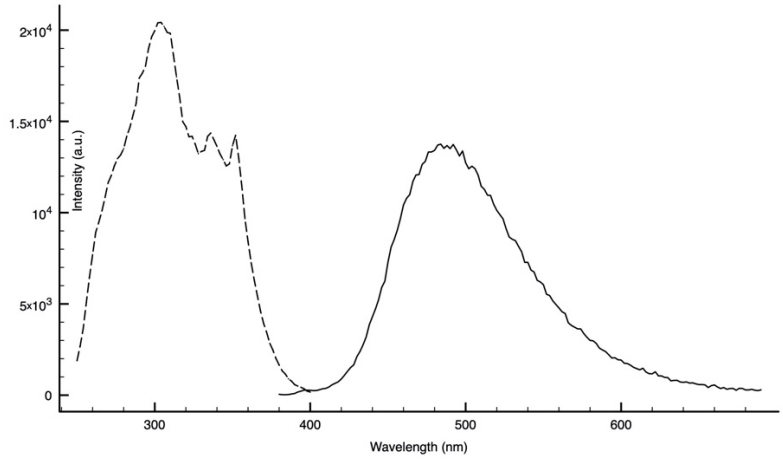


Figure S43: Emission (solid line) and Excitation (dashed line) profiles of compound **4** 10^{-5} M DCM, 298K.

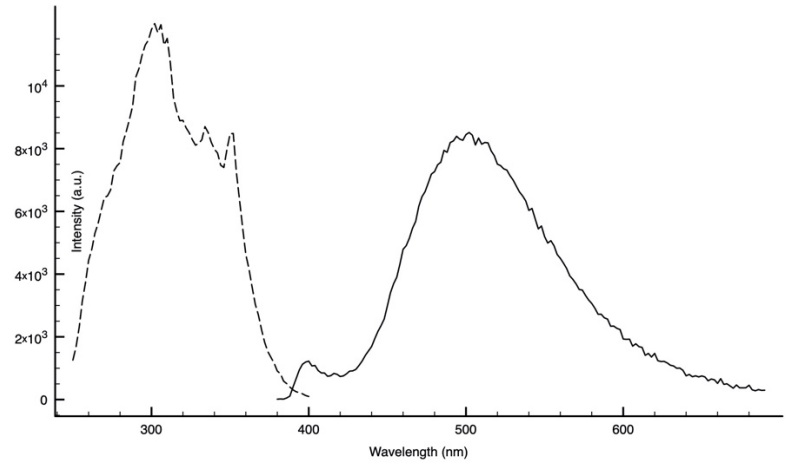


Figure S44: Emission (solid line) and Excitation (dashed line) profiles of compound **4**, 10^{-5} M Acetonitrile, 298K.

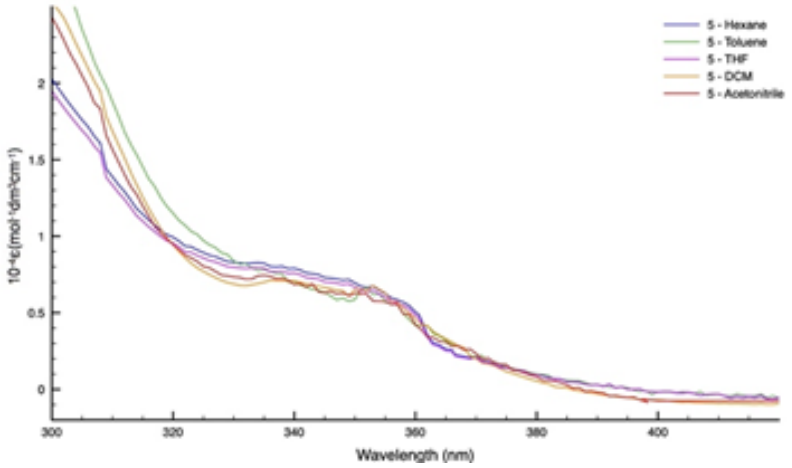


Figure S45: Absorption Profiles of compound **5**, 298 K, 10^{-5} M.

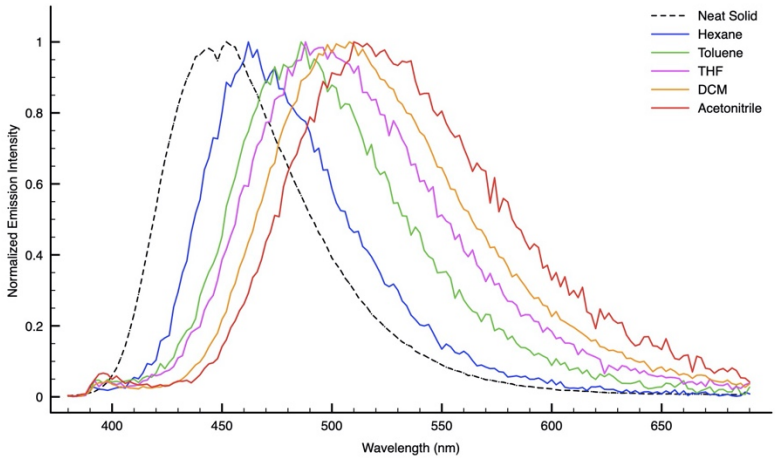


Figure S46: Normalized Emission Profiles of compound **5**, 298K.

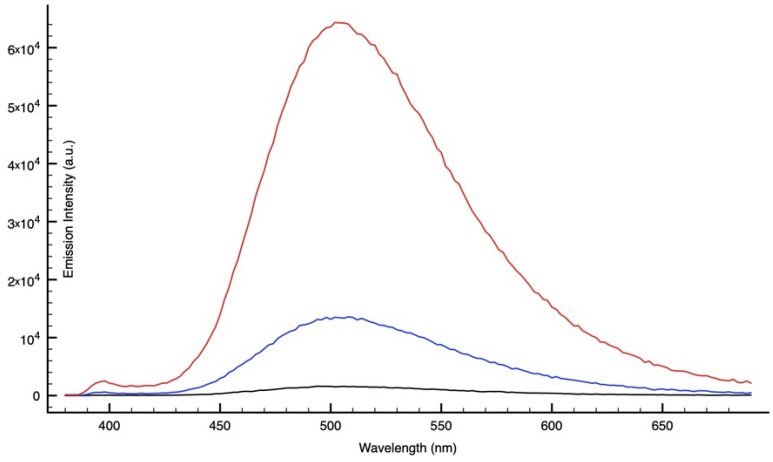


Figure S47: Emission Profiles of compound **5**, 10^{-6} M (black line), 10^{-5} M (blue line) and 10^{-4}M (red line), CH_2Cl_2, λ_{exc} = 350 nm, 298K.

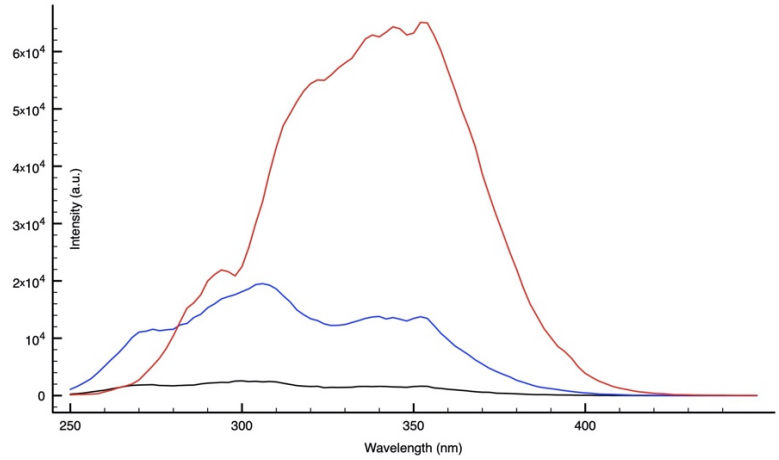


Figure S48: Excitation profiles of compound **5**, 10^{-6} M (black line), 10^{-5} M (blue line) and 10^{-4}M (red line), CH_2Cl_2, λ_{emi} = 504 nm, 298K.

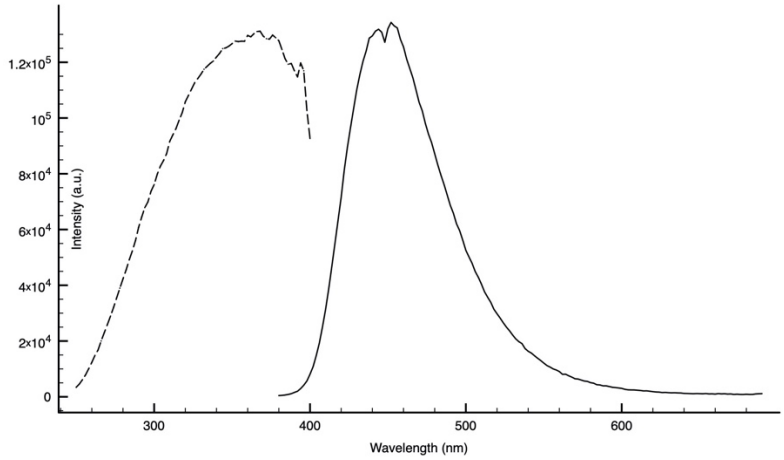


Figure S49: Emission (solid line) and Excitation (dashed line) profiles of compound **5**, Neat solid Matrix, 298K.

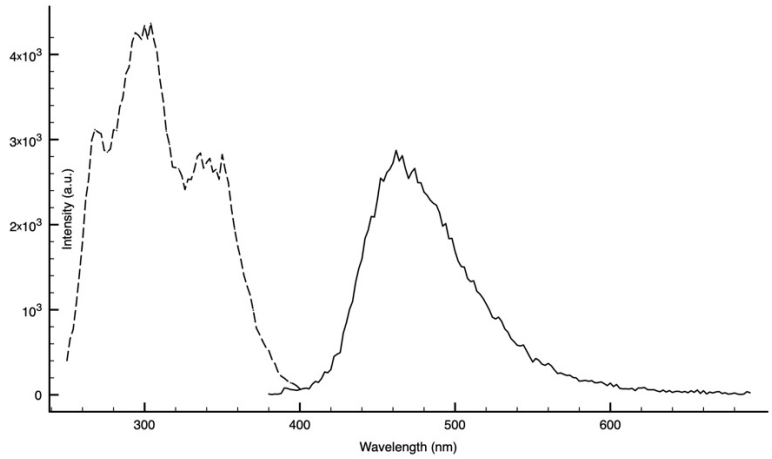


Figure S50: Emission (solid line) and Excitation (dashed line) profiles of compound **5**, 10^{-5} M Hexane, 298K.

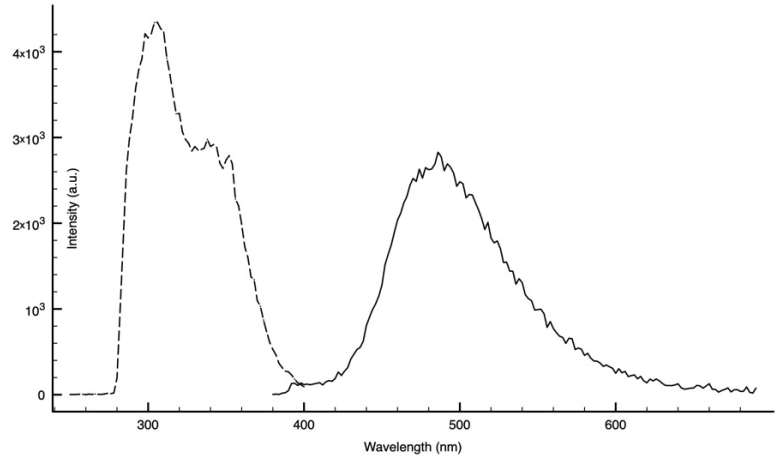


Figure S51: Emission (solid line) and Excitation (dashed line) profiles of compound **5**, 10^{-5} M Toluene, 298K.

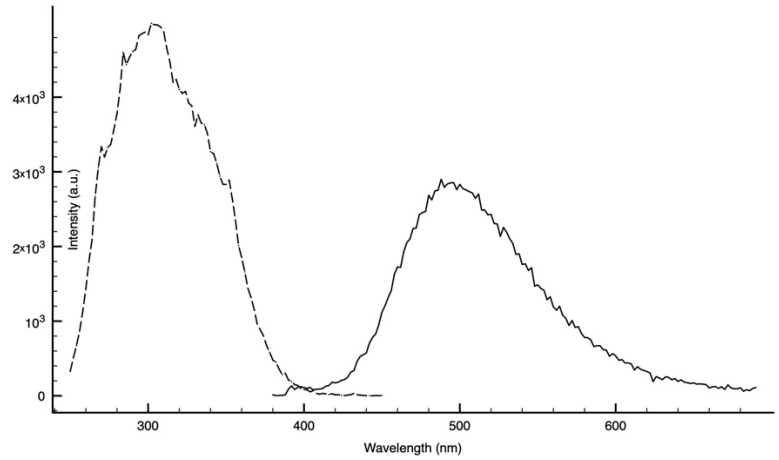


Figure S52: Emission (solid line) and Excitation (dashed line) profiles of compound **5**, 10^{-5} M THF, 298K.

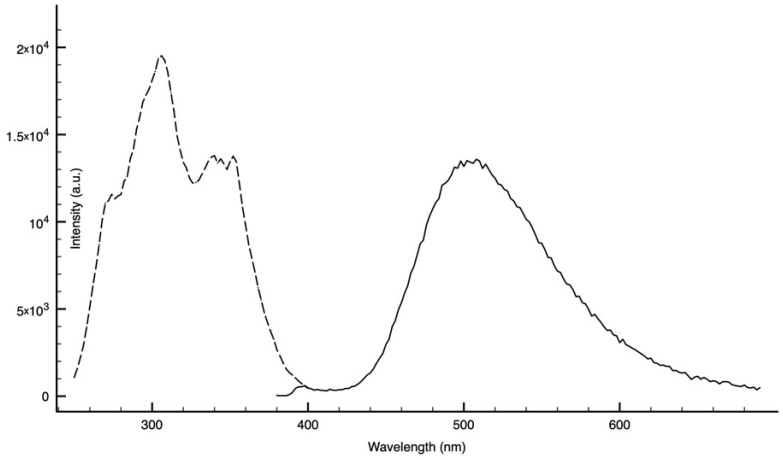


Figure S53: Emission (solid line) and Excitation (dashed line) profiles of compound **5**, 10^{-5} M DCM, 298K.

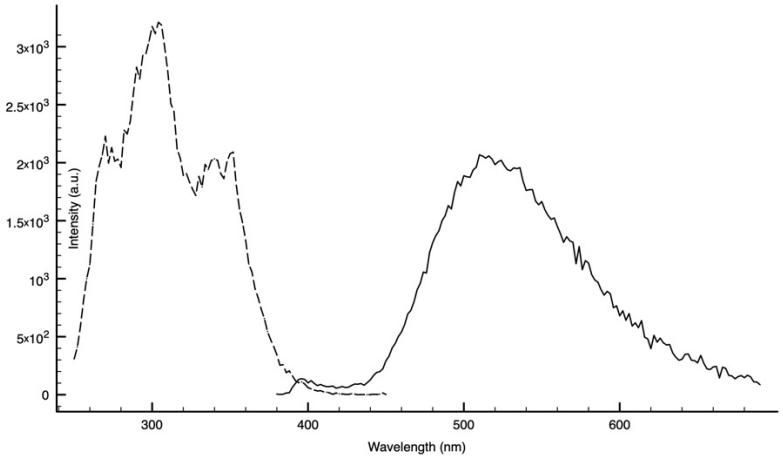


Figure S54: Emission (solid line) and Excitation (dashed line) profiles of compound **5**, 10^{-5} M Acetonitrile, 298K.

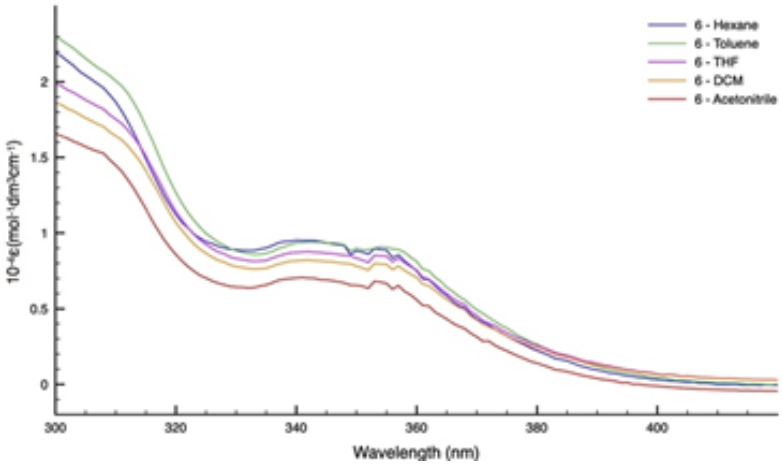


Figure S55: Absorption Profiles of compound **6**, 298 K, 10^{-5} M.

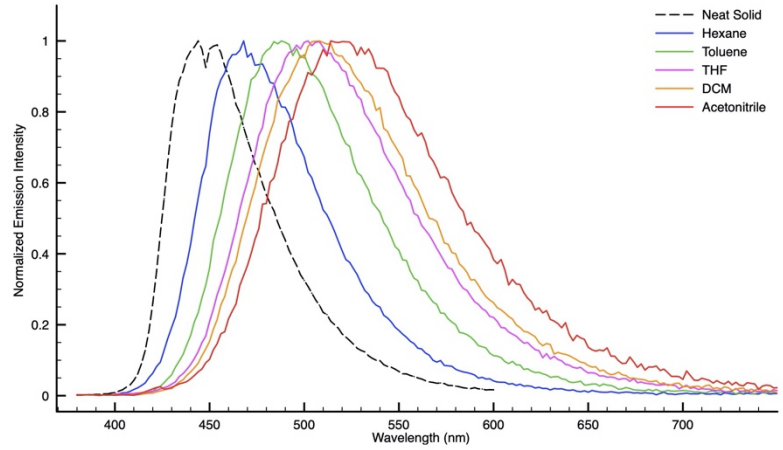


Figure S56: Normalized Emission Profiles of compound **6**, 298K.

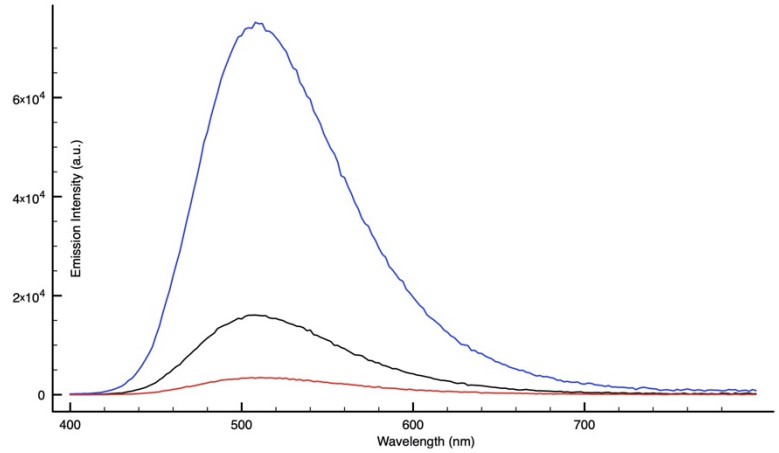


Figure S57: Emission Profiles of compound **6**, $7.02*10^{-6}$ M (black line), $7.02*10^{-5}$ M (blue line) and $7.02*10^{-4}$ M (red line), CH_2Cl_2, λ_{exc} = 350 nm, 298K.

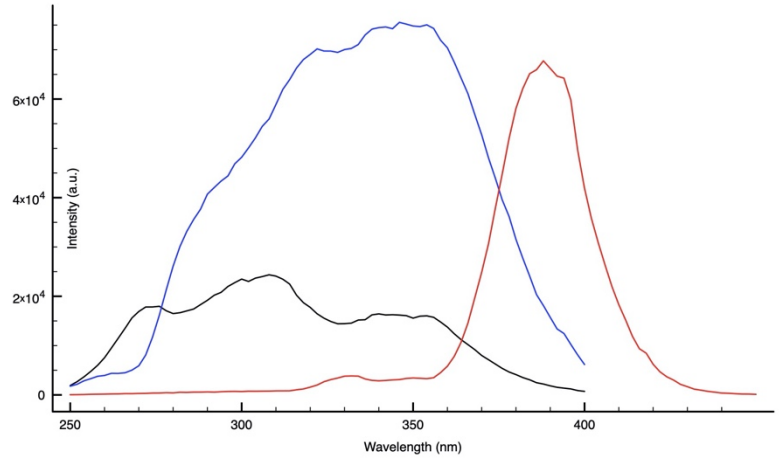


Figure S58: Excitation Profiles of compound **6**, $7.02*10^{-6}$ M (black line), $7.02*10^{-5}$ M (blue line) and $7.02*10^{-4}$ M (red line), CH_2Cl_2, λ_{emi} = 510 nm, 298K.

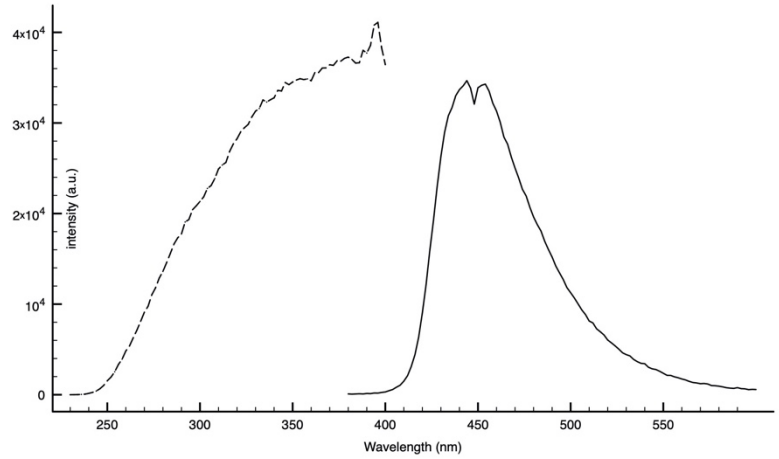


Figure S59: Emission (solid line) and Excitation (dashed line) profiles of compound **6**, Neat solid Matrix, 298K.

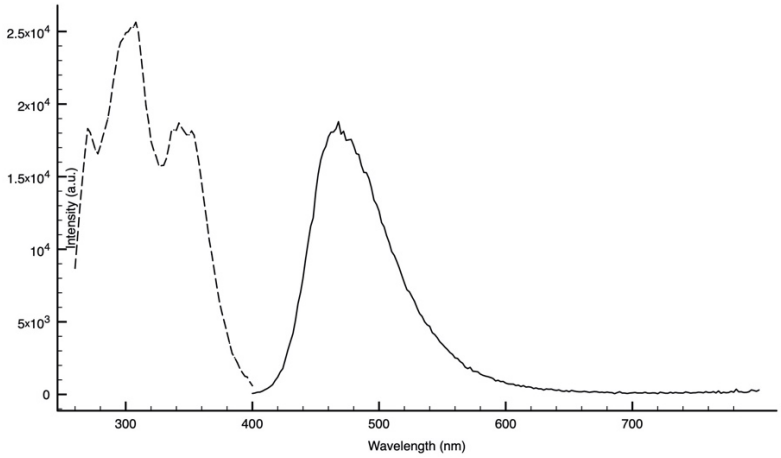


Figure S60: Emission (solid line) and Excitation (dashed line) profiles of compound **6** 10^{-5} M, Hexane, 298K.

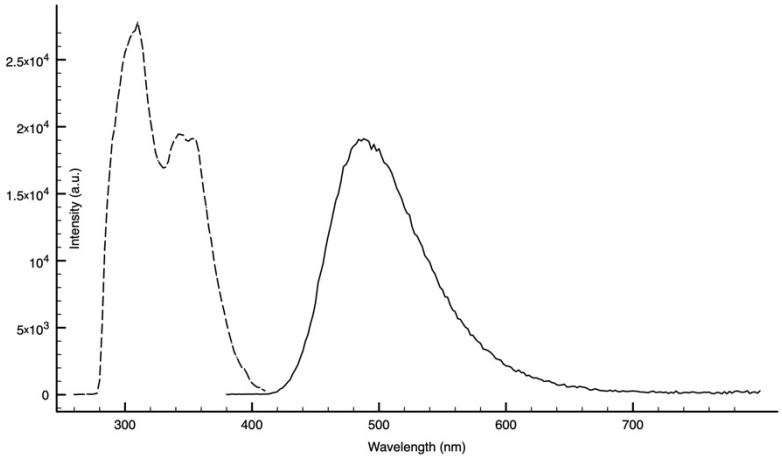


Figure S61: Emission (solid line) and Excitation (dashed line) profiles of compound **6** 10^{-5} M, Toluene, 298K.

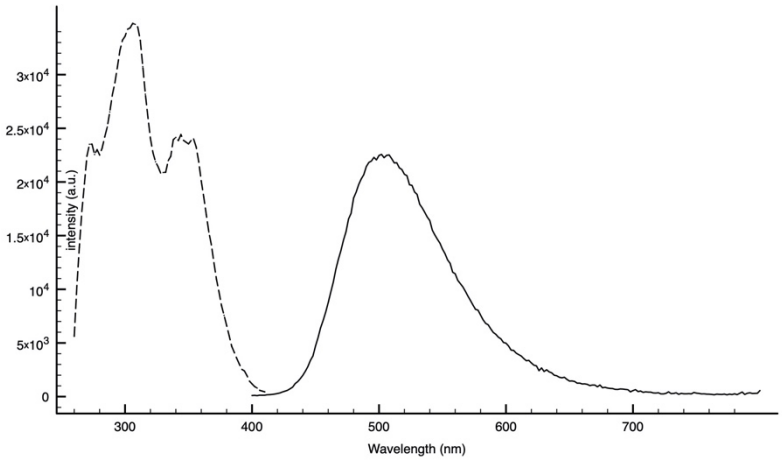


Figure S62: Emission (solid line) and Excitation (dashed line) profiles of compound **6** 10^{-5} M, THF, 298K.

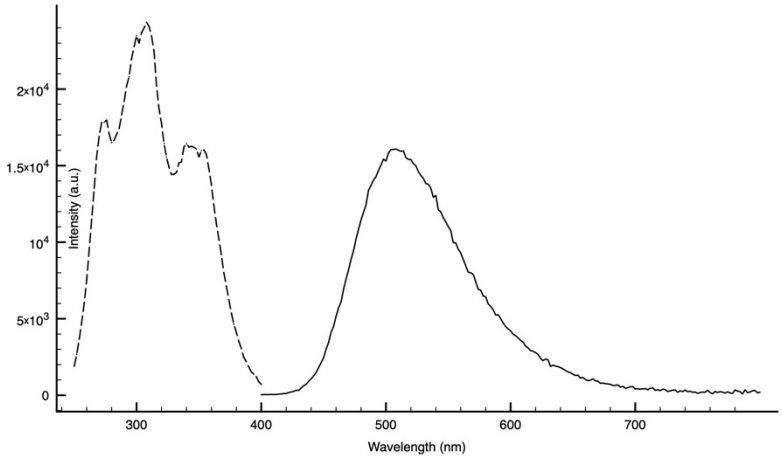


Figure S63: Emission (solid line) and Excitation (dashed line) profiles of compound **6** $7.02*10^{-5}$ M, DCM, 298K.

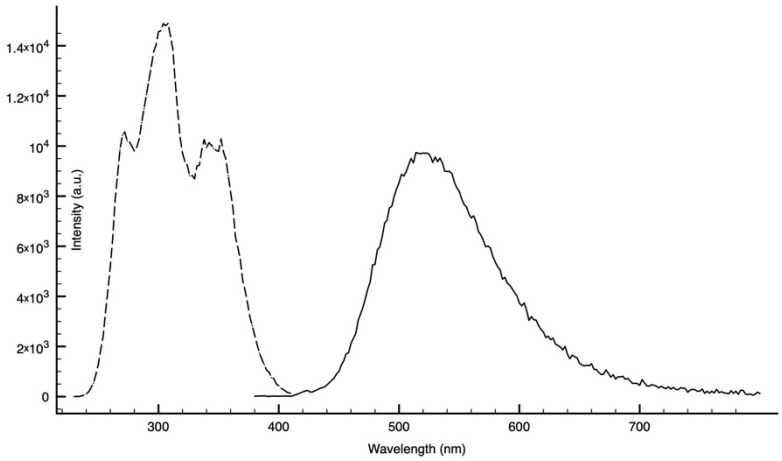


Figure S64: Emission (solid line) and Excitation (dashed line) profiles of compound **6** 10^{-5} M, CH_3CN, 298K.

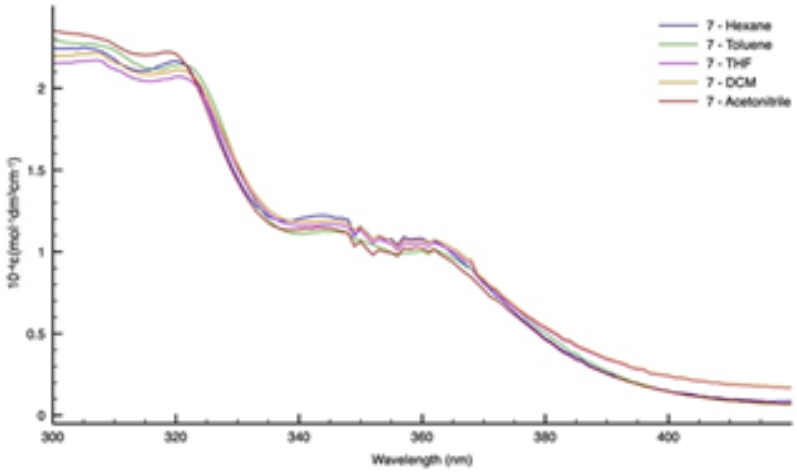


Figure S65: Absorption Profiles of compound **7**, 298 K, 10^{-5} M.

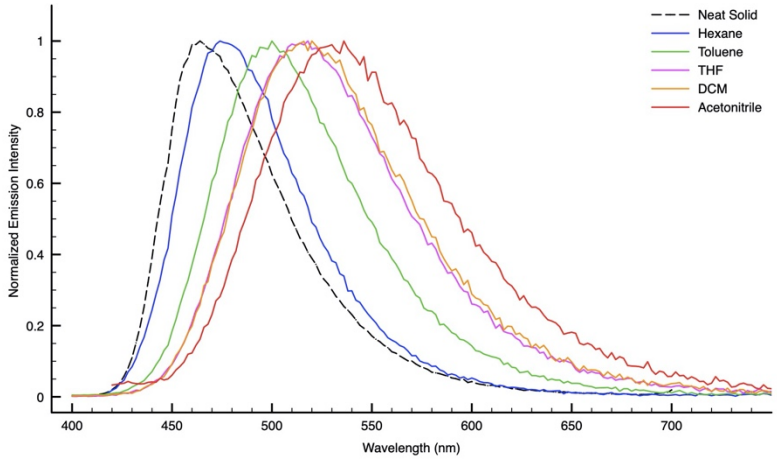


Figure S66: Normalized Emission Profiles of compound **7**, 298K.

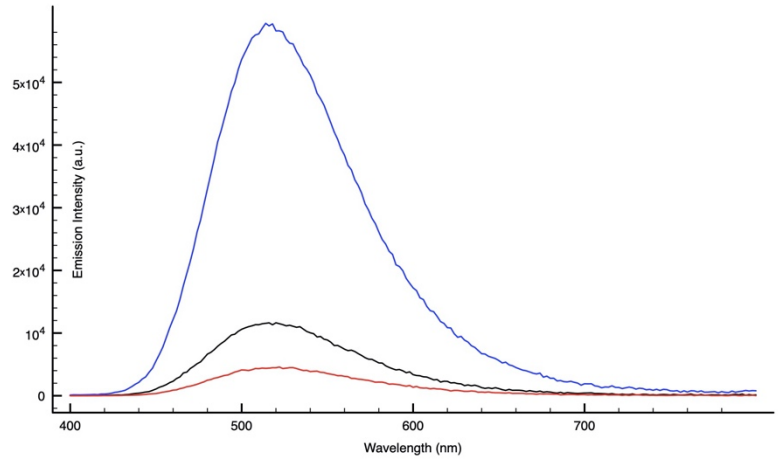


Figure S67: Emission Profiles of compound **7**, $4.9*10^{-6}$ M (black line), $4.9*10^{-5}$ M (blue line) and $4.9*10^{-4}$ M (red line), CH_2Cl_2, λ_{exc} = 350 nm, 298K.

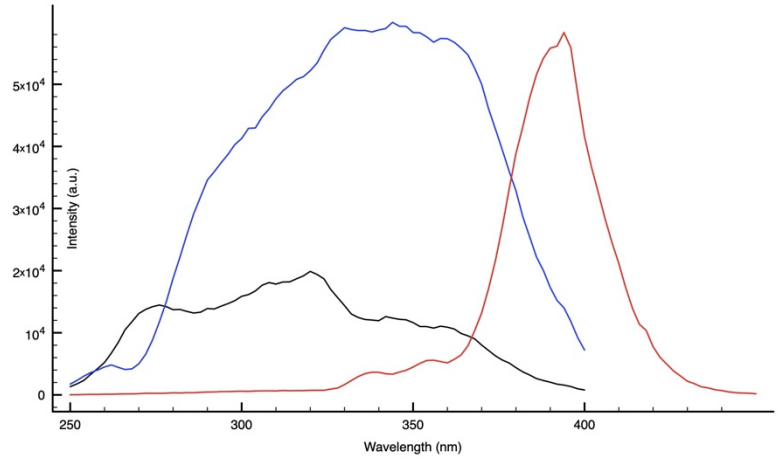


Figure S68: Excitation Profiles of compound **7**, $4.9*10^{-6}$ M (black line), $4.9*10^{-5}$ M (blue line) and $4.9*10^{-4}$ M (red line), CH_2Cl_2, λ_{emi} = 520 nm, 298K.

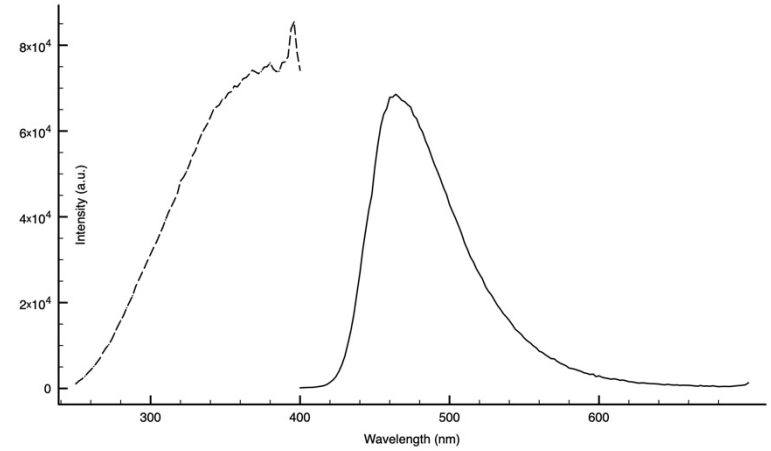


Figure S69: Emission (solid line) and Excitation (dashed line) profiles of compound **7**, Neat solid Matrix, 298K.

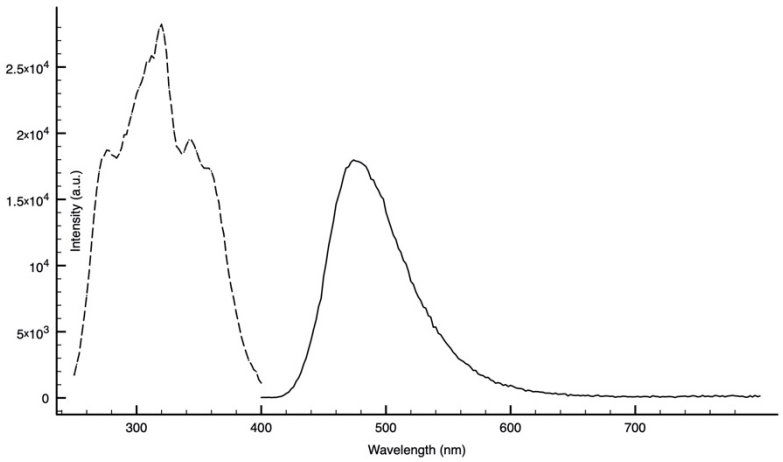


Figure S70: Emission (solid line) and Excitation (dashed line) profiles of compound **7** 10^{-5} M, Hexane, 298K.

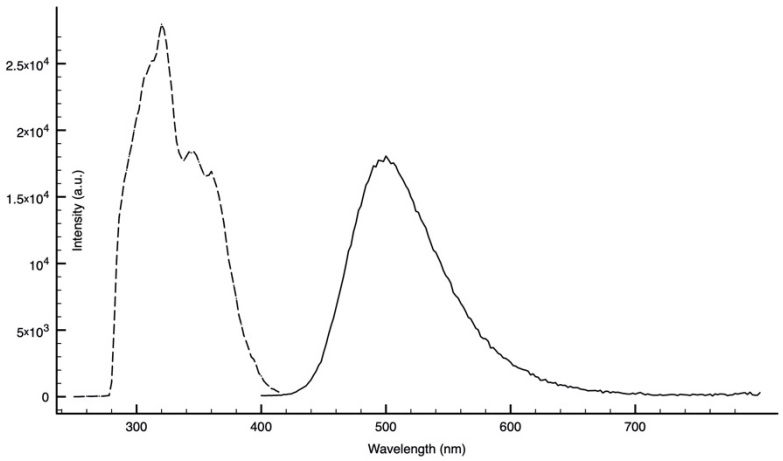


Figure S71: Emission (solid line) and Excitation (dashed line) profiles of compound **7** 10^{-5} M, Toluene, 298K.

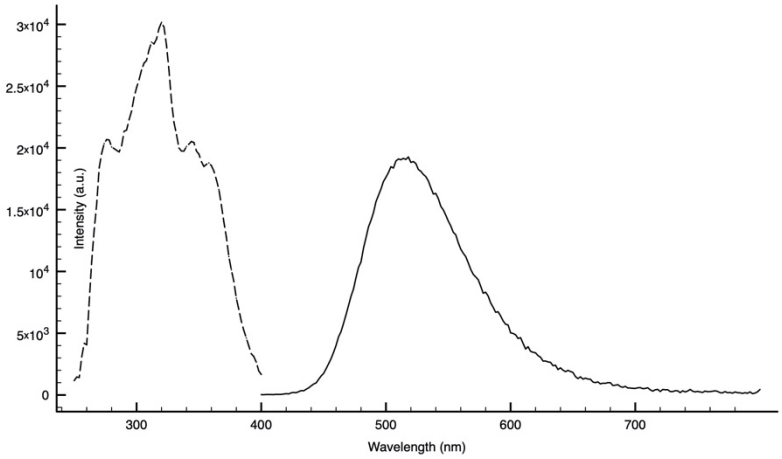


Figure S72: Emission (solid line) and Excitation (dashed line) profiles of compound **7** 10^{-5} M, THF, 298K.

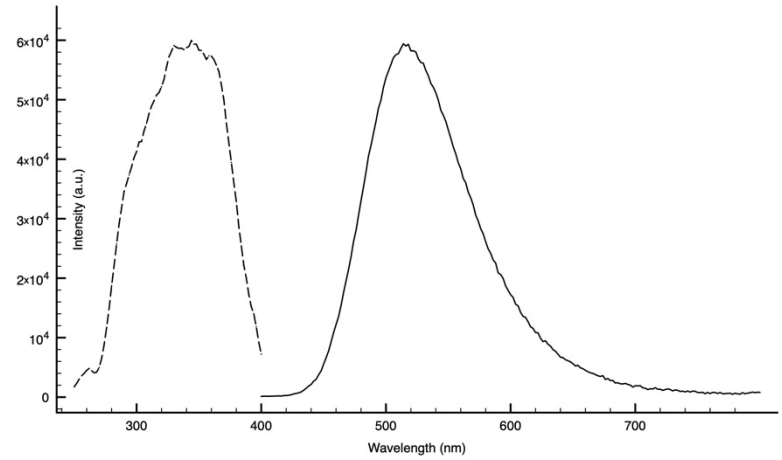


Figure S73: Emission (solid line) and Excitation (dashed line) profiles of compound **7** 4.9*10^{-5} M, DCM, 298K.

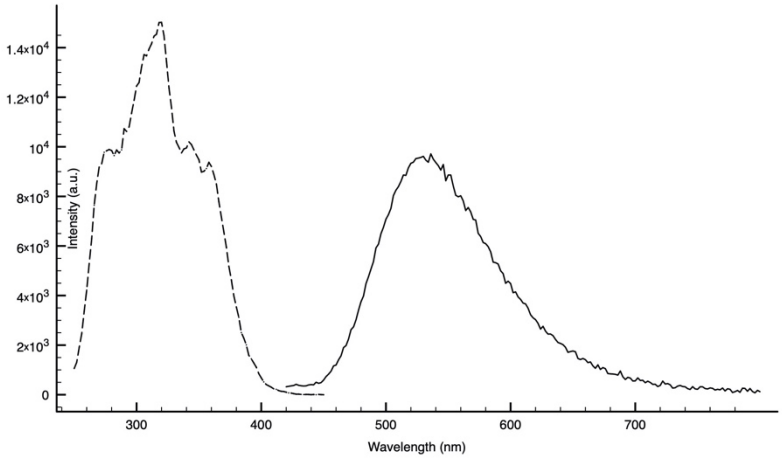


Figure S74: Emission (solid line) and Excitation (dashed line) profiles of compound **7** 10^{-5} M, CH_3CN, 298K.

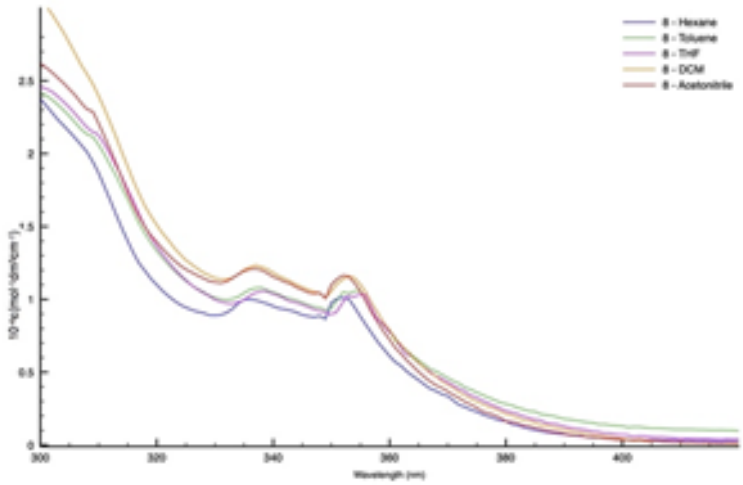


Figure S75: Absorption Profiles of compound **8**, 298 K, 10^{-5} M.

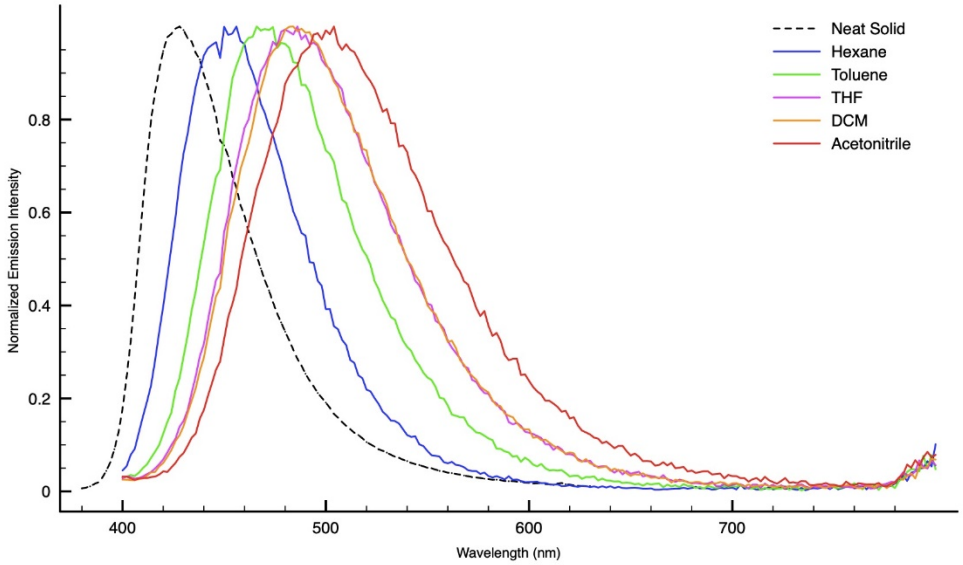


Figure S76: Normalized Emission Profiles of compound **8**, 298K.

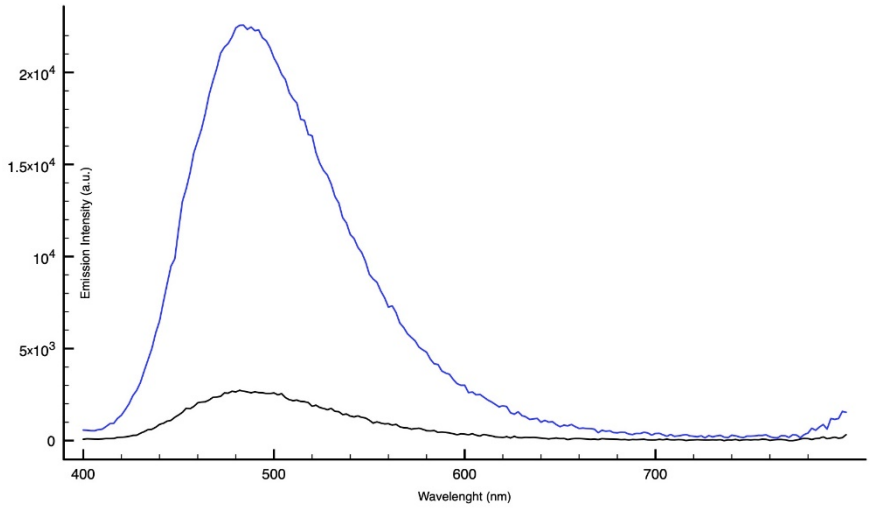


Figure S77: Emission Profiles of compound **8**, 10^{-6} M (black line), 10^{-5} M (blue line) CH_2Cl_2, λ_{exc} = 350 nm, 298K.

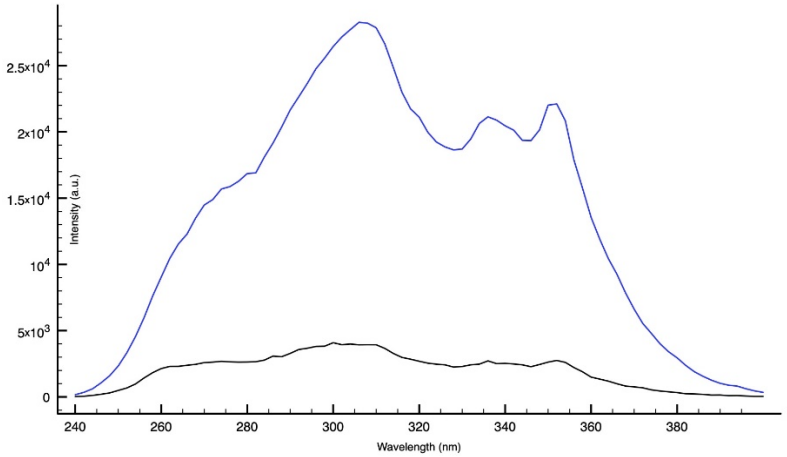


Figure S78: Excitation profiles of compound **8**, 10^{-6} M (black line), 10^{-5} M (blue line), CH_2Cl_2, λ_{emi} = 484 nm, 298K.

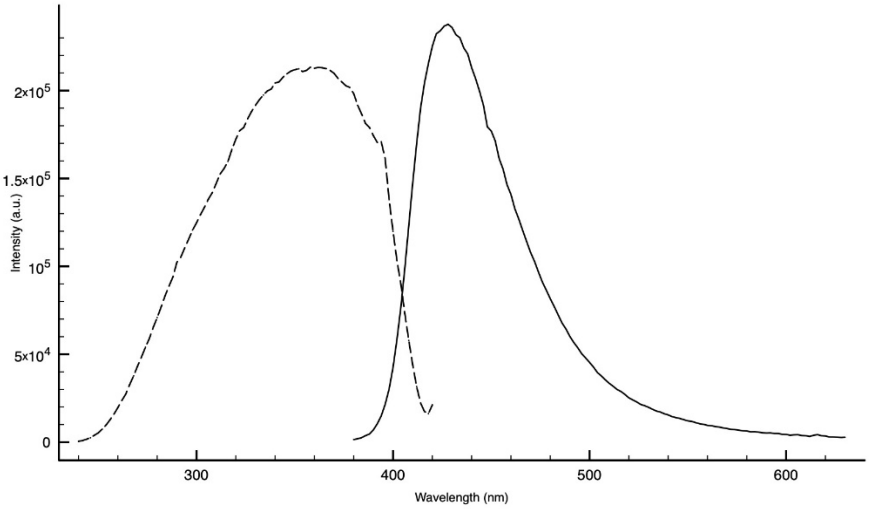


Figure S79: Emission (solid line) and Excitation (dashed line) profiles of compound **8**, Neat solid Matrix, 298K.

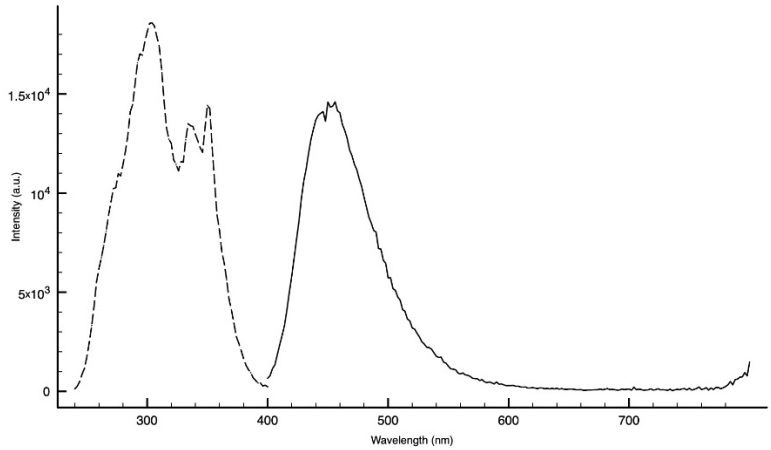


Figure S80: Emission (solid line) and Excitation (dashed line) profiles of compound **8**, 10^{-5} M Hexane, 298K.

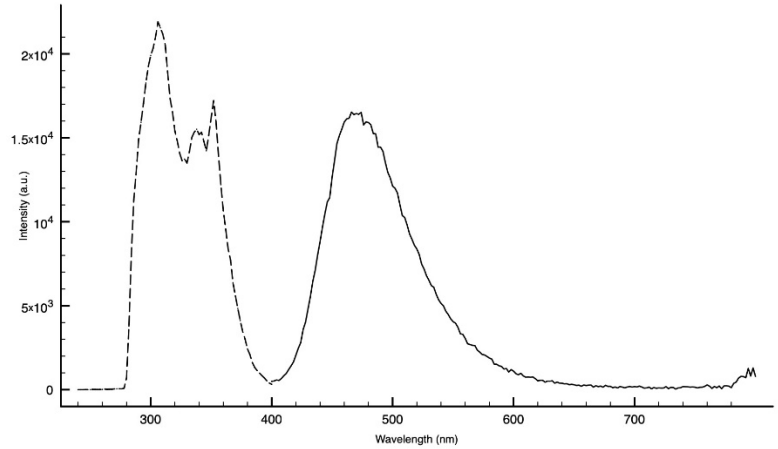


Figure S81: Emission (solid line) and Excitation (dashed line) profiles of compound **8**, 10^{-5} M Toluene, 298K.

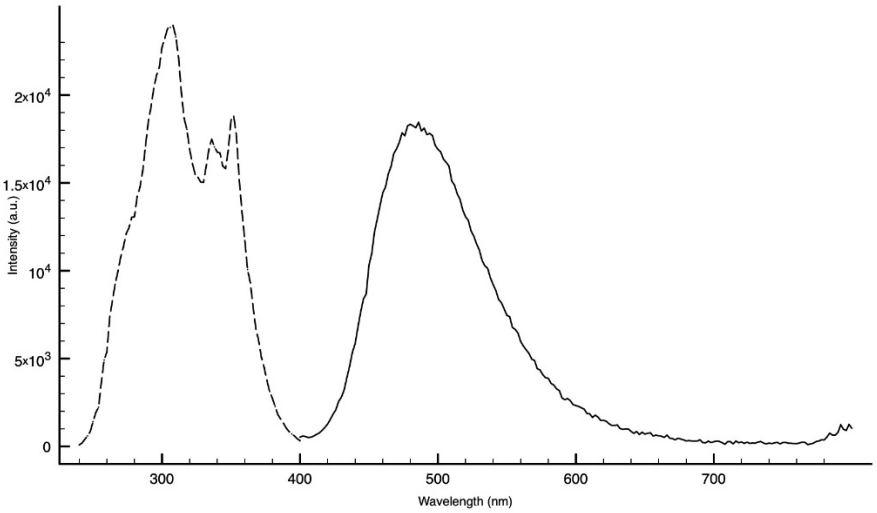


Figure S82: Emission (solid line) and Excitation (dashed line) profiles of compound **8**, 10^{-5} M THF, 298K.

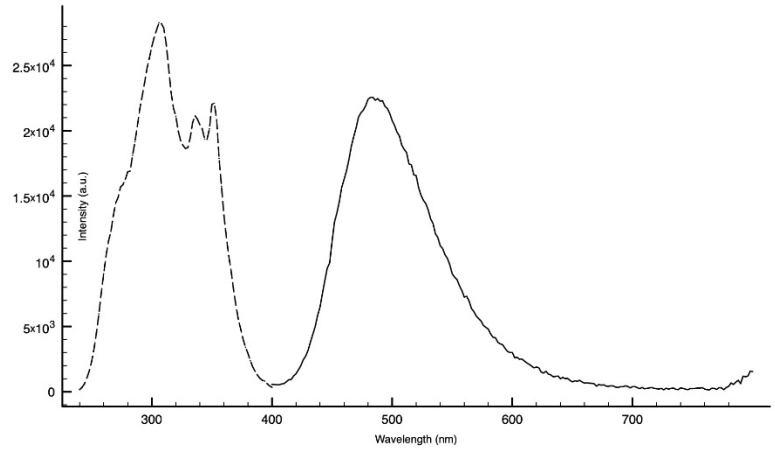


Figure S83: Emission (solid line) and Excitation (dashed line) profiles of compound **8** 10^{-5} M DCM, 298K.

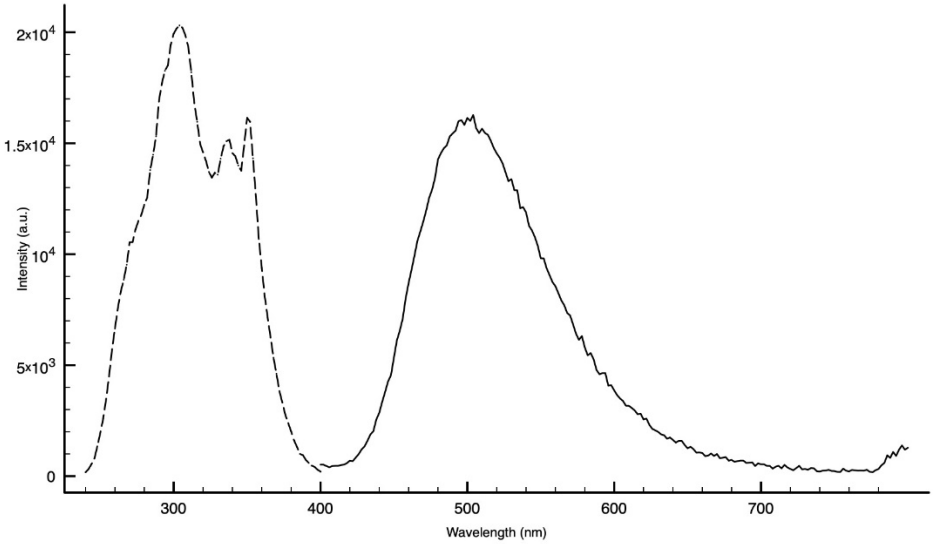


Figure S84: Emission (solid line) and Excitation (dashed line) profiles of compound **8**, 10^{-5} M Acetonitrile, 298K.

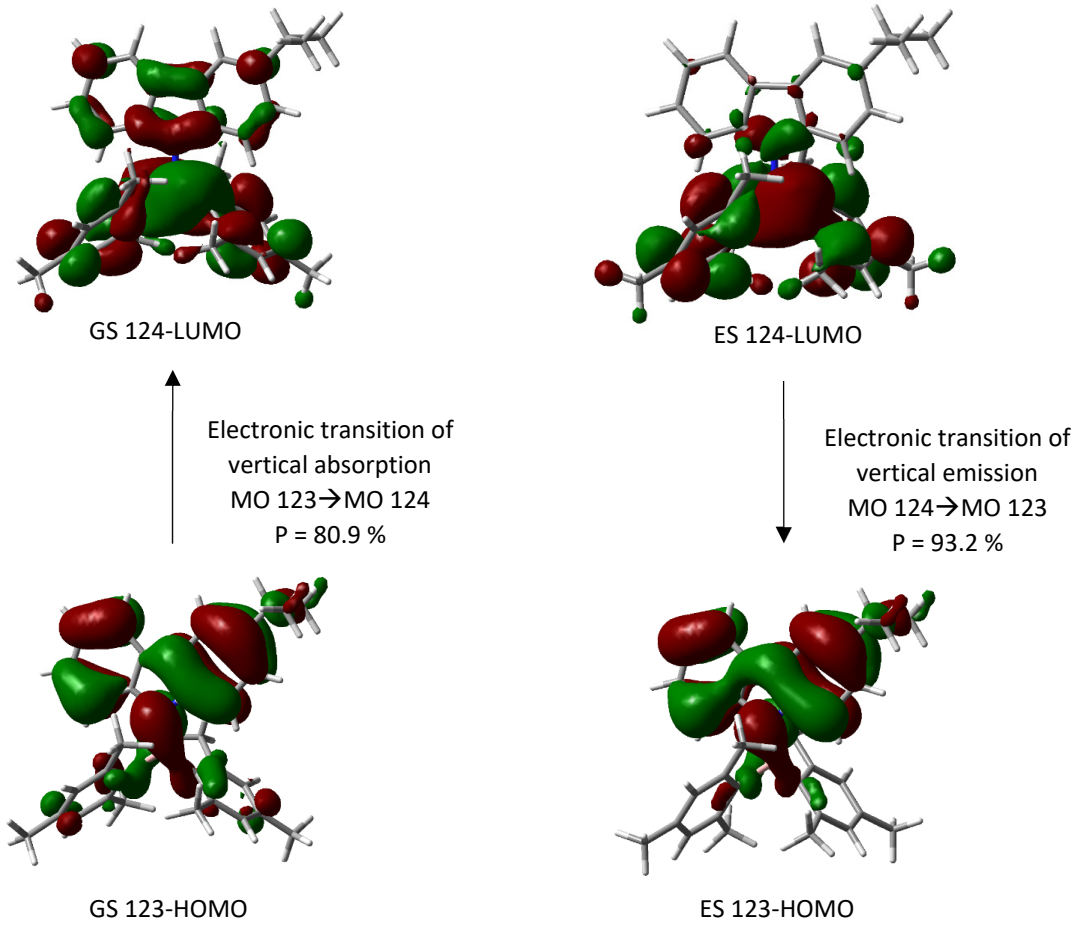
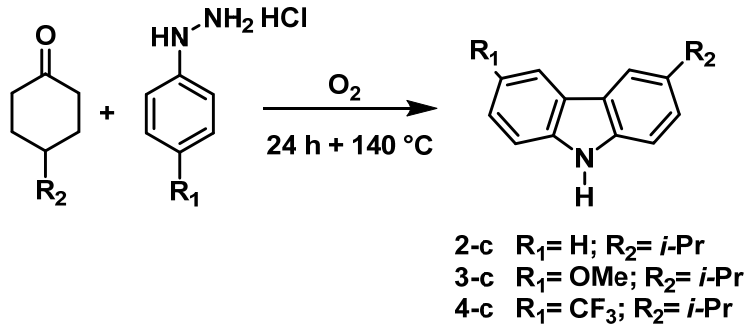


Figure S85: representation of the calculated orbitals HOMO and LUMO of GS and ES most likely involved in the vertical transitions of absorption and emission for compound **2a** in THF.

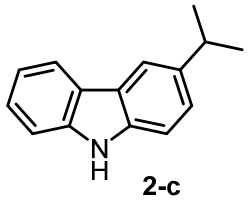
Synthesis of substituted carbazole

Carbazole is commercially available (CAS: 86-74-8). The asymmetric carbazole **2c-4c** were prepared in accordance to the literature.[1]



Scheme S1.

In a 25 mL oven-dried reaction flask cyclohexanone (5 mmol), the appropriate substituted phenylhydrazine hydrochloride (7.5 mmol) and the solvent *N*-methyl-2-pyrrolidone (NMP, 10 mL) were added and the resulting solution was stirred under oxygen (1atm) at +140 °C for 24 h. After cooling to room temperature, the NMP was distilled in high vacuum at +100 °C. The residue was diluted in DCM and filtered on Celite®, then evaporated the solvent. The carbazole product was purified by chromatography separation on silica gel, with eluent *n*-hexane/DCM in 7:3 ratio.



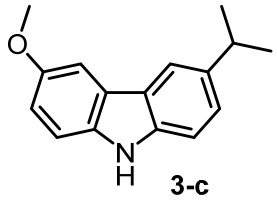
2-c

For compound **2-c** was used cyclohexanone (5 mmol) and (4-*i*-propyl-phenyl)-hydrazine hydrochloride (7.5 mmol). Yield: 38%.

^{1}H-NMR (600 MHz, Chloroform-d, 7.26 ppm +25°C) δ 8.07 (dt, *J* = 7.8, 0.9 Hz, 1H), 7.95 (bs, 1H, NH), 7.93 (bs, 1H), 7.43 – 7.36 (m, 2H), 7.36 (dd, *J* = 8.3, 0.7 Hz, 1H), 7.31 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.22 (dddd, *J* = 8.0, 6.1, 2.2, 0.9 Hz, 1H), 3.11 (dq, *J* = 13.8, 6.9 Hz, 1H), 1.37 (d, *J* = 6.9 Hz, 3H).

^{13}C-NMR (151 MHz, Chloroform-d, 77.0 ppm, +25°C) δ: 140.22 (Cq), 139.85 (Cq), 137.95 (Cq), 125.57 (CH), 124.81 (CH), 123.39 (Cq), 123.35 (Cq), 120.18 (CH), 119.18 (CH), 117.45 (CH), 110.52 (CH), 110.30 (CH), 34.18 (CH), 24.70 ($2CH_3$).

HRMS(ESI-QTOF). Calcd. for $C_{15}H_{16}N^+$ $[M+H]^+$ 210.12773. Found $C_{15}H_{16}N^+$ $[M+H]^+$: 210.1277.



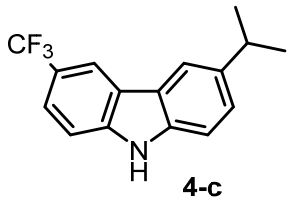
3-c

For compound **3-c** was used (4-*iso*-propyl)-cyclohexanone (5 mmol) and (4-methoxy-phenyl)-hydrazine hydrochloride (7.5 mmol). Yield: 30%.

^{1}H-NMR (600 MHz, Chloroform-d, 7.26 ppm +25 °C) δ 7.89 – 7.86 (m, 1H), 7.81 (s, 1H), 7.55 (d, *J* = 2.5 Hz, 1H), 7.35 – 7.27 (m, 3H), 7.04 (dd, *J* = 8.7, 2.5 Hz, 1H), 3.94 (s, 3H), 3.09 (hept, *J* = 7.0 Hz, 1H), 1.37 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (151 MHz, Chloroform-d, 77.0 ppm, +25 °C) δ 153.75 (Cq), 139.84 (Cq), 138.80 (Cq), 134.79 (Cq), 124.85 (CH), 123.84 (Cq), 123.40 (Cq), 117.30 (CH), 114.90 (CH), 111.25 (CH), 110.48 (CH), 102.99 (CH), 56.06 (CH_3), 34.17 (CH), 24.70 (2 CH_3).

HRMS(ESI-QTOF). Calcd. for $C_{16}H_{18}NO^+$ $[M+H]^+$ 240.13829. Found $C_{16}H_{18}NO^+$ $[M+H]^+$: 240.1385.



4-c

For compound **4-c:** In a 25 mL oven-dried reaction flask (4-trifluoromethyl)-phenylhydrazine hydrochloride (7.5 mmol) was dissolved in 10 mL of NMP. After 10 minutes (4-*i*-propyl)-cyclohexanone (5 mmol) was added and the resulting solution was stirred under oxygen (1 atm) at +140 °C for 24 h. Since the aromatization was not complete, a catalytic amount of iodine was added and the solution was stirred for one hour. After cooling to room temperature, the NMP was distilled in high vacuum at +100 °C. The resulting residue was diluted in DCM and filtered on Celite®, then the mixture was washed with sodium sulphite and extracted with DCM. The combined organic layers were dried with sodium sulphate and then evaporated the solvent. The carbazole product was purified by chromatography separation on silica gel, with eluent *n*-hexane/DCM in 7:3 ratio. Yield: 36%

^{1}H-NMR (600 MHz, Chloroform-d, 7.26 ppm +25°C) δ 8.37 – 8.33 (m, 1H), 8.17 (s, 1H, NH), 7.97 (d, *J* = 1.6 Hz, 1H), 7.63 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.46 (d, *J* = 8.4 Hz, 1H), 7.42 – 7.35 (m, 2H), 3.12 (hept, *J* = 7.0 Hz, 1H), 1.37 (d, *J* = 6.9 Hz, 6H).

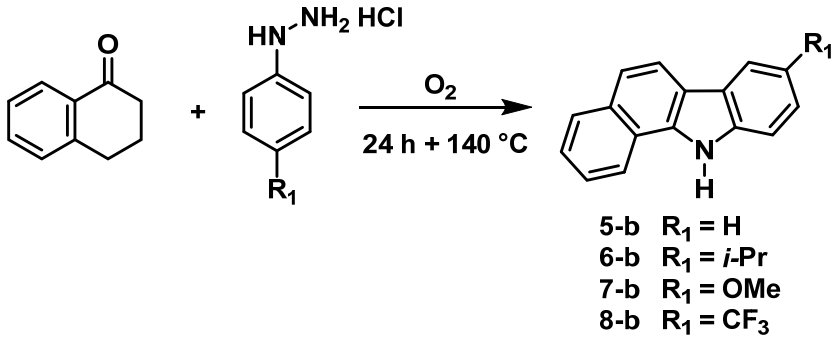
^{13}C-NMR (151 MHz, Chloroform-d, 77.0 ppm, +25°C) δ 141.25 (Cq), 141.18 (Cq), 138.40 (Cq), 125.93 (CH), 125.28 (CF_3, q, *J* = 271.2 Hz), 123.03 (Cq), 122.93 (Cq), 122.42 (CH, q, *J* = 3.6 Hz),

121.51 (Cq, q, J = 32.2 Hz), 117.82 (CH, q, J = 4.1 Hz), 117.67 (CH), 110.68 (CH), 110.55 (CH), 34.17 (CH), 24.61 (2CH_3).

^{19}F NMR (376 MHz, Chloroform-d, rif. BF_3-Et_2O +25 °C) δ -60.16.

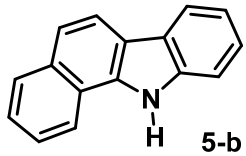
HRMS(ESI-QTOF). Calcd. for $C_{16}H_{15}F_3N^+$ $[M+H]^+$ 278.11511. Found $C_{16}H_{15}F_3N^+$ $[M+H]^+$: 278.1149.

Synthesis of substituted benzocarbazole



Scheme S2.

In a 25 mL oven-dried reaction flask α-tetralone (5 mmol), the appropriate substituted phenylhydrazine hydrochloride (7.5 mmol) and the solvent *N*-methyl-2-pyrrolidone (NMP, 10 mL) were added and the resulting solution was stirred under oxygen (1 atm) at +140 °C for 24 h. After cooling to room temperature, the NMP was distilled in high vacuum at +100 °C. The residue was diluted in DCM and filtered on Celite®, then evaporated the solvent. The products were purified by chromatography separation on silica gel, with eluent *n*-hexane/DCM in 7:3 ratio.



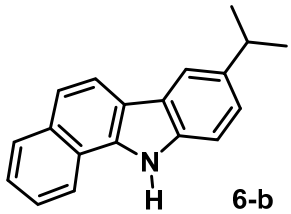
5-b

For compound **5-b** was used α-tetralone (5 mmol) and phenylhydrazine hydrochloride (7.5 mmol). Yield: 59%.

^{1}H-NMR (600 MHz, Chloroform-d, 7.26 ppm, +25 °C) δ 8.78 (s, 1 N-H), 8.17 – 8.11 (m, 3H), 8.02 (d, J = 8.1 Hz, 1H), 7.67 (d, J = 8.5 Hz, 1H), 7.63 – 7.57 (m, 2H), 7.55 (ddd, J = 8.1, 6.9, 1.3 Hz, 1H), 7.45 (ddd, J = 8.2, 7.0, 1.2 Hz, 1H), 7.32 (td, J = 7.5, 1.0 Hz, 1H).

^{13}C-NMR (151 MHz, Chloroform-d, 77 ppm, +25 °C) δ 138.45 (Cq), 134.85 (Cq), 132.42 (Cq), 129.04 (CH), 125.54 (CH), 125.20 (CH), 124.86 (CH), 124.18 (Cq), 121.07 (Cq), 120.44 (CH), 120.21 (CH), 119.97 (CH), 119.90 (CH), 119.31 (CH), 118.43 (Cq), 111.02 (CH).

HRMS(ESI-QTOF). Calcd. for $C_{16}H_{12}N^+$ $[M+H]^+$ 218.09643. Found $C_{16}H_{12}N^+$ $[M+H]^+$: 218.0958.



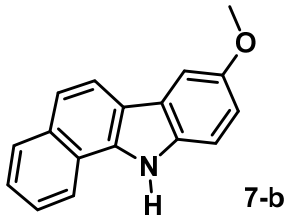
6-b

For compound **6-b** was used α-tetralone (5 mmol) and (4-*i*-propyl-phenyl)-hydrazine hydrochloride (7.5 mmol). Yield: 62%

^{1}H-NMR (600 MHz, Chloroform-d, 7.26 ppm +25°C) δ 8.13 (t, *J* = 8.0 Hz, 2H), 8.03 – 7.96 (m, 2H), 7.65 (d, *J* = 8.5 Hz, 1H), 7.59 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 1H), 7.55 – 7.50 (m, 2H), 7.34 (dd, *J* = 8.3, 1.7 Hz, 1H), 3.14 (hept, *J* = 6.9 Hz, 1H), 1.39 (d, *J* = 7.0 Hz, 6H).

^{13}C-NMR (151 MHz, Chloroform-d, 77.0 ppm, +25°C) δ 140.79 (Cq), 137.00 (Cq), 135.18 (Cq), 132.36 (Cq), 129.03 (CH), 125.42 (CH), 125.05 (CH), 124.24 (Cq), 123.99 (CH), 121.16 (Cq), 120.44 (CH), 119.95 (CH), 119.34 (CH), 118.48 (Cq), 116.96 (CH), 110.77 (CH), 34.29 (CH), 24.72 ($2CH_3$).

HRMS(ESI-QTOF). Calcd. for $C_{19}H_{18}N^+$ $[M+H]^+$ 260.14338. Found $C_{19}H_{18}N^+$ $[M+H]^+$: 260.1430.



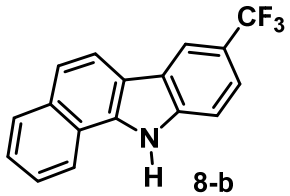
7-b

For compound **7-b** was used α-tetralone (5 mmol) and (4-methoxy-phenyl)-hydrazine hydrochloride (7.5 mmol). Yield: 43%.

^{1}H-NMR (600 MHz, Chloroform-d, TMS +25 °C) δ 8.67 (s, 1H), 8.11 (d, *J* = 8.1 Hz, 1H), 8.09 (d, *J* = 8.5 Hz, 1H), 8.00 (d, *J* = 8.1 Hz, 1H), 7.63 (d, *J* = 8.5 Hz, 1H), 7.62 – 7.56 (m, 2H), 7.53 (ddd, *J* = 8.1, 6.9, 1.3 Hz, 1H), 7.49 (d, *J* = 8.7 Hz, 1H), 7.09 (dd, *J* = 8.7, 2.4 Hz, 1H), 3.97 (s, 3H).

^{13}C-NMR (151 MHz, Chloroform-d, TMS, +25 °C) δ 154.31 (Cq), 135.64 (Cq), 133.39 (Cq), 132.39 (Cq), 129.02 (CH), 125.50 (CH), 125.20 (CH), 124.61 (Cq), 121.23 (Cq), 120.43 (CH), 119.83 (CH), 119.25 (CH), 118.39 (Cq), 114.43 (CH), 111.75 (CH), 102.31 (CH), 56.03 (CH_3).

HRMS(ESI-QTOF). Calcd. for $C_{17}H_{14}NO^+$ $[M+H]^+$ 248.10699. Found $C_{17}H_{14}NO^+$ $[M+H]^+$: 248.1067.



8-b

For compound **8-b:** (4-trifluoromethyl)-phenylhydrazine hydrochloride (7.5 mmol) was dissolved in 10 mL of NMP. The α-tetralone (5 mmol) was added and the resulting solution was stirred under oxygen (1 atm) at +140 °C for 24 h. Since the aromatization was not complete, a catalytic amount of iodine was added and the solution was stirred one hour. After cooling to room temperature, the NMP was distilled in high vacuum at +100 °C. The residue was diluted in DCM and filtered on Celite®, then the mixture was washed with sodium sulphite and extracted with DCM. The combined organic layer was dried with sodium sulphate and then evaporated the solvent. The benzocarbazole product was purified by chromatography separation on silica gel, with eluent *n*-hexane/DCM in 7:3 ratio. Yield: 28%.

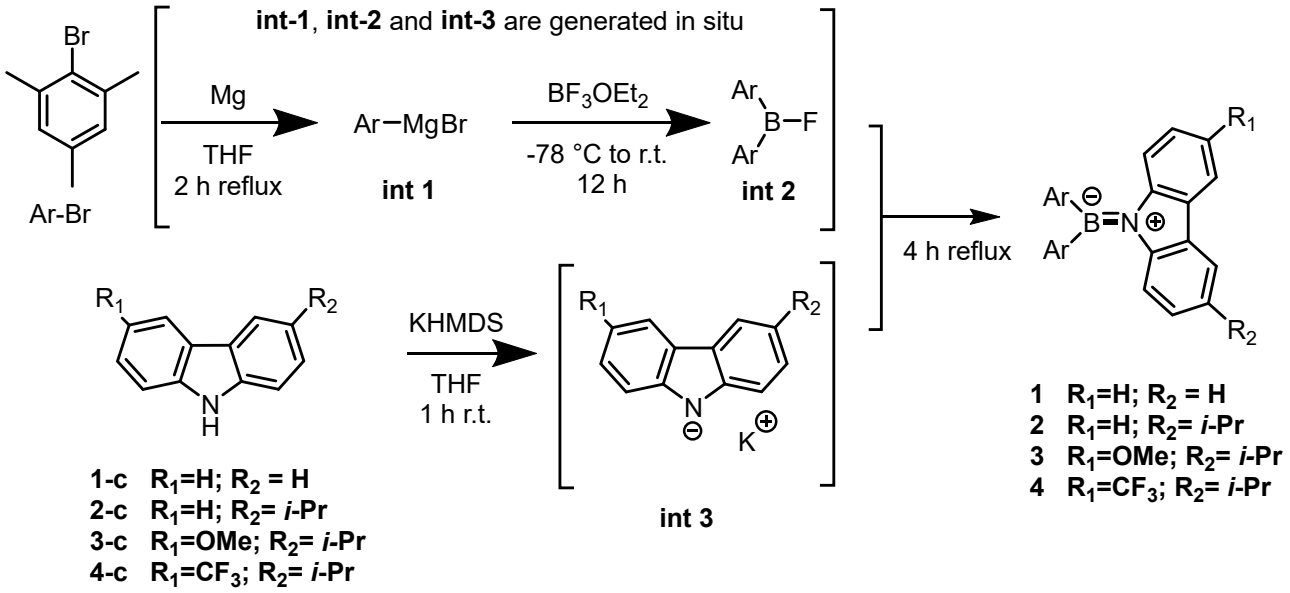
^{1}H NMR (600 MHz, Chloroform-d, 7.26 ppm +25 °C) δ 8.97 (s, 1H), 8.40 (s, 1H), 8.15 (d, J = 8.4 Hz, 2H), 8.04 (d, J = 8.1 Hz, 1H), 7.72 (d, J = 8.6 Hz, 1H), 7.66 (p, J = 8.5 Hz, 3H), 7.61 – 7.56 (m, 1H).

^{13}C NMR (151 MHz, Chloroform-d, TMS, 77.0 ppm, +25 °C) δ 139.80 (Cq), 135.71 (Cq), 132.78 (Cq), 129.18 (CH), 125.97 (CH), 125.84 (CH), 125.23 (Cq, q, $J_{1\text{-}CF}$ = 271.8 Hz), 123.75 (Cq), 122.38 (Cq, q, $J_{2\text{-}CF}$ = 31.7 Hz), 121.6 (CH, q, $J_{4\text{-}CF}$ = 3.0 Hz), 121.19 (CH), 120.98 (Cq), 120.42 (CH), 119.03 (CH), 118.20 (Cq), 117.58 (CH, q, $J_{4\text{-}CF}$ = 3.0 Hz), 111.15 (CH).

^{19}F NMR (376 MHz, Chloroform-d, rif. BF_3-Et_2O +25 °C) δ -62.13.

HRMS(ESI-QTOF). Calcd. for $C_{17}H_{11}F_3N^+$ $[M+H]^+$ 286.08381. Found $C_{17}H_{11}F_3N^+$ $[M+H]^+$: 286.0832.

Synthesis of compounds **1-4**

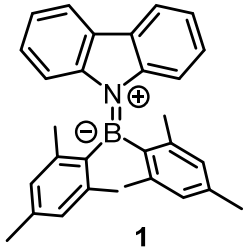


Scheme S3.

In a 25 mL oven-dried reaction flask was added 2-bromomesitylene (0.45 mL, 6 mmol, 2 eq), magnesium (0.2 g) in dry THF (6 mL) and a tip of iodine under nitrogen flow. The mixture was stirred and left to reflux for 2 hours obtaining the Grignard reagent **int-1**. The solution was brought to -78 °C and boron trifluoride diethyl etherate (BF_3OEt_2, 0.41 mL, 3 mmol, 1 eq) was added dropwise. The temperature was slowly increased to room temperature in 12 h obtaining a solution 0.5 M of **int-2**.

In another 25 mL oven-dried reaction flask was added carbazole (1 eq) in dry THF (6 mL). The potassium bis(trimethylsilyl)amide (KHMDS) (1 eq, 0.5 M) was therefore added dropwise and the mixture was stirred at room temperature for 1 h, obtaining **int-3**.

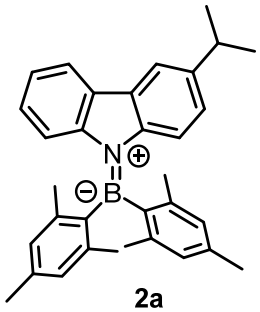
The **int-2** (1 eq) was added dropwise to the **int-3** (1 eq) and the mixture was refluxed 4 hours. After cooling to room temperature, the solvent was removed and the residue was dissolved in DCM, then filtered on Celite®. The product was purified by chromatography separation on silica gel column with *n*-hexane and DCM (7:3) as eluent. Evaporated the solvents, a white solid was obtained. The product was crystallized in acetonitrile/DCM (6:1).



1

Compound **1** was synthesized starting with carbazole **1-c**. Yield: 49%. Spectroscopic data is consistent with previously reported results.[2]

^{1}H NMR (600 MHz, Methylene Chloride-d_2, 5.33 ppm, +25 °C) δ 8.01 (dt, *J* = 7.7, 0.9 Hz, 2H), 7.27 (td, *J* = 7.4, 0.9 Hz, 2H), 7.09 (ddd, *J* = 8.5, 7.2, 1.3 Hz, 2H), 6.95 (dd, *J* = 8.5, 0.9 Hz, 2H), 6.86 (s, 4H), 2.35 (s, 6H), 2.03 (s, 12H).



2a

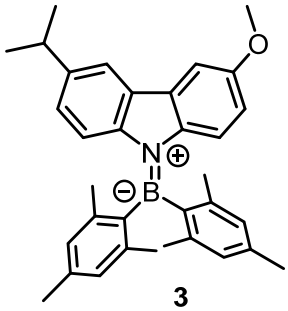
Compound **2a** was synthesized starting with carbazole **2-c**. Yield: 55%.

^{1}H NMR (600 MHz, Methylene Chloride-d_2, 5.33 ppm, +25 °C) δ 7.99 (ddd, *J* = 7.7, 1.4, 0.7 Hz, 1H), 7.85 (d, *J* = 1.8 Hz, 1H), 7.25 (ddd, *J* = 7.8, 7.3, 0.9 Hz, 1H), 7.06 (ddd, *J* = 8.5, 7.2, 1.3 Hz, 1H), 6.97 (dd, *J* = 8.6, 1.9 Hz, 1H), 6.92 (dt, *J* = 8.5, 0.9 Hz, 1H), 6.85 (d, *J* = 4.0 Hz, 4H), 6.82 (dd, *J* = 8.7, 0.6 Hz, 1H), 3.03 (hept, *J* = 6.9 Hz, 1H), 2.34 (d, *J* = 3.2 Hz, 6H), 2.03 (d, *J* = 7.3 Hz, 12H), 1.32 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (151 MHz, Methylene Chloride-d_2, 53.52 ppm, +25 °C) δ 143.67 (Cq), 143.64 (Cq), 141.64 (Cq), 141.06 (Cq), 139.40 (Cq), 139.37 (Cq), 138.36 (Cq-B, broad), 128.76 (CH), 128.73 (CH), 128.39 (Cq), 128.16 (Cq), 126.02 (CH), 125.20 (CH), 122.66 (CH), 119.41 (CH), 116.85 (CH), 115.54 (CH), 115.19 (CH), 34.04 (CH), 24.21 (CH_3), 21.71 (CH_3), 21.11 (CH_3).

^{11}B NMR (192 MHz, Methylene Chloride-d$_2$, ref. BF_3Et_2O, +25 °C) δ 51.97.

HRMS(ESI-QTOF). Calcd. for $C_{33}H_{37}BN^+$ $[M+H]^+$ 458.30136. Found $C_{33}H_{37}BN^+$ $[M+H]^+$: 458.3019.



3

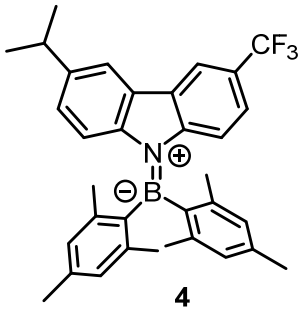
Compound **3** was synthesized starting with carbazole **3-c**. Yield: 88%

^{1}H NMR (600 MHz, Methylene Chloride-*d*$_2$, 5.33 ppm, +25 °C) δ 7.81 (d, *J* = 1.8 Hz, 1H), 7.45 (d, *J* = 2.6 Hz, 1H), 6.97 (dd, *J* = 8.6, 1.8 Hz, 1H), 6.86 (s, 2H), 6.85 (s, 2H), 6.81 (d, *J* = 8.6 Hz, 1H), 6.79 (d, *J* = 9.0 Hz, 1H), 6.66 (dd, *J* = 9.0, 2.6 Hz, 1H), 3.88 (s, 3H), 3.03 (hept, *J* = 6.9 Hz, 1H), 2.35 (s, 3H), 2.34 (s, 3H), 2.04 (s, 6H), 2.03 (s, 6H), 1.32 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (151 MHz, Methylene Chloride-*d*$_2$, 53.52 ppm, +25 °C) δ 156.12 (Cq), 143.51 (Cq), 142.30 (Cq), 141.08 (Cq), 141.05 (Cq), 139.27 (Cq), 139.24 (Cq), 138.38 (Cq-B. broad), 137.94 (Cq), 129.28 (Cq), 128.73 (CH), 128.70 (CH), 128.23 (Cq), 125.30 (CH), 116.73 (Cq), 116.41 (CH), 115.35 (CH), 114.16 (CH), 102.29 (CH), 55.69 (CH_3), 34.04 (CH), 24.22 (CH_3), 21.73 (CH_3), 21.71 (CH_3), 21.11 (CH_3), 21.10 (CH_3).

^{11}B NMR (192 MHz, Methylene Chloride-d$_2$, ref. BF_3Et_2O, +25 °C) δ 51.51.

HRMS(ESI-QTOF). Calcd. for $C_{34}H_{39}BNO^+$ $[M+H]^+$ 488.31192. Found $C_{34}H_{39}BNO^+$ $[M+H]^+$: 488.3115.



4

Compound **4** was synthesized starting with carbazole **4-c**. Yield: 54%

^{1}H NMR (600 MHz, Methylene Chloride-d_2, 5.33 ppm, +25 °C) 8.29 – 8.26 (m, 1H), 7.90 (d, *J* = 1.9 Hz, 1H), 7.31 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.04 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.00 (d, *J* = 8.7 Hz, 1H), 6.87 (s, 4H), 6.85 (d, *J* = 8.6 Hz, 1H), 3.04 (p, *J* = 6.9 Hz, 1H), 2.34 (d, *J* = 2.7 Hz, 6H), 2.01 (d, *J* = 6.5 Hz, 12H), 1.32 (d, *J* = 6.9 Hz, 6H).

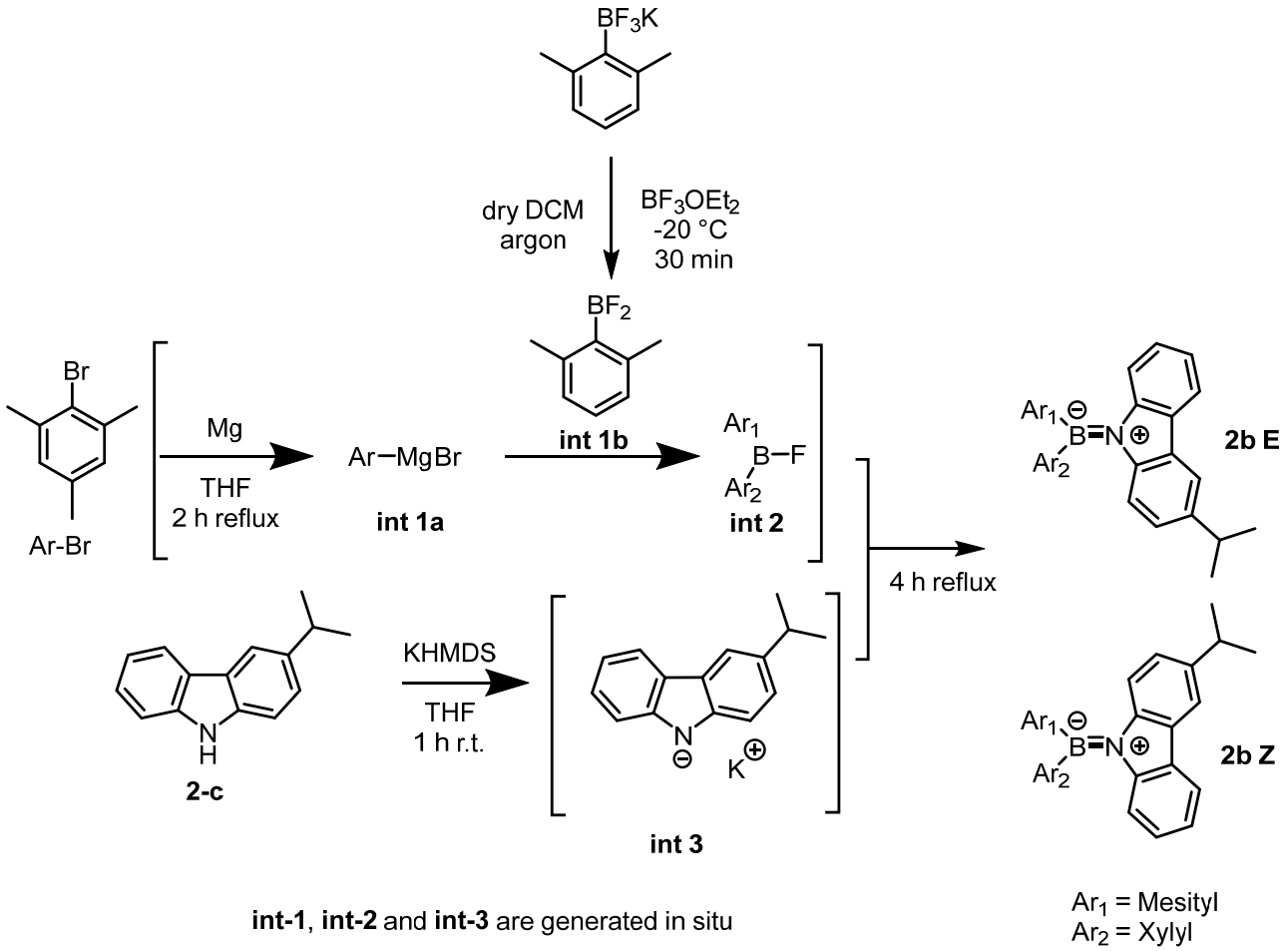
^{13}C NMR (151 MHz, Methylene Chloride-d_2, 53.52 ppm, +25 °C) δ 145.54 (Cq), 144.18 (Cq), 142.23 (Cq), 141.10 (Cq), 141.09 (Cq), 139.93 (Cq), 139.81 (Cq), 137.83 (Cq-B, broad), 128.96 (CH), 128.86 (CH), 128.40 (Cq), 127.20 (Cq), 126.30 (CH), 125.08 (Cq, q, $J_{1\text{-}CF}$ = 271.8 Hz), 124.41 (Cq, q, $J_{2\text{-}CF}$ = 31.7 Hz), 122.64 (CH, q, $J_{3\text{-}CF}$ = 3.0 Hz), 117.12 (CH), 116.87 (CH, q, $J_{3\text{-}CF}$ = 3.0 Hz), 115.72 (CH), 115.34 (CH), 34.03 (CH), 24.14 (CH_3), 21.71 (CH_3), 21.69 (CH_3), 21.13 (CH_3), 21.12 (CH_3).

^{11}B NMR (192 MHz, Methylene Chloride-d_2, ref. BF_3Et_2O, +25 °C) δ 53.19

^{19}F NMR (376 MHz, Methylene Chloride-d_2, ref. BF_3Et_2O, +25 °C) δ -61.35

HRMS(ESI-QTOF). Calcd. for $C_{34}H_{36}BF_3N^+$ $[M+H]^+$ 526.28874. Found $C_{34}H_{36}BF_3N$ $[M+H]^+$: 526.2881.

Synthesis of compounds **2b**

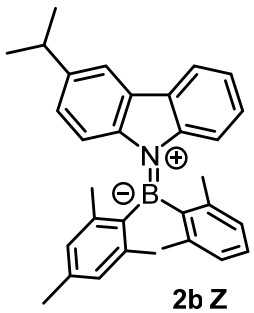


Scheme S4.

In a 25 mL oven-dried reaction flask was added potassium 2,6-dimethylphenyltrifluoroborate (1.27 g, 6 mmol, 2 eq) in 6 mL of dry DCM under argon flow. Boron trifluoride diethyl etherate (BF_3OEt_2, 0.82 mL, 6 mmol, 1 eq) was added dropwise at -20 °C and the mixture was stirred for 30 minutes. The solution was brought to -78 °C and the excess of boron trifluoride diethyl etherate was removed by vacuum. Thereafter the solution was filtered in a dropping funnel under argon flow and was used in the second step (**int-1b**).

In a 25 mL oven-dried reaction flask was added 2-bromomesitylene (0.45 mL, 6 mmol, 2 eq), magnesium (0.2 g), dry THF (6 mL) and a tip of iodine under argon flow. The mixture was stirred and left to reflux for 2 hours obtaining the Grignard reagent **int-1a**. The temperature was then decreased to -78 °C and the solution of **int-1b** in dry DCM (6 mL, 6 mmol, 1 eq) was added dropwise. The temperature was slowly increased to room temperature in 12 h, obtaining a solution 0.5 M of **int-2**.

In another 25 mL oven-dried reaction flask was added carbazole **2-c** (1.25 g, 6 mmol, 2 eq) in dry THF (6 mL) under argon flow. The potassium bis(trimethylsilyl)amide (KHMDS) (2 eq, 0.5 M) was therefore added dropwise and the mixture was stirred at room temperature for 1 h, obtaining **int-3**. The **int-2** (1 eq) was added dropwise to the **int-3** (1 eq) and the mixture was refluxed 4 hours under argon flow. After cooling to room temperature, the solvent was removed and the residue was dissolved in DCM, then was filtered on Celite®. The product was purified by chromatography separation on silica gel column with *n*-hexane and DCM (7:3) as eluent. Evaporated the solvents, a white solid was obtained. The two diastereoisomers E/Z have been purified by CSP-HPLC with AD-H column and 99:1 *n*-hexane/*i*-propanol (flow = 10 mL/min).



2b Z

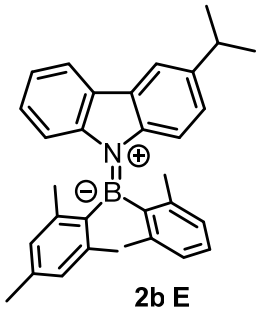
First eluted HPLC AD-H, Compound **2b Z** Yield: 25%

^{1}H NMR (600 MHz, Methylene Chloride-d_2, 5.33 ppm, -10 °C) δ 7.98 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.84 (d, *J* = 1.9 Hz, 1H), 7.25 (td, *J* = 7.5, 3.0 Hz, 2H), 7.03 (ddd, *J* = 8.4, 7.1, 1.4 Hz, 1H), 7.00 (d, *J* = 7.6 Hz, 2H), 6.96 (dd, *J* = 8.6, 1.9 Hz, 1H), 6.87 – 6.82 (m, 3H), 6.81 (d, *J* = 8.5 Hz, 1H), 3.01 (hept, *J* = 7.0 Hz, 1H), 2.33 (s, 3H), 2.02 (d, *J* = 11.4 Hz, 11H), 1.29 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (151 MHz, Methylene Chloride-d_2, 53.52 ppm, -10 °C) 143.47 (Cq), 143.16 (Cq), 141.19 (Cq), 140.77 (Cq), 140.61 (Cq), 139.22 (Cq), 137.61 (Cq-B), 129.16 (CH), 128.50 (CH), 128.05 (Cq), 127.80 (Cq), 127.51 (CH), 125.83 (CH), 125.04 (CH), 122.56 (CH), 119.25 (CH), 116.67 (CH), 115.17 (CH), 114.85 (CH), 33.77 (CH), 24.02 (CH_3), 21.62 (CH_3), 21.52 (CH_3), 20.95 (CH_3).

^{11}B NMR (192 MHz, Methylene Chloride-d_2, ref. BF_3Et_2O, -10 °C) δ 51.72.

HRMS(ESI-QTOF). Calcd. for $C_{32}H_{35}BN^+$ $[M+H]^+$ 444.28571. Found $C_{32}H_{35}BN^+$ $[M+H]^+$: 444.2862.



2b E

Second eluted HPLC AD-H, Compound **2b E** Yield: 25%.

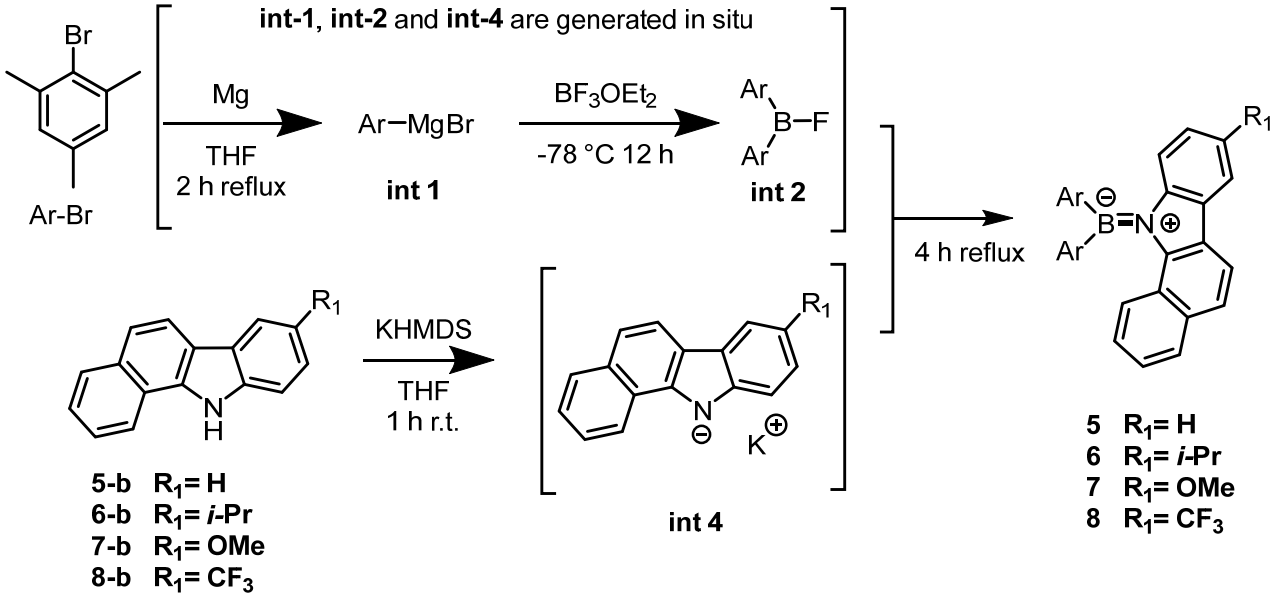
^{1}H NMR (600 MHz, Methylene Chloride-d_2, 5.33 ppm, -10 °C) 7.98 (dd, *J* = 7.9, 1.2 Hz, 1H), 7.84 (d, *J* = 1.9 Hz, 1H), 7.25 (td, *J* = 7.5, 4.5 Hz, 2H), 7.09 – 7.03 (m, 1H), 7.01 (d, *J* = 7.7 Hz, 3H), 6.96 – 6.88 (m, 3H), 6.84 (s, 2H), 6.73 (d, *J* = 8.6 Hz, 1H), 2.99 (h, *J* = 6.9 Hz, 1H), 2.32 (s, 3H), 2.05 (s, 7H), 2.00 (s, 6H), 1.28 (d, *J* = 6.9 Hz, 6H).

^{13}C NMR (151 MHz, Methylene Chloride-d_2, 53.52 ppm, -10 °C) δ 143.46 (Cq), 143.22 (Cq), 141.14 (Cq), 140.78 (Cq), 140.61 (Cq), 139.25 (Cq), 137.54 (Cq-B), 129.15 (CH), 128.53 (CH), 128.04 (Cq), 127.83 (Cq), 127.50 (CH), 125.85 (CH), 125.03 (CH), 122.57 (CH), 119.24 (CH), 116.69 (CH), 115.23 (CH), 114.81 (CH), 33.77 (CH), 24.02 (CH_3), 21.63 (CH_3), 21.53 (CH_3), 20.95 (CH_3).

^{11}B NMR (192 MHz, Methylene Chloride-d_2, ref. BF_3Et_2O, -10 °C) δ 51.83.

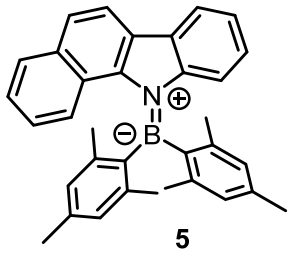
HRMS(ESI-QTOF). Calcd. for $C_{32}H_{35}BN^+$ $[M+H]^+$ 444.28571. Found $C_{32}H_{35}BN^+$ $[M+H]^+$: 444.2853.

Synthesis of compounds **5-8**



Scheme S5.

The compounds **5-8** were prepared with the same general procedure to synthesize compounds **1-4** using benzo[a]carbazole instead of carbazole.



5

Compound **5** was synthesized starting with benzo[a]carbazole **5-b**. Yield: 51%.

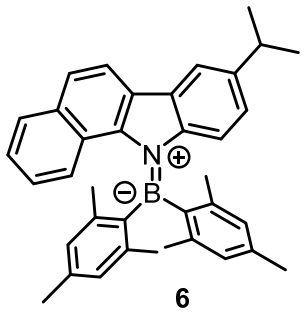
^{1}H NMR (600 MHz, Methylene Chloride-d_2, 5.33 ppm, 0 °C) δ 8.14 (d, *J* = 8.4 Hz, 1H), 8.09 (dt, *J* = 7.8, 1.1 Hz, 1H), 8.03 (dd, *J* = 8.5, 1.1 Hz, 1H), 7.87 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.80 (d, *J* = 8.3 Hz, 1H), 7.33 – 7.26 (m, 2H), 7.13 (dddd, *J* = 20.4, 8.5, 6.9, 1.4 Hz, 2H), 6.99 (s, 1H), 6.95 – 6.89 (m, 2H), 6.79 (s, 1H), 6.29 (s, 1H), 2.52 (s, 3H), 2.40 (s, 3H), 2.34 (s, 3H), 2.09 (s, 3H), 1.79 (s, 3H), 0.94 (s, 3H).

^{13}C NMR (151 MHz, Methylene Chloride-d_2, 53.52 ppm, 0 °C) δ 142.86 (Cq), 142.66 (Cq), 141.29 (Cq), 141.14 (Cq), 140.84 (Cq), 140.03 (Cq), 139.85 (Cq), 139.82 (Cq-B, broad), 139.35 (Cq), 139.00 (Cq-B, broad), 133.06 (Cq), 129.17 (CH), 129.00 (CH), 128.69 (CH), 128.22 (CH), 128.04 (CH), 127.91 (Cq), 125.81 (CH), 125.52 (CH), 125.27 (Cq), 124.28 (CH), 124.13 (CH), 123.71 (Cq),

123.70 (CH), 122.22 (CH), 119.19 (CH), 118.09 (CH), 114.50 (CH), 22.83 (CH_3), 22.71 (CH_3), 21.99 (CH_3), 21.16 (CH_3), 20.77 (CH_3), 19.88 (CH_3).

^{11}B NMR (192 MHz, Methylene Chloride-d$_2$, ref. BF_3Et_2O, +25 °C) δ 54.67.

HRMS(ESI-QTOF). Calcd. for $C_{34}H_{32}BNNa^+$ $[M+Na]^+$ 488.25200. Found $C_{34}H_{32}BNNa^+$ $[M+Na]^+$: 488.2524.



6

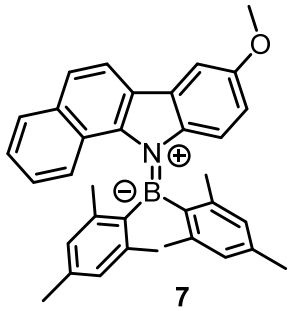
Compound **6** was synthesized starting with carbazole **6-b**.Yield: 54%.

^{1}H NMR (600 MHz, Methylene Chloride-*d*$_2$, 5.33 ppm, +25 °C) δ 8.13 (d, *J* = 8.4 Hz, 1H), 8.02 (dd, *J* = 8.6, 1.0 Hz, 1H), 7.92 (d, *J* = 1.9 Hz, 1H), 7.88 – 7.83 (m, 1H), 7.78 (d, *J* = 8.3 Hz, 1H), 7.27 (ddd, *J* = 8.0, 6.8, 1.1 Hz, 1H), 7.12 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.03 – 6.98 (m, 2H), 6.93 (s, 1H), 6.81 – 6.77 (m, 2H), 6.29 (s, 1H), 3.06 (hept, *J* = 6.9 Hz, 1H), 2.53 (s, 3H), 2.41 (s, 3H), 2.35 (s, 3H), 2.10 (s, 3H), 1.82 (s, 3H), 1.34 (d, *J* = 6.9, 3H), 1.33 (d, *J* = 6.9, 3H), 0.98 (s, 3H).

^{13}C NMR (151 MHz, Methylene Chloride-*d*$_2$, 53.52 ppm, +25 °C) δ 143.15 (Cq), 143.00 (Cq), 141.45 (Cq), 141.37 (Cq), 141.35 (Cq), 141.09 (Cq), 140.90 (Cq), 140.30 (Cq), 140.20 (Cq-B, broad), 140.04 (Cq), 139.43 (Cq), 139.32 (Cq-B, broad), 133.24 (Cq), 129.26 (CH), 129.17 (CH), 128.80 (CH), 128.32 (CH), 128.22 (CH), 128.18 (Cq), 125.71 (Cq), 125.63 (CH), 124.93 (CH), 124.27 (CH), 124.20 (CH), 124.08, 123.73 (CH), 118.16 (CH), 116.54 (CH), 114.51 (CH), 34.02 (CH), 24.29 (CH_3), 24.18 (CH_3), 22.90 (CH_3), 22.80 (CH_3), 22.09 (CH_3), 21.24 (CH_3), 20.85 (CH_3), 20.12 (CH_3).

^{11}B NMR (192 MHz, Methylene Chloride-d$_2$, ref. BF_3Et_2O, +25 °C) δ 54.64.

HRMS(ESI-QTOF). Calcd. for $C_{37}H_{38}BNNa^+$ $[M+Na]^+$ 530.29895. Found $C_{37}H_{38}BNNa^+$ $[M+H]^+$: 530.2996.



7

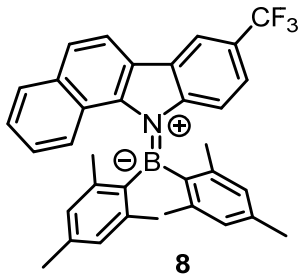
Compound **7** was preparated starting with carbazole **7-b**. Yield: 65%.

^{1}H NMR (600 MHz, Tetrachloroethane-*d*$_2$, 6 ppm, +25 °C) δ 8.09 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 8.5 Hz, 1H), 7.85 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.51 (d, *J* = 2.6 Hz, 1H), 7.28 (ddd, *J* = 8.0, 6.7, 1.1 Hz, 1H), 7.14 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 1H), 6.95 (s, 1H), 6.89 (s, 1H), 6.77 (d, *J* = 9.2 Hz, 1H), 6.74 (s, 1H), 6.72 (dd, J = 9.2, 2.6 Hz, 1H), 6.24 (s, 1H), 3.91 (s, 3H), 2.51 (s, 3H), 2.39 (s, 3H), 2.32 (s, 3H), 2.08 (s, 3H), 1.79 (s, 3H), 0.96 (s, 3H).

^{13}C NMR (151 MHz, Tetrachloroethane-*d*$_2$, 73.78 ppm, +25 °C) δ 154.92 (Cq), 142.54 (Cq), 141.11 (Cq), 140.85 (Cq), 140.70 (Cq), 140.53 (Cq), 139.62 (Cq), 139.52 (Cq-B, broad), 138.99 (Cq), 138.65 (Cq-B, broad), 137.08 (Cq), 132.72 (Cq), 129.07 (CH), 128.92 (CH), 128.56 (CH), 128.01 (Cq), 128.00 (2 CH), 125.34 (CH), 125.03 (Cq), 124.36 (CH), 123.88 (CH), 123.80 (CH), 123.69 (Cq), 118.12 (CH), 115.51 (CH), 113.80 (CH), 101.76 (CH), 53.89 (CH_3), 23.11 (CH_3), 23.01 (CH_3), 22.34 (CH_3), 21.54 (CH_3), 21.13 (CH_3), 20.22 (CH_3).

^{11}B NMR (192 MHz, Tetrachloroethane-d$_2$, ref. BF_3Et_2O, +25 °C) δ 54.57.

HRMS(ESI-QTOF). Calcd. for $C_{35}H_{34}BNONa^+$ $[M+Na]^+$ 518.26257. Found $C_{35}H_{34}BNONa^+$ $[M+Na]^+$: 518.2629.



8

Compound **8** was synthesized starting with carbazole **8-b**. Yield: 31%

^{1}H NMR (600 MHz, Methylene Chloride-d_2, 5.33 ppm, +25 °C) δ 8.39 – 8.36 (m, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.90 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.40 – 7.31 (m, 2H), 7.19 (ddd, *J* = 8.3, 6.8, 1.3 Hz, 1H), 7.05 – 6.99 (m, 2H), 6.97 (s, 1H), 6.82 (s, 1H), 6.30 (s, 1H), 2.50 (s, 3H), 2.41 (s, 3H), 2.37 (s, 3H), 2.10 (s, 3H), 1.84 (s, 3H), 0.95 (s, 3H).

^{13}C NMR (151 MHz, Methylene Chloride-d_2, 53.52 ppm, +25 °C) δ 144.58 (Cq), 143.26 (Cq), 141.77 (Cq), 141.40 (Cq), 141.05 (Cq), 140.77 (Cq), 140.00 (Cq), 139.64 (Cq-B, broad), 138.79 (Cq-B, broad), 133.71 (Cq), 129.55 (CH), 129.32 (CH), 129.13 (CH), 128.51 (CH), 128.44 (CH), 128.06 (Cq), 125.62 (CH), 125.12 (Cq, q, $J_{1\text{-}CF}$ = 271.8 Hz), 125.01 (CH), 124.91 (CH), 124.67 (Cq), 124.21 (Cq, q, $J_{2\text{-}CF}$ = 31.7 Hz), 124.19 (CH), 123.81, 122.48 (CH, q, $J_{3\text{-}CF}$ = 3.0 Hz), 118.02 (CH), 116.78 (CH, q, $J_{3\text{-}CF}$ = 3.0 Hz), 115.08 (CH), 22.90 (CH_3), 22.87 (CH_3), 22.16 (CH_3), 21.26 (CH_3), 20.87 (CH_3), 20.02 (CH_3).

^{11}B NMR (192 MHz, Methylene Chloride-d_2, ref. BF_3Et_2O, +25 °C) δ 55.95

^{19}F NMR (376 MHz, Methylene Chloride-d_2, ref. BF_3Et_2O, +25 °C) δ -61.27.

HRMS(ESI-QTOF). Calcd. for $C_{35}H_{31}BF_3NNa^+$ $[M+Na]^+$ 556.23939. Found $C_{35}H_{31}BF_3NNa^+$ $[M+Na]^+$: 556.2389.

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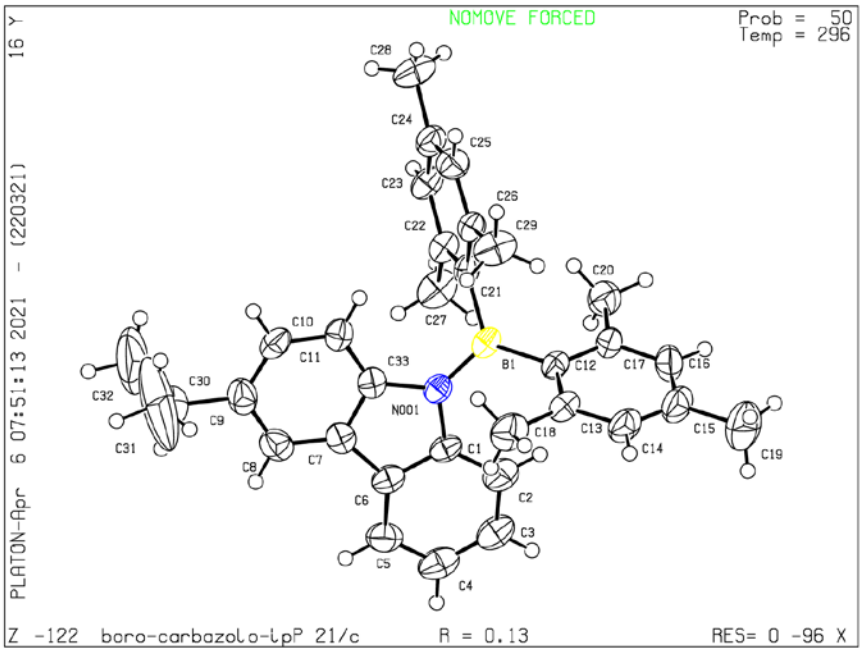
[1] F. Xiao, Y. Liao, M. Wu, G.-J. Deng *Green Chem.* **2012**, *14*, 3277–3280.

[2] T. Taniguchi, J. Wang, S. Irle, S. Yamaguchi *Dalton Trans.,* **2013***, 42,* 620.

Crystal data for 2



A specimen of $C_{33}H_{36}BN$, approximate dimensions 0.150 mm x 0.220 mm x 0.250 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 24.67 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 22831 reflections to a maximum θ angle of 24.92 (0.84 Å resolution), of which 4495 were independent (average redundancy 5.079, completeness = 96.6%, R_{int} = 11.53%, R_{sig} = 9.95%) and 3004 (66.83%) were greater than $2\sigma(F^2)$. The final cell constants of a = 9.81(5) Å, b = 11.79(5) Å, c = 23.06(10) Å, β = 92.61(10) , volume = 2660.(20) $Å^3$, are based upon the refinement of the XYZ-centroids of 6219 reflections above 20 σ(I) with 4.94 < 2θ < 49.62 . Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.945. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9840 and 0.9900. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z = 4 for the formula unit, $C_{33}H_{36}BN$. The final anisotropic full-matrix least-squares refinement on F^2 with 324 variables converged at R1 = 13.19%, for the observed data and wR2 = 28.58% for all data. The goodness-of-fit was 1.184. The largest peak in the final difference electron density synthesis was 0.337 $e^-/Å^3$ and the largest hole was -0.284 $e^-/Å^3$ with an RMS deviation of 0.059 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.140 g/cm^3 and F(000), 984 e^-. CCDC deposition number: 2080360.

Table 1. Sample and crystal data

Identification code	mazza1907	
Chemical formula	$C_{33}H_{36}BN$	
Formula weight	457.44 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.150 x 0.220 x 0.250 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 9.81(5) Å	α = 90°
	b = 11.79(5) Å	β = 92.61(10)°
	c = 23.06(10) Å	γ = 90°
Volume	2660.(20) $Å^3$	
Z	4	
Density (calculated)	1.140 g/cm^3	
Absorption coefficient	0.064 mm^{-1}	
F(000)	984	

Table 2. Data collection and structure refinement

Theta range for data collection	1.94 to 24.92°
Index ranges	-11<=h<=11, -13<=k<=13, -27<=l<=27
Reflections collected	22831
Independent reflections	4495 [R(int) = 0.1153]
Coverage of independent reflections	96.6%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9900 and 0.9840
Structure solution technique	direct methods
Structure solution program	XT, VERSION 2014/5
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)

Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	4495 / 0 / 324	
Goodness-of-fit on F^2	1.184	
Final R indices	3004 data; $I>2\sigma(I)$	R1 = 0.1319, wR2 = 0.2645
	all data	R1 = 0.1913, wR2 = 0.2858
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0499P)^2+9.5587P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.337 and -0.284 eÅ^{-3}	
R.M.S. deviation from mean	0.059 eÅ^{-3}	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
N001	0.2761(4)	0.2575(4)	0.49871(19)	0.0351(11)
C1	0.1436(5)	0.2281(5)	0.4773(2)	0.0367(13)
C33	0.3608(6)	0.2497(4)	0.4513(2)	0.0355(13)
C21	0.4636(5)	0.2446(4)	0.5795(2)	0.0335(13)
C6	0.1444(6)	0.2059(4)	0.4190(3)	0.0394(14)
C13	0.1629(5)	0.4539(5)	0.5778(3)	0.0408(14)
C26	0.5648(5)	0.3197(5)	0.6005(2)	0.0357(13)
C12	0.2162(5)	0.3479(5)	0.5963(2)	0.0355(13)
C7	0.2830(6)	0.2229(4)	0.4018(2)	0.0388(14)
C22	0.4932(5)	0.1286(4)	0.5789(2)	0.0368(13)
C17	0.1836(6)	0.3099(5)	0.6508(3)	0.0436(15)
C11	0.4985(6)	0.2745(5)	0.4479(2)	0.0395(14)
C23	0.6215(6)	0.0910(5)	0.5993(3)	0.0430(15)
C14	0.0779(6)	0.5138(6)	0.6122(3)	0.0537(17)
C5	0.0263(6)	0.1688(5)	0.3896(3)	0.0531(17)
C24	0.7215(6)	0.1640(5)	0.6190(3)	0.0448(15)

	x/a	y/b	z/c	U(eq)
C25	0.6919(6)	0.2779(5)	0.6190(3)	0.0455(15)
C10	0.5535(6)	0.2690(5)	0.3951(3)	0.0451(15)
C9	0.4811(7)	0.2404(6)	0.3449(3)	0.0529(17)
C8	0.3425(7)	0.2173(5)	0.3489(3)	0.0502(16)
C27	0.3922(6)	0.0413(5)	0.5577(3)	0.0562(18)
C16	0.0967(6)	0.3727(6)	0.6837(3)	0.0565(18)
C2	0.0260(6)	0.2151(6)	0.5074(3)	0.0537(17)
C15	0.0440(7)	0.4758(6)	0.6648(3)	0.0576(18)
C4	0.9099(7)	0.1557(6)	0.4193(3)	0.0580(18)
C29	0.5399(7)	0.4445(5)	0.6021(3)	0.0589(19)
B1	0.3162(6)	0.2828(5)	0.5574(3)	0.0338(15)
C20	0.2338(7)	0.1967(6)	0.6741(3)	0.0563(18)
C3	0.9105(6)	0.1777(6)	0.4773(3)	0.0583(18)
C18	0.1955(7)	0.5044(6)	0.5205(3)	0.0624(19)
C28	0.8565(7)	0.1193(7)	0.6421(3)	0.076(2)
C30	0.5433(8)	0.2355(7)	0.2867(3)	0.073(2)
C19	0.9498(9)	0.5415(8)	0.7021(4)	0.094(3)
C31	0.5997(17)	0.3458(12)	0.2714(5)	0.206(8)
C32	0.6425(16)	0.1431(14)	0.2825(5)	0.209(9)

Table 4. Bond lengths (Å)

N001-C33	1.407(8)	N001-C1	1.412(9)
N001-B1	1.423(10)	C1-C6	1.371(10)
C1-C2	1.381(9)	C33-C7	1.381(9)
C33-C11	1.388(10)	C21-C22	1.398(9)
C21-C26	1.401(8)	C21-B1	1.577(10)
C6-C5	1.386(9)	C6-C7	1.447(10)
C13-C14	1.373(9)	C13-C12	1.414(9)
C13-C18	1.496(10)	C26-C25	1.390(9)
C26-C29	1.493(10)	C12-C17	1.384(9)
C12-B1	1.562(9)	C7-C8	1.377(10)
C22-C23	1.396(9)	C22-C27	1.496(9)
C17-C16	1.384(9)	C17-C20	1.513(10)
C11-C10	1.355(9)	C11-H11	0.93
C23-C24	1.368(9)	C23-H23	0.93
C14-C15	1.348(10)	C14-H14	0.93

C5-C4	1.368(10)	C5-H5	0.93
C24-C25	1.375(10)	C24-C28	1.501(10)
C25-H25	0.93	C10-C9	1.372(10)
C10-H10	0.93	C9-C8	1.393(11)
C9-C30	1.502(11)	C8-H8	0.93
C27-H27A	0.96	C27-H27B	0.96
C27-H27C	0.96	C16-C15	1.384(11)
C16-H16	0.93	C2-C3	1.374(10)
C2-H2	0.93	C15-C19	1.505(10)
C4-C3	1.362(11)	C4-H4	0.93
C29-H29A	0.96	C29-H29B	0.96
C29-H29C	0.96	C20-H20A	0.96
C20-H20B	0.96	C20-H20C	0.96
C3-H3	0.93	C18-H18A	0.96
C18-H18B	0.96	C18-H18C	0.96
C28-H28A	0.96	C28-H28B	0.96
C28-H28C	0.96	C30-C31	1.462(14)
C30-C32	1.467(13)	C30-H30	0.98
C19-H19A	0.96	C19-H19B	0.96
C19-H19C	0.96	C31-H31A	0.96
C31-H31B	0.96	C31-H31C	0.96
C32-H32A	0.96	C32-H32B	0.96
C32-H32C	0.96		

Table 5. Bond angles (°)

C33-N001-C1	106.2(5)	C33-N001-B1	127.2(5)
C1-N001-B1	126.4(5)	C6-C1-C2	120.9(5)
C6-C1-N001	110.1(5)	C2-C1-N001	129.0(6)
C7-C33-C11	120.3(6)	C7-C33-N001	109.5(6)
C11-C33-N001	129.9(5)	C22-C21-C26	118.5(5)
C22-C21-B1	117.7(5)	C26-C21-B1	123.8(5)
C1-C6-C5	119.8(6)	C1-C6-C7	106.9(5)
C5-C6-C7	133.2(6)	C14-C13-C12	120.4(6)
C14-C13-C18	117.8(6)	C12-C13-C18	121.9(5)
C25-C26-C21	119.6(6)	C25-C26-C29	119.2(5)
C21-C26-C29	121.2(6)	C17-C12-C13	117.6(5)
C17-C12-B1	122.6(5)	C13-C12-B1	119.6(5)

C8-C7-C33	120.1(6)	C8-C7-C6	132.7(6)
C33-C7-C6	107.2(6)	C23-C22-C21	119.5(5)
C23-C22-C27	117.7(6)	C21-C22-C27	122.8(6)
C16-C17-C12	119.9(6)	C16-C17-C20	118.4(6)
C12-C17-C20	121.6(5)	C10-C11-C33	118.0(6)
C10-C11-H11	121.0	C33-C11-H11	121.0
C24-C23-C22	122.3(6)	C24-C23-H23	118.9
C22-C23-H23	118.9	C15-C14-C13	122.0(7)
C15-C14-H14	119.0	C13-C14-H14	119.0
C4-C5-C6	119.3(7)	C4-C5-H5	120.3
C6-C5-H5	120.3	C23-C24-C25	117.8(6)
C23-C24-C28	120.4(7)	C25-C24-C28	121.7(6)
C24-C25-C26	122.2(6)	C24-C25-H25	118.9
C26-C25-H25	118.9	C11-C10-C9	123.9(7)
C11-C10-H10	118.1	C9-C10-H10	118.1
C10-C9-C8	117.5(6)	C10-C9-C30	123.2(7)
C8-C9-C30	119.3(6)	C7-C8-C9	120.2(6)
C7-C8-H8	119.9	C9-C8-H8	119.9
C22-C27-H27A	109.5	C22-C27-H27B	109.5
H27A-C27-H27B	109.5	C22-C27-H27C	109.5
H27A-C27-H27C	109.5	H27B-C27-H27C	109.5
C17-C16-C15	121.9(7)	C17-C16-H16	119.1
C15-C16-H16	119.1	C3-C2-C1	118.2(7)
C3-C2-H2	120.9	C1-C2-H2	120.9
C14-C15-C16	118.1(6)	C14-C15-C19	121.7(7)
C16-C15-C19	120.1(7)	C3-C4-C5	120.3(6)
C3-C4-H4	119.9	C5-C4-H4	119.9
C26-C29-H29A	109.5	C26-C29-H29B	109.5
H29A-C29-H29B	109.5	C26-C29-H29C	109.5
H29A-C29-H29C	109.5	H29B-C29-H29C	109.5
N001-B1-C12	119.7(5)	N001-B1-C21	117.2(5)
C12-B1-C21	123.1(6)	C17-C20-H20A	109.5
C17-C20-H20B	109.5	H20A-C20-H20B	109.5

C17-C20-H20C	109.5	H20A-C20-H20C	109.5
H20B-C20-H20C	109.5	C4-C3-C2	121.5(6)
C4-C3-H3	119.2	C2-C3-H3	119.2
C13-C18-H18A	109.5	C13-C18-H18B	109.5
H18A-C18-H18B	109.5	C13-C18-H18C	109.5
H18A-C18-H18C	109.5	H18B-C18-H18C	109.5
C24-C28-H28A	109.5	C24-C28-H28B	109.5
H28A-C28-H28B	109.5	C24-C28-H28C	109.5
H28A-C28-H28C	109.5	H28B-C28-H28C	109.5
C31-C30-C32	112.7(11)	C31-C30-C9	110.9(7)
C32-C30-C9	112.6(7)	C31-C30-H30	106.8
C32-C30-H30	106.8	C9-C30-H30	106.8
C15-C19-H19A	109.5	C15-C19-H19B	109.5
H19A-C19-H19B	109.5	C15-C19-H19C	109.5
H19A-C19-H19C	109.5	H19B-C19-H19C	109.5
C30-C31-H31A	109.5	C30-C31-H31B	109.5
H31A-C31-H31B	109.5	C30-C31-H31C	109.5
H31A-C31-H31C	109.5	H31B-C31-H31C	109.5
C30-C32-H32A	109.5	C30-C32-H32B	109.5
H32A-C32-H32B	109.5	C30-C32-H32C	109.5
H32A-C32-H32C	109.5	H32B-C32-H32C	109.5

Table 6. Torsion angles (°)

C33-N001-C1-C6	-1.6(6)	B1-N001-C1-C6	-177.9(5)
C33-N001-C1-C2	175.0(6)	B1-N001-C1-C2	-1.4(9)

C1-N001-C33-C7	3.3(6)	B1-N001-C33-C7	179.7(5)
C1-N001-C33-C11	176.7(5)	B1-N001-C33-C11	-7.0(9)
C2-C1-C6-C5	-0.6(9)	N001-C1-C6-C5	176.2(5)
C2-C1-C6-C7	-177.6(5)	N001-C1-C6-C7	-0.7(6)
C22-C21-C26-C25	1.3(8)	B1-C21-C26-C25	180.0(5)
C22-C21-C26-C29	179.8(5)	B1-C21-C26-C29	-1.5(8)
C14-C13-C12-C17	-2.3(8)	C18-C13-C12-C17	178.0(6)
C14-C13-C12-B1	-178.1(5)	C18-C13-C12-B1	2.2(8)
C11-C33-C7-C8	2.0(8)	N001-C33-C7-C8	176.1(5)
C11-C33-C7-C6	-177.9(5)	N001-C33-C7-C6	-3.8(6)
C1-C6-C7-C8	-177.1(6)	C5-C6-C7-C8	6.6(11)
C1-C6-C7-C33	2.7(6)	C5-C6-C7-C33	-173.6(6)
C26-C21-C22-C23	0.2(8)	B1-C21-C22-C23	-178.5(5)
C26-C21-C22-C27	179.6(5)	B1-C21-C22-C27	0.8(8)
C13-C12-C17-C16	2.8(8)	B1-C12-C17-C16	178.6(5)
C13-C12-C17-C20	178.9(5)	B1-C12-C17-C20	-5.3(9)
C7-C33-C11-C10	-1.5(8)	N001-C33-C11-C10	-174.2(5)
C21-C22-C23-C24	-1.3(9)	C27-C22-C23-C24	179.3(6)
C12-C13-C14-C15	1.1(10)	C18-C13-C14-C15	-179.2(6)
C1-C6-C5-C4	0.6(9)	C7-C6-C5-C4	176.5(6)
C22-C23-C24-C25	0.8(9)	C22-C23-C24-C28	178.3(6)

C23-C24-C25-C26	0.8(9)	C28-C24-C25-C26	-176.6(6)
C21-C26-C25-C24	-1.9(9)	C29-C26-C25-C24	179.6(6)
C33-C11-C10-C9	0.0(9)	C11-C10-C9-C8	0.9(9)
C11-C10-C9-C30	179.5(6)	C33-C7-C8-C9	-1.1(9)
C6-C7-C8-C9	178.8(6)	C10-C9-C8-C7	-0.4(9)
C30-C9-C8-C7	-179.0(6)	C12-C17-C16-C15	-2.3(9)
C20-C17-C16-C15	-178.5(6)	C6-C1-C2-C3	1.0(9)
N001-C1-C2-C3	-175.3(6)	C13-C14-C15-C16	-0.4(10)
C13-C14-C15-C19	-179.4(7)	C17-C16-C15-C14	1.0(10)
C17-C16-C15-C19	-180.0(7)	C6-C5-C4-C3	-0.8(10)
C33-N001-B1-C12	148.3(5)	C1-N001-B1-C12	-36.1(8)
C33-N001-B1-C21	-30.5(8)	C1-N001-B1-C21	145.1(5)
C17-C12-B1-N001	129.1(6)	C13-C12-B1-N001	-55.2(7)
C17-C12-B1-C21	-52.2(8)	C13-C12-B1-C21	123.5(6)
C22-C21-B1-N001	-61.4(7)	C26-C21-B1-N001	119.9(6)
C22-C21-B1-C12	119.9(6)	C26-C21-B1-C12	-58.8(8)
C5-C4-C3-C2	1.2(11)	C1-C2-C3-C4	-1.2(10)
C10-C9-C30-C31	-59.5(12)	C8-C9-C30-C31	119.1(10)
C10-C9-C30-C32	67.8(13)	C8-C9-C30-C32	-113.7(11)

Table 7. Anisotropic atomic displacement parameters ($Å^2$).

The anisotropic atomic displacement factor exponent takes the form:
$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N001	0.033(2)	0.031(3)	0.041(3)	0.001(2)	0.005(2)	0.001(2)
C1	0.028(3)	0.032(3)	0.050(4)	0.005(3)	0.001(3)	-0.002(2)
C33	0.048(3)	0.019(3)	0.040(3)	0.003(2)	0.005(3)	0.008(2)
C21	0.037(3)	0.030(3)	0.035(3)	0.002(2)	0.010(2)	-0.001(2)
C6	0.037(3)	0.028(3)	0.053(4)	0.002(3)	-0.001(3)	0.005(2)
C13	0.032(3)	0.037(3)	0.054(4)	-0.004(3)	0.005(3)	0.001(3)
C26	0.035(3)	0.033(3)	0.040(3)	0.001(2)	0.006(3)	-0.001(2)
C12	0.030(3)	0.033(3)	0.043(3)	-0.006(2)	0.004(2)	0.001(2)
C7	0.050(4)	0.028(3)	0.039(3)	0.003(2)	0.002(3)	0.005(3)
C22	0.036(3)	0.027(3)	0.048(4)	0.000(2)	0.008(3)	-0.002(2)
C17	0.035(3)	0.056(4)	0.040(4)	-0.008(3)	0.007(3)	0.003(3)
C11	0.044(3)	0.033(3)	0.043(4)	0.002(2)	0.009(3)	0.003(3)
C23	0.039(3)	0.029(3)	0.062(4)	0.004(3)	0.010(3)	0.008(3)
C14	0.047(4)	0.048(4)	0.066(5)	-0.012(3)	0.005(3)	0.014(3)
C5	0.048(4)	0.054(4)	0.056(4)	-0.007(3)	-0.011(3)	0.006(3)
C24	0.042(3)	0.046(4)	0.047(4)	0.005(3)	0.007(3)	0.011(3)
C25	0.038(3)	0.050(4)	0.049(4)	0.001(3)	0.001(3)	-0.011(3)
C10	0.036(3)	0.043(4)	0.056(4)	0.008(3)	0.010(3)	0.010(3)
C9	0.068(5)	0.050(4)	0.041(4)	0.008(3)	0.010(3)	0.015(3)
C8	0.063(4)	0.043(4)	0.044(4)	0.002(3)	-0.005(3)	0.013(3)
C27	0.056(4)	0.027(3)	0.087(5)	-0.002(3)	0.008(4)	-0.001(3)
C16	0.050(4)	0.078(5)	0.042(4)	-0.010(3)	0.013(3)	-0.005(4)
C2	0.038(4)	0.059(4)	0.065(4)	-0.001(3)	0.003(3)	-0.007(3)
C15	0.048(4)	0.060(5)	0.066(5)	-0.021(4)	0.010(3)	0.009(3)
C4	0.039(4)	0.051(4)	0.084(5)	-0.004(4)	-0.005(4)	-0.002(3)
C29	0.051(4)	0.037(4)	0.088(5)	-0.003(3)	-0.006(4)	-0.006(3)

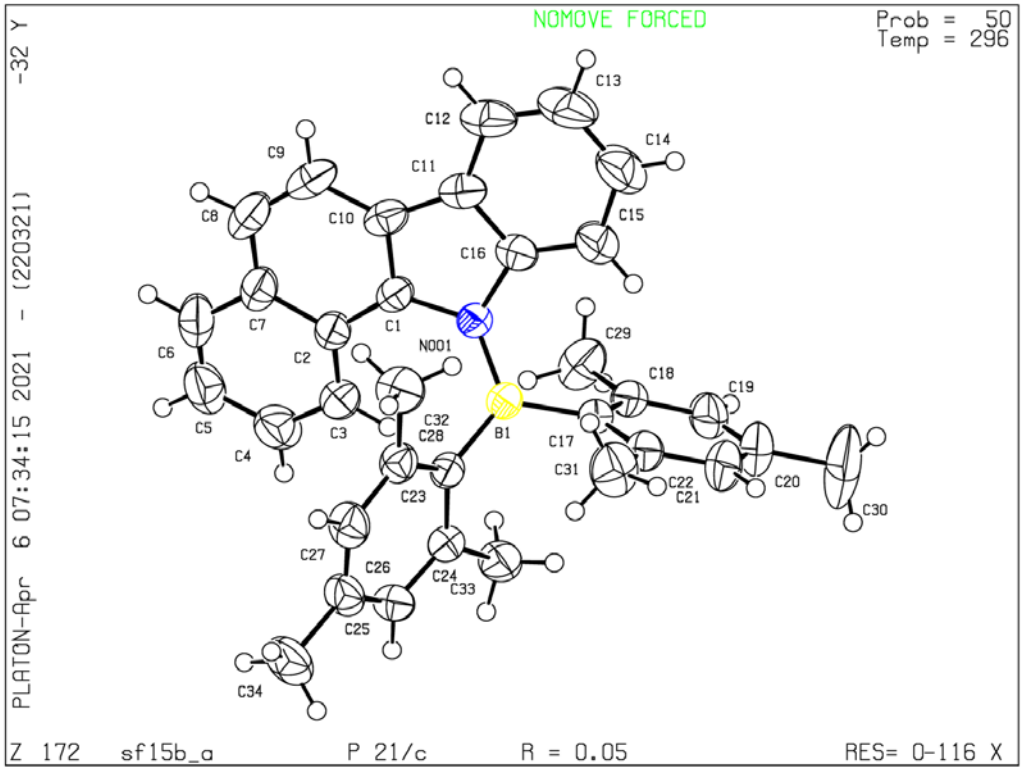
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B1	0.034(3)	0.020(3)	0.048(4)	0.006(3)	0.009(3)	0.003(3)
C20	0.055(4)	0.064(5)	0.051(4)	0.011(3)	0.009(3)	0.004(3)
C3	0.035(4)	0.061(5)	0.079(5)	0.003(4)	0.008(3)	-0.008(3)
C18	0.069(5)	0.043(4)	0.075(5)	0.008(3)	0.007(4)	0.022(3)
C28	0.048(4)	0.090(6)	0.091(6)	0.005(5)	-0.004(4)	0.029(4)
C30	0.069(5)	0.097(6)	0.053(5)	0.001(4)	0.014(4)	0.014(5)
C19	0.096(7)	0.095(7)	0.093(6)	-0.031(5)	0.025(5)	0.026(5)
C31	0.34(2)	0.196(15)	0.088(8)	-0.029(9)	0.127(11)	-0.126(15)
C32	0.275(18)	0.280(19)	0.076(7)	0.006(9)	0.062(9)	0.193(16)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$)

	x/a	y/b	z/c	U(eq)
H11	0.5514	0.2943	0.4808	0.047
H23	0.6395	0.0136	0.5995	0.052
H14	0.0428	0.5828	0.5989	0.064
H5	0.0263	0.1529	0.3501	0.064
H25	0.7591	0.3287	0.6319	0.055
H10	0.6457	0.2855	0.3928	0.054
H8	0.2901	0.1981	0.3158	0.06
H27A	0.3902	0.0385	0.5160	0.084
H27B	0.3032	0.0609	0.5702	0.084
H27C	0.4182	-0.0315	0.5731	0.084
H16	0.0730	0.3449	0.7196	0.068
H2	0.0250	0.2312	0.5468	0.064
H4	-0.1701	0.1318	0.3999	0.07
H29A	0.6192	0.4820	0.6189	0.088
H29B	0.4630	0.4599	0.6252	0.088
H29C	0.5216	0.4720	0.5634	0.088
H20A	0.2209	0.1932	0.7151	0.084
H20B	0.3289	0.1884	0.6671	0.084
H20C	0.1832	0.1367	0.6549	0.084

	x/a	y/b	z/c	U(eq)
H3	-0.1691	0.1671	0.4971	0.07
H18A	0.1379	0.4710	0.4904	0.094
H18B	0.2893	0.4898	0.5130	0.094
H18C	0.1802	0.5847	0.5215	0.094
H28A	0.9165	0.1817	0.6514	0.114
H28B	0.8960	0.0725	0.6133	0.114
H28C	0.8434	0.0753	0.6764	0.114
H30	0.4689	0.2195	0.2581	0.087
H19A	-0.0156	0.6170	0.7078	0.141
H19B	-0.0556	0.5045	0.7390	0.141
H19C	-0.1394	0.5448	0.6833	0.141
H31A	0.6837	0.3582	0.2934	0.309
H31B	0.5358	0.4044	0.2800	0.309
H31C	0.6165	0.3470	0.2307	0.309
H32A	0.6721	0.1385	0.2435	0.313
H32B	0.6006	0.0728	0.2928	0.313
H32C	0.7197	0.1576	0.3086	0.313

Crystal data for 5



A specimen of $C_{34}H_{32}BN$, approximate dimensions 0.350 mm x 0.400 mm x 0.500 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 6.67 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 36617 reflections to a maximum θ angle of 26.00° (0.81 Å resolution), of which 5218 were independent (average redundancy 7.017, completeness = 99.0%, R_{int} = 2.63%, R_{sig} = 1.49%) and 4720 (90.46%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.5407(6) Å, b = 8.4893(5) Å, c = 27.6625(15) Å, β = 98.960(2)°, volume = 2677.1(3) $Å^3$, are based upon the refinement of the XYZ-centroids of 9963 reflections above 20 σ(I) with 5.024° < 2θ < 61.09°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.940. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9680 and 0.9770. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z = 4 for the formula unit, $C_{34}H_{32}BN$. The final anisotropic full-matrix least-squares refinement on F^2 with 331 variables converged at R1 = 5.09%, for the observed data and wR2 = 13.44% for all data. The goodness-of-fit was 1.037. The largest peak in the final difference electron density synthesis was 0.245 $e^-/Å^3$ and the largest hole was -0.178 $e^-/Å^3$ with an RMS deviation of 0.029 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.155 g/cm^3 and F(000), 992 e^-. CCDC number: 208357

Table 1. Sample and crystal data

Identification code	mazza1906	
Chemical formula	$C_{34}H_{32}BN$	
Formula weight	465.41 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.350 x 0.400 x 0.500 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 11.5407(6) Å	α = 90°
	b = 8.4893(5) Å	β = 98.960(2)°
	c = 27.6625(15) Å	γ = 90°
Volume	2677.1(3) $Å^3$	
Z	4	
Density (calculated)	1.155 g/cm^3	
Absorption coefficient	0.065 mm^{-1}	
F(000)	992	

Table 2. Data collection and structure refinement

Theta range for data collection	2.51 to 26.00°
Index ranges	-14<=h<=14, -10<=k<=10, -34<=l<=34
Reflections collected	36617
Independent reflections	5218 [R(int) = 0.0263]
Coverage of independent reflections	99.0%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9770 and 0.9680
Structure solution technique	direct methods
Structure solution program	XT, VERSION 2014/5
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)

Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5218 / 0 / 331	
Goodness-of-fit on F^2	1.037	
Δ/σ_{max}	0.001	
Final R indices	4720 data; $I>2\sigma(I)$	R1 = 0.0509, wR2 = 0.1312
	all data	R1 = 0.0553, wR2 = 0.1344
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0634P)^2+0.7797P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.245 and -0.178 eÅ^{-3}	
R.M.S. deviation from mean	0.029 eÅ^{-3}	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
N001	0.29918(10)	0.74757(13)	0.65886(4)	0.0399(3)
C17	0.15636(12)	0.54080(16)	0.61290(5)	0.0406(3)
C23	0.29780(11)	0.72064(16)	0.56406(5)	0.0387(3)
C1	0.40510(12)	0.83377(15)	0.67153(5)	0.0403(3)
C18	0.18030(13)	0.40544(17)	0.64187(5)	0.0456(3)
C2	0.51720(12)	0.80668(17)	0.65725(5)	0.0432(3)
C24	0.33173(12)	0.60807(17)	0.53147(5)	0.0425(3)
C16	0.22485(13)	0.79629(17)	0.69299(5)	0.0458(3)
C11	0.27955(15)	0.91896(17)	0.72165(5)	0.0503(4)
C25	0.37283(13)	0.6563(2)	0.48940(5)	0.0506(4)
C10	0.39278(14)	0.94275(16)	0.70761(5)	0.0473(3)
C28	0.29841(13)	0.88018(17)	0.55008(5)	0.0458(3)
C22	0.04618(13)	0.5525(2)	0.58269(6)	0.0508(4)
C7	0.60903(14)	0.91157(19)	0.67726(5)	0.0524(4)
C3	0.54678(13)	0.6788(2)	0.62927(5)	0.0524(4)

	x/a	y/b	z/c	U(eq)
C27	0.33656(14)	0.92188(19)	0.50661(6)	0.0552(4)
C19	0.09673(16)	0.2878(2)	0.64017(7)	0.0606(4)
C26	0.37642(14)	0.8129(2)	0.47622(5)	0.0543(4)
C33	0.32651(16)	0.43325(18)	0.54074(6)	0.0567(4)
C8	0.58822(17)	0.0346(2)	0.70917(6)	0.0629(5)
C32	0.25329(17)	0.00982(19)	0.57938(7)	0.0623(4)
C9	0.48430(17)	0.04791(19)	0.72549(6)	0.0609(5)
B1	0.25342(13)	0.67088(17)	0.61285(6)	0.0376(3)
C15	0.11466(16)	0.7433(2)	0.69979(7)	0.0639(5)
C29	0.29603(17)	0.3785(2)	0.67423(7)	0.0682(5)
C5	0.74741(16)	0.7638(3)	0.63811(7)	0.0726(6)
C31	0.01198(16)	0.6956(3)	0.55167(8)	0.0730(5)
C6	0.72316(15)	0.8856(3)	0.66610(7)	0.0673(5)
C12	0.22521(19)	0.9881(2)	0.75778(6)	0.0691(5)
C21	0.96555(15)	0.4316(3)	0.58291(7)	0.0700(5)
C4	0.65874(15)	0.6584(3)	0.61994(6)	0.0674(5)
C20	0.98935(17)	0.2986(3)	0.61103(8)	0.0749(6)
C34	0.41929(18)	0.8623(3)	0.42966(7)	0.0747(6)
C14	0.0633(2)	0.8134(3)	0.73633(8)	0.0832(6)
C13	0.1178(2)	0.9341(3)	0.76504(8)	0.0841(6)
C30	0.9011(3)	0.1662(4)	0.61051(14)	0.1426(13)

Table 4. Bond lengths (Å)

N001-C1	1.4209(17)	N001-C16	1.4320(17)
N001-B1	1.4538(18)	C17-C18	1.404(2)
C17-C22	1.412(2)	C17-B1	1.5731(19)
C23-C28	1.4088(19)	C23-C24	1.4105(19)
C23-B1	1.5740(19)	C1-C10	1.3844(19)
C1-C2	1.429(2)	C18-C19	1.384(2)
C18-C29	1.505(2)	C2-C3	1.406(2)
C2-C7	1.428(2)	C24-C25	1.385(2)
C24-C33	1.509(2)	C16-C15	1.389(2)
C16-C11	1.398(2)	C11-C12	1.390(2)
C11-C10	1.434(2)	C25-C26	1.381(2)
C25-H25	0.93	C10-C9	1.412(2)

C28-C27	1.389(2)	C28-C32	1.507(2)
C22-C21	1.386(2)	C22-C31	1.504(3)
C7-C8	1.412(3)	C7-C6	1.416(3)
C3-C4	1.368(2)	C3-H3	0.93
C27-C26	1.376(2)	C27-H27	0.93
C19-C20	1.372(3)	C19-H19	0.93
C26-C34	1.509(2)	C33-H33A	0.96
C33-H33B	0.96	C33-H33C	0.96
C8-C9	1.350(3)	C8-H8	0.93
C32-H32A	0.96	C32-H32B	0.96
C32-H32C	0.96	C9-H9	0.93
C15-C14	1.384(2)	C15-H15	0.93
C29-H29A	0.96	C29-H29B	0.96
C29-H29C	0.96	C5-C6	1.347(3)
C5-C4	1.393(3)	C5-H5	0.93
C31-H31A	0.96	C31-H31B	0.96
C31-H31C	0.96	C6-H6	0.93
C12-C13	1.366(3)	C12-H12	0.93
C21-C20	1.374(3)	C21-H21	0.93
C4-H4	0.93	C20-C30	1.516(3)
C34-H34A	0.96	C34-H34B	0.96
C34-H34C	0.96	C14-C13	1.386(3)
C14-H14	0.93	C13-H13	0.93
C30-H30A	0.96	C30-H30B	0.96
C30-H30C	0.96		

Table 5. Bond angles (°)

C1-N001-C16	105.63(11)	C1-N001-B1	128.88(11)
C16-N001-B1	122.23(12)	C18-C17-C22	118.32(13)
C18-C17-B1	119.89(12)	C22-C17-B1	121.73(13)
C28-C23-C24	117.52(12)	C28-C23-B1	120.64(12)
C24-C23-B1	121.74(12)	C10-C1-N001	109.93(12)
C10-C1-C2	120.38(13)	N001-C1-C2	129.06(12)
C19-C18-C17	119.81(15)	C19-C18-C29	117.37(15)
C17-C18-C29	122.79(13)	C3-C2-C7	117.75(14)
C3-C2-C1	125.76(13)	C7-C2-C1	116.22(14)
C25-C24-C23	120.13(13)	C25-C24-C33	117.50(13)
C23-C24-C33	122.37(13)	C15-C16-C11	120.42(14)
C15-C16-N001	130.61(14)	C11-C16-N001	108.96(13)
C12-C11-C16	120.51(16)	C12-C11-C10	131.86(16)
C16-C11-C10	107.53(13)	C26-C25-C24	122.33(15)
C26-C25-H25	118.8	C24-C25-H25	118.8
C1-C10-C9	121.32(15)	C1-C10-C11	107.53(13)
C9-C10-C11	131.10(15)	C27-C28-C23	119.89(14)
C27-C28-C32	117.53(14)	C23-C28-C32	122.51(13)
C21-C22-C17	119.25(16)	C21-C22-C31	118.94(16)
C17-C22-C31	121.76(14)	C8-C7-C6	120.39(15)
C8-C7-C2	121.02(15)	C6-C7-C2	118.53(16)
C4-C3-C2	121.31(16)	C4-C3-H3	119.3
C2-C3-H3	119.3	C26-C27-C28	122.59(15)
C26-C27-H27	118.7	C28-C27-H27	118.7
C20-C19-C18	122.17(17)	C20-C19-H19	118.9
C18-C19-H19	118.9	C27-C26-C25	117.33(14)
C27-C26-C34	121.34(17)	C25-C26-C34	121.31(17)
C24-C33-H33A	109.5	C24-C33-H33B	109.5
H33A-C33-H33B	109.5	C24-C33-H33C	109.5
H33A-C33-H33C	109.5	H33B-C33-H33C	109.5
C9-C8-C7	121.14(15)	C9-C8-H8	119.4
C7-C8-H8	119.4	C28-C32-H32A	109.5
C28-C32-H32B	109.5	H32A-C32-H32B	109.5

C28-C32-H32C	109.5	H32A-C32-H32C	109.5
H32B-C32-H32C	109.5	C8-C9-C10	119.00(15)
C8-C9-H9	120.5	C10-C9-H9	120.5
N001-B1-C17	118.37(12)	N001-B1-C23	120.54(12)
C17-B1-C23	121.06(12)	C14-C15-C16	117.75(18)
C14-C15-H15	121.1	C16-C15-H15	121.1
C18-C29-H29A	109.5	C18-C29-H29B	109.5
H29A-C29-H29B	109.5	C18-C29-H29C	109.5
H29A-C29-H29C	109.5	H29B-C29-H29C	109.5
C6-C5-C4	119.60(18)	C6-C5-H5	120.2
C4-C5-H5	120.2	C22-C31-H31A	109.5
C22-C31-H31B	109.5	H31A-C31-H31B	109.5
C22-C31-H31C	109.5	H31A-C31-H31C	109.5
H31B-C31-H31C	109.5	C5-C6-C7	121.90(16)
C5-C6-H6	119.1	C7-C6-H6	119.1
C13-C12-C11	119.05(18)	C13-C12-H12	120.5
C11-C12-H12	120.5	C20-C21-C22	122.39(17)
C20-C21-H21	118.8	C22-C21-H21	118.8
C3-C4-C5	120.84(19)	C3-C4-H4	119.6
C5-C4-H4	119.6	C19-C20-C21	118.03(16)
C19-C20-C30	120.0(2)	C21-C20-C30	121.9(2)
C26-C34-H34A	109.5	C26-C34-H34B	109.5
H34A-C34-H34B	109.5	C26-C34-H34C	109.5
H34A-C34-H34C	109.5	H34B-C34-H34C	109.5
C15-C14-C13	121.9(2)	C15-C14-H14	119.1
C13-C14-H14	119.1	C12-C13-C14	120.37(17)
C12-C13-H13	119.8	C14-C13-H13	119.8

C20-C30-H30A	109.5	C20-C30-H30B	109.5
H30A-C30-H30B	109.5	C20-C30-H30C	109.5
H30A-C30-H30C	109.5	H30B-C30-H30C	109.5

Table 6. Torsion angles (°)

C16-N001-C1-C10	-6.50(15)	B1-N001-C1-C10	153.06(13)
C16-N001-C1-C2	164.36(13)	B1-N001-C1-C2	-36.1(2)
C22-C17-C18-C19	0.1(2)	B1-C17-C18-C19	-177.07(13)
C22-C17-C18-C29	178.13(15)	B1-C17-C18-C29	0.9(2)
C10-C1-C2-C3	165.74(14)	N001-C1-C2-C3	-4.3(2)
C10-C1-C2-C7	-8.10(19)	N001-C1-C2-C7	-178.12(12)
C28-C23-C24-C25	5.1(2)	B1-C23-C24-C25	-178.56(13)
C28-C23-C24-C33	-175.63(14)	B1-C23-C24-C33	0.7(2)
C1-N001-C16-C15	-175.27(17)	B1-N001-C16-C15	23.5(2)
C1-N001-C16-C11	5.94(15)	B1-N001-C16-C11	-155.31(13)
C15-C16-C11-C12	0.9(2)	N001-C16-C11-C12	179.85(14)
C15-C16-C11-C10	177.78(15)	N001-C16-C11-C10	-3.28(16)
C23-C24-C25-C26	-3.6(2)	C33-C24-C25-C26	177.08(15)
N001-C1-C10-C9	-177.62(13)	C2-C1-C10-C9	10.6(2)
N001-C1-C10-C11	4.59(15)	C2-C1-C10-C11	-167.18(12)
C12-C11-C10-C1	175.60(17)	C16-C11-C10-C1	-0.77(16)

C12-C11-C10-C9	-1.9(3)	C16-C11-C10-C9	-178.26(15)
C24-C23-C28-C27	-2.8(2)	B1-C23-C28-C27	-179.23(13)
C24-C23-C28-C32	174.09(14)	B1-C23-C28-C32	-2.3(2)
C18-C17-C22-C21	0.5(2)	B1-C17-C22-C21	177.67(15)
C18-C17-C22-C31	178.10(15)	B1-C17-C22-C31	-4.8(2)
C3-C2-C7-C8	-174.53(14)	C1-C2-C7-C8	-0.2(2)
C3-C2-C7-C6	2.8(2)	C1-C2-C7-C6	177.16(13)
C7-C2-C3-C4	-2.3(2)	C1-C2-C3-C4	-176.07(15)
C23-C28-C27-C26	-1.1(2)	C32-C28-C27-C26	-178.15(15)
C17-C18-C19-C20	-0.4(3)	C29-C18-C19-C20	-178.47(18)
C28-C27-C26-C25	2.7(2)	C28-C27-C26-C34	-178.91(15)
C24-C25-C26-C27	-0.3(2)	C24-C25-C26-C34	-178.73(15)
C6-C7-C8-C9	-170.85(15)	C2-C7-C8-C9	6.4(2)
C7-C8-C9-C10	-4.2(2)	C1-C10-C9-C8	-4.3(2)
C11-C10-C9-C8	172.94(16)	C1-N001-B1-C17	161.19(13)
C16-N001-B1-C17	-42.24(18)	C1-N001-B1-C23	-20.5(2)
C16-N001-B1-C23	136.11(13)	C18-C17-B1-N001	-59.91(17)
C22-C17-B1-N001	123.00(15)	C18-C17-B1-C23	121.75(14)
C22-C17-B1-C23	-55.35(19)	C28-C23-B1-N001	-51.06(19)
C24-C23-B1-N001	132.69(14)	C28-C23-B1-C17	127.25(14)

C24-C23-B1-C17	-49.00(19)	C11-C16-C15-C14	-1.5(3)
N001-C16-C15-C14	179.82(17)	C4-C5-C6-C7	-0.9(3)
C8-C7-C6-C5	176.08(16)	C2-C7-C6-C5	-1.3(2)
C16-C11-C12-C13	0.3(3)	C10-C11-C12-C13	-175.72(18)
C17-C22-C21-C20	-1.0(3)	C31-C22-C21-C20	-178.66(19)
C2-C3-C4-C5	0.2(3)	C6-C5-C4-C3	1.4(3)
C18-C19-C20-C21	-0.1(3)	C18-C19-C20-C30	179.9(2)
C22-C21-C20-C19	0.8(3)	C22-C21-C20-C30	-179.2(2)
C16-C15-C14-C13	1.0(3)	C11-C12-C13-C14	-0.8(3)
C15-C14-C13-C12	0.2(4)		

Table 7. Anisotropic atomic displacement parameters ($Å^2$)

The anisotropic atomic displacement factor exponent takes the form:
$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N001	0.0456(6)	0.0374(6)	0.0375(6)	-0.0034(5)	0.0092(5)	-0.0062(5)
C17	0.0430(7)	0.0433(7)	0.0367(6)	-0.0047(5)	0.0095(5)	-0.0073(6)
C23	0.0393(7)	0.0385(7)	0.0379(7)	-0.0005(5)	0.0041(5)	-0.0058(5)
C1	0.0510(8)	0.0346(6)	0.0332(6)	0.0026(5)	0.0003(5)	-0.0073(6)
C18	0.0544(8)	0.0425(7)	0.0411(7)	-0.0029(6)	0.0114(6)	-0.0099(6)
C2	0.0467(8)	0.0466(7)	0.0345(6)	0.0084(6)	0.0005(5)	-0.0093(6)
C24	0.0435(7)	0.0436(7)	0.0400(7)	-0.0028(6)	0.0053(5)	-0.0048(6)
C16	0.0567(8)	0.0429(7)	0.0396(7)	0.0000(6)	0.0129(6)	0.0028(6)
C11	0.0704(10)	0.0420(8)	0.0379(7)	-0.0024(6)	0.0063(7)	0.0054(7)
C25	0.0517(8)	0.0609(9)	0.0400(7)	-0.0051(7)	0.0095(6)	-0.0033(7)
C10	0.0644(9)	0.0376(7)	0.0368(7)	0.0000(6)	-0.0022(6)	-0.0020(6)
C28	0.0497(8)	0.0407(7)	0.0463(8)	0.0041(6)	0.0050(6)	-0.0048(6)
C22	0.0409(7)	0.0631(9)	0.0489(8)	-0.0044(7)	0.0080(6)	-0.0048(7)

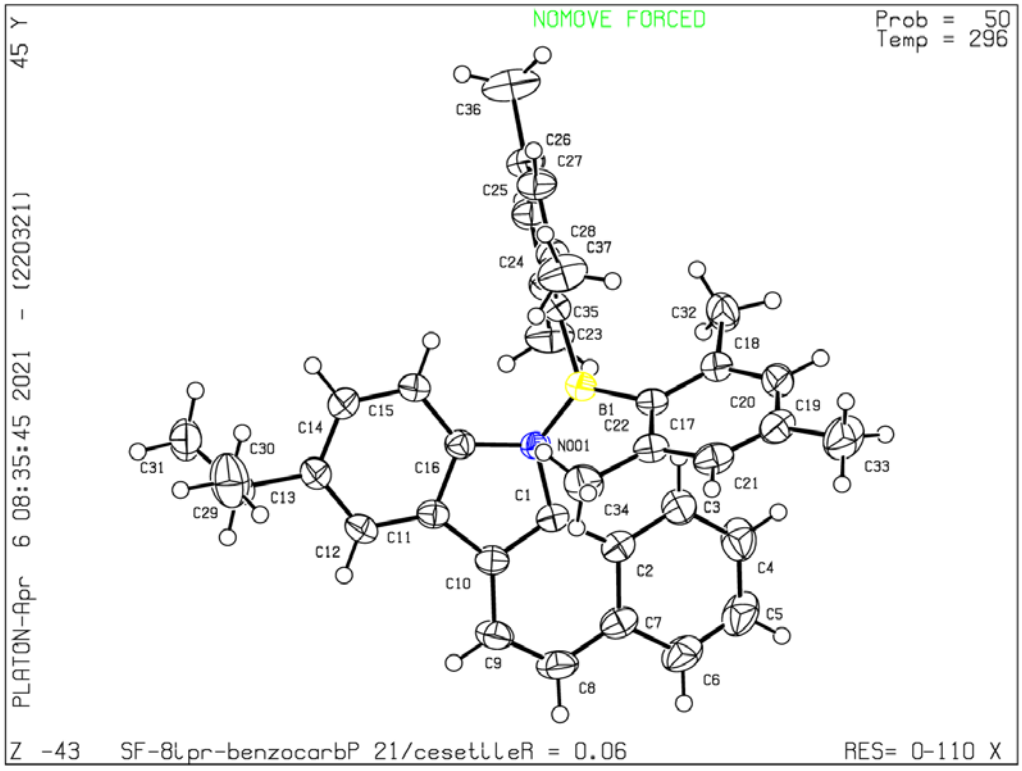
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C7	0.0567(9)	0.0549(9)	0.0414(7)	0.0146(7)	-0.0054(6)	-0.0185(7)
C3	0.0458(8)	0.0645(10)	0.0454(8)	-0.0036(7)	0.0029(6)	-0.0060(7)
C27	0.0617(9)	0.0498(9)	0.0534(9)	0.0154(7)	0.0070(7)	-0.0060(7)
C19	0.0706(11)	0.0503(9)	0.0651(10)	0.0014(8)	0.0237(8)	-0.0168(8)
C26	0.0508(8)	0.0710(10)	0.0410(8)	0.0109(7)	0.0065(6)	-0.0064(7)
C33	0.0704(10)	0.0424(8)	0.0612(9)	-0.0088(7)	0.0227(8)	-0.0035(7)
C8	0.0730(11)	0.0527(9)	0.0549(9)	0.0040(8)	-0.0153(8)	-0.0240(8)
C32	0.0845(12)	0.0374(8)	0.0669(10)	0.0046(7)	0.0174(9)	0.0037(8)
C9	0.0854(12)	0.0430(8)	0.0471(8)	-0.0071(7)	-0.0124(8)	-0.0079(8)
B1	0.0388(7)	0.0329(7)	0.0406(8)	-0.0004(6)	0.0049(6)	0.0006(6)
C15	0.0648(10)	0.0667(11)	0.0660(10)	-0.0124(9)	0.0278(8)	-0.0065(8)
C29	0.0814(12)	0.0513(9)	0.0647(10)	0.0135(8)	-0.0113(9)	-0.0101(9)
C5	0.0472(9)	0.1076(16)	0.0632(11)	0.0174(11)	0.0092(8)	-0.0102(10)
C31	0.0513(10)	0.0882(14)	0.0758(12)	0.0142(10)	-0.0020(8)	0.0050(9)
C6	0.0527(9)	0.0845(13)	0.0609(10)	0.0241(10)	-0.0034(8)	-0.0270(9)
C12	0.0982(14)	0.0598(10)	0.0514(9)	-0.0128(8)	0.0183(9)	0.0107(10)
C21	0.0404(8)	0.0912(14)	0.0775(12)	-0.0061(11)	0.0063(8)	-0.0193(9)
C4	0.0531(9)	0.0944(14)	0.0550(9)	-0.0021(9)	0.0099(7)	0.0026(9)
C20	0.0579(10)	0.0769(13)	0.0925(14)	-0.0049(11)	0.0202(10)	-0.0315(10)
C34	0.0756(12)	0.0999(15)	0.0510(10)	0.0217(10)	0.0177(8)	-0.0061(11)
C14	0.0831(14)	0.0906(15)	0.0870(14)	-0.0135(12)	0.0477(12)	0.0006(12)
C13	0.1078(17)	0.0854(14)	0.0680(12)	-0.0180(11)	0.0413(12)	0.0162(12)
C30	0.099(2)	0.127(2)	0.198(4)	0.021(2)	0.011(2)	-0.0743(19)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$)

	x/a	y/b	z/c	U(eq)
H25	0.3989	0.5806	0.4693	0.061

	x/a	y/b	z/c	U(eq)
H3	0.4891	0.6068	0.6168	0.063
H27	0.3351	1.0276	0.4977	0.066
H19	0.1139	0.1985	0.6594	0.073
H33A	0.2462	0.4014	0.5391	0.085
H33B	0.3689	0.4096	0.5726	0.085
H33C	0.3612	0.3775	0.5164	0.085
H8	0.6471	1.1078	0.7191	0.075
H32A	0.3168	1.0514	0.6024	0.093
H32B	0.1940	0.9684	0.5967	0.093
H32C	0.2203	1.0922	0.5577	0.093
H9	0.4732	1.1251	0.7482	0.073
H15	0.0767	0.6635	0.6804	0.077
H29A	0.2922	0.4184	0.7064	0.102
H29B	0.3570	0.4322	0.6608	0.102
H29C	0.3128	0.2677	0.6761	0.102
H5	0.8229	0.7502	0.6310	0.087
H31A	-0.0689	0.6875	0.5371	0.11
H31B	0.0600	0.7022	0.5264	0.11
H31C	0.0230	0.7883	0.5717	0.11
H6	0.7831	0.9546	0.6784	0.081
H12	0.2615	1.0700	0.7767	0.083
H21	-0.1073	0.4408	0.5633	0.084
H4	0.6759	0.5730	0.6012	0.081
H34A	0.3950	0.9685	0.4217	0.112
H34B	0.3868	0.7934	0.4035	0.112
H34C	0.5033	0.8562	0.4342	0.112
H14	-0.0100	0.7784	0.7418	0.1
H13	0.0810	0.9785	0.7894	0.101
H30A	-0.0656	0.0833	0.6319	0.214
H30B	-0.1188	0.1261	0.5778	0.214
H30C	-0.1684	0.2053	0.6215	0.214

Crystal data for 6



A specimen of $C_{37}H_{38}BN$, approximate dimensions 0.300 mm x 0.400 mm x 0.500 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 20.33 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 37031 reflections to a maximum θ angle of 25.00° (0.84 Å resolution), of which 5136 were independent (average redundancy 7.210, completeness = 99.7%, R_{int} = 4.28%, R_{sig} = 2.65%) and 4716 (91.82%) were greater than $2\sigma(F^2)$. The final cell constants of a = 15.957(3) Å, b = 8.378(2) Å, c = 22.580(5) Å, α = 90.00(3)°, β = 104.29(3)°, γ = 90.00(3)°, volume = 2925.3(12) $Å^3$, are based upon the refinement of the XYZ-centroids of 9970 reflections above 20 σ(I) with 5.049° < 2θ < 56.54°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.936. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9680 and 0.9810. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z = 1 for the formula unit, $C_{148}H_{152}B_4N_4$. The final anisotropic full-matrix least-squares refinement on F^2 with 360 variables converged at R1 = 6.24%, for the observed data and wR2 = 15.29% for all data. The goodness-of-fit was 1.094. The largest peak in the final difference electron density synthesis was 0.270 $e^-/Å^3$ and the largest hole was -0.255 $e^-/Å^3$ with an RMS deviation of 0.046 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.152 g/cm^3 and F(000), 1088 e^-. CCDC number: 208359

Table 1. Sample and crystal data

Identification code	mazza1913	
Chemical formula	$C_{37}H_{38}B_4N_4$	
Formula weight	2029.97 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.300 x 0.400 x 0.500 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 15.957(3) Å	α = 90.00(3)°
	b = 8.378(2) Å	β = 104.29(3)°
	c = 22.580(5) Å	γ = 90.00(3)°
Volume	2925.3(12) $Å^3$	
Z	4	
Density (calculated)	1.152 g/cm^3	
Absorption coefficient	0.065 mm^{-1}	
F(000)	1088	

Table 2. Data collection and structure refinement

Theta range for data collection	2.53 to 25.00°
Index ranges	-18<=h<=18, -9<=k<=9, -26<=l<=26
Reflections collected	37031
Independent reflections	5136 [R(int) = 0.0428]
Coverage of independent reflections	99.7%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9810 and 0.9680
Structure solution technique	direct methods
Structure solution program	XT, VERSION 2014/5
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)

Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5136 / 0 / 360	
Goodness-of-fit on F^2	1.094	
Δ/σ_{max}	0.021	
Final R indices	4716 data; $I>2\sigma(I)$	R1 = 0.0624, wR2 = 0.1498
	all data	R1 = 0.0667, wR2 = 0.1529
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0651P)^2+1.7643P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.270 and -0.255 $eÅ^{-3}$	
R.M.S. deviation from mean	0.046 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
N001	0.21911(10)	0.76631(18)	0.31913(7)	0.0305(4)
C16	0.16401(11)	0.8239(2)	0.26380(8)	0.0316(4)
C1	0.19210(12)	0.8466(2)	0.36656(8)	0.0309(4)
C17	0.38634(12)	0.7330(2)	0.36734(8)	0.0318(4)
C23	0.30047(11)	0.5514(2)	0.27096(8)	0.0306(4)
C24	0.24541(12)	0.4186(2)	0.26737(9)	0.0338(4)
C11	0.11026(11)	0.9440(2)	0.27663(8)	0.0320(4)
C12	0.05466(12)	0.0278(2)	0.22993(9)	0.0366(4)
C10	0.12792(12)	0.9559(2)	0.34202(9)	0.0337(4)
C28	0.35945(12)	0.5530(2)	0.23345(9)	0.0363(4)
C22	0.41159(13)	0.8944(2)	0.37488(9)	0.0358(4)
C2	0.21552(12)	0.8148(2)	0.43071(9)	0.0347(4)
C25	0.25105(13)	0.2935(2)	0.22835(9)	0.0398(5)
C18	0.44351(12)	0.6174(2)	0.40008(9)	0.0360(4)
C13	0.05231(13)	0.9938(3)	0.16987(9)	0.0388(5)

	x/a	y/b	z/c	U(eq)
C19	0.51939(13)	0.6642(3)	0.44062(9)	0.0429(5)
C15	0.16143(13)	0.7862(3)	0.20325(9)	0.0414(5)
C21	0.48969(14)	0.9347(3)	0.41502(10)	0.0435(5)
C9	0.08989(14)	0.0520(3)	0.37953(10)	0.0442(5)
C27	0.36198(14)	0.4260(3)	0.19480(10)	0.0447(5)
C7	0.17553(14)	0.9144(3)	0.46768(9)	0.0419(5)
C3	0.26864(13)	0.6900(3)	0.45956(9)	0.0432(5)
C20	0.54393(13)	0.8231(3)	0.44879(9)	0.0444(5)
C14	0.10564(14)	0.8708(3)	0.15797(9)	0.0455(5)
C8	0.11525(16)	0.0334(3)	0.44093(10)	0.0506(6)
C26	0.30892(15)	0.2943(3)	0.19190(10)	0.0447(5)
C34	0.35972(15)	0.0264(3)	0.33825(11)	0.0493(6)
C35	0.18165(15)	0.4017(3)	0.30649(11)	0.0533(6)
C32	0.42624(16)	0.4405(3)	0.39261(11)	0.0520(6)
C29	0.99699(14)	0.0908(3)	0.11818(10)	0.0479(5)
C31	0.94268(16)	0.9887(3)	0.06791(10)	0.0563(6)
C4	0.28530(16)	0.6673(3)	0.52121(10)	0.0565(6)
C5	0.24941(17)	0.7686(4)	0.55742(11)	0.0620(7)
C6	0.19584(16)	0.8876(3)	0.53126(10)	0.0551(6)
B1	0.30041(14)	0.6849(2)	0.31983(9)	0.0301(4)
C37	0.41916(17)	0.6923(3)	0.23251(12)	0.0586(7)
C33	0.62924(16)	0.8696(4)	0.49072(12)	0.0658(7)
C36	0.3143(2)	0.1547(3)	0.15096(14)	0.0769(9)
C30	0.0531(2)	0.2050(4)	0.09200(14)	0.0758(9)

Table 4. Bond lengths (Å)

N001-C1	1.419(2)	N001-C16	1.423(2)
N001-B1	1.462(3)	C16-C15	1.394(3)
C16-C11	1.398(3)	C1-C10	1.383(3)
C1-C2	1.429(3)	C17-C18	1.409(3)
C17-C22	1.409(3)	C17-B1	1.571(3)
C23-C28	1.413(3)	C23-C24	1.408(3)
C23-B1	1.571(3)	C24-C25	1.386(3)
C24-C35	1.510(3)	C11-C12	1.389(3)
C11-C10	1.437(3)	C12-C13	1.377(3)
C12-H12	0.93	C10-C9	1.410(3)

C28-C27	1.383(3)	C28-C37	1.510(3)
C22-C21	1.390(3)	C22-C34	1.502(3)
C2-C3	1.401(3)	C2-C7	1.437(3)
C25-C26	1.380(3)	C25-H25	0.93
C18-C19	1.382(3)	C18-C32	1.509(3)
C13-C14	1.404(3)	C13-C29	1.514(3)
C19-C20	1.387(3)	C19-H19	0.93
C15-C14	1.375(3)	C15-H15	0.93
C21-C20	1.371(3)	C21-H21	0.93
C9-C8	1.354(3)	C9-H9	0.93
C27-C26	1.383(3)	C27-H27	0.93
C7-C6	1.410(3)	C7-C8	1.413(3)
C3-C4	1.364(3)	C3-H3	0.93
C20-C33	1.505(3)	C14-H14	0.93
C8-H8	0.93	C26-C36	1.506(3)
C34-H34A	0.96	C34-H34B	0.96
C34-H34C	0.96	C35-H35A	0.96
C35-H35B	0.96	C35-H35C	0.96
C32-H32A	0.96	C32-H32B	0.96
C32-H32C	0.96	C29-C31	1.512(3)
C29-C30	1.526(4)	C29-H29	0.98
C31-H31A	0.96	C31-H31B	0.96
C31-H31C	0.96	C4-C5	1.395(4)
C4-H4	0.93	C5-C6	1.351(4)
C5-H5	0.93	C6-H6	0.93
C37-H37A	0.96	C37-H37B	0.96
C37-H37C	0.96	C33-H33A	0.96
C33-H33B	0.96	C33-H33C	0.96
C36-H36A	0.96	C36-H36B	0.96
C36-H36C	0.96	C30-H30A	0.96
C30-H30B	0.96	C30-H30C	0.96

Table 5. Bond angles (°)

C1-N001-C16	105.35(15)	C1-N001-B1	130.32(16)
C16-N001-B1	121.46(15)	C15-C16-C11	119.69(18)
C15-C16-N001	130.28(17)	C11-C16-N001	109.88(16)

C10-C1-N001	110.14(16)	C10-C1-C2	120.81(17)
N001-C1-C2	128.63(17)	C18-C17-C22	117.88(18)
C18-C17-B1	121.68(17)	C22-C17-B1	120.26(17)
C28-C23-C24	118.13(17)	C28-C23-B1	122.01(17)
C24-C23-B1	119.64(16)	C25-C24-C23	119.79(18)
C25-C24-C35	117.36(18)	C23-C24-C35	122.80(17)
C12-C11-C16	121.05(17)	C12-C11-C10	132.20(17)
C16-C11-C10	106.74(16)	C13-C12-C11	120.01(18)
C13-C12-H12	120.0	C11-C12-H12	120.0
C1-C10-C9	121.55(18)	C1-C10-C11	107.69(16)
C9-C10-C11	130.74(18)	C27-C28-C23	119.89(19)
C27-C28-C37	117.96(19)	C23-C28-C37	122.13(18)
C21-C22-C17	119.71(19)	C21-C22-C34	117.64(19)
C17-C22-C34	122.55(18)	C3-C2-C1	125.98(18)
C3-C2-C7	117.89(18)	C1-C2-C7	115.99(18)
C26-C25-C24	122.22(19)	C26-C25-H25	118.9
C24-C25-H25	118.9	C19-C18-C17	120.03(19)
C19-C18-C32	117.30(19)	C17-C18-C32	122.67(18)
C12-C13-C14	118.02(18)	C12-C13-C29	121.12(18)
C14-C13-C29	120.80(18)	C18-C19-C20	122.2(2)
C18-C19-H19	118.9	C20-C19-H19	118.9
C14-C15-C16	118.00(18)	C14-C15-H15	121.0
C16-C15-H15	121.0	C20-C21-C22	122.6(2)
C20-C21-H21	118.7	C22-C21-H21	118.7
C8-C9-C10	119.0(2)	C8-C9-H9	120.5
C10-C9-H9	120.5	C28-C27-C26	122.08(19)
C28-C27-H27	119.0	C26-C27-H27	119.0
C6-C7-C8	120.6(2)	C6-C7-C2	118.4(2)
C8-C7-C2	120.96(19)	C4-C3-C2	121.4(2)
C4-C3-H3	119.3	C2-C3-H3	119.3
C21-C20-C19	117.52(19)	C21-C20-C33	121.5(2)
C19-C20-C33	120.9(2)	C15-C14-C13	123.21(19)
C15-C14-H14	118.4	C13-C14-H14	118.4
C9-C8-C7	121.3(2)	C9-C8-H8	119.4
C7-C8-H8	119.4	C25-C26-C27	117.87(19)
C25-C26-C36	120.7(2)	C27-C26-C36	121.5(2)
C22-C34-H34A	109.5	C22-C34-H34B	109.5

H34A-C34-H34B	109.5	C22-C34-H34C	109.5
H34A-C34-H34C	109.5	H34B-C34-H34C	109.5
C24-C35-H35A	109.5	C24-C35-H35B	109.5
H35A-C35-H35B	109.5	C24-C35-H35C	109.5
H35A-C35-H35C	109.5	H35B-C35-H35C	109.5
C18-C32-H32A	109.5	C18-C32-H32B	109.5
H32A-C32-H32B	109.5	C18-C32-H32C	109.5
H32A-C32-H32C	109.5	H32B-C32-H32C	109.5
C13-C29-C31	113.09(19)	C13-C29-C30	110.44(19)
C31-C29-C30	110.3(2)	C13-C29-H29	107.6
C31-C29-H29	107.6	C30-C29-H29	107.6
C29-C31-H31A	109.5	C29-C31-H31B	109.5
H31A-C31-H31B	109.5	C29-C31-H31C	109.5
H31A-C31-H31C	109.5	H31B-C31-H31C	109.5
C3-C4-C5	120.5(2)	C3-C4-H4	119.7
C5-C4-H4	119.7	C6-C5-C4	120.0(2)
C6-C5-H5	120.0	C4-C5-H5	120.0
C5-C6-C7	121.6(2)	C5-C6-H6	119.2
C7-C6-H6	119.2	N001-B1-C17	120.68(16)
N001-B1-C23	118.60(17)	C17-B1-C23	120.70(16)
C28-C37-H37A	109.5	C28-C37-H37B	109.5
H37A-C37-H37B	109.5	C28-C37-H37C	109.5
H37A-C37-H37C	109.5	H37B-C37-H37C	109.5
C20-C33-H33A	109.5	C20-C33-H33B	109.5
H33A-C33-H33B	109.5	C20-C33-H33C	109.5

H33A-C33-H33C	109.5	H33B-C33-H33C	109.5
C26-C36-H36A	109.5	C26-C36-H36B	109.5
H36A-C36-H36B	109.5	C26-C36-H36C	109.5
H36A-C36-H36C	109.5	H36B-C36-H36C	109.5
C29-C30-H30A	109.5	C29-C30-H30B	109.5
H30A-C30-H30B	109.5	C29-C30-H30C	109.5
H30A-C30-H30C	109.5	H30B-C30-H30C	109.5

Table 6. Torsion angles (°)

C1-N001-C16-C15	180.0(2)	B1-N001-C16-C15	17.3(3)
C1-N001-C16-C11	4.6(2)	B1-N001-C16-C11	-158.04(16)
C16-N001-C1-C10	-3.9(2)	B1-N001-C1-C10	156.66(18)
C16-N001-C1-C2	168.61(18)	B1-N001-C1-C2	-30.8(3)
C28-C23-C24-C25	0.8(3)	B1-C23-C24-C25	-173.94(18)
C28-C23-C24-C35	178.23(19)	B1-C23-C24-C35	3.4(3)
C15-C16-C11-C12	-0.6(3)	N001-C16-C11-C12	175.32(17)
C15-C16-C11-C10	-179.57(18)	N001-C16-C11-C10	-3.7(2)
C16-C11-C12-C13	-0.4(3)	C10-C11-C12-C13	178.2(2)
N001-C1-C10-C9	-179.88(18)	C2-C1-C10-C9	6.9(3)
N001-C1-C10-C11	1.7(2)	C2-C1-C10-C11	-171.44(16)
C12-C11-C10-C1	-177.6(2)	C16-C11-C10-C1	1.2(2)

C12-C11-C10-C9	4.2(4)	C16-C11-C10-C9	-177.0(2)
C24-C23-C28-C27	-0.2(3)	B1-C23-C28-C27	174.47(18)
C24-C23-C28-C37	178.0(2)	B1-C23-C28-C37	-7.3(3)
C18-C17-C22-C21	-1.8(3)	B1-C17-C22-C21	-177.05(17)
C18-C17-C22-C34	174.45(18)	B1-C17-C22-C34	-0.8(3)
C10-C1-C2-C3	168.94(19)	N001-C1-C2-C3	-2.9(3)
C10-C1-C2-C7	-6.5(3)	N001-C1-C2-C7	-178.28(18)
C23-C24-C25-C26	-0.5(3)	C35-C24-C25-C26	-178.0(2)
C22-C17-C18-C19	3.5(3)	B1-C17-C18-C19	178.69(17)
C22-C17-C18-C32	-175.91(19)	B1-C17-C18-C32	-0.7(3)
C11-C12-C13-C14	1.6(3)	C11-C12-C13-C29	-175.70(19)
C17-C18-C19-C20	-2.8(3)	C32-C18-C19-C20	176.7(2)
C11-C16-C15-C14	0.4(3)	N001-C16-C15-C14	-174.5(2)
C17-C22-C21-C20	-0.8(3)	C34-C22-C21-C20	-177.21(19)
C1-C10-C9-C8	-1.9(3)	C11-C10-C9-C8	176.1(2)
C23-C28-C27-C26	-0.9(3)	C37-C28-C27-C26	-179.1(2)
C3-C2-C7-C6	3.8(3)	C1-C2-C7-C6	179.57(19)
C3-C2-C7-C8	-174.3(2)	C1-C2-C7-C8	1.5(3)
C1-C2-C3-C4	-178.2(2)	C7-C2-C3-C4	-2.9(3)
C22-C21-C20-C19	1.6(3)	C22-C21-C20-C33	178.4(2)

C18-C19-C20-C21	0.2(3)	C18-C19-C20-C33	-176.6(2)
C16-C15-C14-C13	0.8(3)	C12-C13-C14-C15	-1.8(3)
C29-C13-C14-C15	175.5(2)	C10-C9-C8-C7	-3.3(4)
C6-C7-C8-C9	-174.7(2)	C2-C7-C8-C9	3.4(3)
C24-C25-C26-C27	-0.5(3)	C24-C25-C26-C36	178.8(2)
C28-C27-C26-C25	1.2(3)	C28-C27-C26-C36	-178.1(2)
C12-C13-C29-C31	-131.8(2)	C14-C13-C29-C31	51.0(3)
C12-C13-C29-C30	104.1(3)	C14-C13-C29-C30	-73.1(3)
C2-C3-C4-C5	0.1(4)	C3-C4-C5-C6	1.8(4)
C4-C5-C6-C7	-0.8(4)	C8-C7-C6-C5	176.1(2)
C2-C7-C6-C5	-2.0(4)	C1-N001-B1-C17	-25.7(3)
C16-N001-B1-C17	132.17(18)	C1-N001-B1-C23	155.85(18)
C16-N001-B1-C23	-46.3(2)	C18-C17-B1-N001	134.87(19)
C22-C17-B1-N001	-50.1(3)	C18-C17-B1-C23	-46.7(3)
C22-C17-B1-C23	128.35(19)	C28-C23-B1-N001	127.75(19)
C24-C23-B1-N001	-57.7(2)	C28-C23-B1-C17	-50.7(3)
C24-C23-B1-C17	123.89(19)		

Table 7. Anisotropic atomic displacement parameters (Å^2)

The anisotropic atomic displacement factor exponent takes the form:
$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N001	0.0310(8)	0.0322(8)	0.0294(8)	-0.0031(6)	0.0092(6)	0.0010(6)
C16	0.0295(9)	0.0331(10)	0.0332(9)	-0.0013(8)	0.0093(7)	0.0001(8)
C1	0.0325(9)	0.0299(9)	0.0326(9)	-0.0038(8)	0.0124(8)	-0.0043(8)
C17	0.0330(9)	0.0324(10)	0.0325(9)	-0.0030(8)	0.0130(8)	0.0006(8)
C23	0.0288(9)	0.0307(9)	0.0314(9)	0.0009(7)	0.0059(7)	0.0032(7)
C24	0.0317(9)	0.0337(10)	0.0362(10)	-0.0017(8)	0.0088(8)	0.0008(8)
C11	0.0302(9)	0.0313(10)	0.0365(10)	-0.0026(8)	0.0123(8)	-0.0013(8)
C12	0.0316(10)	0.0355(10)	0.0438(11)	-0.0008(9)	0.0114(8)	0.0060(8)
C10	0.0347(10)	0.0320(10)	0.0375(10)	-0.0016(8)	0.0148(8)	-0.0013(8)
C28	0.0359(10)	0.0387(11)	0.0364(10)	0.0005(8)	0.0128(8)	0.0009(8)
C22	0.0390(10)	0.0338(10)	0.0380(10)	-0.0048(8)	0.0161(8)	-0.0031(8)
C2	0.0338(10)	0.0381(11)	0.0344(10)	-0.0033(8)	0.0128(8)	-0.0079(8)
C25	0.0433(11)	0.0326(10)	0.0438(11)	-0.0052(9)	0.0112(9)	-0.0038(9)
C18	0.0367(10)	0.0375(11)	0.0343(10)	-0.0028(8)	0.0096(8)	0.0024(8)
C13	0.0345(10)	0.0423(11)	0.0389(11)	0.0009(9)	0.0078(8)	0.0055(9)
C19	0.0351(10)	0.0529(13)	0.0400(11)	-0.0016(10)	0.0079(9)	0.0058(9)
C15	0.0441(11)	0.0456(12)	0.0350(10)	-0.0036(9)	0.0105(9)	0.0146(9)
C21	0.0448(12)	0.0413(12)	0.0479(12)	-0.0119(9)	0.0185(10)	-0.0125(10)
C9	0.0481(12)	0.0405(12)	0.0488(12)	-0.0014(9)	0.0211(10)	0.0102(10)
C27	0.0483(12)	0.0495(13)	0.0435(12)	-0.0040(10)	0.0250(10)	0.0018(10)
C7	0.0460(11)	0.0460(12)	0.0382(11)	-0.0053(9)	0.0191(9)	-0.0061(10)
C3	0.0422(11)	0.0518(13)	0.0397(11)	0.0073(10)	0.0178(9)	0.0037(10)
C20	0.0337(10)	0.0607(14)	0.0401(11)	-0.0112(10)	0.0118(9)	-0.0069(10)
C14	0.0482(12)	0.0564(14)	0.0310(10)	-0.0024(9)	0.0083(9)	0.0124(10)
C8	0.0638(14)	0.0486(13)	0.0465(12)	-0.0088(10)	0.0271(11)	0.0075(11)
C26	0.0551(13)	0.0397(12)	0.0419(11)	-0.0083(9)	0.0172(10)	0.0013(10)
C34	0.0559(13)	0.0319(11)	0.0591(14)	0.0008(10)	0.0125(11)	-0.0054(10)
C35	0.0528(13)	0.0472(13)	0.0709(16)	-0.0139(12)	0.0365(12)	-0.0150(11)
C32	0.0569(14)	0.0378(12)	0.0531(13)	0.0026(10)	-0.0020(11)	0.0076(10)

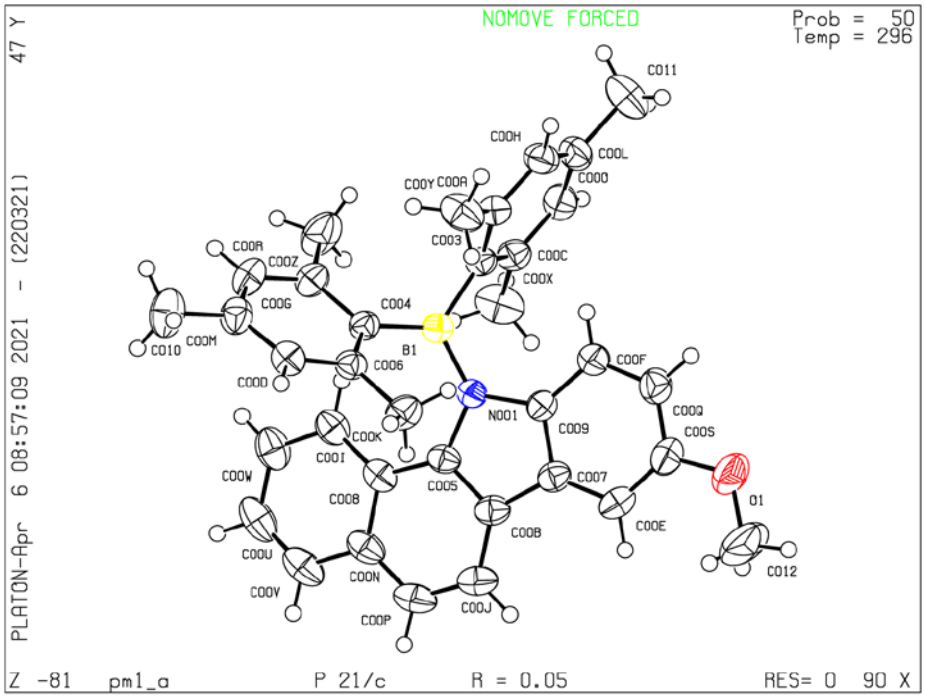
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C29	0.0461(12)	0.0535(13)	0.0432(12)	0.0057(10)	0.0091(10)	0.0167(10)
C31	0.0499(13)	0.0716(16)	0.0431(12)	0.0082(12)	0.0032(10)	0.0100(12)
C4	0.0521(13)	0.0758(17)	0.0441(12)	0.0181(12)	0.0168(11)	0.0092(12)
C5	0.0627(15)	0.094(2)	0.0330(11)	0.0082(12)	0.0179(11)	-0.0007(15)
C6	0.0607(14)	0.0714(16)	0.0392(12)	-0.0067(11)	0.0235(11)	-0.0027(13)
B1	0.0340(11)	0.0261(10)	0.0328(10)	0.0035(8)	0.0130(9)	-0.0002(8)
C37	0.0653(15)	0.0586(15)	0.0637(15)	-0.0094(12)	0.0382(13)	-0.0191(12)
C33	0.0448(13)	0.086(2)	0.0616(16)	-0.0186(14)	0.0039(12)	-0.0144(13)
C36	0.102(2)	0.0606(17)	0.0821(19)	-0.0319(15)	0.0504(18)	-0.0119(16)
C30	0.0756(19)	0.0666(18)	0.0763(19)	0.0270(15)	0.0018(15)	-0.0014(15)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$)

	x/a	y/b	z/c	U(eq)
H12	0.0190	1.1068	0.2392	0.044
H25	0.2146	0.2061	0.2267	0.048
H19	0.5552	0.5866	0.4632	0.052
H15	0.1964	0.7062	0.1938	0.05
H21	0.5058	1.0416	0.4191	0.052
H9	0.0480	1.1271	0.3624	0.053
H27	0.4006	0.4293	0.1700	0.054
H3	0.2931	0.6211	0.4362	0.052
H14	0.1031	0.8453	0.1175	0.055
H8	0.0926	1.1001	0.4660	0.061
H34A	0.3163	1.0619	0.3581	0.074
H34B	0.3324	0.9880	0.2981	0.074
H34C	0.3973	1.1139	0.3352	0.074
H35A	0.1310	0.4639	0.2893	0.08
H35B	0.2077	0.4388	0.3471	0.08

	x/a	y/b	z/c	U(eq)
H35C	0.1658	0.2915	0.3080	0.08
H32A	0.4313	0.4073	0.3529	0.078
H32B	0.3689	0.4181	0.3966	0.078
H32C	0.4675	0.3835	0.4235	0.078
H29	-0.0426	1.1553	0.1353	0.058
H31A	-0.0202	0.9230	0.0506	0.085
H31B	-0.0914	1.0561	0.0367	0.085
H31C	-0.0949	0.9220	0.0845	0.085
H4	0.3209	0.5837	0.5392	0.068
H5	0.2624	0.7541	0.5995	0.074
H6	0.1718	0.9535	0.5558	0.066
H37A	0.4424	0.6846	0.1972	0.088
H37B	0.4656	0.6906	0.2688	0.088
H37C	0.3875	0.7903	0.2309	0.088
H33A	0.6735	0.8663	0.4687	0.099
H33B	0.6434	0.7965	0.5245	0.099
H33C	0.6252	0.9757	0.5058	0.099
H36A	0.2863	0.0639	0.1635	0.115
H36B	0.3739	0.1298	0.1538	0.115
H36C	0.2861	0.1815	0.1095	0.115
H30A	0.0829	1.2762	0.1235	0.114
H30B	0.0171	1.2657	0.0594	0.114
H30C	0.0944	1.1451	0.0766	0.114

Crystal data for 7



A specimen of $C_{35}H_{34}BNO$, approximate dimensions 0.350 mm x 0.350 mm x 0.450 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 13.56 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 39480 reflections to a maximum θ angle of 26.00° (0.81 Å resolution), of which 5507 were independent (average redundancy 7.169, completeness = 99.0%, R_{int} = 2.45%, R_{sig} = 1.31%) and 5051 (91.72%) were greater than $2\sigma(F^2)$. The final cell constants of a = 13.0781(10) Å, b = 8.4879(6) Å, c = 25.5536(19) Å, β = 93.325(2)°, volume = 2831.8(4) $Å^3$, are based upon the refinement of the XYZ-centroids of 9935 reflections above 20 σ(I) with 5.057° < 2θ < 56.70°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.938. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9700 and 0.9770. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z = 4 for the formula unit, $C_{35}H_{34}BNO$. The final anisotropic full-matrix least-squares refinement on F^2 with 350 variables converged at R1 = 4.89%, for the observed data and wR2 = 13.39% for all data. The goodness-of-fit was 1.030. The largest peak in the final difference electron density synthesis was 0.214 $e^-/Å^3$ and the largest hole was -0.180 $e^-/Å^3$ with an RMS deviation of 0.034 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.162 g/cm^3 and F(000), 1056 e^-. CCDC number: 208358.

Table 1. Sample and crystal data

Identification code	mazza2002	
Chemical formula	$C_{35}H_{34}BNO$	
Formula weight	495.44 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.350 x 0.350 x 0.450 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 13.0781(10) Å	α = 90°
	b = 8.4879(6) Å	β = 93.325(2)°
	c = 25.5536(19) Å	γ = 90°
Volume	2831.8(4) $Å^3$	
Z	4	
Density (calculated)	1.162 g/cm^3	
Absorption coefficient	0.068 mm^{-1}	
F(000)	1056	

Table 2. Data collection and structure refinement

Theta range for data collection	1.60 to 26.00°
Index ranges	-16<=h<=16, -10<=k<=10, -31<=l<=31
Reflections collected	39480
Independent reflections	5507 [R(int) = 0.0245]
Coverage of independent reflections	99.0%
Absorption correction	Multi-Scan
Max. and min. transmission	0.9770 and 0.9700
Structure solution technique	direct methods
Structure solution program	XT, VERSION 2014/5
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)

Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	5507 / 0 / 350	
Goodness-of-fit on F^2	1.030	
Δ/σ_{max}	0.001	
Final R indices	5051 data; $I>2\sigma(I)$	R1 = 0.0489, wR2 = 0.1306
	all data	R1 = 0.0522, wR2 = 0.1339
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0678P)^2+0.9105P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.214 and -0.180 eÅ^{-3}	
R.M.S. deviation from mean	0.034 eÅ^{-3}	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2)

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
N001	0.67643(8)	0.25163(13)	0.35235(4)	0.0345(2)
O1	0.71456(11)	0.03754(19)	0.14897(5)	0.0759(4)
C003	0.80821(10)	0.47518(15)	0.36076(5)	0.0356(3)
C004	0.79069(10)	0.25938(15)	0.44099(5)	0.0355(3)
C005	0.59152(9)	0.16083(15)	0.36572(5)	0.0357(3)
C006	0.81409(10)	0.09747(15)	0.44634(5)	0.0363(3)
C007	0.62290(10)	0.09947(16)	0.28098(5)	0.0383(3)
C008	0.53518(10)	0.16846(16)	0.41188(5)	0.0388(3)
C009	0.69104(10)	0.21738(16)	0.29847(5)	0.0362(3)
C00A	0.91536(10)	0.48313(16)	0.35666(5)	0.0394(3)
C00B	0.55835(10)	0.06651(16)	0.32341(6)	0.0398(3)
C00C	0.74756(11)	0.59556(16)	0.33698(5)	0.0407(3)
C00D	0.85282(11)	0.03902(17)	0.49423(6)	0.0431(3)
C00E	0.62687(11)	0.03443(18)	0.23068(6)	0.0468(3)
C00F	0.76317(11)	0.27496(18)	0.26489(5)	0.0437(3)

	x/a	y/b	z/c	U(eq)
C00G	0.80933(11)	0.35629(17)	0.48564(6)	0.0449(3)
C00H	0.95695(11)	0.60223(18)	0.32744(6)	0.0456(3)
C00I	0.55222(11)	0.27715(18)	0.45318(6)	0.0446(3)
C00J	0.47385(11)	0.96428(19)	0.32648(7)	0.0499(4)
C00K	0.80309(12)	0.98332(17)	0.40126(6)	0.0466(3)
C00L	0.89728(13)	0.71706(18)	0.30256(6)	0.0484(4)
C00M	0.86713(11)	0.1326(2)	0.53819(6)	0.0479(4)
C00N	0.45065(10)	0.06239(18)	0.41413(6)	0.0464(3)
C00O	0.79263(12)	0.71251(17)	0.30842(6)	0.0464(3)
C00P	0.42377(11)	0.96047(19)	0.37129(7)	0.0541(4)
C00Q	0.76488(12)	0.2118(2)	0.21540(6)	0.0480(4)
C00R	0.84496(12)	0.2908(2)	0.53302(6)	0.0514(4)
C00S	0.69917(12)	0.0912(2)	0.19864(6)	0.0491(4)
B1	0.75576(11)	0.32901(17)	0.38589(6)	0.0344(3)
C00U	0.41224(13)	0.1681(2)	0.49827(7)	0.0592(5)
C00V	0.39227(12)	0.0651(2)	0.45881(7)	0.0565(4)
C00W	0.49234(14)	0.2773(2)	0.49548(7)	0.0547(4)
C00X	0.63295(13)	0.6044(2)	0.34201(9)	0.0652(5)
C00Y	0.98713(12)	0.3606(2)	0.38061(8)	0.0598(4)
C00Z	0.78992(18)	0.5312(2)	0.48394(7)	0.0695(5)
C010	0.90409(17)	0.0630(3)	0.59030(7)	0.0727(5)
C011	0.94383(17)	0.8444(3)	0.27056(9)	0.0772(6)
C012	0.6546(3)	0.9100(4)	0.13088(10)	0.1276(13)

Table 4. Bond lengths (Å)

N001-C005	1.4100(16)	N001-C009	1.4307(16)
N001-B1	1.4627(18)	O1-C00S	1.3743(18)
O1-C012	1.400(3)	C003-C00C	1.4094(19)
C003-C00A	1.4129(18)	C003-B1	1.5727(19)
C004-C006	1.4129(19)	C004-C00G	1.4161(19)
C004-B1	1.570(2)	C005-C00B	1.3942(19)

C005-C008	1.4281(19)	C006-C00D	1.3887(19)
C006-C00K	1.5057(19)	C007-C009	1.3961(19)
C007-C00E	1.403(2)	C007-C00B	1.440(2)
C008-C00I	1.410(2)	C008-C00N	1.4294(19)
C009-C00F	1.3996(19)	C00A-C00H	1.387(2)
C00A-C00Y	1.507(2)	C00B-C00J	1.4108(19)
C00C-C00O	1.384(2)	C00C-C00X	1.514(2)
C00D-C00M	1.380(2)	C00D-H00D	0.93
C00E-C00S	1.373(2)	C00E-H00E	0.93
C00F-C00Q	1.375(2)	C00F-H00F	0.93
C00G-C00R	1.388(2)	C00G-C00Z	1.507(2)
C00H-C00L	1.380(2)	C00H-H00H	0.93
C00I-C00W	1.371(2)	C00I-H00I	0.93
C00J-C00P	1.352(2)	C00J-H00J	0.93
C00K-H00A	0.96	C00K-H00B	0.96
C00K-H00C	0.96	C00L-C00O	1.386(2)
C00L-C011	1.505(2)	C00M-C00R	1.378(2)
C00M-C010	1.510(2)	C00N-C00V	1.410(2)
C00N-C00P	1.423(2)	C00O-H00O	0.93
C00P-H00P	0.93	C00Q-C00S	1.388(2)

C00Q-H00Q	0.93	C00R-H00R	0.93
C00U-C00V	1.349(3)	C00U-C00W	1.403(3)
C00U-H00U	0.93	C00V-H00V	0.93
C00W-H00W	0.93	C00X-H00G	0.96
C00X-H00K	0.96	C00X-H00L	0.96
C00Y-H00M	0.96	C00Y-H00N	0.96
C00Y-H00S	0.96	C00Z-H00T	0.96
C00Z-H00$	0.96	C00Z-H00	0.96
C010-H01A	0.96	C010-H01B	0.96
C010-H01C	0.96	C011-H01D	0.96
C011-H01E	0.96	C011-H01F	0.96
C012-H01G	0.96	C012-H01H	0.96
C012-H01I	0.96		

Table 5. Bond angles (°)

C005-N001-C009	105.86(10)	C005-N001-B1	130.18(11)
C009-N001-B1	121.70(11)	C00S-O1-C012	116.91(16)
C00C-C003-C00A	117.98(12)	C00C-C003-B1	120.01(12)
C00A-C003-B1	121.73(12)	C006-C004-C00G	117.44(12)
C006-C004-B1	120.20(11)	C00G-C004-B1	122.09(12)
C00B-C005-N001	109.87(11)	C00B-C005-C008	120.96(12)

N001-C005-C008	128.82(12)	C00D-C006-C004	119.91(12)
C00D-C006-C00K	117.26(12)	C004-C006-C00K	122.78(12)
C009-C007-C00E	121.24(13)	C009-C007-C00B	106.83(12)
C00E-C007-C00B	131.92(13)	C00I-C008-C005	125.54(12)
C00I-C008-C00N	118.11(13)	C005-C008-C00N	116.23(13)
C007-C009-C00F	119.64(12)	C007-C009-N001	109.59(11)
C00F-C009-N001	130.64(12)	C00H-C00A-C003	119.77(13)
C00H-C00A-C00Y	117.86(13)	C003-C00A-C00Y	122.28(13)
C005-C00B-C00J	121.30(14)	C005-C00B-C007	107.62(12)
C00J-C00B-C007	131.06(13)	C00O-C00C-C003	120.08(13)
C00O-C00C-C00X	117.62(13)	C003-C00C-C00X	122.30(13)
C00M-C00D-C006	122.49(14)	C00M-C00D-H00D	118.8
C006-C00D-H00D	118.8	C00S-C00E-C007	118.12(14)
C00S-C00E-H00E	120.9	C007-C00E-H00E	120.9
C00Q-C00F-C009	118.37(14)	C00Q-C00F-H00F	120.8
C009-C00F-H00F	120.8	C00R-C00G-C004	120.22(14)
C00R-C00G-C00Z	117.86(14)	C004-C00G-C00Z	121.90(14)
C00L-C00H-C00A	122.26(14)	C00L-C00H-H00H	118.9
C00A-C00H-H00H	118.9	C00W-C00I-C008	121.19(15)
C00W-C00I-H00I	119.4	C008-C00I-H00I	119.4

C00P-C00J-C00B	118.77(15)	C00P-C00J-H00J	120.6
C00B-C00J-H00J	120.6	C006-C00K-H00A	109.5
C006-C00K-H00B	109.5	H00A-C00K-H00B	109.5
C006-C00K-H00C	109.5	H00A-C00K-H00C	109.5
H00B-C00K-H00C	109.5	C00H-C00L-C00O	117.78(13)
C00H-C00L-C011	121.43(16)	C00O-C00L-C011	120.79(16)
C00R-C00M-C00D	117.70(14)	C00R-C00M-C010	121.35(15)
C00D-C00M-C010	120.94(16)	C00V-C00N-C00P	120.77(14)
C00V-C00N-C008	118.59(15)	C00P-C00N-C008	120.59(14)
C00C-C00O-C00L	122.03(14)	C00C-C00O-H00O	119.0
C00L-C00O-H00O	119.0	C00J-C00P-C00N	121.78(14)
C00J-C00P-H00P	119.1	C00N-C00P-H00P	119.1
C00F-C00Q-C00S	121.90(14)	C00F-C00Q-H00Q	119.0
C00S-C00Q-H00Q	119.0	C00M-C00R-C00G	122.14(14)
C00M-C00R-H00R	118.9	C00G-C00R-H00R	118.9
C00E-C00S-O1	125.22(15)	C00E-C00S-C00Q	120.68(13)
O1-C00S-C00Q	114.10(14)	N001-B1-C004	121.07(11)
N001-B1-C003	115.23(11)	C004-B1-C003	123.50(11)
C00V-C00U-C00W	120.18(15)	C00V-C00U-H00U	119.9
C00W-C00U-H00U	119.9	C00U-C00V-C00N	121.70(15)

C00U-C00V-H00V	119.1	C00N-C00V-H00V	119.1
C00I-C00W-C00U	120.12(17)	C00I-C00W-H00W	119.9
C00U-C00W-H00W	119.9	C00C-C00X-H00G	109.5
C00C-C00X-H00K	109.5	H00G-C00X-H00K	109.5
C00C-C00X-H00L	109.5	H00G-C00X-H00L	109.5
H00K-C00X-H00L	109.5	C00A-C00Y-H00M	109.5
C00A-C00Y-H00N	109.5	H00M-C00Y-H00N	109.5
C00A-C00Y-H00S	109.5	H00M-C00Y-H00S	109.5
H00N-C00Y-H00S	109.5	C00G-C00Z-H00T	109.5
C00G-C00Z-H00$	109.5	H00T-C00Z-H00$	109.5
C00G-C00Z-H00	109.5	H00T-C00Z-H00	109.5
H00$-C00Z-H00	109.5	C00M-C010-H01A	109.5
C00M-C010-H01B	109.5	H01A-C010-H01B	109.5
C00M-C010-H01C	109.5	H01A-C010-H01C	109.5
H01B-C010-H01C	109.5	C00L-C011-H01D	109.5
C00L-C011-H01E	109.5	H01D-C011-H01E	109.5
C00L-C011-H01F	109.5	H01D-C011-H01F	109.5
H01E-C011-H01F	109.5	O1-C012-H01G	109.5
O1-C012-H01H	109.5	H01G-C012-H01H	109.5
O1-C012-H01I	109.5	H01G-C012-H01I	109.5

H01H-C012-H01I	109.5

Table 6. Torsion angles (°)

C009-N001-C005-C00B	3.60(14)	B1-N001-C005-C00B	-159.11(13)
C009-N001-C005-C008	-169.46(13)	B1-N001-C005-C008	27.8(2)
C00G-C004-C006-C00D	0.63(19)	B1-C004-C006-C00D	174.80(12)
C00G-C004-C006-C00K	-176.74(13)	B1-C004-C006-C00K	-2.56(19)
C00B-C005-C008-C00I	-169.42(13)	N001-C005-C008-C00I	3.0(2)
C00B-C005-C008-C00N	6.47(19)	N001-C005-C008-C00N	178.86(12)
C00E-C007-C009-C00F	1.6(2)	C00B-C007-C009-C00F	-179.36(12)
C00E-C007-C009-N001	-174.66(12)	C00B-C007-C009-N001	4.38(14)
C005-N001-C009-C007	-4.95(14)	B1-N001-C009-C007	159.57(12)
C005-N001-C009-C00F	179.34(14)	B1-N001-C009-C00F	-16.1(2)
C00C-C003-C00A-C00H	-3.47(19)	B1-C003-C00A-C00H	170.41(13)
C00C-C003-C00A-C00Y	-179.95(14)	B1-C003-C00A-C00Y	-6.1(2)
N001-C005-C00B-C00J	-179.76(12)	C008-C005-C00B-C00J	-6.1(2)
N001-C005-C00B-C007	-0.99(15)	C008-C005-C00B-C007	172.70(11)
C009-C007-C00B-C005	-2.10(15)	C00E-C007-C00B-C005	176.80(14)
C009-C007-C00B-C00J	176.51(14)	C00E-C007-C00B-C00J	-4.6(3)
C00A-C003-C00C-C00O	3.17(19)	B1-C003-C00C-C00O	-170.81(12)
C00A-C003-C00C-C00X	-175.88(14)	B1-C003-C00C-C00X	10.1(2)

C004-C006-C00D-C00M	1.9(2)	C00K-C006-C00D-C00M	179.44(13)
C009-C007-C00E-C00S	-0.7(2)	C00B-C007-C00E-C00S	-179.49(14)
C007-C009-C00F-C00Q	-0.5(2)	N001-C009-C00F-C00Q	174.90(13)
C006-C004-C00G-C00R	-2.8(2)	B1-C004-C00G-C00R	-176.82(13)
C006-C004-C00G-C00Z	178.29(15)	B1-C004-C00G-C00Z	4.2(2)
C003-C00A-C00H-C00L	1.3(2)	C00Y-C00A-C00H-C00L	177.91(15)
C005-C008-C00I-C00W	178.53(14)	C00N-C008-C00I-C00W	2.7(2)
C005-C00B-C00J-C00P	1.0(2)	C007-C00B-C00J-C00P	-177.47(15)
C00A-C00H-C00L-C00O	1.3(2)	C00A-C00H-C00L-C011	-179.36(16)
C006-C00D-C00M-C00R	-2.3(2)	C006-C00D-C00M-C010	176.69(15)
C00I-C008-C00N-C00V	-3.7(2)	C005-C008-C00N-C00V	-179.91(13)
C00I-C008-C00N-C00P	173.97(13)	C005-C008-C00N-C00P	-2.2(2)
C003-C00C-C00O-C00L	-0.6(2)	C00X-C00C-C00O-C00L	178.45(15)
C00H-C00L-C00O-C00C	-1.6(2)	C011-C00L-C00O-C00C	179.03(16)
C00B-C00J-C00P-C00N	3.4(2)	C00V-C00N-C00P-C00J	174.93(15)
C008-C00N-C00P-C00J	-2.7(2)	C009-C00F-C00Q-C00S	-1.5(2)
C00D-C00M-C00R-C00G	0.0(2)	C010-C00M-C00R-C00G	-178.93(16)
C004-C00G-C00R-C00M	2.5(2)	C00Z-C00G-C00R-C00M	-178.51(17)
C007-C00E-C00S-O1	178.32(15)	C007-C00E-C00S-C00Q	-1.3(2)
C012-O1-C00S-C00E	-3.1(3)	C012-O1-C00S-C00Q	176.5(2)

C00F-C00Q-C00S-C00E	2.5(2)	C00F-C00Q-C00S-O1	-177.17(15)
C005-N001-B1-C004	30.5(2)	C009-N001-B1-C004	-129.85(13)
C005-N001-B1-C003	-154.44(12)	C009-N001-B1-C003	45.19(16)
C006-C004-B1-N001	47.79(18)	C00G-C004-B1-N001	-138.32(13)
C006-C004-B1-C003	-126.84(14)	C00G-C004-B1-C003	47.06(19)
C00C-C003-B1-N001	50.08(17)	C00A-C003-B1-N001	-123.67(13)
C00C-C003-B1-C004	-135.01(13)	C00A-C003-B1-C004	51.24(18)
C00W-C00U-C00V-C00N	0.5(2)	C00P-C00N-C00V-C00U	-175.48(15)
C008-C00N-C00V-C00U	2.2(2)	C008-C00I-C00W-C00U	-0.1(2)
C00V-C00U-C00W-C00I	-1.6(2)		

Table 7. Anisotropic atomic displacement parameters (Å^2)

The anisotropic atomic displacement factor exponent takes the form:
$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

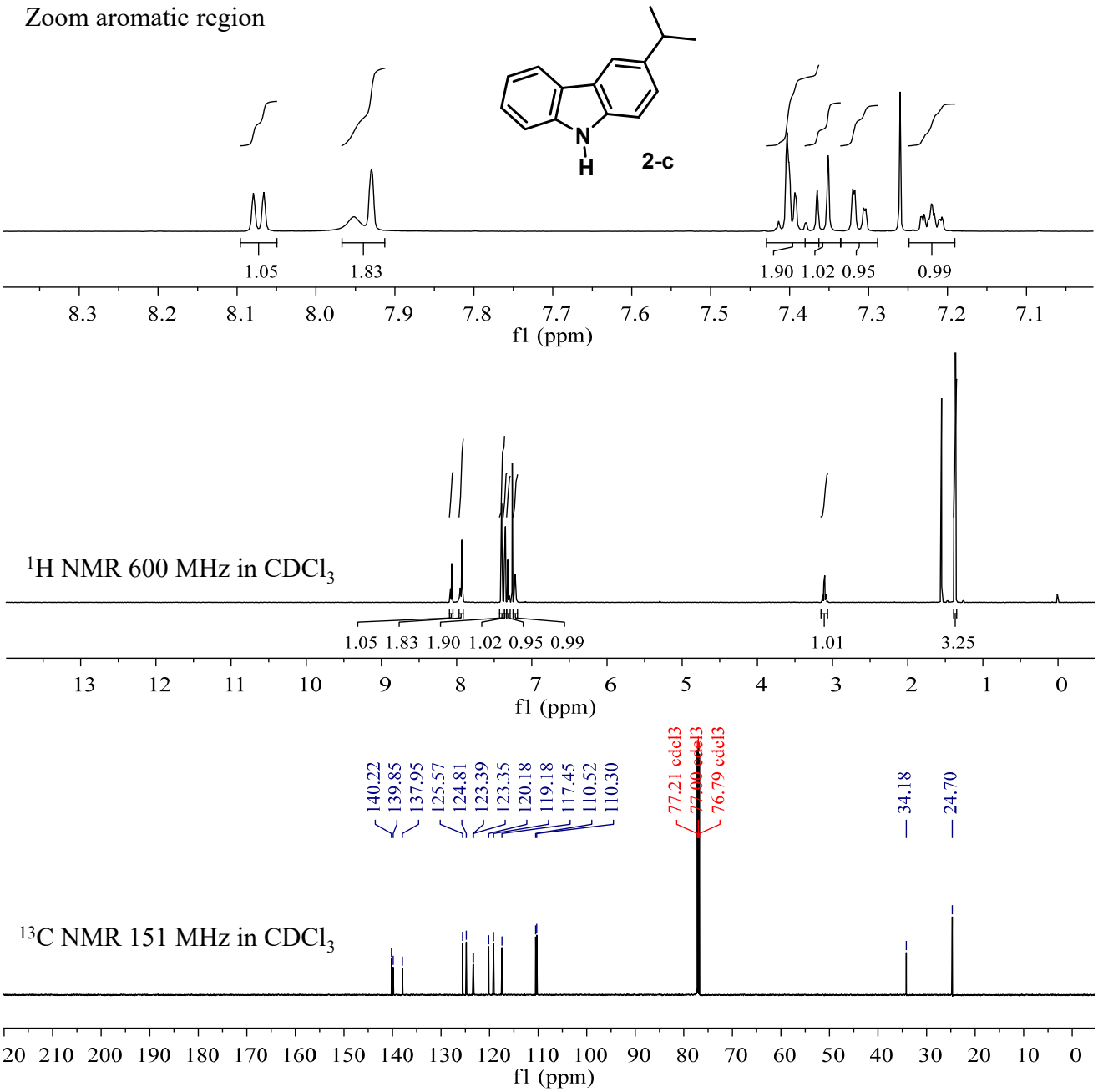
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N001	0.0337(5)	0.0350(5)	0.0350(5)	-0.0005(4)	0.0042(4)	-0.0034(4)
O1	0.0775(9)	0.1025(11)	0.0486(7)	-0.0303(7)	0.0113(6)	-0.0202(8)
C003	0.0376(7)	0.0314(6)	0.0374(6)	-0.0028(5)	0.0005(5)	-0.0023(5)
C004	0.0352(6)	0.0348(6)	0.0366(7)	-0.0035(5)	0.0031(5)	-0.0013(5)
C005	0.0296(6)	0.0334(6)	0.0441(7)	0.0034(5)	0.0008(5)	0.0000(5)
C006	0.0337(6)	0.0359(7)	0.0397(7)	-0.0019(5)	0.0048(5)	-0.0013(5)
C007	0.0342(6)	0.0385(7)	0.0415(7)	-0.0006(5)	-0.0042(5)	0.0015(5)
C008	0.0334(6)	0.0365(7)	0.0467(7)	0.0082(6)	0.0051(5)	0.0046(5)
C009	0.0355(6)	0.0372(7)	0.0356(6)	-0.0016(5)	-0.0002(5)	0.0014(5)
C00A	0.0381(7)	0.0369(7)	0.0430(7)	-0.0018(6)	0.0005(5)	-0.0039(5)
C00B	0.0331(6)	0.0371(7)	0.0486(8)	0.0000(6)	-0.0029(5)	-0.0002(5)
C00C	0.0430(7)	0.0341(7)	0.0446(7)	-0.0031(6)	-0.0001(6)	0.0015(5)
C00D	0.0410(7)	0.0415(7)	0.0468(8)	0.0039(6)	0.0038(6)	0.0042(6)

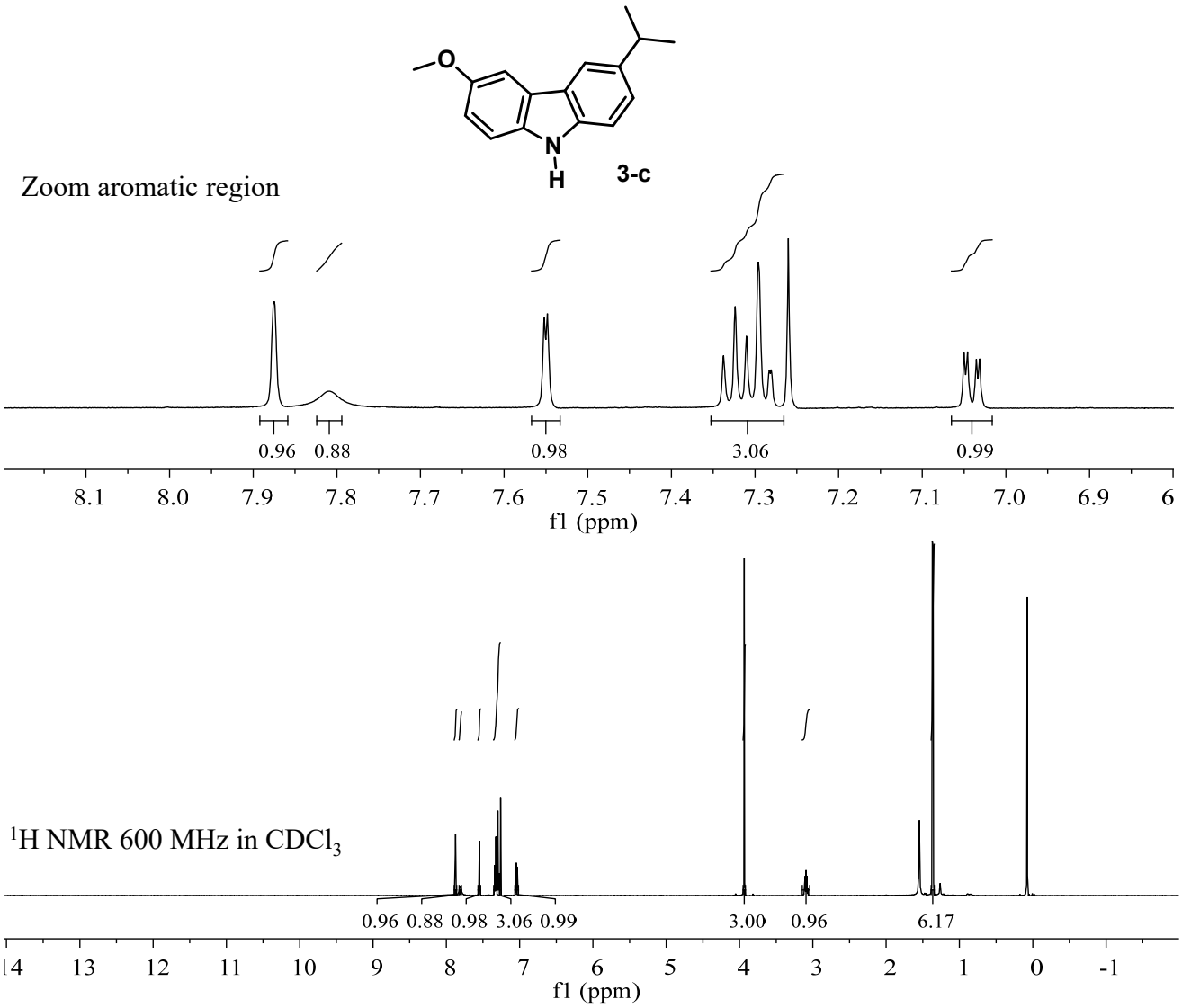
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C00E	0.0430(7)	0.0487(8)	0.0473(8)	-0.0095(6)	-0.0083(6)	-0.0024(6)
C00F	0.0430(7)	0.0476(8)	0.0408(7)	-0.0033(6)	0.0054(6)	-0.0067(6)
C00G	0.0497(8)	0.0418(7)	0.0430(7)	-0.0085(6)	0.0006(6)	0.0007(6)
C00H	0.0427(7)	0.0447(8)	0.0499(8)	-0.0015(6)	0.0078(6)	-0.0076(6)
C00I	0.0431(7)	0.0429(7)	0.0487(8)	0.0042(6)	0.0105(6)	0.0045(6)
C00J	0.0393(7)	0.0461(8)	0.0636(9)	-0.0022(7)	-0.0033(7)	-0.0087(6)
C00K	0.0540(8)	0.0351(7)	0.0503(8)	-0.0070(6)	-0.0001(6)	0.0050(6)
C00L	0.0616(9)	0.0399(7)	0.0446(8)	0.0019(6)	0.0100(7)	-0.0068(7)
C00M	0.0433(7)	0.0602(9)	0.0399(7)	0.0019(7)	-0.0005(6)	0.0033(7)
C00N	0.0339(7)	0.0437(8)	0.0621(9)	0.0144(7)	0.0077(6)	0.0020(6)
C00O	0.0598(9)	0.0341(7)	0.0451(8)	0.0026(6)	0.0006(6)	0.0048(6)
C00P	0.0371(7)	0.0480(8)	0.0771(11)	0.0059(8)	0.0032(7)	-0.0114(6)
C00Q	0.0455(8)	0.0576(9)	0.0415(8)	-0.0022(7)	0.0073(6)	-0.0008(7)
C00R	0.0569(9)	0.0579(9)	0.0388(7)	-0.0123(7)	-0.0031(6)	0.0021(7)
C00S	0.0472(8)	0.0608(9)	0.0389(7)	-0.0087(7)	-0.0006(6)	0.0034(7)
B1	0.0327(7)	0.0307(7)	0.0401(7)	-0.0048(6)	0.0053(6)	0.0019(5)
C00U	0.0537(9)	0.0615(10)	0.0653(10)	0.0208(9)	0.0277(8)	0.0150(8)
C00V	0.0421(8)	0.0547(9)	0.0743(11)	0.0201(8)	0.0180(7)	0.0038(7)
C00W	0.0605(9)	0.0534(9)	0.0519(9)	0.0062(7)	0.0180(7)	0.0133(7)
C00X	0.0460(9)	0.0521(9)	0.0971(14)	0.0128(9)	0.0020(9)	0.0106(7)
C00Y	0.0383(8)	0.0615(10)	0.0796(12)	0.0190(9)	0.0034(7)	0.0029(7)
C00Z	0.1039(15)	0.0446(9)	0.0587(10)	-0.0176(8)	-0.0070(10)	0.0085(9)
C010	0.0793(13)	0.0898(14)	0.0474(9)	0.0087(9)	-0.0094(8)	0.0140(11)
C011	0.0866(14)	0.0669(12)	0.0801(13)	0.0276(10)	0.0212(11)	-0.0074(10)
C012	0.133(2)	0.171(3)	0.0822(16)	-0.0773(19)	0.0305(15)	-0.071(2)

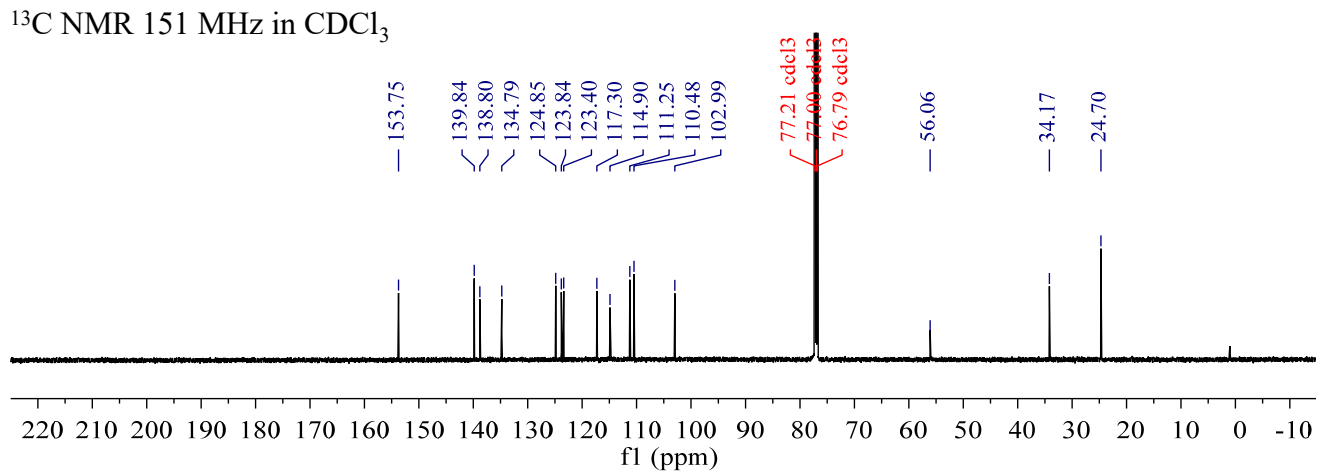
Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$)

	x/a	y/b	z/c	U(eq)
H00D	0.8698	-0.0672	0.4968	0.052
H00E	0.5818	-0.0449	0.2193	0.056

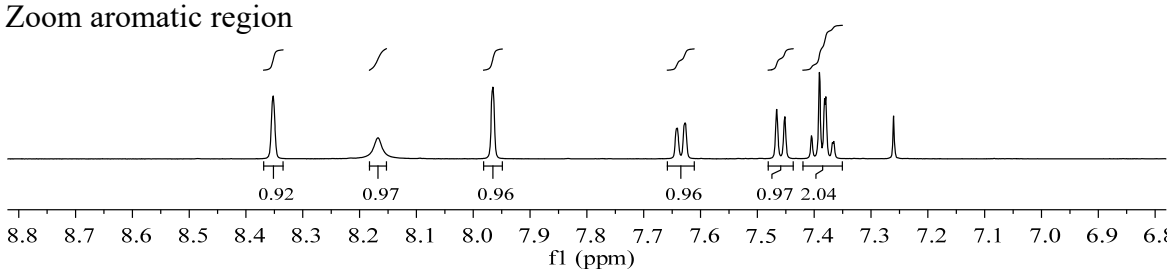
	x/a	y/b	z/c	U(eq)
H00F	0.8088	0.3540	0.2758	0.052
H00H	1.0275	0.6048	0.3245	0.055
H00I	0.6050	0.3501	0.4517	0.054
H00J	0.4530	-0.0993	0.2982	0.06
H00A	0.8408	-0.1110	0.4100	0.07
H00B	0.8294	0.0304	0.3706	0.07
H00C	0.7321	-0.0422	0.3944	0.07
H00O	0.7514	0.7905	0.2927	0.056
H00P	0.3703	-0.1107	0.3742	0.065
H00Q	0.8114	0.2510	0.1925	0.058
H00R	0.8542	0.3557	0.5622	0.062
H00U	0.3728	0.1668	0.5274	0.071
H00V	0.3386	-0.0060	0.4611	0.068
H00W	0.5048	0.3498	0.5224	0.066
H00G	0.6113	0.7124	0.3401	0.098
H00K	0.6162	0.5605	0.3751	0.098
H00L	0.5987	0.5458	0.3140	0.098
H00M	1.0555	0.3811	0.3706	0.09
H00N	0.9660	0.2580	0.3684	0.09
H00S	0.9857	0.3645	0.4181	0.09
H00T	0.7859	0.5705	0.5190	0.104
H00$	0.7266	0.5518	0.4643	0.104
H00	0.8449	0.5829	0.4675	0.104
H01A	0.8464	0.0264	0.6085	0.109
H01B	0.9401	0.1421	0.6110	0.109
H01C	0.9493	-0.0236	0.5846	0.109
H01D	0.9875	0.9094	0.2930	0.116
H01E	0.8904	0.9077	0.2541	0.116
H01F	0.9833	0.7972	0.2442	0.116
H01G	0.6651	-0.1774	0.1544	0.191
H01H	0.6740	-0.1199	0.0966	0.191
H01I	0.5837	-0.0604	0.1292	0.191


Zoom aromatic region
2-c
1.05
1.83
1.90 1.02 0.95
0.99
f1 (ppm)
^{1}H NMR 600 MHz in CDCl$_3$
1.05 1.83 1.90 1.02 0.95 0.99
1.01
3.25
f1 (ppm)
^{13}C NMR 151 MHz in CDCl$_3$
140.22
139.85
137.95
125.57
124.81
123.39
123.35
120.18
119.18
117.45
110.52
110.30
77.21 cdcl3
77.00 cdcl3
76.79 cdcl3
34.18
24.70
f1 (ppm)

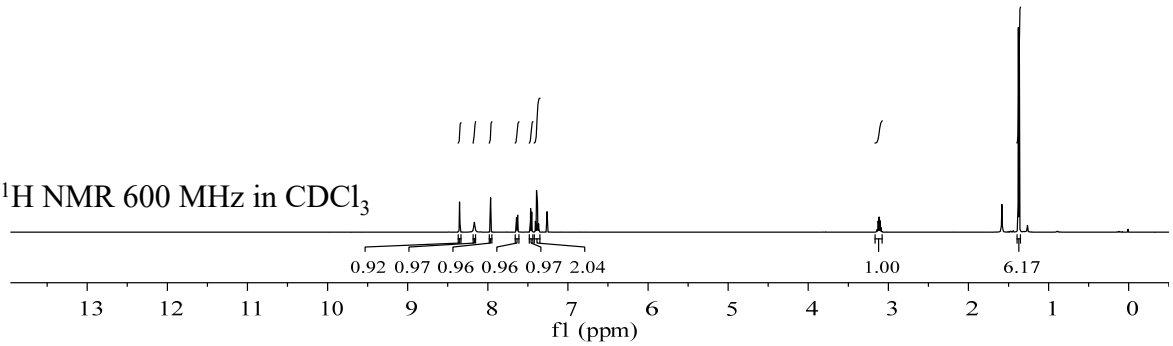

3-c
Zoom aromatic region
0.96 0.88 0.98 3.06 0.99
f1 (ppm)
^{1}H NMR 600 MHz in CDCl$_3$
0.96 0.88 0.98 3.06 0.99 3.00 0.96 6.17
f1 (ppm)

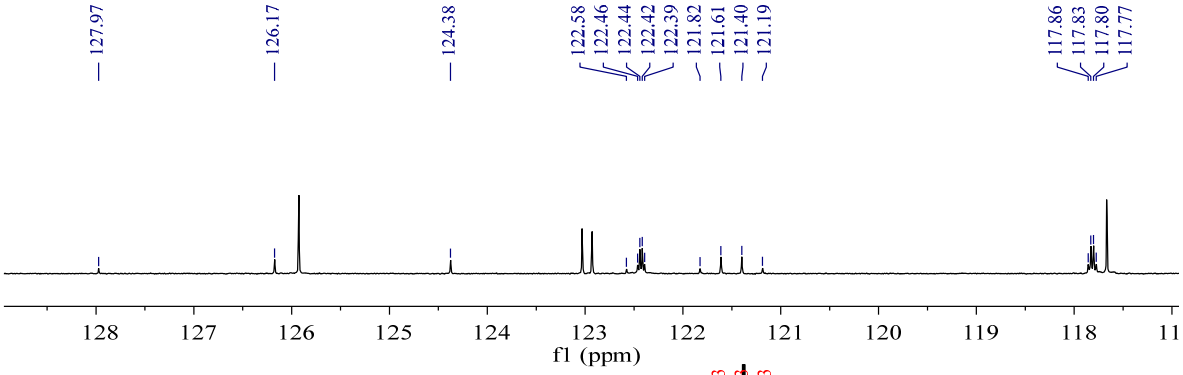

^{13}C NMR 151 MHz in CDCl$_3$
153.75
139.84
138.80
134.79
124.85
123.84
123.40
117.30
114.90
111.25
110.48
102.99
77.21 cdcl3
76.79 cdcl3
56.06
34.17
24.70
f1 (ppm)

Zoom aromatic region

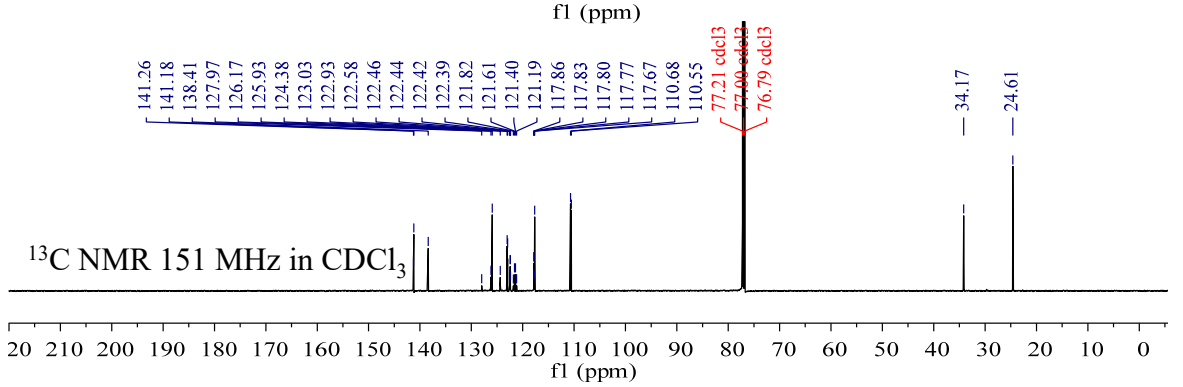


^{1}H NMR 600 MHz in $CDCl_3$

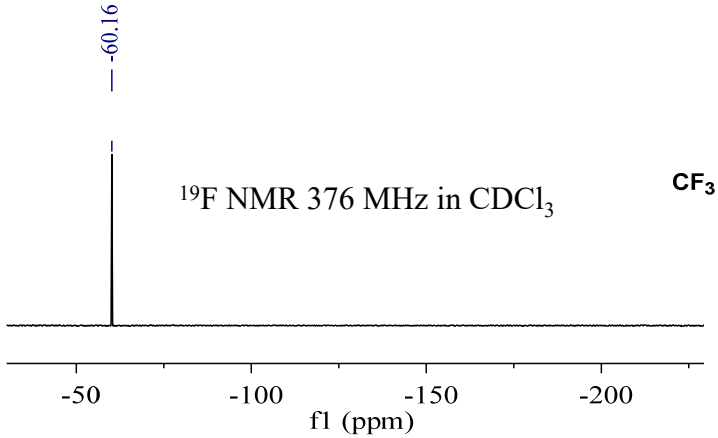


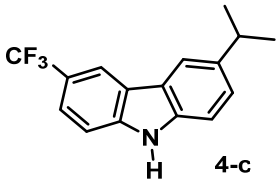


^{13}C NMR 151 MHz in $CDCl_3$



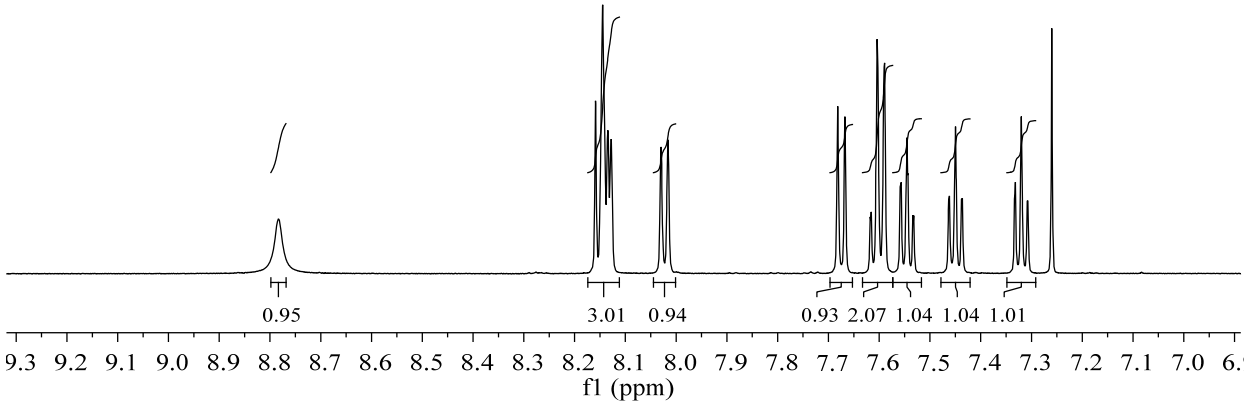
^{19}F NMR 376 MHz in $CDCl_3$



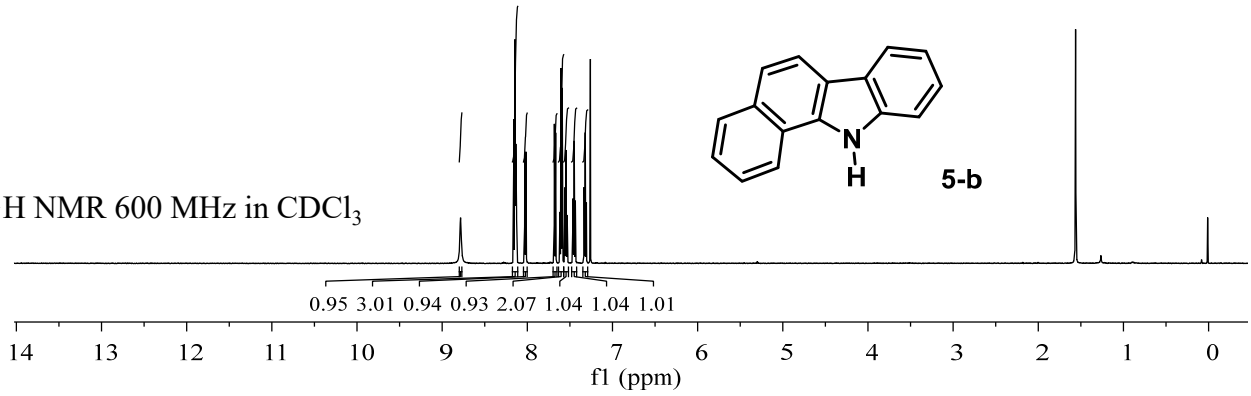


4-c

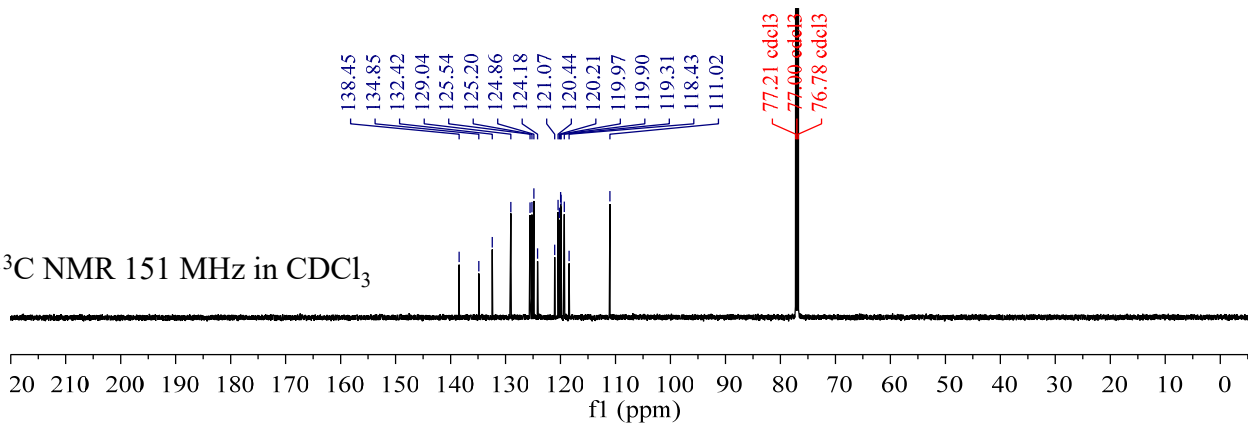
Zoom aromatic region

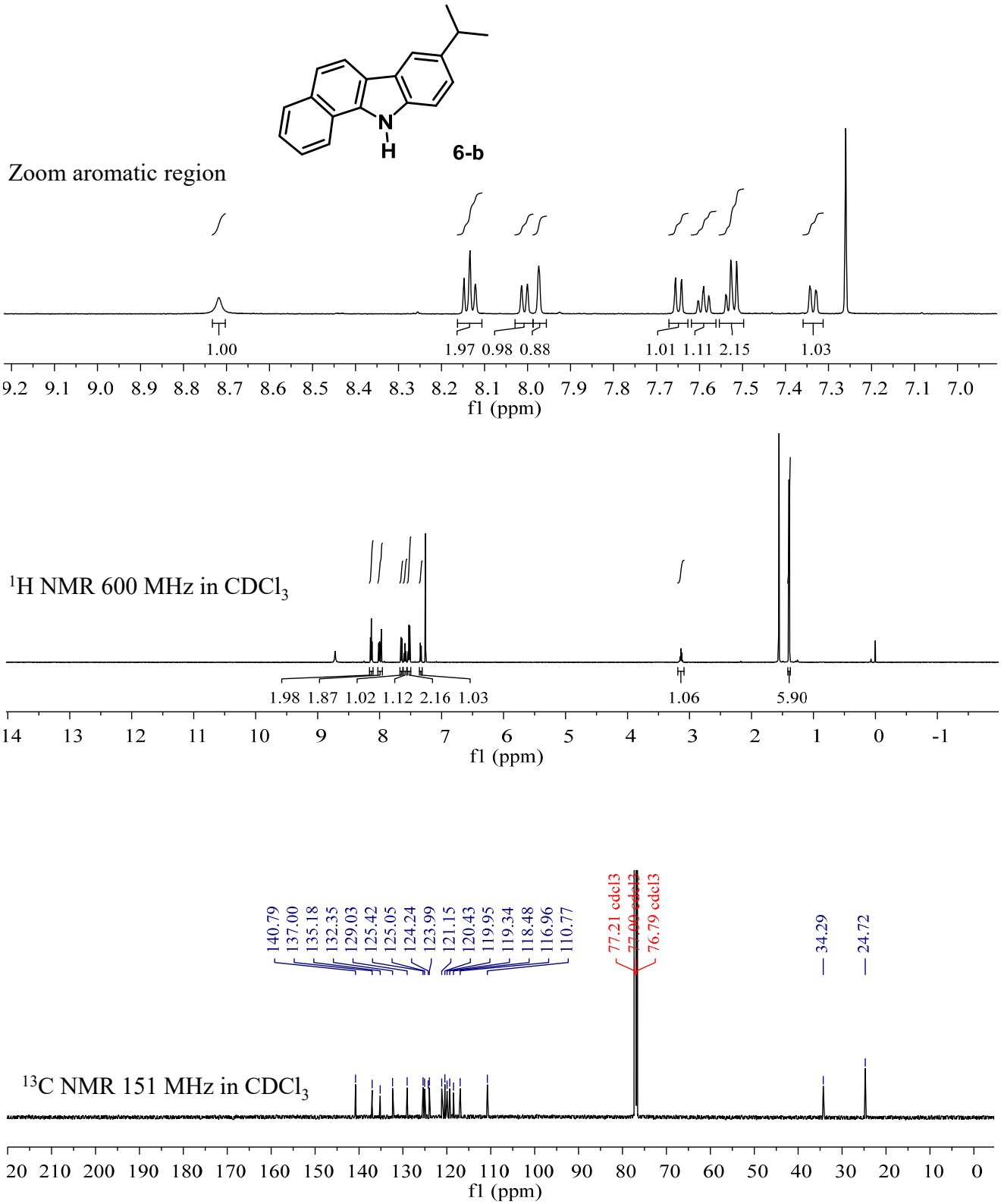


^{1}H NMR 600 MHz in $CDCl_3$

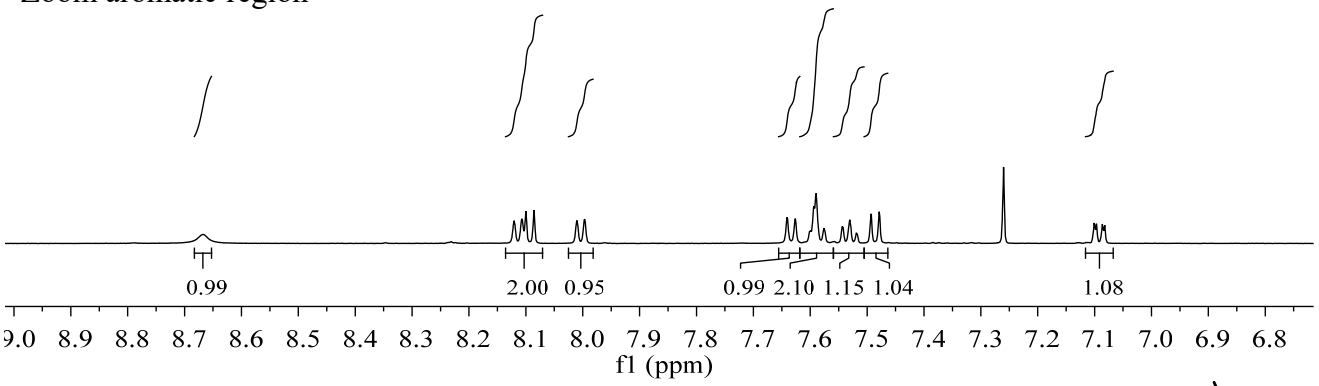


^{13}C NMR 151 MHz in $CDCl_3$

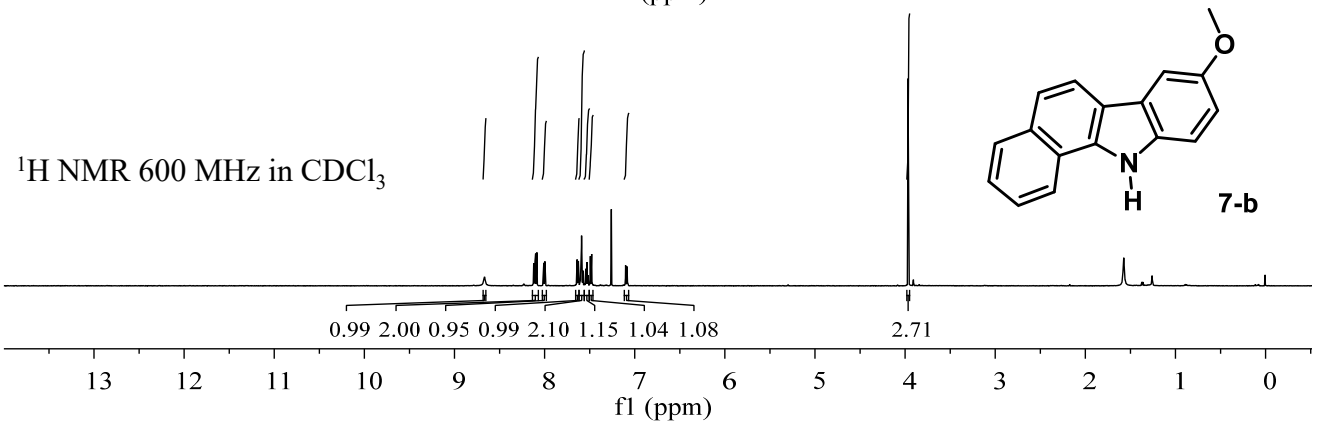



6-b
Zoom aromatic region
1.00
1.97 0.98 0.88
1.01 1.11 2.15
1.03
f1 (ppm)
^{1}H NMR 600 MHz in CDCl$_3$
1.98 1.87 1.02 1.12 2.16 1.03
1.06
5.90
f1 (ppm)
^{13}C NMR 151 MHz in CDCl$_3$
140.79
137.00
135.18
132.35
129.03
125.42
125.05
124.24
123.99
121.15
120.43
119.95
119.34
118.48
116.96
110.77
77.21 cdcl3
77.00 cdcl3
76.79 cdcl3
34.29
24.72
f1 (ppm)

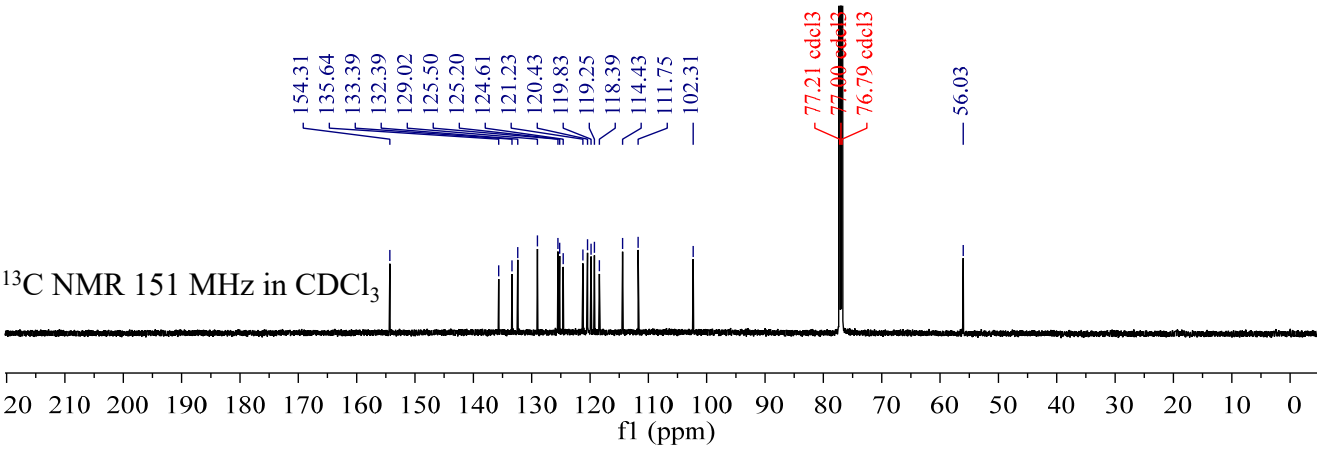
Zoom aromatic region

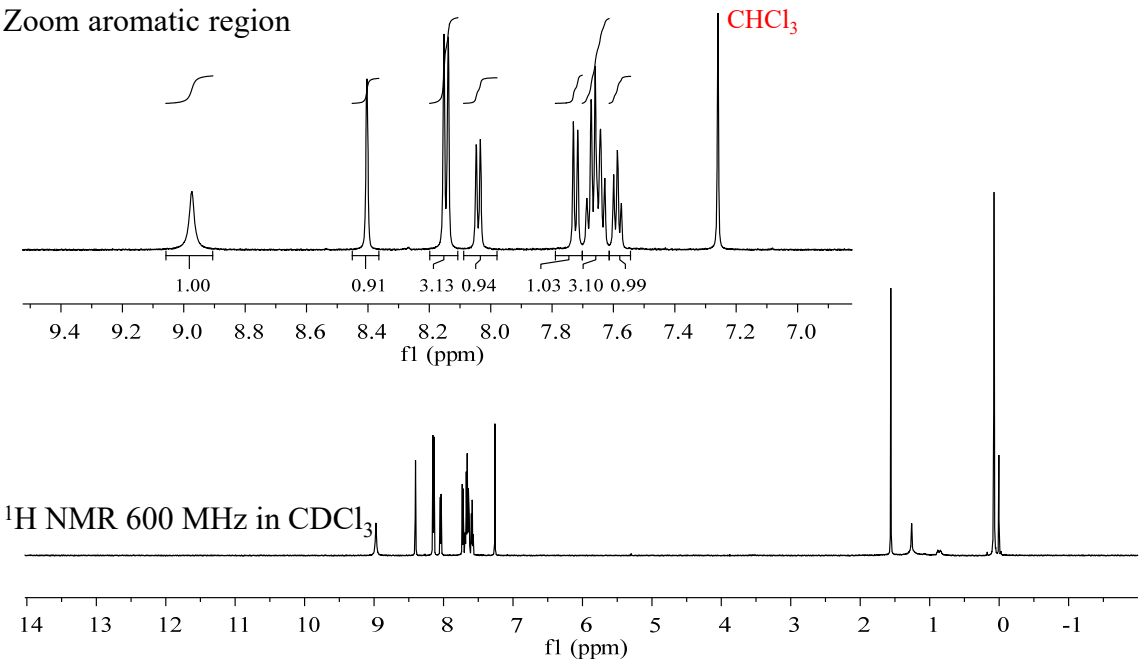


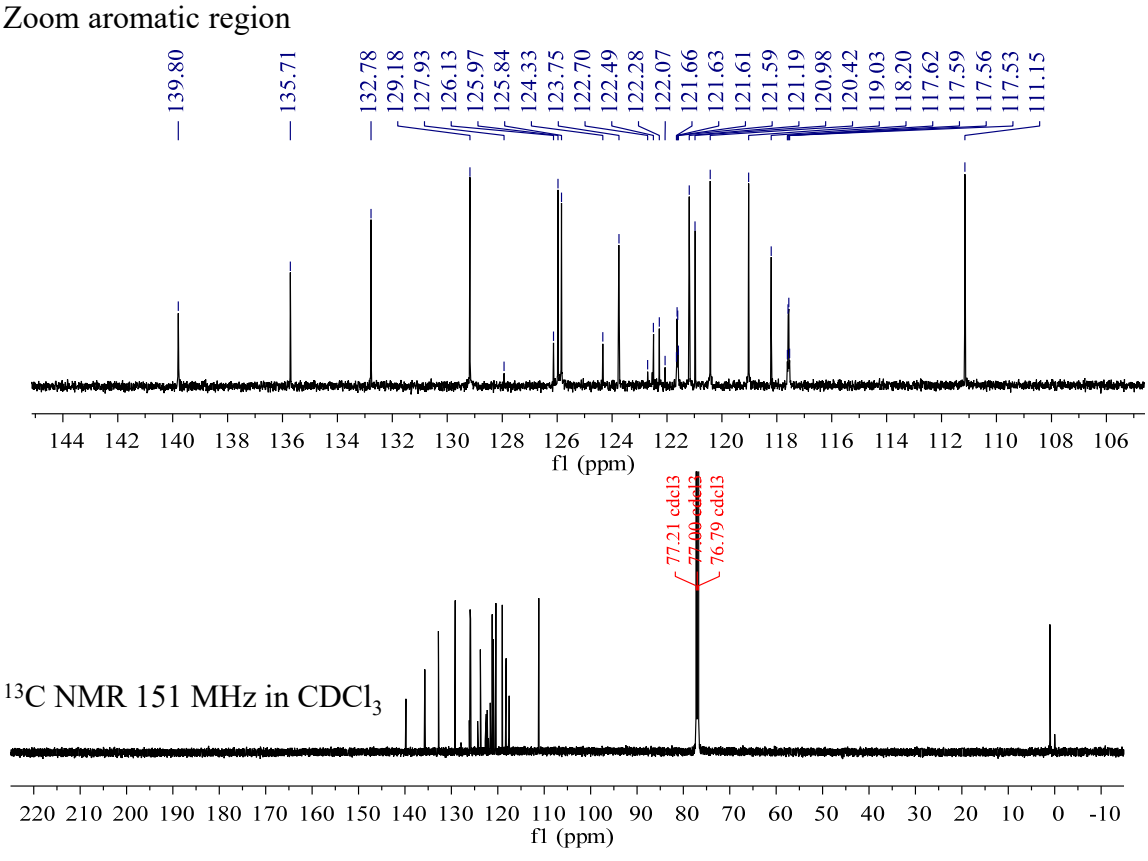
^{1}H NMR 600 MHz in $CDCl_3$

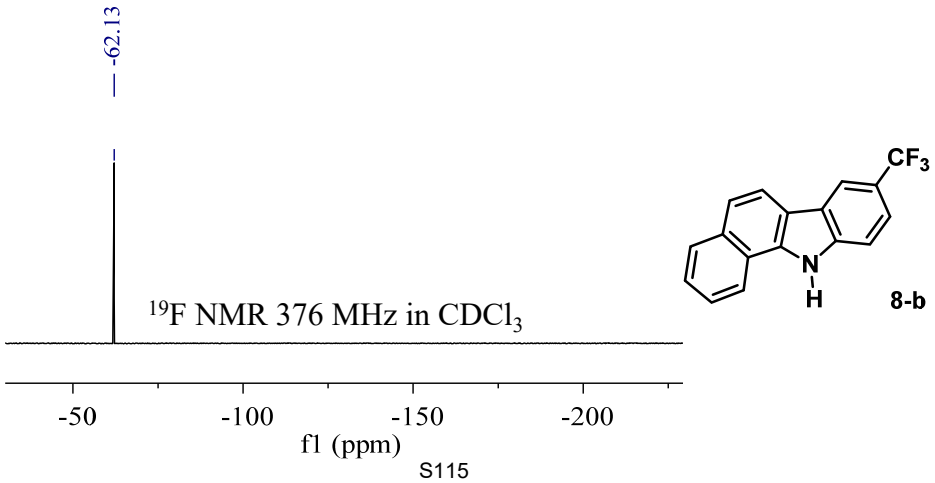


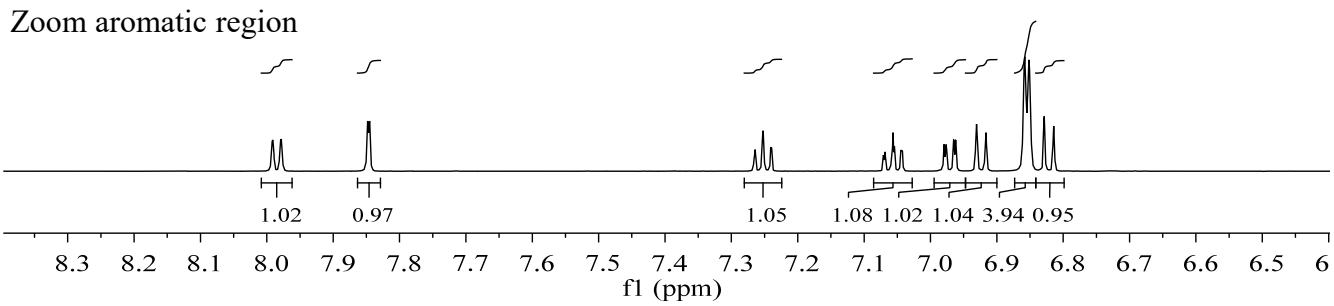
^{13}C NMR 151 MHz in $CDCl_3$

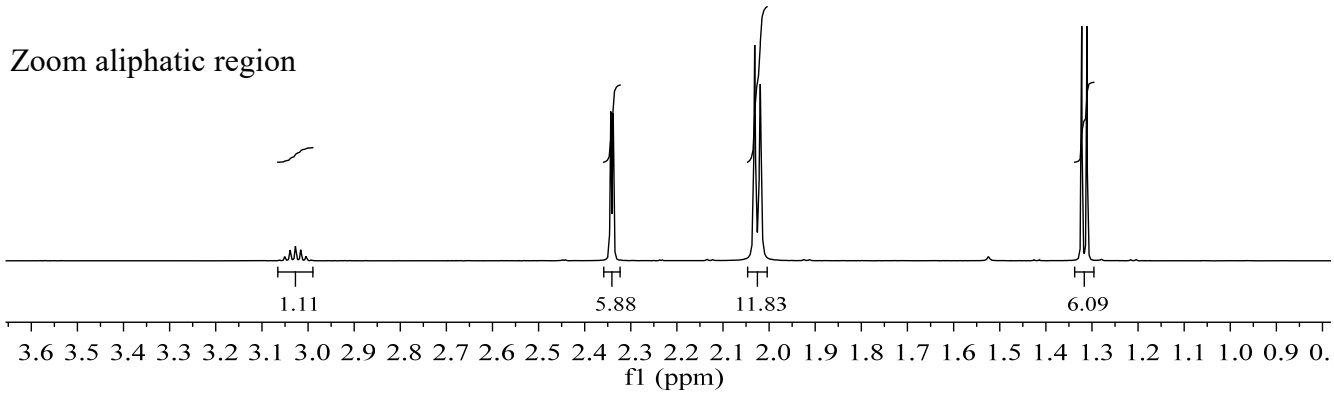


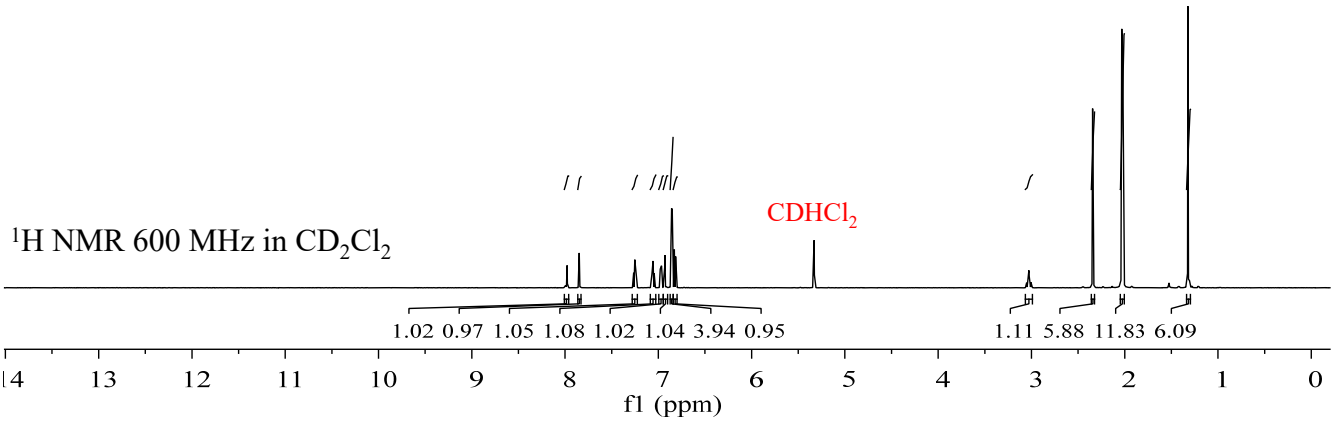

Zoom aromatic region
CHCl3
1.00
0.91
3.13 0.94
1.03 3.10 0.99
9.4 9.2 9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0
f1 (ppm)
1H NMR 600 MHz in CDCl3
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

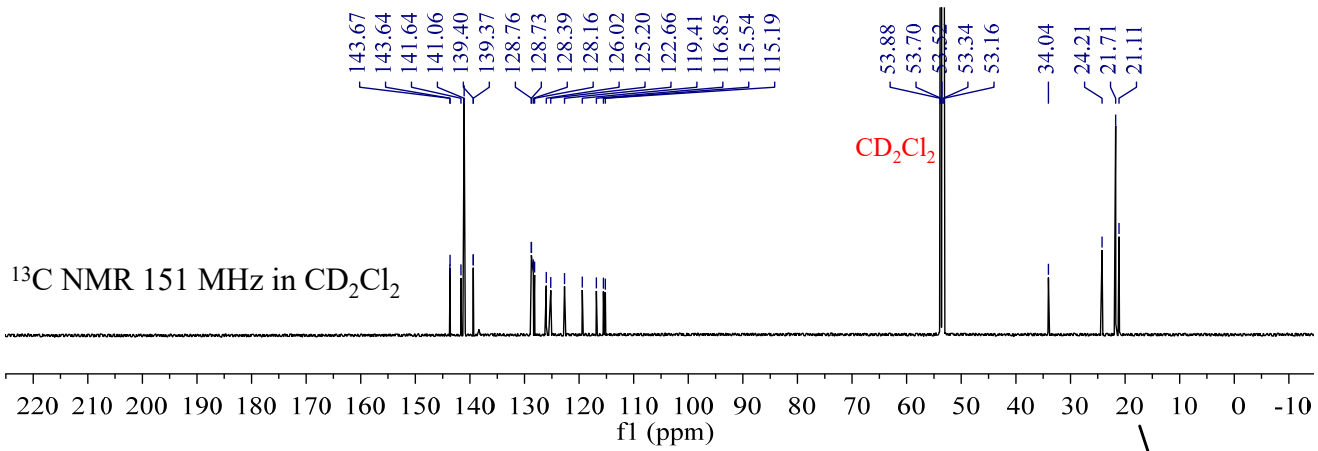

Zoom aromatic region
139.80
135.71
132.78
129.18
127.93
126.13
125.97
125.84
124.33
123.75
122.70
122.49
122.28
122.07
121.66
121.63
121.61
121.59
121.19
120.98
120.42
119.03
118.20
117.62
117.59
117.56
117.53
111.15
144 142 140 138 136 134 132 130 128 126 124 122 120 118 116 114 112 110 108 106
f1 (ppm)
77.21 cdcl3
77.00 cdcl3
76.79 cdcl3
13C NMR 151 MHz in CDCl3
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

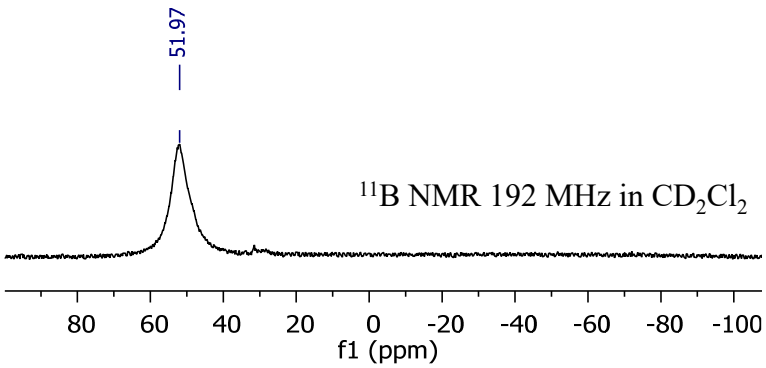

-62.13
19F NMR 376 MHz in CDCl3
-50 -100 -150 -200
f1 (ppm)
CF3
N
H
8-b

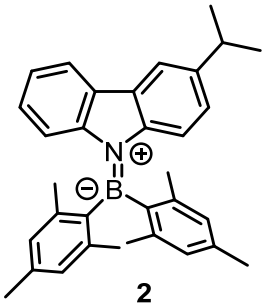

Zoom aromatic region
1.02
0.97
1.05
1.08 1.02 1.04 3.94 0.95
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6
f1 (ppm)


Zoom aliphatic region
1.11
5.88
11.83
6.09
3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8 2.7 2.6 2.5 2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 1.5 1.4 1.3 1.2 1.1 1.0 0.9 0.
f1 (ppm)


CDHCl2
1H NMR 600 MHz in CD2Cl2
1.02 0.97 1.05 1.08 1.02 1.04 3.94 0.95
1.11 5.88 11.83 6.09
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

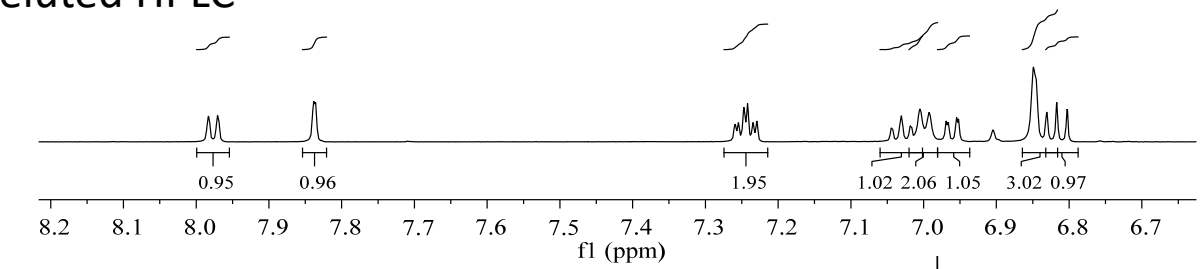

143.67
143.64
141.64
141.06
139.40
139.37
128.76
128.73
128.39
128.16
126.02
125.20
122.66
119.41
116.85
115.54
115.19
53.88
53.70
53.52
53.34
53.16
34.04
24.21
21.71
21.11
CD2Cl2
13C NMR 151 MHz in CD2Cl2
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

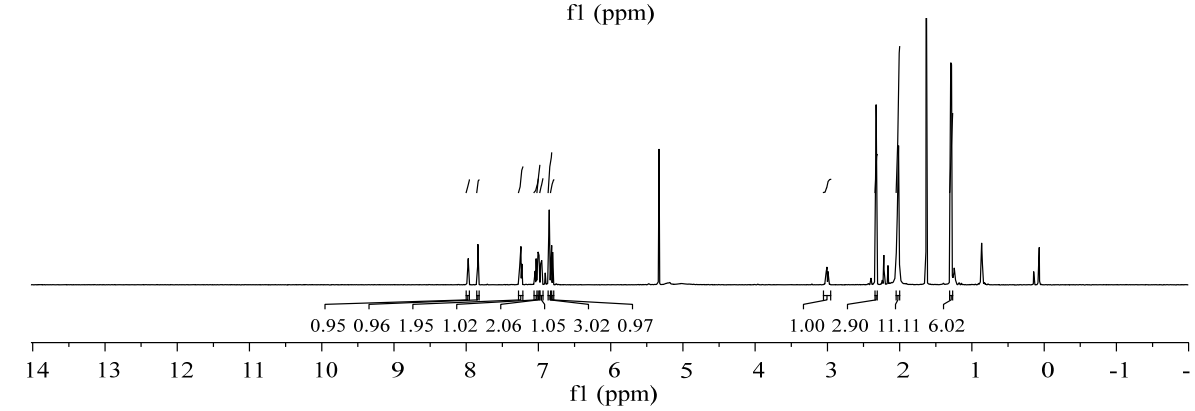

51.97
11B NMR 192 MHz in CD2Cl2
80 60 40 20 0 -20 -40 -60 -80 -100
f1 (ppm)

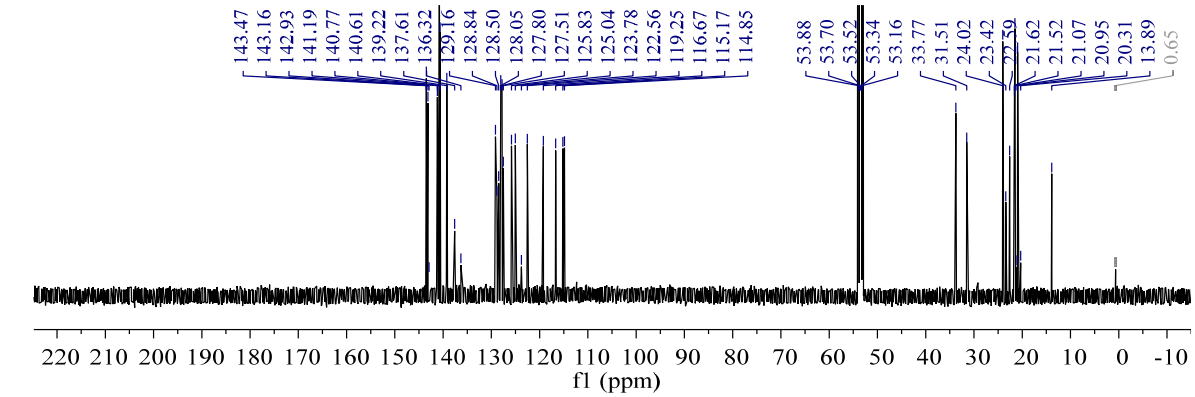

N
B

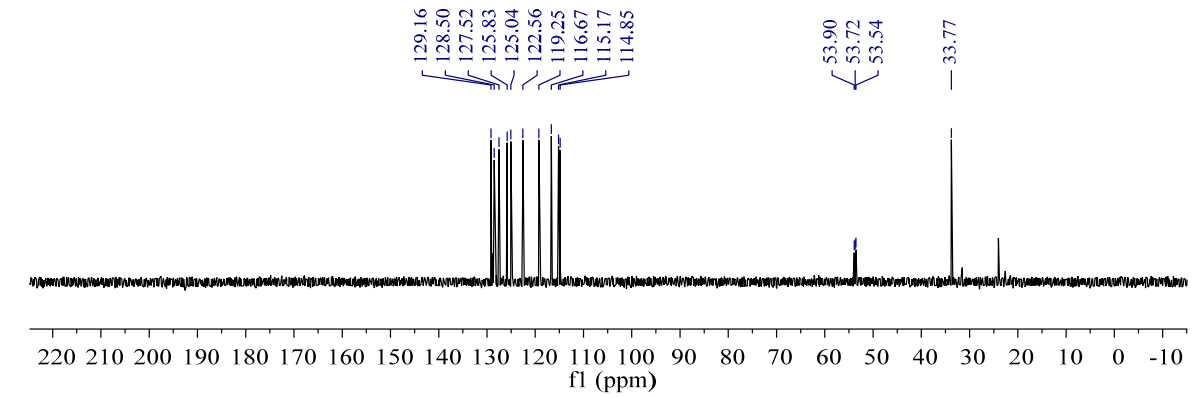
2

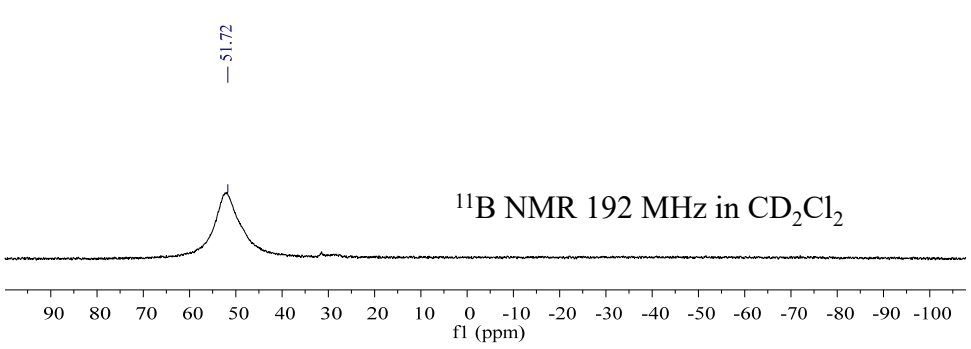
1° eluted HPLC

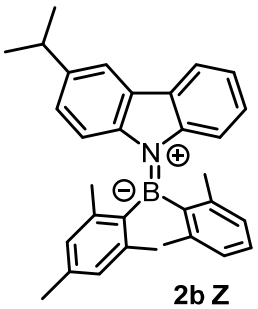






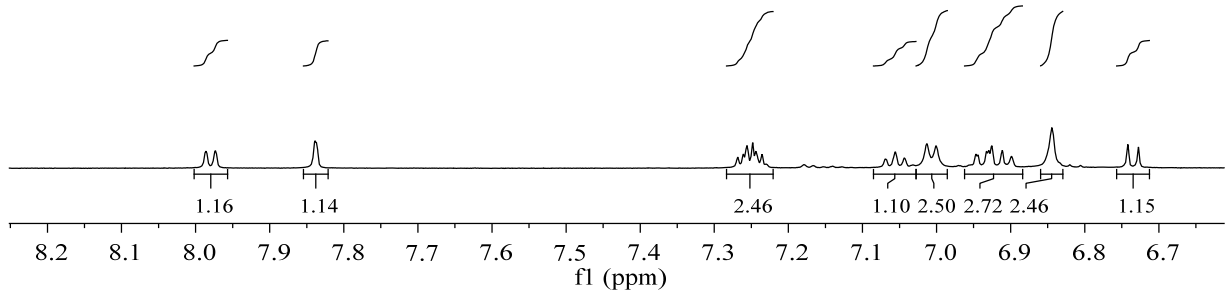


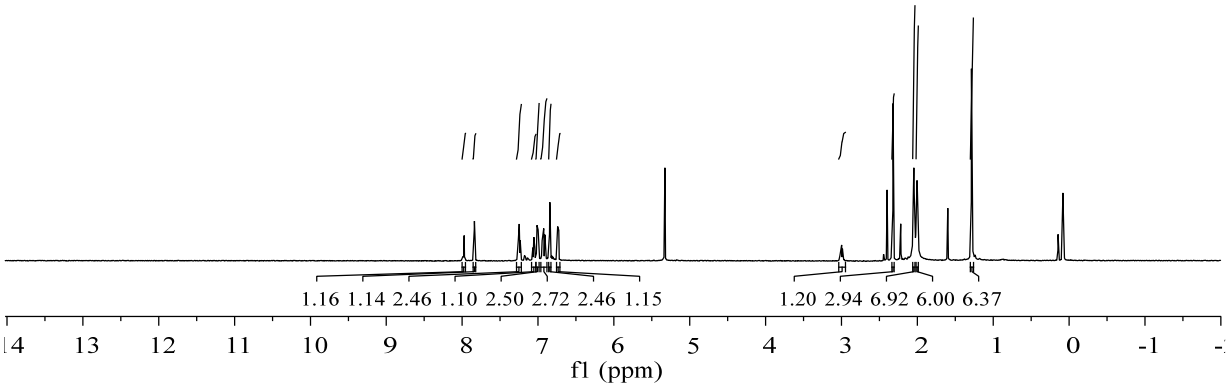


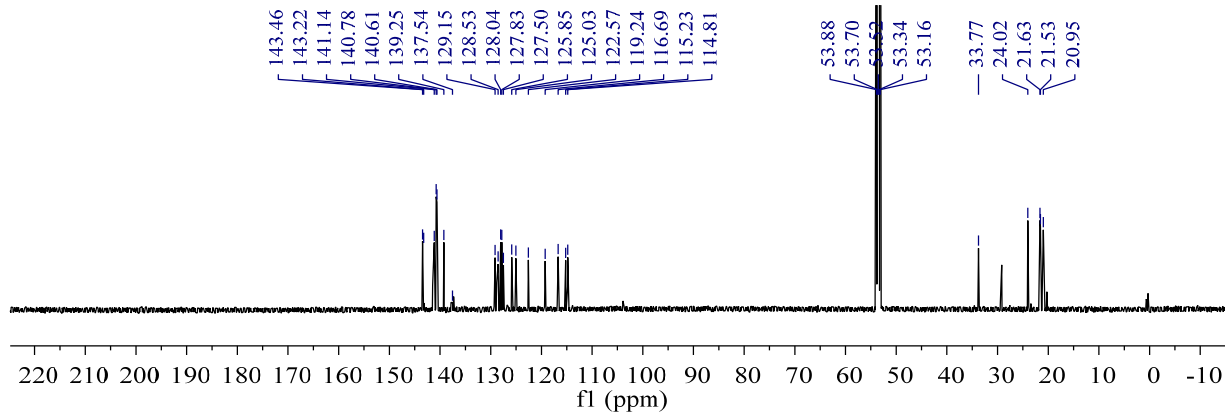


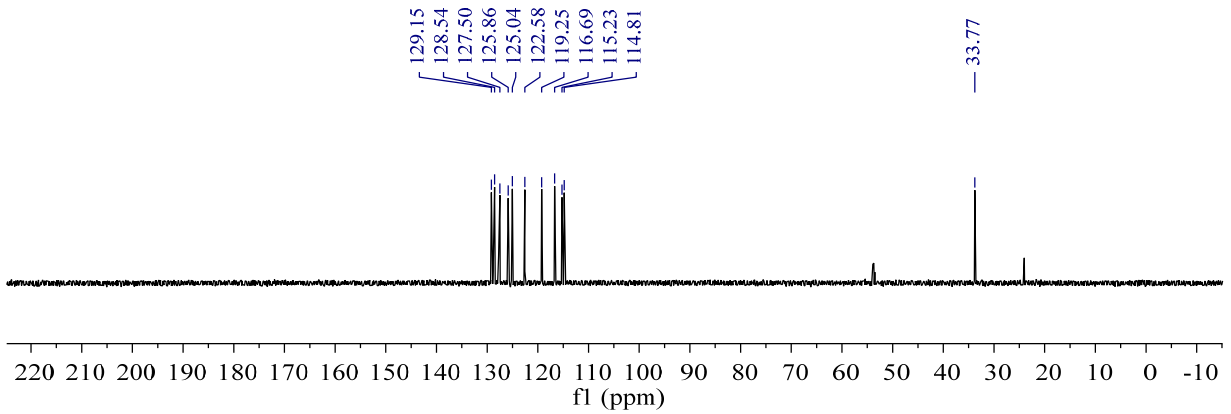
2b Z

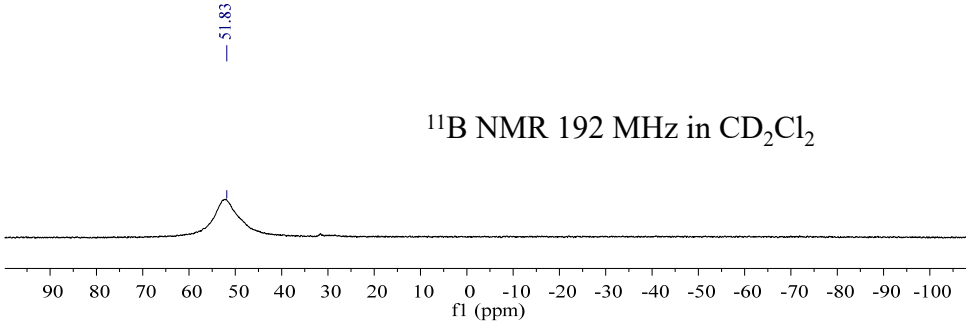
2° eluted HPLC



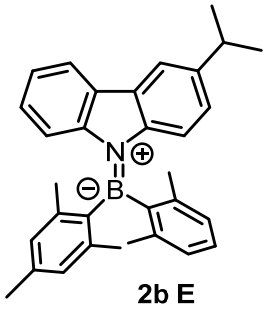






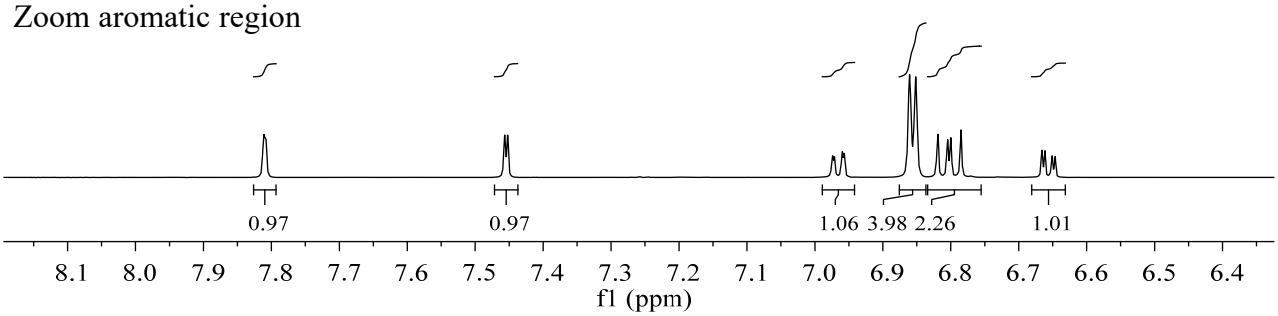


^{11}B NMR 192 MHz in CD_2Cl_2

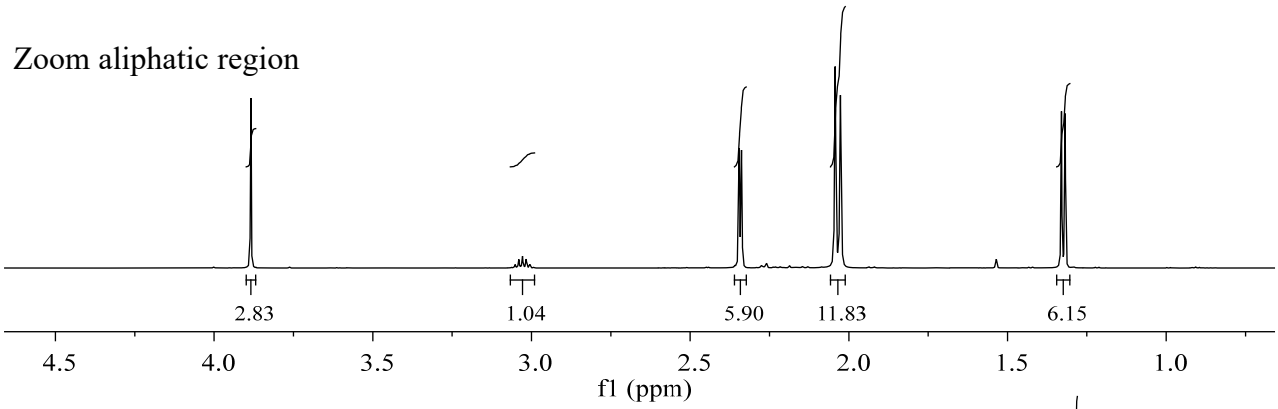


2b E

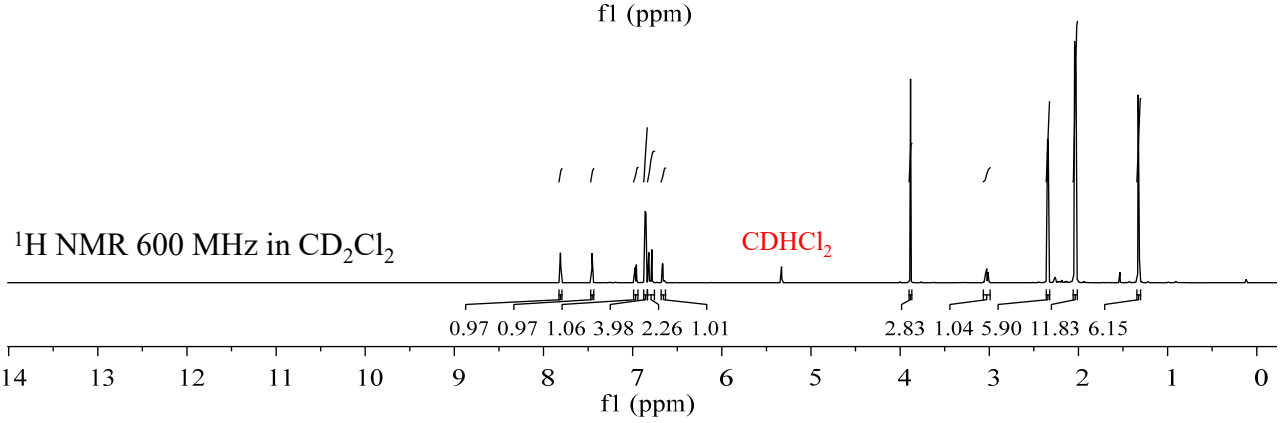
Zoom aromatic region



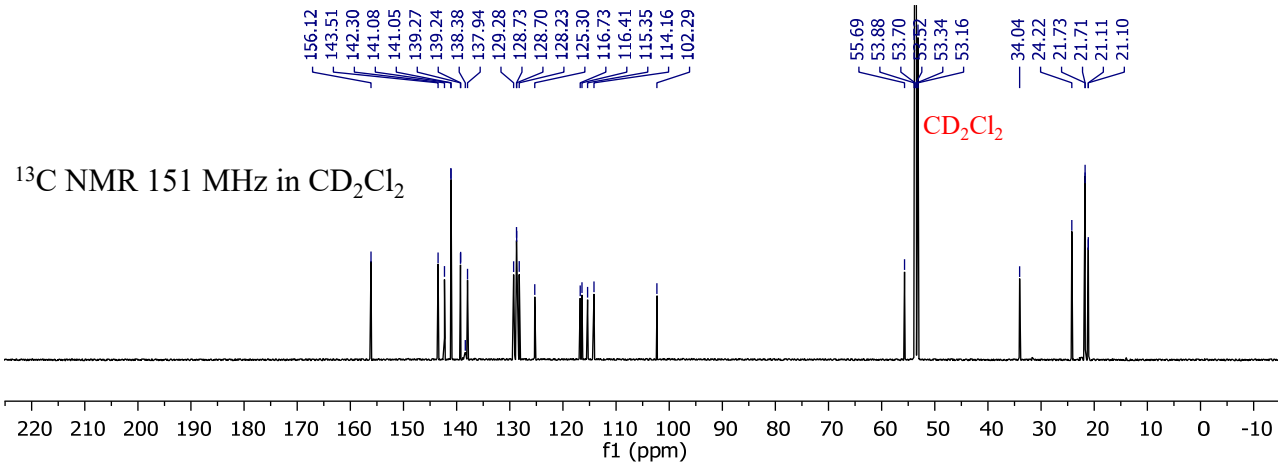
Zoom aliphatic region



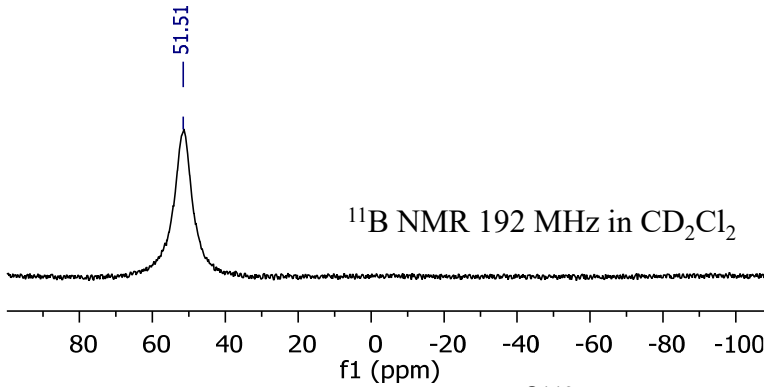
^{1}H NMR 600 MHz in CD_2Cl_2

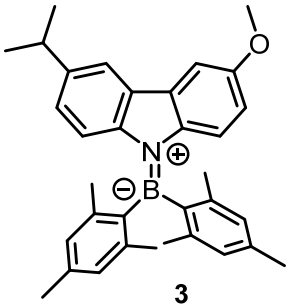


^{13}C NMR 151 MHz in CD_2Cl_2

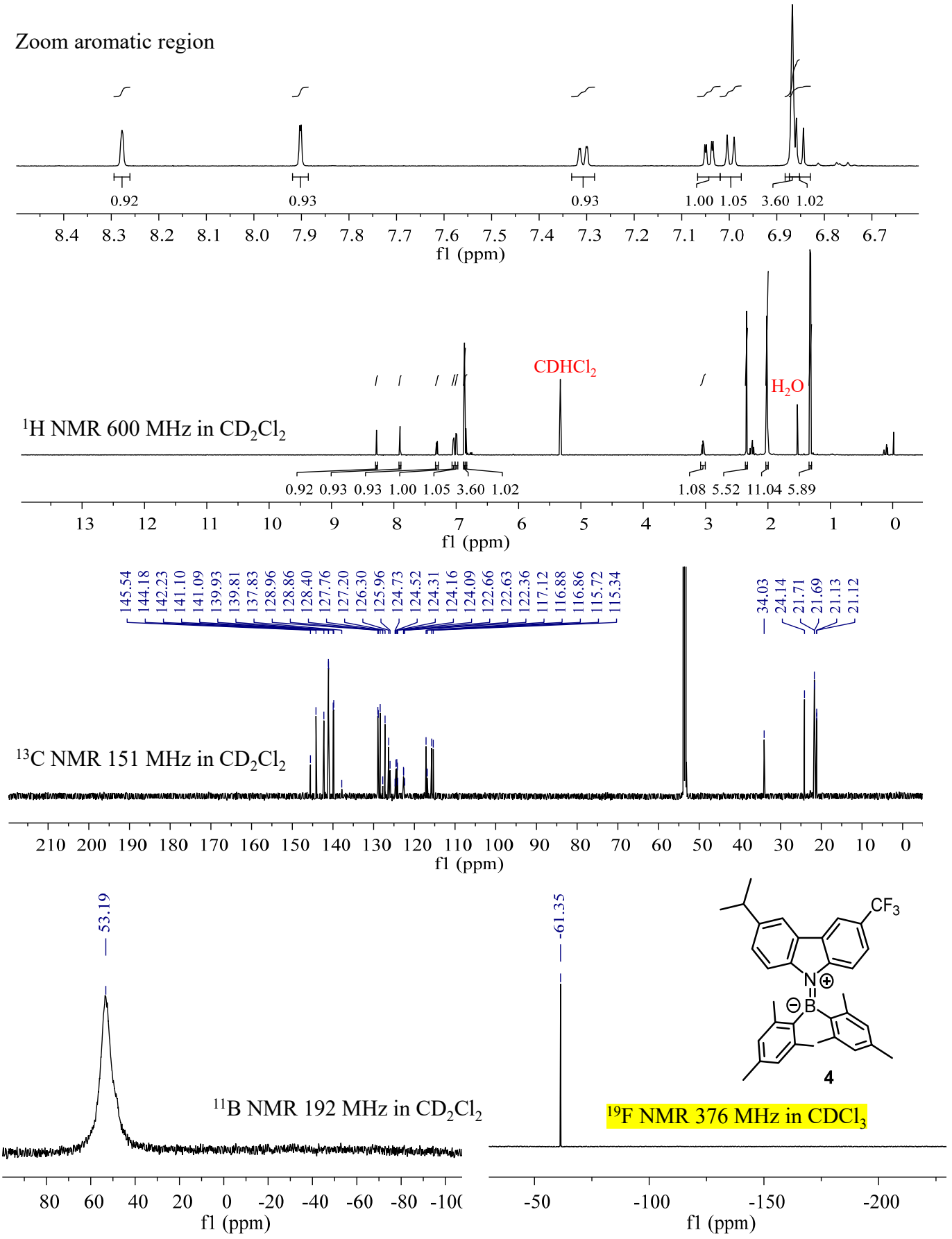


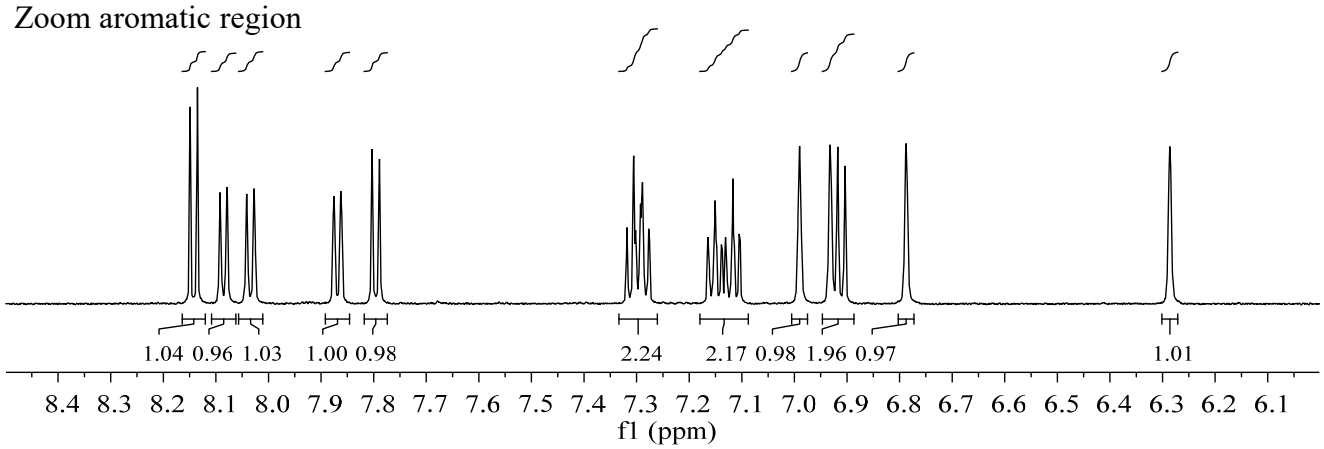
^{11}B NMR 192 MHz in CD_2Cl_2

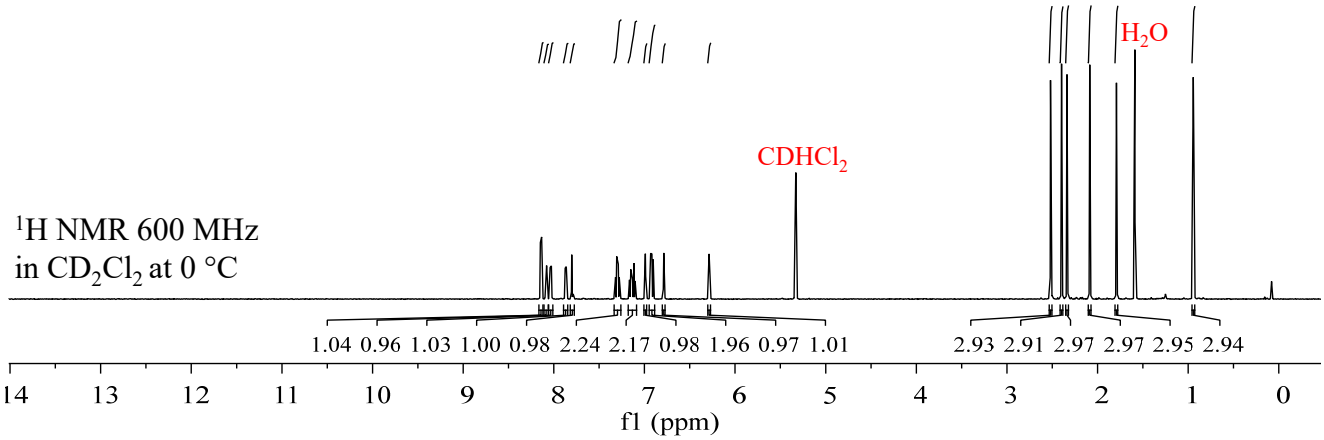


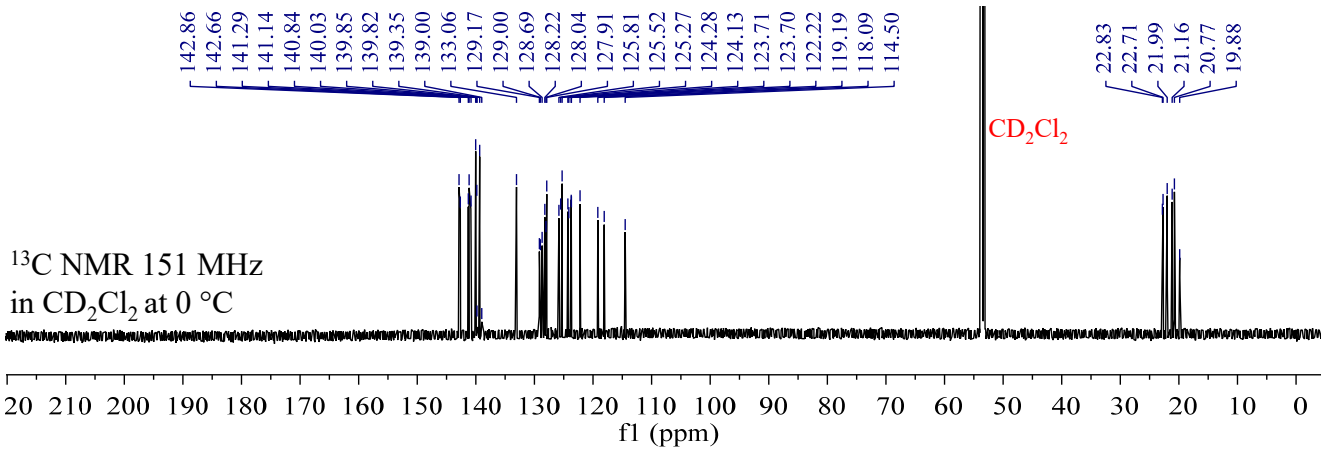


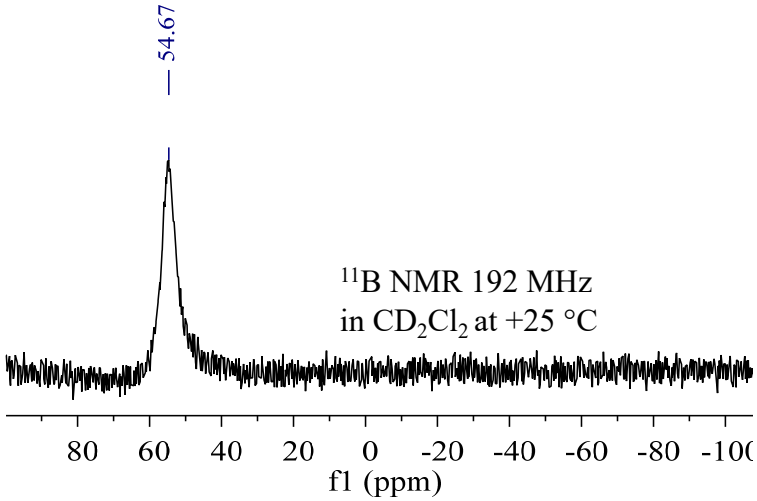
3

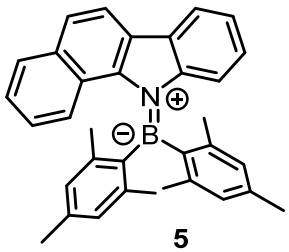

Zoom aromatic region
0.92
0.93
0.93
1.00 1.05
3.60 1.02
f1 (ppm)
CDHCl2
H2O
1H NMR 600 MHz in CD2Cl2
0.92 0.93 0.93 1.00 1.05 3.60 1.02
1.08 5.52 11.04 5.89
f1 (ppm)
13C NMR 151 MHz in CD2Cl2
f1 (ppm)
53.19
11B NMR 192 MHz in CD2Cl2
f1 (ppm)
-61.35
19F NMR 376 MHz in CDCl3
f1 (ppm)
CF3
4


Zoom aromatic region
1.04 0.96 1.03 1.00 0.98 2.24 2.17 0.98 1.96 0.97 1.01
f1 (ppm)


^{1}H NMR 600 MHz
in CD_2Cl_2 at 0 °C
$CDHCl_2$
H_2O
1.04 0.96 1.03 1.00 0.98 2.24 2.17 0.98 1.96 0.97 1.01
2.93 2.91 2.97 2.97 2.95 2.94
f1 (ppm)

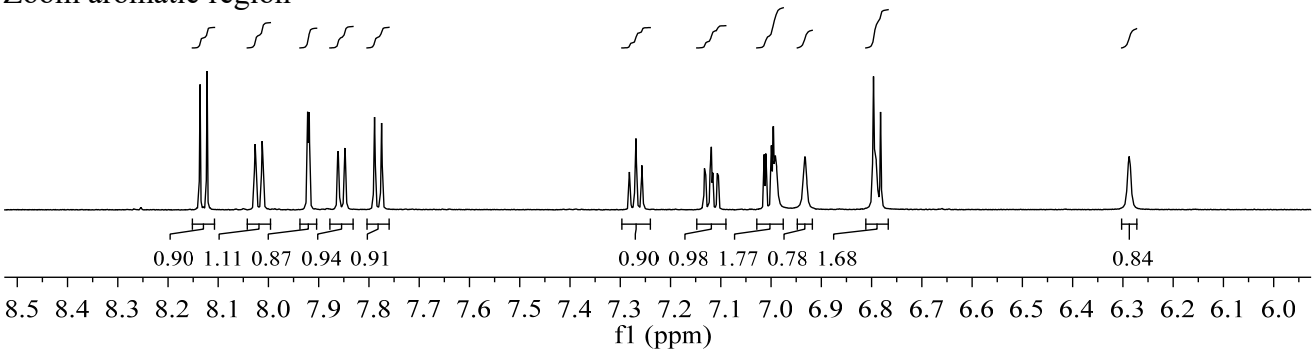

142.86 142.66 141.29 141.14 140.84 140.03 139.85 139.82 139.35 139.00 133.06 129.17 129.00 128.69 128.22 128.04 127.91 125.81 125.52 125.27 124.28 124.13 123.71 123.70 122.22 119.19 118.09 114.50
22.83 22.71 21.99 21.16 20.77 19.88
CD_2Cl_2
^{13}C NMR 151 MHz
in CD_2Cl_2 at 0 °C
f1 (ppm)


54.67
^{11}B NMR 192 MHz
in CD_2Cl_2 at +25 °C
f1 (ppm)

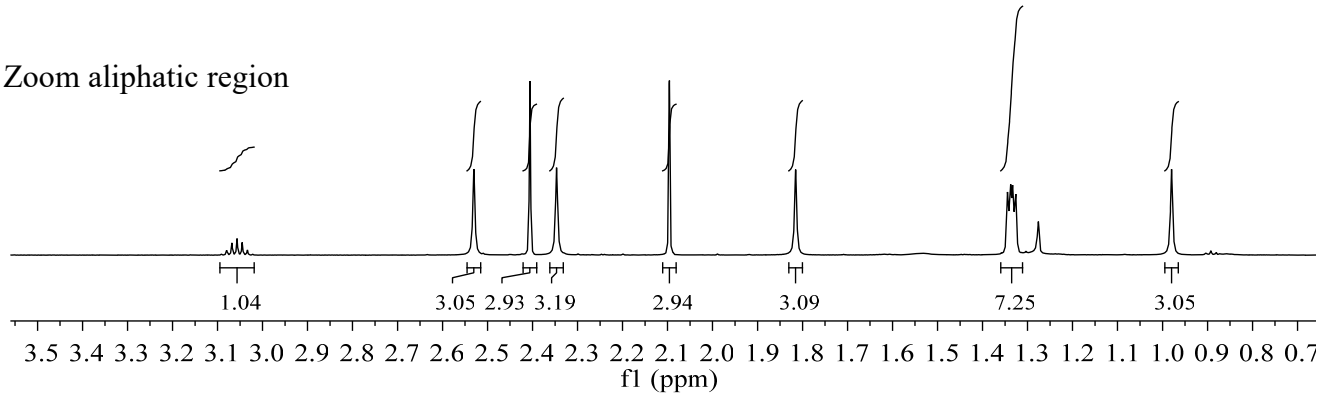

N
B

5

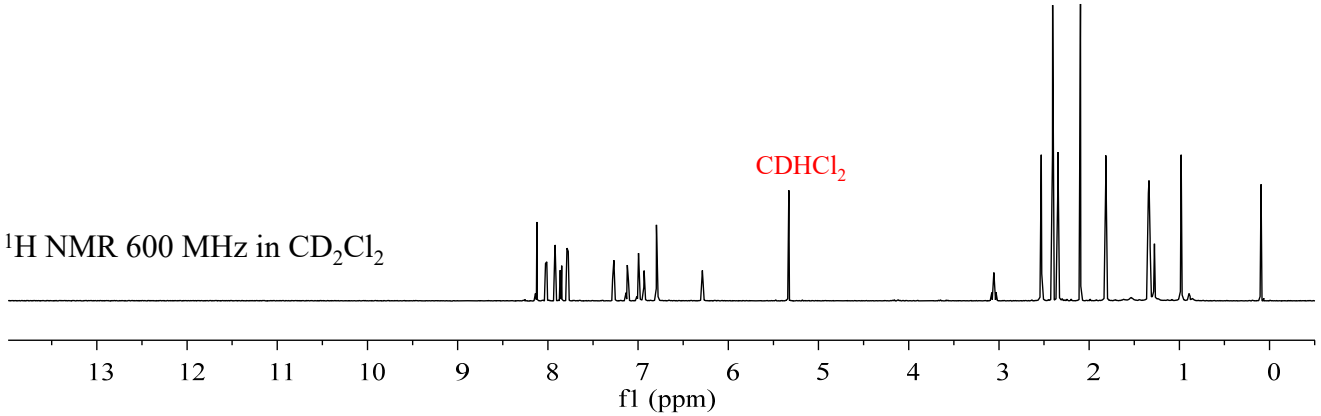
Zoom aromatic region



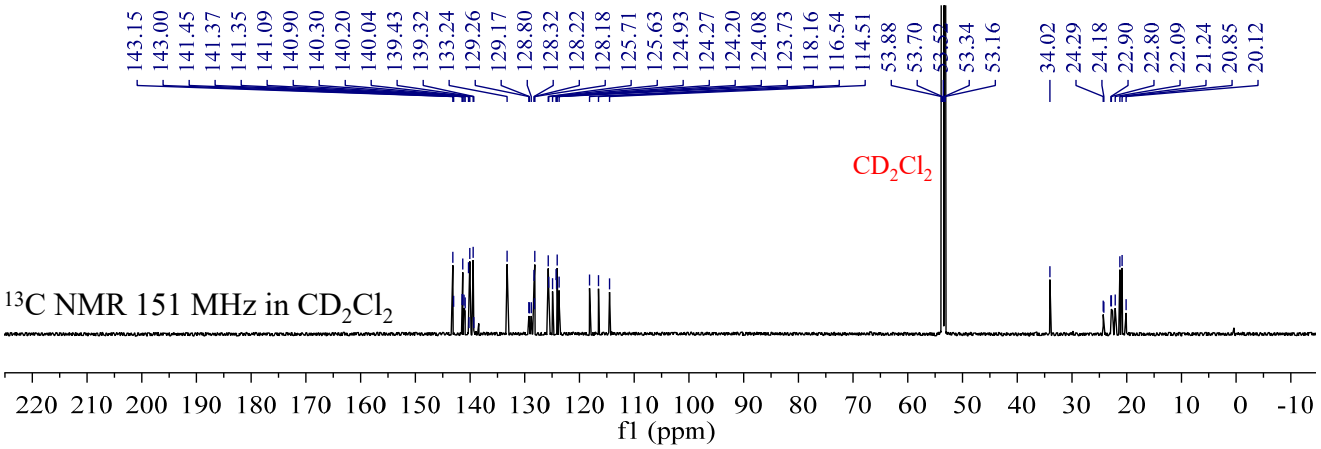
Zoom aliphatic region



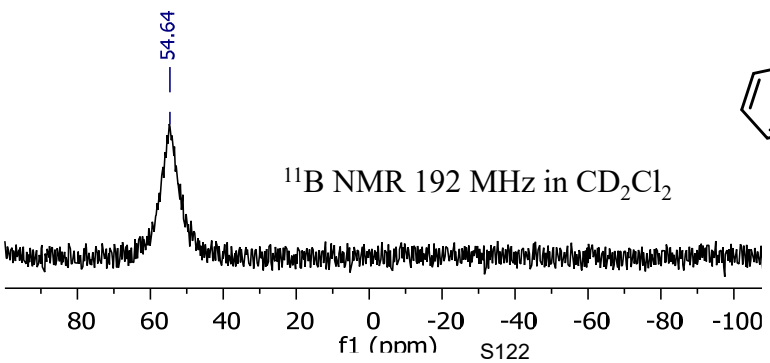
^{1}H NMR 600 MHz in CD_2Cl_2

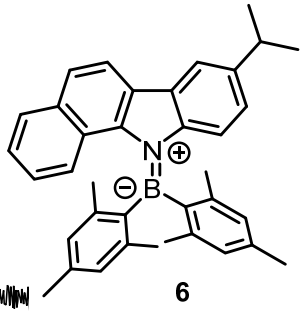


^{13}C NMR 151 MHz in CD_2Cl_2



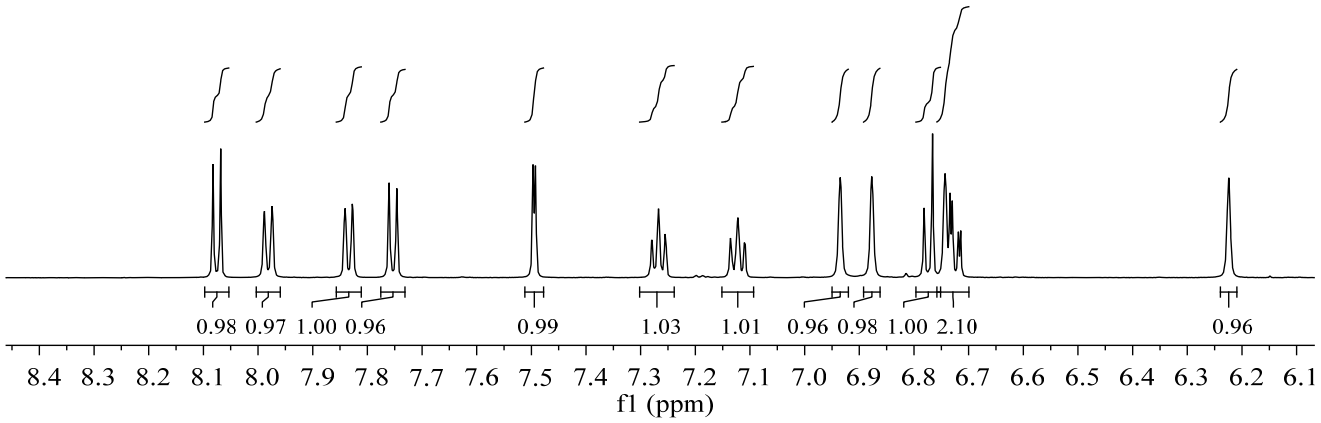
^{11}B NMR 192 MHz in CD_2Cl_2

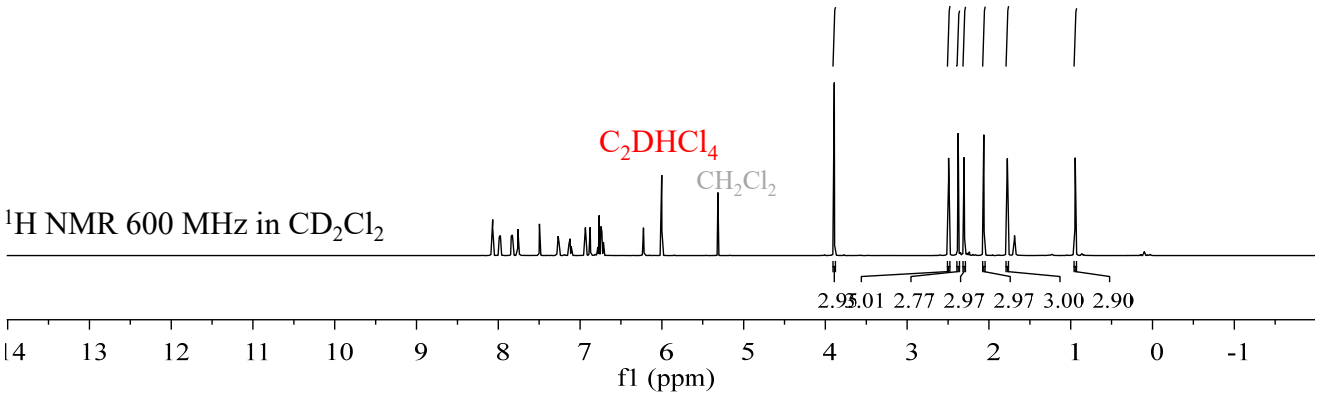


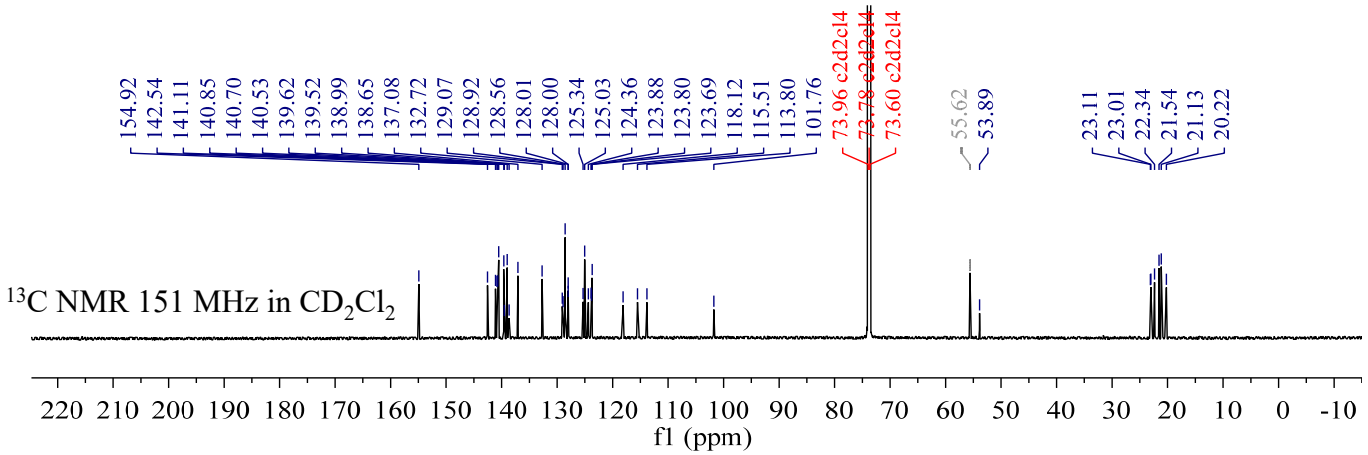


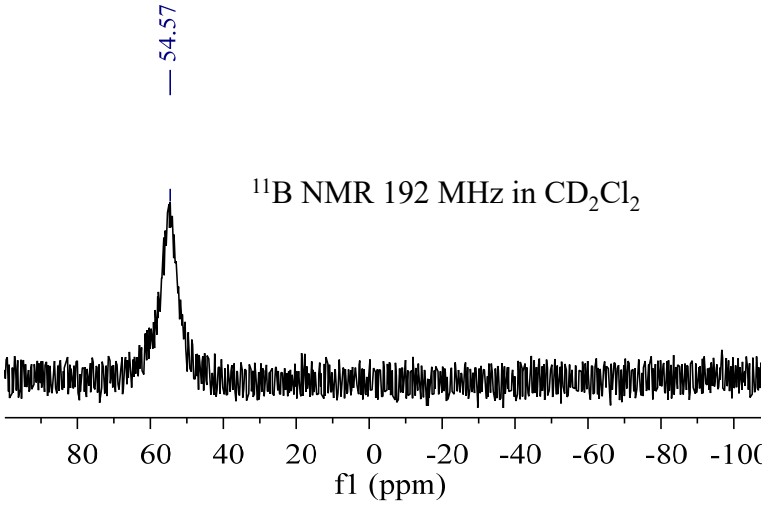
6

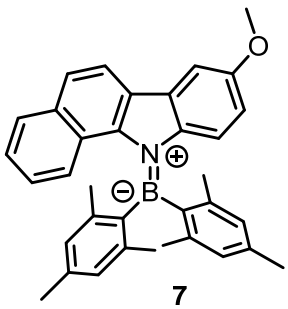
Zoom aromatic region





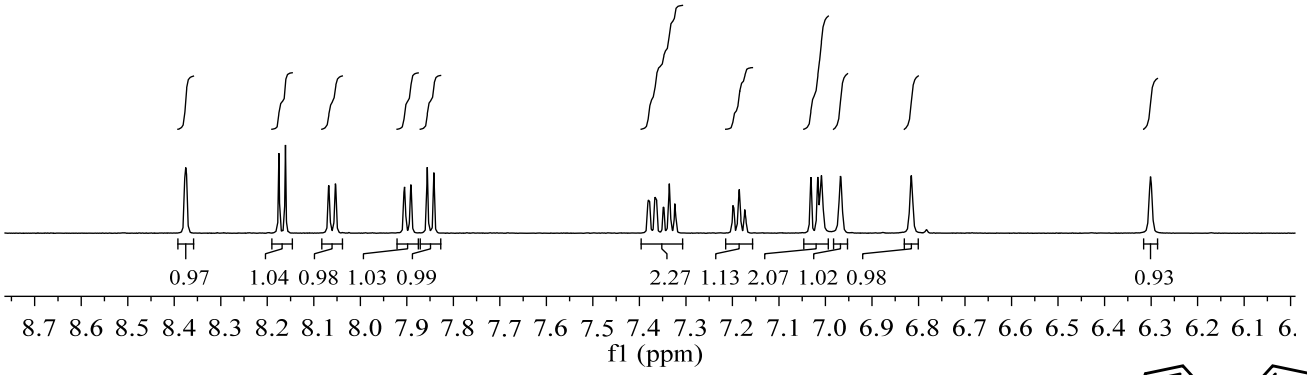


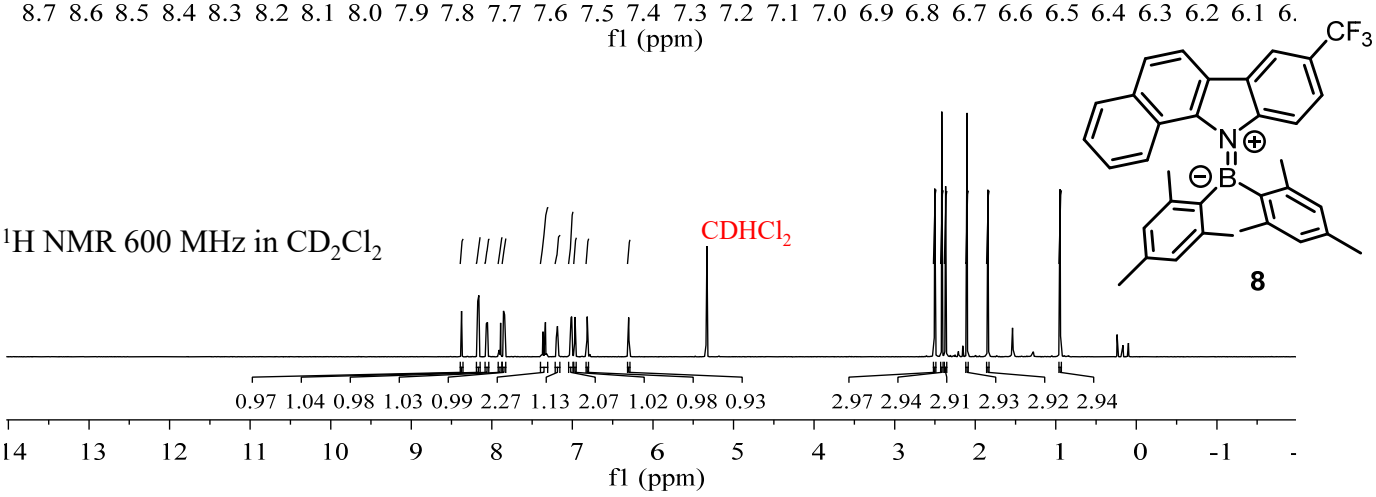


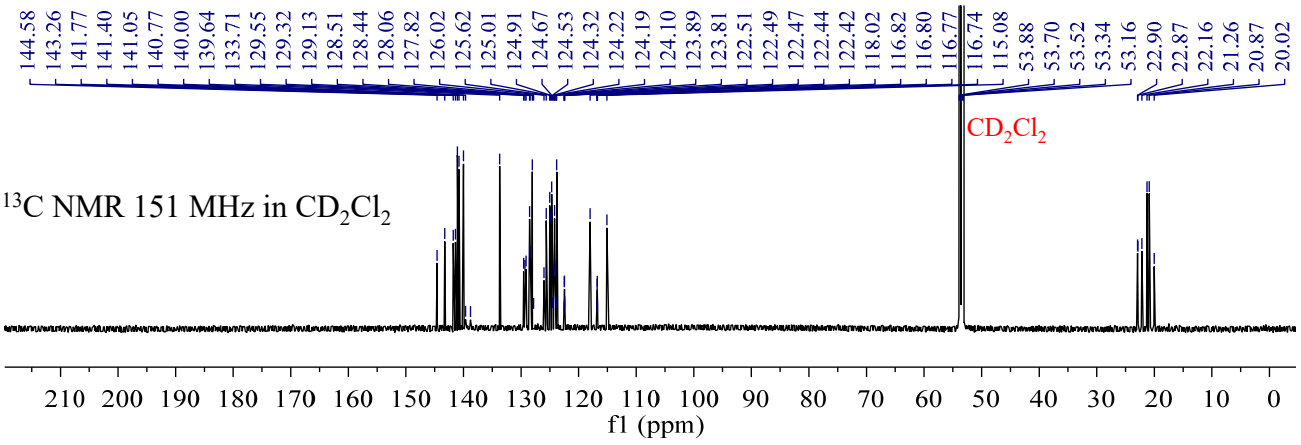


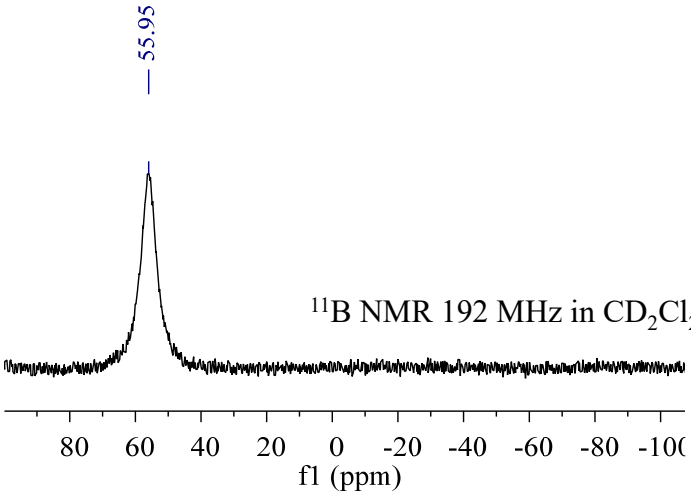
7

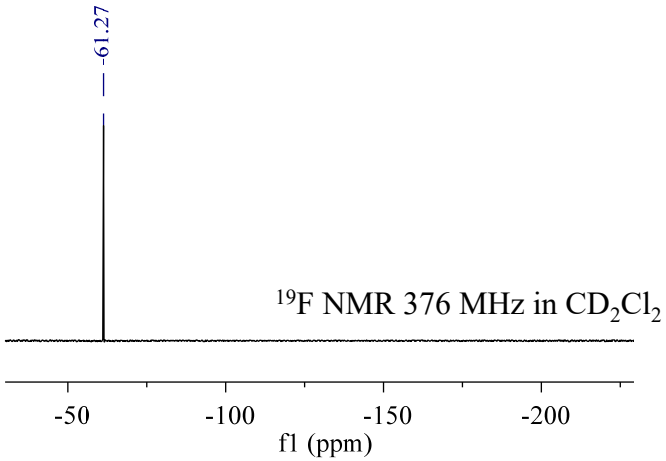
Zoom aromatic region











Compound 1 GS1

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1241.25757084 A.U. after 1 cycles
Lowest frequency = 27.6254

Zero-point correction= 0.515838
(Hartree/Particle)
Thermal correction to Energy= 0.546101
Thermal correction to Enthalpy= 0.547045
Thermal correction to Gibbs Free Energy= 0.453089
Sum of electronic and zero-point Energies= -1240.741733
Sum of electronic and thermal Energies= -1240.711470
Sum of electronic and thermal Enthalpies= -1240.710526
Sum of electronic and thermal Free Energies= -1240.804482

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000056	-0.346726	0.000005
2	6	0	-0.929597	-2.390363	-2.084873
3	1	0	-0.793081	-1.492298	-2.694729
4	1	0	0.065465	-2.761524	-1.831419
5	1	0	-1.419597	-3.137539	-2.712131
6	6	0	0.930319	-2.390014	2.084950
7	1	0	1.420503	-3.137082	2.712192
8	1	0	0.793642	-1.491973	2.694805
9	1	0	-0.064675	-2.761386	1.831540
10	6	0	1.926674	0.117525	-2.287144
11	1	0	0.868748	0.165053	-2.549784
12	1	0	2.219767	1.119525	-1.958873
13	1	0	2.485039	-0.105437	-3.198781
14	6	0	5.038902	-3.430241	-0.599630
15	1	0	5.488241	-3.690041	0.361898
16	1	0	4.827068	-4.368475	-1.124541
17	1	0	5.782715	-2.887793	-1.187764
18	6	0	3.780268	-2.617677	-0.417902
19	6	0	2.947837	-2.815602	0.683281
20	1	0	3.231299	-3.545893	1.435845
21	6	0	1.756007	-2.107704	0.847581
22	6	0	1.372322	-1.131222	-0.105476
23	6	0	2.224247	-0.915098	-1.218439
24	6	0	3.394807	-1.664141	-1.357795
25	1	0	4.025564	-1.492018	-2.225446
26	6	0	-2.223988	-0.915687	1.218439
27	6	0	-3.394359	-1.665038	1.357791
28	1	0	-4.025170	-1.493065	2.225430
29	6	0	-3.779552	-2.618688	0.417913
30	6	0	-2.947040	-2.816426	-0.683248
31	1	0	-3.230293	-3.546819	-1.435794
32	6	0	-1.755395	-2.108226	-0.847539
33	6	0	-1.371992	-1.131604	0.105497
34	6	0	-1.926710	0.117026	2.287141
35	1	0	-2.220013	1.118953	1.958840
36	1	0	-2.485073	-0.106050	3.198752
37	1	0	-0.868809	0.164796	2.549840
38	6	0	-5.037986	-3.431573	0.599603
39	1	0	-5.487559	-3.690964	-0.361930

40	1	0	-4.825836	-4.370038	1.123969
41	1	0	-5.781726	-2.889551	1.188220
42	7	0	-0.000153	1.103615	-0.000003
43	6	0	-1.044553	1.959517	-0.453543
44	6	0	1.044009	1.959820	0.453519
45	6	0	-2.264702	1.639140	-1.052680
46	6	0	-0.661425	3.308494	-0.294513
47	6	0	2.264256	1.639795	1.052647
48	6	0	0.660487	3.308685	0.294497
49	6	0	-3.099148	2.680464	-1.449265
50	1	0	-2.567882	0.614117	-1.203699
51	6	0	-1.509351	4.340929	-0.701825
52	6	0	3.098402	2.681360	1.449229
53	1	0	2.567731	0.614860	1.203663
54	6	0	1.508116	4.341366	0.701808
55	6	0	-2.733186	4.020794	-1.274156
56	1	0	-4.052100	2.441837	-1.907887
57	1	0	-1.211897	5.376269	-0.577942
58	6	0	2.732048	4.021584	1.274128
59	1	0	4.051426	2.443009	1.907845
60	1	0	1.210362	5.376619	0.577929
61	1	0	-3.404694	4.808542	-1.595727
62	1	0	3.403329	4.809526	1.595698

Compound 1 1RF-C-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1241.18493043 A.U. after 1 cycles
Lowest frequency = -44.2678

Zero-point correction= 0.515645
(Hartree/Particle)
Thermal correction to Energy= 0.544452
Thermal correction to Enthalpy= 0.545397
Thermal correction to Gibbs Free Energy= 0.456369
Sum of electronic and zero-point Energies= -1240.669285
Sum of electronic and thermal Energies= -1240.640478
Sum of electronic and thermal Enthalpies= -1240.639534
Sum of electronic and thermal Free Energies= -1240.728561

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.466840	-2.109991	-0.243714
2	6	0	1.317798	-2.595524	-0.980619
3	6	0	0.174606	-1.989754	-0.409128
4	7	0	0.586823	-0.928252	0.489609
5	6	0	1.968879	-1.209491	0.722021
6	6	0	2.722439	-0.953110	1.860439
7	6	0	4.036591	-1.415889	1.922517
8	6	0	3.788035	-2.553253	-0.192764
9	6	0	1.199449	-3.615942	-1.923606
10	6	0	-1.187609	-3.563823	-1.606357
11	6	0	-1.083107	-2.528173	-0.677172
12	1	0	2.287947	-0.449319	2.708695
13	1	0	4.628109	-1.211695	2.807952
14	1	0	4.168192	-3.237100	-0.943346

15	1	0	2.086322	-4.061968	-2.359904
16	1	0	-2.167271	-3.982529	-1.808127
17	1	0	-1.966204	-2.183040	-0.167702
18	5	0	-0.151032	0.361653	0.535429
19	6	0	-1.732761	0.172610	0.470951
20	6	0	-2.495942	0.157759	-0.713671
21	6	0	-2.401314	-0.017792	1.703121
22	6	0	-3.880841	-0.024963	-0.647890
23	6	0	-3.784254	-0.197111	1.731576
24	6	0	-4.548080	-0.200306	0.561897
25	1	0	-4.452185	-0.033576	-1.572659
26	1	0	-4.278029	-0.337886	2.689319
27	6	0	0.475797	1.834164	0.391290
28	6	0	1.840591	2.248797	0.563438
29	6	0	-0.310630	2.784282	-0.352277
30	6	0	2.425783	3.166690	-0.302861
31	6	0	0.312820	3.701074	-1.208145
32	6	0	1.692839	3.838240	-1.281682
33	1	0	3.472839	3.419059	-0.157928
34	1	0	-0.317296	4.359893	-1.799122
35	6	0	-1.630740	-0.025979	3.007061
36	1	0	-0.908871	-0.848059	3.038761
37	1	0	-1.069179	0.903970	3.147023
38	1	0	-2.302035	-0.138783	3.860704
39	6	0	-1.870835	0.292610	-2.087201
40	1	0	-0.843629	0.655308	-2.047979
41	1	0	-1.856565	-0.673369	-2.600262
42	1	0	-2.445103	0.982613	-2.712572
43	6	0	-6.048052	-0.364995	0.615872
44	1	0	-6.451152	-0.665747	-0.353640
45	1	0	-6.340544	-1.117790	1.352809
46	1	0	-6.537499	0.573287	0.899416
47	6	0	-1.800909	3.030178	-0.173408
48	1	0	-2.402293	2.726277	-1.031077
49	1	0	-2.211303	2.554720	0.710854
50	1	0	-1.930039	4.111243	-0.060217
51	6	0	2.638003	1.973827	1.821957
52	1	0	2.045355	1.468143	2.578328
53	1	0	3.557800	1.416603	1.648636
54	1	0	2.916586	2.944957	2.244265
55	6	0	2.353178	4.750185	-2.281038
56	1	0	1.666607	5.522728	-2.634674
57	1	0	3.233844	5.239689	-1.857440
58	1	0	2.687616	4.182209	-3.156503
59	6	0	4.584699	-2.170696	0.881680
60	1	0	5.609220	-2.518363	0.948481
61	6	0	-0.065741	-4.084858	-2.255342
62	1	0	-0.179023	-4.884567	-2.978161

Compound 1 1RF-N-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1241.15830093 A.U. after 1 cycles
Lowest frequency = -68.8685

Zero-point correction= 0.516310
(Hartree/Particle)
Thermal correction to Energy= 0.544409
Thermal correction to Enthalpy= 0.545353

Thermal correction to Gibbs Free Energy= 0.459050
Sum of electronic and zero-point Energies= -1240.641991
Sum of electronic and thermal Energies= -1240.613892
Sum of electronic and thermal Enthalpies= -1240.612948
Sum of electronic and thermal Free Energies= -1240.699251

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.000001	0.820932	0.000000
2	6	0	-5.729280	1.740767	-0.122326
3	1	0	-6.309329	1.141662	-0.828287
4	1	0	-5.950304	1.363031	0.882421
5	1	0	-6.086161	2.772276	-0.168968
6	6	0	-4.253719	1.650944	-0.403804
7	6	0	-3.683660	0.520632	-0.985066
8	1	0	-4.330442	-0.266277	-1.361723
9	6	0	-1.392155	1.357665	-0.599977
10	6	0	-3.398405	2.731789	-0.205189
11	1	0	-3.821112	3.709107	0.012216
12	6	0	3.398407	2.731787	0.205189
13	1	0	3.821114	3.709105	-0.012216
14	6	0	4.253721	1.650942	0.403804
15	6	0	3.683661	0.520630	0.985066
16	1	0	4.330443	-0.266279	1.361722
17	6	0	1.392156	1.357664	0.599977
18	6	0	5.729282	1.740764	0.122325
19	1	0	6.309332	1.141670	0.828295
20	1	0	5.950308	1.363015	-0.882416
21	1	0	6.086161	2.772275	0.168954
22	6	0	2.020217	2.635146	0.396993
23	6	0	-2.306034	0.374695	-1.138051
24	6	0	-1.890181	-0.777568	-2.033423
25	1	0	-0.888977	-0.658832	-2.437668
26	1	0	-1.952870	-1.752242	-1.544739
27	1	0	-2.582681	-0.800141	-2.880296
28	6	0	1.335049	3.955631	0.662237
29	1	0	1.915594	4.458750	1.442096
30	1	0	1.308922	4.632731	-0.194063
31	1	0	0.335421	3.820802	1.055553
32	6	0	2.306036	0.374694	1.138050
33	6	0	1.890182	-0.777569	2.033422
34	1	0	0.888978	-0.658833	2.437667
35	1	0	1.952871	-1.752244	1.544737
36	1	0	2.582682	-0.800143	2.880295
37	6	0	-2.020215	2.635147	-0.396993
38	6	0	-1.335046	3.955632	-0.662237
39	1	0	-1.308919	4.632732	0.194063
40	1	0	-0.335418	3.820803	-1.055553
41	1	0	-1.915592	4.458752	-1.442096
42	7	0	0.000000	-0.702440	0.000000
43	6	0	0.838490	-1.533935	-0.748334
44	6	0	-0.838491	-1.533934	0.748334
45	6	0	0.533822	-2.893913	-0.487261
46	6	0	1.816036	-1.186947	-1.686693
47	6	0	-0.533825	-2.893912	0.487261
48	6	0	1.229282	-3.906796	-1.155989
49	6	0	2.493993	-2.210886	-2.337493

50	1	0	2.047154	-0.150638	-1.899663
51	6	0	-1.229286	-3.906794	1.155990
52	1	0	1.001852	-4.949344	-0.961117
53	1	0	3.257555	-1.958889	-3.065128
54	6	0	-2.209662	-3.560708	2.076042
55	1	0	-1.001858	-4.949342	0.961118
56	1	0	-2.755577	-4.334879	2.602870
57	6	0	2.209658	-3.560711	-2.076041
58	1	0	2.755572	-4.334883	-2.602869
59	6	0	-2.493995	-2.210882	2.337494
60	1	0	-3.257557	-1.958884	3.065128
61	6	0	-1.816037	-1.186944	1.686693
62	1	0	-2.047153	-0.150635	1.899663

Compound 1 2RF-CC-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1241.23979905 A.U. after 1 cycles
Lowest frequency = -60.0680

Zero-point correction= 0.516215
(Hartree/Particle)
Thermal correction to Energy= 0.545376
Thermal correction to Enthalpy= 0.546320
Thermal correction to Gibbs Free Energy= 0.455472
Sum of electronic and zero-point Energies= -1240.723584
Sum of electronic and thermal Energies= -1240.694423
Sum of electronic and thermal Enthalpies= -1240.693479
Sum of electronic and thermal Free Energies= -1240.784327

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.232261	-0.000826	0.000015
2	6	0	3.840116	4.752182	0.000356
3	1	0	4.865484	4.365919	0.000440
4	1	0	3.730346	5.383860	-0.884542
5	1	0	3.730197	5.383848	0.885245
6	6	0	2.839925	3.622759	0.000263
7	6	0	2.346138	3.087960	-1.185620
8	1	0	2.636239	3.538586	-2.131189
9	6	0	1.050692	1.386883	0.000096
10	6	0	2.345945	3.087936	1.186056
11	1	0	2.635892	3.538544	2.131681
12	6	0	2.531891	-2.947206	1.186374
13	1	0	2.853092	-3.377073	2.131750
14	6	0	3.070244	-3.437286	0.000210
15	6	0	2.532084	-2.947182	-1.186031
16	1	0	2.853439	-3.377029	-2.131364
17	6	0	1.115354	-1.347083	0.000072
18	6	0	4.161820	-4.478658	0.000289
19	1	0	4.105710	-5.117346	-0.884617
20	1	0	5.150998	-4.007367	0.000376
21	1	0	4.105564	-5.117365	0.885171
22	7	0	-1.206216	-0.032335	-0.000100
23	6	0	-2.048008	-1.196839	-0.000177
24	6	0	-2.101258	1.091980	-0.000157

25	6	0	-3.402174	-0.806930	-0.000275
26	6	0	-1.713004	-2.551815	-0.000167
27	6	0	-3.435855	0.639219	-0.000263
28	6	0	-4.423068	-1.758651	-0.000363
29	6	0	-2.742668	-3.490585	-0.000256
30	1	0	-0.687417	-2.881567	-0.000094
31	6	0	-4.500123	1.542123	-0.000335
32	6	0	-4.087046	-3.105838	-0.000353
33	1	0	-5.461786	-1.447888	-0.000439
34	1	0	-2.486799	-4.544089	-0.000249
35	1	0	-5.523170	1.183123	-0.000416
36	1	0	-4.865084	-3.860515	-0.000421
37	6	0	-2.902499	3.350666	-0.000196
38	1	0	-2.696094	4.414954	-0.000170
39	6	0	-1.829905	2.461214	-0.000123
40	1	0	-0.821108	2.838970	-0.000043
41	6	0	1.561739	-1.942107	1.206721
42	6	0	1.459266	2.008497	-1.206653
43	6	0	0.901949	1.631009	-2.563310
44	1	0	1.601123	1.021911	-3.140683
45	1	0	-0.040507	1.089666	-2.491243
46	1	0	0.708599	2.535778	-3.145309
47	6	0	0.946027	-1.637501	2.557159
48	1	0	0.663462	-2.574418	3.045782
49	1	0	1.644404	-1.127349	3.225277
50	1	0	0.043664	-1.034252	2.481864
51	6	0	1.561936	-1.942083	-1.206515
52	6	0	0.946443	-1.637448	-2.557048
53	1	0	0.044064	-1.034208	-2.481886
54	1	0	1.644926	-1.127273	-3.225038
55	1	0	0.663967	-2.574355	-3.045741
56	6	0	1.459070	2.008473	1.206923
57	6	0	0.901533	1.630958	2.563483
58	1	0	-0.040918	1.089628	2.491253
59	1	0	1.600608	1.021835	3.140950
60	1	0	0.708103	2.535714	3.145475
61	6	0	-4.227388	2.903548	-0.000301
62	1	0	-5.039845	3.621045	-0.000355

Compound 1 2RF-CN-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1241.22183830 A.U. after 1 cycles
Lowest frequency = -41.9425

Zero-point correction= 0.516219
(Hartree/Particle)
Thermal correction to Energy= 0.545036
Thermal correction to Enthalpy= 0.545980
Thermal correction to Gibbs Free Energy= 0.456573
Sum of electronic and zero-point Energies= -1240.705619
Sum of electronic and thermal Energies= -1240.676802
Sum of electronic and thermal Enthalpies= -1240.675858
Sum of electronic and thermal Free Energies= -1240.765265

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	0.500299	0.129800	-0.010954
2	6	0	5.972960	-2.176056	0.013135
3	1	0	6.004819	-3.162000	-0.455352
4	1	0	6.689717	-1.527649	-0.495644
5	1	0	6.315139	-2.293392	1.047490
6	6	0	4.583867	-1.594615	-0.020231
7	6	0	3.459199	-2.413588	-0.024542
8	1	0	3.597916	-3.489852	-0.030200
9	6	0	1.933455	-0.486283	-0.021295
10	6	0	4.378856	-0.217828	-0.024302
11	1	0	5.242337	0.439579	-0.029829
12	6	0	-0.570986	3.712169	-1.171862
13	1	0	-0.721988	4.233087	-2.113730
14	6	0	-0.838547	4.376442	0.021809
15	6	0	-0.546487	3.701227	1.203532
16	1	0	-0.678100	4.213415	2.153065
17	6	0	0.127559	1.688258	-0.000554
18	6	0	-1.405766	5.774616	0.034107
19	1	0	-1.082725	6.329499	0.918329
20	1	0	-1.100574	6.337834	-0.851185
21	1	0	-2.501128	5.751878	0.045046
22	7	0	-0.725156	-0.776772	-0.004121
23	6	0	-1.477452	-1.124801	1.124623
24	6	0	-1.499371	-1.114165	-1.121159
25	6	0	-2.754733	-1.603251	0.732631
26	6	0	-1.096683	-1.157165	2.470184
27	6	0	-2.768786	-1.596473	-0.708866
28	6	0	-3.670851	-2.032574	1.696651
29	6	0	-2.021927	-1.594258	3.412191
30	1	0	-0.099822	-0.877780	2.780202
31	6	0	-3.703491	-2.017016	-1.658811
32	6	0	-3.306309	-2.013404	3.036280
33	1	0	-4.649635	-2.392574	1.398683
34	1	0	-1.734992	-1.624369	4.457529
35	1	0	-4.676287	-2.379945	-1.345203
36	1	0	-4.005490	-2.347370	3.794047
37	6	0	-2.088204	-1.562745	-3.401956
38	1	0	-1.821597	-1.583253	-4.452893
39	6	0	-1.144822	-1.134228	-2.474111
40	1	0	-0.154193	-0.851876	-2.800948
41	6	0	-0.088690	2.401801	-1.203431
42	6	0	2.158566	-1.909337	-0.024708
43	6	0	1.073879	-2.968434	-0.032425
44	1	0	0.433059	-2.914681	0.848020
45	1	0	0.427440	-2.896951	-0.907342
46	1	0	1.535896	-3.957181	-0.043692
47	6	0	0.249601	1.833972	-2.566851
48	1	0	0.672924	2.614709	-3.204585
49	1	0	0.986110	1.029370	-2.508843
50	1	0	-0.634969	1.442026	-3.073961
51	6	0	-0.063705	2.390661	1.213137
52	6	0	0.302206	1.810407	2.564166
53	1	0	-0.571880	1.413232	3.085216
54	1	0	1.037808	1.006939	2.483926
55	1	0	0.737728	2.585551	3.200495
56	6	0	3.106060	0.349705	-0.024344
57	6	0	3.087606	1.864331	-0.031664
58	1	0	2.573285	2.270834	-0.902341
59	1	0	2.589176	2.279285	0.844374

60	1	0	4.111901	2.241024	-0.042666
61	6	0	-3.365075	-1.985444	-3.005044
62	1	0	-4.078858	-2.312524	-3.752123

Compound 1 3RF-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1241.17771446 A.U. after 1 cycles
Lowest frequency = -62.3403

Zero-point correction= 0.516372
(Hartree/Particle)
Thermal correction to Energy= 0.545387
Thermal correction to Enthalpy= 0.546331
Thermal correction to Gibbs Free Energy= 0.455417
Sum of electronic and zero-point Energies= -1240.661342
Sum of electronic and thermal Energies= -1240.632328
Sum of electronic and thermal Enthalpies= -1240.631384
Sum of electronic and thermal Free Energies= -1240.722297

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.041736	-1.406796	-0.551981
2	6	0	3.249879	-0.757706	0.715435
3	6	0	1.967210	-0.471884	1.238794
4	7	0	0.952386	-0.832850	0.312585
5	6	0	1.641311	-1.511618	-0.735152
6	6	0	1.151736	-2.253759	-1.809011
7	6	0	2.048798	-2.818880	-2.711232
8	6	0	3.930946	-1.971455	-1.468792
9	6	0	4.402675	-0.530951	1.470692
10	6	0	3.006820	0.120920	3.325972
11	6	0	1.851663	-0.095768	2.580275
12	1	0	0.102245	-2.440522	-1.924880
13	1	0	1.659857	-3.404023	-3.537237
14	1	0	5.000579	-1.879034	-1.315859
15	1	0	5.379703	-0.749283	1.054054
16	1	0	2.912369	0.414737	4.365365
17	1	0	0.892325	-0.023922	3.065492
18	5	0	-0.361717	-0.087510	0.093378
19	6	0	-1.811316	-0.834127	0.232628
20	6	0	-2.606217	-1.620147	-0.657108
21	6	0	-2.410350	-0.578486	1.500742
22	6	0	-3.911324	-1.989876	-0.300202
23	6	0	-3.706280	-0.981894	1.817528
24	6	0	-4.500127	-1.674293	0.915627
25	1	0	-4.486338	-2.566670	-1.018437
26	1	0	-4.094712	-0.741075	2.803463
27	6	0	-0.325128	1.504597	-0.295389
28	6	0	-0.563426	1.759260	-1.680388
29	6	0	-0.096178	2.666663	0.501782
30	6	0	-0.606459	3.051826	-2.200838
31	6	0	-0.169523	3.946450	-0.067630
32	6	0	-0.433412	4.177597	-1.407817
33	1	0	-0.774768	3.171031	-3.267286
34	1	0	0.006286	4.799115	0.581097

35	6	0	-1.653457	0.075680	2.627228
36	1	0	-1.267040	-0.682856	3.316609
37	1	0	-0.812631	0.662451	2.280815
38	1	0	-2.294728	0.748362	3.202021
39	6	0	-2.192202	-2.231862	-1.984677
40	1	0	-1.468035	-1.664463	-2.550280
41	1	0	-1.786928	-3.236289	-1.819117
42	1	0	-3.069523	-2.352658	-2.623715
43	6	0	-5.924507	-2.053592	1.232863
44	1	0	-6.611487	-1.236958	0.984884
45	1	0	-6.240054	-2.931072	0.663824
46	1	0	-6.050999	-2.273912	2.295739
47	6	0	0.229426	2.713476	1.982893
48	1	0	-0.674680	2.726364	2.598878
49	1	0	0.863915	1.899936	2.312497
50	1	0	0.771042	3.635391	2.202010
51	6	0	-0.781082	0.663149	-2.694229
52	1	0	-0.114165	-0.186022	-2.545984
53	1	0	-1.815406	0.314599	-2.671339
54	1	0	-0.585353	1.035331	-3.701714
55	6	0	-0.525096	5.571313	-1.975799
56	1	0	-0.062610	5.629884	-2.964597
57	1	0	-1.569959	5.881426	-2.086898
58	1	0	-0.033092	6.299314	-1.327089
59	6	0	3.431355	-2.666418	-2.560969
60	1	0	4.107659	-3.114503	-3.279407
61	6	0	4.278635	-0.064339	2.771612
62	1	0	5.161791	0.110333	3.374971

Compound 2a GS1

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.23226478 A.U. after 1 cycles
Lowest frequency = 20.3061

Zero-point correction= 0.599596
(Hartree/Particle)
Thermal correction to Energy= 0.634376
Thermal correction to Enthalpy= 0.635320
Thermal correction to Gibbs Free Energy= 0.530947
Sum of electronic and zero-point Energies= -1358.632668
Sum of electronic and thermal Energies= -1358.597889
Sum of electronic and thermal Enthalpies= -1358.596945
Sum of electronic and thermal Free Energies= -1358.701318

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.941061	0.239899	-0.066015
2	6	0	3.354360	0.898133	-1.835695
3	1	0	2.677123	0.418903	-2.548960
4	1	0	2.949466	1.889799	-1.623885
5	1	0	4.316205	1.025411	-2.336194
6	6	0	1.578389	2.250838	2.156275
7	1	0	1.730460	3.101015	2.824052
8	1	0	0.913398	1.549171	2.668601
9	1	0	2.538419	1.747339	2.025809

10	6	0	-0.344429	1.426067	-2.535716
11	1	0	0.342282	0.597755	-2.716470
12	1	0	-1.329554	0.988549	-2.346729
13	1	0	-0.414352	2.006572	-3.458072
14	6	0	0.055474	6.076557	-0.709846
15	1	0	-0.175378	6.572545	0.236032
16	1	0	0.967154	6.537928	-1.105673
17	1	0	-0.751735	6.292539	-1.413554
18	6	0	0.240362	4.590593	-0.522045
19	6	0	0.777793	4.074842	0.656873
20	1	0	1.036456	4.756211	1.462412
21	6	0	1.000273	2.708110	0.833736
22	6	0	0.650489	1.792748	-0.190353
23	6	0	0.088280	2.311545	-1.384411
24	6	0	-0.093051	3.688738	-1.530321
25	1	0	-0.512399	4.065464	-2.459065
26	6	0	2.649362	-1.081489	1.380435
27	6	0	3.952082	-1.475884	1.693912
28	1	0	4.116966	-2.074355	2.585532
29	6	0	5.042026	-1.131794	0.897282
30	6	0	4.796441	-0.361660	-0.239083
31	1	0	5.627983	-0.088771	-0.882602
32	6	0	3.513998	0.075981	-0.574358
33	6	0	2.406146	-0.284621	0.232961
34	6	0	1.540362	-1.546667	2.302777
35	1	0	1.034034	-2.427359	1.895693
36	1	0	1.946374	-1.823274	3.278125
37	1	0	0.775101	-0.786338	2.465550
38	6	0	6.443817	-1.551302	1.266734
39	1	0	7.059406	-1.711743	0.378313
40	1	0	6.937104	-0.781129	1.870231
41	1	0	6.443185	-2.473872	1.851793
42	7	0	-0.143670	-0.707723	-0.226048
43	6	0	-0.046794	-2.053582	-0.682402
44	6	0	-1.525203	-0.481181	0.039597
45	6	0	-1.328691	-2.644573	-0.706614
46	6	0	1.065832	-2.764287	-1.137362
47	6	0	-2.265560	-1.647553	-0.234166
48	6	0	-1.497338	-3.957190	-1.153268
49	6	0	0.880087	-4.072623	-1.575490
50	1	0	2.051497	-2.324064	-1.147567
51	6	0	-3.645043	-1.683307	-0.015883
52	6	0	-0.385991	-4.670968	-1.581649
53	1	0	-2.483245	-4.408294	-1.170533
54	1	0	1.739262	-4.635255	-1.922880
55	6	0	-4.303691	-0.563751	0.484869
56	1	0	-4.204810	-2.588143	-0.230973
57	1	0	-0.497572	-5.690982	-1.931023
58	6	0	-3.541081	0.584046	0.772037
59	1	0	-4.033364	1.462925	1.174003
60	6	0	-2.167099	0.641378	0.566507
61	1	0	-1.623449	1.542656	0.807166
62	6	0	-5.807171	-0.589737	0.722044
63	1	0	-6.155639	-1.587532	0.431391
64	6	0	-6.161813	-0.394659	2.207329
65	1	0	-7.241450	-0.483879	2.361419
66	1	0	-5.665244	-1.141037	2.832344
67	1	0	-5.856644	0.594099	2.562451
68	6	0	-6.546911	0.430400	-0.162412
69	1	0	-6.255980	1.455431	0.085712

70	1	0	-6.325665	0.268236	-1.220284
71	1	0	-7.629256	0.349165	-0.023540

Compound 2a GS2

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.23206247 A.U. after 1 cycles
Lowest frequency = 18.8925

Zero-point correction= 0.599560
(Hartree/Particle)
Thermal correction to Energy= 0.634349
Thermal correction to Enthalpy= 0.635293
Thermal correction to Gibbs Free Energy= 0.530756
Sum of electronic and zero-point Energies= -1358.632502
Sum of electronic and thermal Energies= -1358.597713
Sum of electronic and thermal Enthalpies= -1358.596769
Sum of electronic and thermal Free Energies= -1358.701306

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.979303	0.201280	-0.052237
2	6	0	3.421566	0.564886	-1.867463
3	1	0	2.676677	0.188291	-2.574923
4	1	0	3.150052	1.596019	-1.632679
5	1	0	4.383043	0.577612	-2.384404
6	6	0	1.914546	2.069734	2.189835
7	1	0	2.200441	2.879887	2.863460
8	1	0	1.166958	1.462873	2.709488
9	1	0	2.789858	1.436566	2.031670
10	6	0	-0.181532	1.592180	-2.475937
11	1	0	0.381113	0.679655	-2.678245
12	1	0	-1.215392	1.292720	-2.277879
13	1	0	-0.182438	2.191063	-3.389178
14	6	0	0.859662	6.114939	-0.583776
15	1	0	0.710749	6.619155	0.374129
16	1	0	1.817819	6.460035	-0.988175
17	1	0	0.076960	6.447990	-1.269262
18	6	0	0.850456	4.614313	-0.423742
19	6	0	1.335887	4.010582	0.735806
20	1	0	1.696334	4.636971	1.546853
21	6	0	1.379342	2.623448	0.886271
22	6	0	0.894181	1.781032	-0.145148
23	6	0	0.384593	2.391337	-1.319327
24	6	0	0.383631	3.782909	-1.439552
25	1	0	0.001543	4.228543	-2.353766
26	6	0	2.526830	-1.360238	1.334653
27	6	0	3.771484	-1.930360	1.611521
28	1	0	3.873791	-2.561488	2.489901
29	6	0	4.880506	-1.720150	0.794823
30	6	0	4.715986	-0.903742	-0.323680
31	1	0	5.562726	-0.732366	-0.982267
32	6	0	3.496655	-0.293242	-0.622327
33	6	0	2.367997	-0.517545	0.205203
34	6	0	1.385115	-1.689282	2.275449
35	1	0	0.753233	-2.482853	1.864780

36	1	0	1.770640	-2.040372	3.235007
37	1	0	0.735958	-0.834601	2.471473
38	6	0	6.221268	-2.329246	1.124840
39	1	0	6.789488	-2.557133	0.219748
40	1	0	6.827032	-1.641368	1.725313
41	1	0	6.109974	-3.252248	1.698495
42	7	0	-0.223985	-0.591632	-0.203084
43	6	0	-0.315203	-1.931081	-0.679815
44	6	0	-1.557943	-0.188855	0.096805
45	6	0	-1.663604	-2.348380	-0.682510
46	6	0	0.684335	-2.773806	-1.170502
47	6	0	-2.452235	-1.244834	-0.175565
48	6	0	-2.012807	-3.619762	-1.142999
49	6	0	0.318964	-4.039064	-1.622150
50	1	0	1.718843	-2.466487	-1.197999
51	6	0	-3.818095	-1.105990	0.071320
52	6	0	-1.014445	-4.466154	-1.606873
53	1	0	-3.049617	-3.937329	-1.143760
54	1	0	1.089173	-4.703446	-1.997378
55	6	0	-4.314179	0.085204	0.601311
56	1	0	-4.487744	-1.931605	-0.145424
57	1	0	-1.266679	-5.456722	-1.967526
58	6	0	-3.402876	1.115926	0.884485
59	1	0	-3.776599	2.042933	1.307416
60	6	0	-2.035128	0.998445	0.650453
61	1	0	-1.374668	1.818185	0.890414
62	6	0	-5.799342	0.273905	0.879908
63	1	0	-5.918346	1.282202	1.292606
64	6	0	-6.640277	0.203265	-0.407653
65	1	0	-7.693857	0.406672	-0.193266
66	1	0	-6.295092	0.932805	-1.144491
67	1	0	-6.579873	-0.788043	-0.866749
68	6	0	-6.319804	-0.717935	1.935947
69	1	0	-6.247195	-1.750243	1.580853
70	1	0	-5.746066	-0.643754	2.863095
71	1	0	-7.370669	-0.519729	2.167765

Compound 2a 1RF-C1-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.15973694 A.U. after 1 cycles
Lowest frequency = -41.3058

Zero-point correction= 0.599407
(Hartree/Particle)
Thermal correction to Energy= 0.632723
Thermal correction to Enthalpy= 0.633667
Thermal correction to Gibbs Free Energy= 0.534326
Sum of electronic and zero-point Energies= -1358.560330
Sum of electronic and thermal Energies= -1358.527014
Sum of electronic and thermal Enthalpies= -1358.526070
Sum of electronic and thermal Free Energies= -1358.625411

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.234194	-1.227164	-0.646754

2	6	0	1.205536	-2.000947	-1.311909
3	6	0	-0.000939	-1.774685	-0.608669
4	7	0	0.176725	-0.670503	0.315386
5	6	0	1.598438	-0.544220	0.408316
6	6	0	2.366279	-0.127200	1.488527
7	6	0	3.754931	-0.197137	1.405658
8	6	0	3.625446	-1.272426	-0.735493
9	6	0	1.291786	-2.978557	-2.302577
10	6	0	0.187971	-3.784274	-2.553929
11	6	0	-0.965972	-3.635486	-1.781012
12	6	0	-1.071187	-2.646983	-0.801781
13	1	0	1.901259	0.200073	2.404620
14	1	0	4.339291	0.137692	2.255923
15	1	0	4.100881	-1.792126	-1.561335
16	1	0	2.221447	-3.131307	-2.839490
17	1	0	-1.799308	-4.314364	-1.924051
18	1	0	-1.960944	-2.592900	-0.198568
19	5	0	-0.892097	0.344077	0.503988
20	6	0	-2.351298	-0.296193	0.558705
21	6	0	-3.188442	-0.488656	-0.558411
22	6	0	-2.814874	-0.719796	1.826329
23	6	0	-4.449325	-1.070230	-0.392292
24	6	0	-4.078493	-1.296144	1.955567
25	6	0	-4.918217	-1.478134	0.854029
26	1	0	-5.080256	-1.210864	-1.266316
27	1	0	-4.416251	-1.611189	2.939224
28	6	0	-0.735227	1.940490	0.402317
29	6	0	0.462880	2.729048	0.481189
30	6	0	-1.834257	2.646764	-0.203844
31	6	0	0.666162	3.812266	-0.367987
32	6	0	-1.593131	3.739458	-1.046073
33	6	0	-0.326447	4.278339	-1.230175
34	1	0	1.605790	4.353925	-0.298852
35	1	0	-2.443793	4.207408	-1.533676
36	6	0	-1.952544	-0.551229	3.060039
37	1	0	-1.023083	-1.123328	2.978444
38	1	0	-1.675101	0.496987	3.215133
39	1	0	-2.475801	-0.891105	3.956025
40	6	0	-2.763731	-0.125512	-1.966705
41	1	0	-1.878107	0.509615	-1.988314
42	1	0	-2.533725	-1.026043	-2.543529
43	1	0	-3.565061	0.400699	-2.494027
44	6	0	-6.295232	-2.075318	1.018891
45	1	0	-6.681913	-2.453454	0.069972
46	1	0	-6.288916	-2.900969	1.735495
47	1	0	-7.006392	-1.329207	1.390310
48	6	0	-3.305727	2.436621	0.118923
49	1	0	-3.877388	2.000782	-0.701369
50	1	0	-3.468678	1.828770	1.002332
51	1	0	-3.730204	3.426714	0.313138
52	6	0	1.434004	2.646397	1.640734
53	1	0	1.091786	1.961409	2.410628
54	1	0	2.449941	2.384570	1.347714
55	1	0	1.470078	3.638939	2.101829
56	6	0	-0.064009	5.383266	-2.218521
57	1	0	-0.976189	5.936005	-2.454550
58	1	0	0.679543	6.090456	-1.842172
59	1	0	0.324207	4.973880	-3.157988
60	6	0	4.409247	-0.722594	0.278883
61	6	0	5.928352	-0.769443	0.195660

62	1	0	6.177418	-1.253509	-0.755621
63	6	0	6.548185	-1.620001	1.319114
64	1	0	7.632815	-1.691692	1.194104
65	1	0	6.356819	-1.181840	2.303035
66	1	0	6.137166	-2.632539	1.319391
67	6	0	6.542052	0.642234	0.167086
68	1	0	7.627371	0.589720	0.038020
69	1	0	6.129438	1.234805	-0.653260
70	1	0	6.343104	1.178624	1.099728
71	1	0	0.237696	-4.556828	-3.312603

Compound 2a 1RF-C1-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.15965177 A.U. after 1 cycles
Lowest frequency = -41.0584

Zero-point correction= 0.599413
(Hartree/Particle)
Thermal correction to Energy= 0.632729
Thermal correction to Enthalpy= 0.633673
Thermal correction to Gibbs Free Energy= 0.534289
Sum of electronic and zero-point Energies= -1358.560239
Sum of electronic and thermal Energies= -1358.526923
Sum of electronic and thermal Enthalpies= -1358.525979
Sum of electronic and thermal Free Energies= -1358.625362

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.325920	-1.078945	-0.414842
2	6	0	1.377317	-1.908411	-1.131543
3	6	0	0.121342	-1.736976	-0.503861
4	7	0	0.187666	-0.616796	0.415886
5	6	0	1.593148	-0.420465	0.594742
6	6	0	2.271148	0.042394	1.712724
7	6	0	3.666297	0.044154	1.708857
8	6	0	3.718281	-1.056783	-0.422417
9	6	0	1.570646	-2.888526	-2.104204
10	6	0	0.524952	-3.750534	-2.411702
11	6	0	-0.678902	-3.653342	-1.710209
12	6	0	-0.891012	-2.663245	-0.749995
13	1	0	1.737756	0.353358	2.596608
14	1	0	4.190389	0.417424	2.582972
15	1	0	4.258460	-1.564602	-1.214271
16	1	0	2.537060	-2.999212	-2.583475
17	1	0	-1.467785	-4.373972	-1.894969
18	1	0	-1.816957	-2.648182	-0.201493
19	5	0	-0.938206	0.345418	0.528116
20	6	0	-2.364908	-0.365988	0.500367
21	6	0	-3.120997	-0.608177	-0.663935
22	6	0	-2.884061	-0.803367	1.741442
23	6	0	-4.359204	-1.251136	-0.569435
24	6	0	-4.123090	-1.441538	1.798904
25	6	0	-4.883172	-1.673295	0.649969
26	1	0	-4.927286	-1.429495	-1.478966
27	1	0	-4.504815	-1.766161	2.763170

28	6	0	-0.853753	1.947016	0.419298
29	6	0	0.297567	2.794648	0.559630
30	6	0	-1.948526	2.593295	-0.257484
31	6	0	0.496738	3.880283	-0.287517
32	6	0	-1.712426	3.690455	-1.095297
33	6	0	-0.465159	4.290215	-1.210793
34	1	0	1.403012	4.468342	-0.169478
35	1	0	-2.554950	4.111839	-1.636544
36	6	0	-2.108803	-0.583323	3.023877
37	1	0	-1.149987	-1.110784	3.006040
38	1	0	-1.891441	0.478221	3.183997
39	1	0	-2.669888	-0.940531	3.889732
40	6	0	-2.628351	-0.234572	-2.047140
41	1	0	-1.779585	0.448900	-2.020936
42	1	0	-2.312754	-1.126120	-2.596863
43	1	0	-3.422405	0.241184	-2.630399
44	6	0	-6.236564	-2.337297	0.736069
45	1	0	-6.539445	-2.751410	-0.228185
46	1	0	-6.237060	-3.148703	1.468728
47	1	0	-7.007440	-1.622113	1.043784
48	6	0	-3.424365	2.312035	-0.020120
49	1	0	-3.923336	1.840281	-0.867546
50	1	0	-3.609348	1.704663	0.859293
51	1	0	-3.908687	3.281068	0.136654
52	6	0	1.202740	2.769536	1.774040
53	1	0	0.848983	2.076561	2.531434
54	1	0	2.245106	2.553294	1.543229
55	1	0	1.165609	3.767135	2.223990
56	6	0	-0.199730	5.399435	-2.193518
57	1	0	-1.122397	5.905210	-2.487094
58	1	0	0.485736	6.144831	-1.782243
59	1	0	0.261491	5.002698	-3.104991
60	6	0	4.411881	-0.455845	0.632127
61	6	0	5.933342	-0.413628	0.661973
62	1	0	6.218233	0.074295	1.601127
63	6	0	6.502010	0.436056	-0.488925
64	1	0	7.591405	0.507658	-0.415387
65	1	0	6.261458	-0.004142	-1.461216
66	1	0	6.091601	1.448788	-0.472008
67	6	0	6.555882	-1.821633	0.670272
68	1	0	7.644413	-1.761100	0.763280
69	1	0	6.174722	-2.416375	1.504051
70	1	0	6.332242	-2.361610	-0.254435
71	1	0	0.658108	-4.525742	-3.157490

Compound 2a 1-RF-C-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.15967642 A.U. after 1 cycles
Lowest frequency = -43.9232

Zero-point correction= 0.599361
(Hartree/Particle)
Thermal correction to Energy= 0.632706
Thermal correction to Enthalpy= 0.633650
Thermal correction to Gibbs Free Energy= 0.534108
Sum of electronic and zero-point Energies= -1358.560315
Sum of electronic and thermal Energies= -1358.526970
Sum of electronic and thermal Enthalpies= -1358.526026

Sum of electronic and thermal Free Energies= -1358.625569

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.904102	-2.803014	-0.483204
2	6	0	1.813160	-1.801351	0.035566
3	6	0	1.310616	-0.543450	-0.360827
4	7	0	-0.032514	-0.698695	-0.888418
5	6	0	-0.124128	-2.101078	-1.148577
6	6	0	-0.860149	-2.750994	-2.131089
7	6	0	-0.717402	-4.129685	-2.286020
8	6	0	1.030727	-4.184924	-0.621638
9	6	0	3.072667	-1.926035	0.622006
10	6	0	3.891301	-0.808741	0.769675
11	6	0	3.421401	0.415591	0.268277
12	6	0	2.157687	0.562313	-0.300653
13	6	0	5.269242	-0.931545	1.404225
14	6	0	6.396713	-0.586001	0.414573
15	6	0	5.385271	-0.092671	2.689839
16	1	0	-1.495147	-2.196599	-2.802898
17	1	0	-1.295806	-4.639019	-3.048675
18	1	0	1.816050	-4.720197	-0.099795
19	1	0	3.431286	-2.903792	0.928361
20	1	0	4.065398	1.288002	0.299467
21	1	0	1.871383	1.517593	-0.705992
22	1	0	5.394141	-1.983100	1.687582
23	1	0	7.376636	-0.745894	0.874553
24	1	0	6.336152	-1.205540	-0.483625
25	1	0	6.344175	0.460905	0.101564
26	1	0	6.358927	-0.245579	3.165314
27	1	0	4.608295	-0.364158	3.408878
28	1	0	5.283407	0.975419	2.475743
29	5	0	-1.094550	0.291997	-0.575915
30	6	0	-0.568039	1.796532	-0.619568
31	6	0	-0.044235	2.499403	0.483816
32	6	0	-0.613636	2.451437	-1.872667
33	6	0	0.397120	3.816837	0.325084
34	6	0	-0.164865	3.766501	-1.994858
35	6	0	0.343271	4.473068	-0.902153
36	1	0	0.798091	4.342139	1.188252
37	1	0	-0.212390	4.251720	-2.966048
38	6	0	-2.556760	-0.016438	0.016087
39	6	0	-3.280407	-1.257587	0.018483
40	6	0	-3.057660	0.927724	0.981353
41	6	0	-4.002569	-1.664335	1.135943
42	6	0	-3.789752	0.483698	2.089762
43	6	0	-4.185116	-0.838452	2.245344
44	1	0	-4.500117	-2.630047	1.106153
45	1	0	-4.096861	1.218919	2.828343
46	6	0	-1.152015	1.740331	-3.096803
47	1	0	-0.549018	0.861276	-3.344815
48	1	0	-2.179563	1.394740	-2.940397
49	1	0	-1.153565	2.399937	-3.966862
50	6	0	0.105101	1.870412	1.854079
51	1	0	-0.454365	0.940175	1.953357
52	1	0	1.155053	1.643348	2.060435
53	1	0	-0.238675	2.552340	2.637570

54	6	0	0.794597	5.906665	-1.047332
55	1	0	1.459183	6.199895	-0.231646
56	1	0	1.324995	6.064541	-1.990182
57	1	0	-0.060358	6.591761	-1.037697
58	6	0	-3.027248	2.441334	0.834739
59	1	0	-2.363095	2.938256	1.542962
60	1	0	-2.760941	2.770293	-0.163923
61	1	0	-4.040829	2.798158	1.043389
62	6	0	-3.562703	-2.055603	-1.238125
63	1	0	-3.194044	-1.556978	-2.129583
64	1	0	-3.181089	-3.075412	-1.208150
65	1	0	-4.651003	-2.114788	-1.343517
66	6	0	-4.877604	-1.324343	3.490677
67	1	0	-5.348419	-0.502554	4.034996
68	1	0	-5.644236	-2.068353	3.259661
69	1	0	-4.159458	-1.798768	4.168973
70	6	0	0.187199	-4.852827	-1.503575
71	1	0	0.280830	-5.924383	-1.637867

Compound 2a 1-RF-C-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.15957180 A.U. after 1 cycles
Lowest frequency = -44.1321

Zero-point correction= 0.599302
(Hartree/Particle)
Thermal correction to Energy= 0.632679
Thermal correction to Enthalpy= 0.633623
Thermal correction to Gibbs Free Energy= 0.533728
Sum of electronic and zero-point Energies= -1358.560270
Sum of electronic and thermal Energies= -1358.526893
Sum of electronic and thermal Enthalpies= -1358.525949
Sum of electronic and thermal Free Energies= -1358.625844

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.587200	-2.360034	-0.605642
2	6	0	2.212095	-1.173168	-0.056279
3	6	0	1.391047	-0.076766	-0.405391
4	7	0	0.126039	-0.561902	-0.926490
5	6	0	0.401177	-1.929622	-1.238243
6	6	0	-0.154633	-2.715563	-2.239607
7	6	0	0.340944	-4.002847	-2.446128
8	6	0	2.068433	-3.654859	-0.795885
9	6	0	3.467457	-0.986732	0.517287
10	6	0	3.967107	0.303588	0.702320
11	6	0	3.187291	1.375113	0.247950
12	6	0	1.919647	1.207472	-0.311795
13	6	0	5.334345	0.549101	1.324900
14	6	0	5.394193	0.063931	2.784616
15	6	0	6.471870	-0.066974	0.490319
16	1	0	-0.923199	-2.324147	-2.886171
17	1	0	-0.096245	-4.619660	-3.223317
18	1	0	2.974526	-3.983399	-0.299234
19	1	0	4.066693	-1.851997	0.780680

20	1	0	3.588823	2.381488	0.313618
21	1	0	1.388778	2.068675	-0.679722
22	1	0	5.487361	1.634347	1.334155
23	1	0	6.361982	0.306391	3.234104
24	1	0	4.611408	0.530676	3.387728
25	1	0	5.260373	-1.020207	2.846994
26	1	0	7.446158	0.181508	0.922084
27	1	0	6.450318	0.301727	-0.538179
28	1	0	6.393391	-1.157666	0.455245
29	5	0	-1.152284	0.104493	-0.569020
30	6	0	-1.036684	1.694661	-0.557537
31	6	0	-0.695475	2.469031	0.569184
32	6	0	-1.271798	2.359989	-1.783613
33	6	0	-0.614658	3.860840	0.459625
34	6	0	-1.182378	3.750020	-1.856937
35	6	0	-0.857439	4.524403	-0.740510
36	1	0	-0.349763	4.440836	1.340088
37	1	0	-1.370363	4.241061	-2.807967
38	6	0	-2.474212	-0.594693	0.020554
39	6	0	-2.848484	-1.981284	-0.017032
40	6	0	-3.190536	0.153588	1.021147
41	6	0	-3.424200	-2.598970	1.088758
42	6	0	-3.766390	-0.502408	2.116450
43	6	0	-3.801158	-1.886288	2.227184
44	1	0	-3.652577	-3.659689	1.027367
45	1	0	-4.244517	0.102434	2.881910
46	6	0	-1.627228	1.577864	-3.030994
47	1	0	-0.820355	0.896312	-3.317922
48	1	0	-2.526259	0.970438	-2.880855
49	1	0	-1.815733	2.245251	-3.874298
50	6	0	-0.365225	1.850867	1.912448
51	1	0	-0.657233	0.802599	1.976311
52	1	0	0.710349	1.902367	2.105088
53	1	0	-0.865719	2.387191	2.724220
54	6	0	-0.796254	6.030323	-0.832495
55	1	0	-0.224029	6.457213	-0.005882
56	1	0	-0.333173	6.354470	-1.768317
57	1	0	-1.799963	6.468288	-0.798896
58	6	0	-3.557240	1.626914	0.929038
59	1	0	-3.034754	2.255670	1.651048
60	1	0	-3.400315	2.047355	-0.058415
61	1	0	-4.625556	1.700214	1.156030
62	6	0	-2.928991	-2.784447	-1.299201
63	1	0	-2.717597	-2.177558	-2.174514
64	1	0	-2.291905	-3.667960	-1.307355
65	1	0	-3.964651	-3.125157	-1.400676
66	6	0	-4.326175	-2.576702	3.457705
67	1	0	-4.988820	-1.925144	4.031873
68	1	0	-4.874045	-3.487839	3.204122
69	1	0	-3.500218	-2.867814	4.116454
70	6	0	1.415103	-4.490148	-1.696550
71	1	0	1.783463	-5.494628	-1.870737

Compound 2a 1-RF-N-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.13257745 A.U. after 1 cycles
Lowest frequency = -68.6512

Zero-point correction= 0.600039
(Hartree/Particle)
Thermal correction to Energy= 0.632644
Thermal correction to Enthalpy= 0.633588
Thermal correction to Gibbs Free Energy= 0.537002
Sum of electronic and zero-point Energies= -1358.532538
Sum of electronic and thermal Energies= -1358.499934
Sum of electronic and thermal Enthalpies= -1358.498989
Sum of electronic and thermal Free Energies= -1358.595575

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.112749	0.788170	-0.018843
2	6	0	-6.012247	-2.191805	-0.911834
3	1	0	-5.930214	-3.105626	-1.505076
4	1	0	-6.180405	-2.493654	0.128201
5	1	0	-6.899046	-1.644600	-1.240105
6	6	0	-4.769489	-1.350039	-1.019428
7	6	0	-3.518549	-1.913266	-1.260605
8	1	0	-3.449609	-2.969608	-1.503125
9	6	0	-2.365795	0.233994	-0.860780
10	6	0	-4.817984	0.041656	-0.998336
11	1	0	-5.782175	0.539316	-1.059892
12	6	0	0.266411	4.441382	0.078815
13	1	0	0.043058	5.428847	-0.316340
14	6	0	1.528906	4.192606	0.610999
15	6	0	1.650551	3.036052	1.377787
16	1	0	2.535380	2.896721	1.991880
17	6	0	-0.514044	2.157989	0.575361
18	6	0	2.660380	5.174712	0.469809
19	1	0	3.305243	5.173026	1.351820
20	1	0	3.286889	4.914913	-0.391034
21	1	0	2.293645	6.191561	0.311410
22	6	0	-0.766636	3.506352	0.144925
23	6	0	-2.345216	-1.161034	-1.240390
24	6	0	-1.128577	-1.876272	-1.797637
25	1	0	-0.345764	-1.193691	-2.115680
26	1	0	-0.695404	-2.600975	-1.104888
27	1	0	-1.453547	-2.433948	-2.681247
28	6	0	-2.150844	4.099728	0.020588
29	1	0	-2.192604	4.946115	0.713538
30	1	0	-2.387479	4.494393	-0.969679
31	1	0	-2.918847	3.403180	0.332308
32	6	0	0.656693	2.059702	1.418330
33	6	0	0.837877	1.021571	2.510023
34	1	0	-0.088440	0.518825	2.772966
35	1	0	1.586336	0.263630	2.269040
36	1	0	1.189616	1.544876	3.404280
37	6	0	-3.665467	0.826621	-1.026541
38	6	0	-3.883769	2.235005	-1.529083
39	1	0	-4.469496	2.869301	-0.860518
40	1	0	-2.950875	2.724872	-1.777860
41	1	0	-4.453418	2.150416	-2.460072
42	7	0	-0.184980	-0.366370	0.333473
43	6	0	1.128257	-0.543686	-0.114619
44	6	0	-0.480275	-1.450016	1.165292
45	6	0	1.669176	-1.737603	0.418052

46	6	0	1.875890	0.234218	-1.004055
47	6	0	0.641286	-2.313886	1.255211
48	6	0	2.966066	-2.134308	0.072551
49	6	0	3.159531	-0.184278	-1.327724
50	1	0	1.473567	1.145566	-1.429116
51	6	0	0.583142	-3.452072	2.066583
52	1	0	3.380144	-3.050651	0.482425
53	1	0	3.739756	0.422475	-2.014790
54	1	0	1.436650	-4.117487	2.140156
55	6	0	-1.677184	-2.846486	2.695898
56	1	0	-2.573042	-3.063720	3.267083
57	6	0	-1.643463	-1.709202	1.897769
58	1	0	-2.499919	-1.048673	1.843464
59	6	0	3.728019	-1.363185	-0.800114
60	6	0	5.139204	-1.790595	-1.180538
61	1	0	5.339852	-2.726542	-0.646251
62	6	0	5.269433	-2.086138	-2.685857
63	1	0	6.272560	-2.453517	-2.923750
64	1	0	4.545390	-2.841141	-3.002202
65	1	0	5.095089	-1.186540	-3.283723
66	6	0	6.196588	-0.768311	-0.725359
67	1	0	6.064608	0.191913	-1.233057
68	1	0	6.131186	-0.587676	0.350542
69	1	0	7.205645	-1.127129	-0.950932
70	6	0	-0.577769	-3.715734	2.780810
71	1	0	-0.636343	-4.593057	3.414710

Compound 2a 1-RF-N-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.13230363 A.U. after 1 cycles
Lowest frequency = -68.6670

Zero-point correction= 0.599993
(Hartree/Particle)
Thermal correction to Energy= 0.632617
Thermal correction to Enthalpy= 0.633561
Thermal correction to Gibbs Free Energy= 0.536690
Sum of electronic and zero-point Energies= -1358.532311
Sum of electronic and thermal Energies= -1358.499686
Sum of electronic and thermal Enthalpies= -1358.498742
Sum of electronic and thermal Free Energies= -1358.595613

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-1.214047	0.704984	-0.028939
2	6	0	-5.695741	-2.920722	-0.698885
3	1	0	-5.516520	-3.819401	-1.293868
4	1	0	-5.775236	-3.234801	0.348061
5	1	0	-6.662291	-2.501428	-0.987968
6	6	0	-4.584868	-1.918939	-0.863208
7	6	0	-3.280342	-2.309256	-1.156808
8	1	0	-3.078677	-3.348600	-1.398743
9	6	0	-2.414554	-0.021754	-0.814462
10	6	0	-4.821336	-0.546599	-0.844533
11	1	0	-5.846027	-0.185093	-0.865643

12	6	0	-0.342324	4.512357	-0.004363
13	1	0	-0.714550	5.456533	-0.393079
14	6	0	0.963665	4.442415	0.473661
15	6	0	1.273925	3.320513	1.238821
16	1	0	2.194545	3.308710	1.814837
17	6	0	-0.782925	2.148966	0.533942
18	6	0	1.944032	5.567621	0.280040
19	1	0	2.619929	5.661770	1.133327
20	1	0	2.562916	5.387059	-0.606210
21	1	0	1.436072	6.523769	0.134013
22	6	0	-1.234717	3.446351	0.109888
23	6	0	-2.220564	-1.404468	-1.189961
24	6	0	-0.942514	-1.952600	-1.796879
25	1	0	-0.273543	-1.172800	-2.149373
26	1	0	-0.386534	-2.606506	-1.121600
27	1	0	-1.225463	-2.556199	-2.664638
28	6	0	-2.690862	3.844914	0.043812
29	1	0	-2.818041	4.683743	0.735553
30	1	0	-3.020835	4.195180	-0.936398
31	1	0	-3.342926	3.053168	0.390399
32	6	0	0.424816	2.218687	1.325935
33	6	0	0.791519	1.225239	2.412625
34	1	0	-0.045297	0.602627	2.715958
35	1	0	1.626595	0.575078	2.143054
36	1	0	1.104492	1.800024	3.289531
37	6	0	-3.788632	0.387375	-0.925567
38	6	0	-4.217801	1.748198	-1.423316
39	1	0	-4.855530	2.303378	-0.732326
40	1	0	-3.371716	2.357896	-1.714162
41	1	0	-4.809658	1.578044	-2.328385
42	7	0	-0.124246	-0.309808	0.287750
43	6	0	1.181047	-0.311691	-0.215918
44	6	0	-0.235027	-1.415854	1.135281
45	6	0	1.901315	-1.417912	0.298496
46	6	0	1.778258	0.549835	-1.138291
47	6	0	0.995457	-2.119585	1.180963
48	6	0	3.222558	-1.641936	-0.097552
49	6	0	3.094178	0.301967	-1.512796
50	1	0	1.240918	1.394782	-1.550944
51	6	0	1.125512	-3.247503	1.997813
52	1	0	3.764177	-2.492742	0.303339
53	1	0	3.567008	0.969656	-2.226249
54	1	0	2.063530	-3.790859	2.037654
55	6	0	-1.167865	-2.947451	2.719554
56	1	0	-2.001916	-3.278508	3.328472
57	6	0	-1.321216	-1.823187	1.916823
58	1	0	-2.260782	-1.285114	1.896095
59	6	0	3.837345	-0.781772	-1.006755
60	6	0	5.276154	-0.999147	-1.458252
61	1	0	5.508624	-0.198845	-2.170355
62	6	0	6.273078	-0.876616	-0.291487
63	1	0	7.303245	-0.971715	-0.648727
64	1	0	6.173835	0.088782	0.211162
65	1	0	6.106569	-1.658937	0.455112
66	6	0	5.456055	-2.336406	-2.199358
67	1	0	5.255719	-3.185543	-1.539101
68	1	0	4.774447	-2.409270	-3.050519
69	1	0	6.480143	-2.439452	-2.571499
70	6	0	0.041428	-3.659353	2.761335
71	1	0	0.128415	-4.530763	3.400082

Compound 2a 2-RF-CC-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.21462189 A.U. after 1 cycles
Lowest frequency = -60.4223

Zero-point correction= 0.599943
(Hartree/Particle)
Thermal correction to Energy= 0.633611
Thermal correction to Enthalpy= 0.634555
Thermal correction to Gibbs Free Energy= 0.533460
Sum of electronic and zero-point Energies= -1358.614679
Sum of electronic and thermal Energies= -1358.581011
Sum of electronic and thermal Enthalpies= -1358.580067
Sum of electronic and thermal Free Energies= -1358.681162

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.884899	0.117398	-0.000038
2	6	0	-0.751722	6.084708	-0.000210
3	1	0	-1.794210	6.422062	-0.000249
4	1	0	-0.272043	6.510146	0.884693
5	1	0	-0.271993	6.510094	-0.885111
6	6	0	-0.673953	4.578065	-0.000163
7	6	0	-0.621779	3.851973	1.185644
8	1	0	-0.568478	4.385117	2.131278
9	6	0	-0.668286	1.713985	-0.000078
10	6	0	-0.621700	3.851902	-1.185923
11	1	0	-0.568336	4.384991	-2.131585
12	6	0	-4.514001	-0.777044	-1.186354
13	1	0	-5.032348	-0.916247	-2.131694
14	6	0	-5.240162	-0.828478	-0.000165
15	6	0	-4.514086	-0.776971	1.186073
16	1	0	-5.032499	-0.916115	2.131385
17	6	0	-2.411114	-0.396015	-0.000078
18	6	0	-6.742137	-0.970381	-0.000214
19	1	0	-7.093495	-1.506732	0.884676
20	1	0	-7.227208	0.012125	-0.000257
21	1	0	-7.093433	-1.506778	-0.885100
22	7	0	0.226829	-0.794540	0.000029
23	6	0	0.172071	-2.230115	0.000076
24	6	0	1.625239	-0.462816	0.000069
25	6	0	1.479281	-2.757600	0.000145
26	6	0	-0.926884	-3.090428	0.000062
27	6	0	2.396681	-1.638874	0.000141
28	6	0	1.696102	-4.136406	0.000201
29	6	0	-0.694924	-4.464453	0.000119
30	1	0	-1.937616	-2.717357	0.000010
31	6	0	3.791599	-1.584111	0.000191
32	6	0	0.600913	-4.990045	0.000188
33	1	0	2.705514	-4.532180	0.000254
34	1	0	-1.545765	-5.136342	0.000108
35	6	0	4.443417	-0.353938	0.000171
36	1	0	4.369685	-2.502773	0.000247
37	1	0	0.748339	-6.063925	0.000231

38	6	0	3.656150	0.810514	0.000098
39	1	0	4.140182	1.781096	0.000080
40	6	0	2.264843	0.777859	0.000047
41	1	0	1.710861	1.701940	-0.000009
42	6	0	5.963698	-0.280152	0.000226
43	1	0	6.330402	-1.313117	0.000281
44	6	0	6.507351	0.400094	-1.269272
45	1	0	7.601349	0.382764	-1.277958
46	1	0	6.151083	-0.104999	-2.170527
47	1	0	6.191193	1.445862	-1.325931
48	6	0	6.507255	0.400196	1.269709
49	1	0	6.191093	1.445970	1.326260
50	1	0	6.150919	-0.104824	2.170979
51	1	0	7.601252	0.382867	1.278480
52	6	0	-3.129889	-0.588179	-1.206626
53	6	0	-0.601371	2.455001	1.206609
54	6	0	-0.405882	1.812238	2.563802
55	1	0	-1.338682	1.752293	3.128965
56	1	0	0.013181	0.809142	2.493153
57	1	0	0.290690	2.410298	3.156820
58	6	0	-2.457153	-0.734187	-2.556368
59	1	0	-2.803773	-1.654521	-3.035369
60	1	0	-2.701989	0.088795	-3.232572
61	1	0	-1.374046	-0.804091	-2.481715
62	6	0	-3.129975	-0.588105	1.206432
63	6	0	-2.457335	-0.734033	2.556230
64	1	0	-1.374221	-0.803915	2.481660
65	1	0	-2.702240	0.088975	3.232376
66	1	0	-2.803968	-1.654352	3.035248
67	6	0	-0.601290	2.454930	-1.206803
68	6	0	-0.405707	1.812086	-2.563945
69	1	0	0.013326	0.808984	-2.493208
70	1	0	-1.338463	1.752133	-3.129180
71	1	0	0.290926	2.410097	-3.156940

Compound 2a 2-RF-CC-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.21448733 A.U. after 1 cycles
Lowest frequency = -58.2549

Zero-point correction= 0.599961
(Hartree/Particle)
Thermal correction to Energy= 0.633616
Thermal correction to Enthalpy= 0.634560
Thermal correction to Gibbs Free Energy= 0.533600
Sum of electronic and zero-point Energies= -1358.614526
Sum of electronic and thermal Energies= -1358.580871
Sum of electronic and thermal Enthalpies= -1358.579927
Sum of electronic and thermal Free Energies= -1358.680887

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.909449	0.092190	0.000038
2	6	0	1.552036	6.026477	0.000225
3	1	0	2.629446	6.225932	0.000280

4	1	0	1.131524	6.510479	-0.884678
5	1	0	1.131444	6.510432	0.885116
6	6	0	1.279620	4.542617	0.000174
7	6	0	1.133860	3.829462	-1.185657
8	1	0	1.150502	4.365015	-2.131284
9	6	0	0.901790	1.703665	0.000081
10	6	0	1.133763	3.829398	1.185954
11	1	0	1.150328	4.364900	2.131611
12	6	0	4.392527	-1.262928	1.186368
13	1	0	4.888617	-1.467823	2.131699
14	6	0	5.106166	-1.406851	0.000167
15	6	0	4.392622	-1.262866	-1.186084
16	1	0	4.888788	-1.467710	-2.131387
17	6	0	2.356134	-0.614435	0.000078
18	6	0	6.577520	-1.740206	0.000217
19	1	0	6.857186	-2.317184	-0.884678
20	1	0	7.184564	-0.828010	0.000260
21	1	0	6.857118	-2.317224	0.885108
22	7	0	-0.311006	-0.667779	-0.000032
23	6	0	-0.443327	-2.098470	-0.000072
24	6	0	-1.654465	-0.156620	-0.000073
25	6	0	-1.807649	-2.452173	-0.000134
26	6	0	0.534834	-3.093995	-0.000057
27	6	0	-2.573463	-1.224015	-0.000135
28	6	0	-2.201189	-3.791129	-0.000181
29	6	0	0.126871	-4.426441	-0.000105
30	1	0	1.585423	-2.855267	-0.000010
31	6	0	-3.947932	-0.992380	-0.000184
32	6	0	-1.226020	-4.779712	-0.000167
33	1	0	-3.253359	-4.052907	-0.000229
34	1	0	0.883560	-5.202834	-0.000095
35	6	0	-4.435155	0.314809	-0.000173
36	1	0	-4.631843	-1.834462	-0.000231
37	1	0	-1.511483	-5.825388	-0.000203
38	6	0	-3.504786	1.364494	-0.000112
39	1	0	-3.868528	2.387011	-0.000103
40	6	0	-2.126899	1.154537	-0.000062
41	1	0	-1.459197	2.000092	-0.000016
42	6	0	-5.929114	0.607961	-0.000226
43	1	0	-6.037558	1.698493	-0.000203
44	6	0	-6.620091	0.077847	-1.269607
45	1	0	-7.677859	0.357565	-1.279075
46	1	0	-6.152438	0.481460	-2.171075
47	1	0	-6.564620	-1.013426	-1.325334
48	6	0	-6.620194	0.077783	1.269073
49	1	0	-6.564727	-1.013492	1.324750
50	1	0	-6.152614	0.481351	2.170599
51	1	0	-7.677962	0.357501	1.278470
52	6	0	3.044132	-0.897874	1.206633
53	6	0	0.932262	2.446969	-1.206619
54	6	0	0.655828	1.834839	-2.563879
55	1	0	1.573444	1.654646	-3.128326
56	1	0	0.110534	0.894364	-2.493447
57	1	0	0.042932	2.517967	-3.157384
58	6	0	2.357652	-0.957011	2.556068
59	1	0	2.584208	-1.913901	3.035270
60	1	0	2.704568	-0.171772	3.232460
61	1	0	1.274451	-0.888808	2.480571
62	6	0	3.044229	-0.897810	-1.206438
63	6	0	2.357857	-0.956875	-2.555930

64	1	0	1.274649	-0.888682	-2.480515
65	1	0	2.704821	-0.171595	-3.232250
66	1	0	2.584457	-1.913736	-3.035169
67	6	0	0.932164	2.446904	1.206825
68	6	0	0.655620	1.834700	2.564028
69	1	0	0.110321	0.894235	2.493502
70	1	0	1.573191	1.654464	3.128535
71	1	0	0.042686	2.517800	3.157527

Compound 2a 2-RF-CN-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.19619590 A.U. after 1 cycles
Lowest frequency = -39.0984

Zero-point correction= 0.599970
(Hartree/Particle)
Thermal correction to Energy= 0.633291
Thermal correction to Enthalpy= 0.634235
Thermal correction to Gibbs Free Energy= 0.534611
Sum of electronic and zero-point Energies= -1358.596225
Sum of electronic and thermal Energies= -1358.562905
Sum of electronic and thermal Enthalpies= -1358.561961
Sum of electronic and thermal Free Energies= -1358.661585

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.102454	-0.025810	-0.008633
2	6	0	4.835373	-4.510216	-1.116243
3	1	0	4.309988	-5.458415	-1.248204
4	1	0	5.442219	-4.324052	-2.005181
5	1	0	5.522334	-4.630707	-0.271078
6	6	0	3.874866	-3.378935	-0.858390
7	6	0	2.643415	-3.602413	-0.250919
8	1	0	2.369487	-4.618463	0.014100
9	6	0	2.068821	-1.213194	-0.310130
10	6	0	4.197529	-2.068281	-1.198613
11	1	0	5.149519	-1.872413	-1.681527
12	6	0	1.009414	3.481170	-1.746437
13	1	0	0.672235	3.892402	-2.694326
14	6	0	1.531789	4.338228	-0.781947
15	6	0	2.031812	3.757296	0.380064
16	1	0	2.508519	4.388530	1.125438
17	6	0	1.358061	1.522617	-0.332681
18	6	0	1.568888	5.831778	-0.993568
19	1	0	2.412578	6.288924	-0.470766
20	1	0	1.648963	6.083660	-2.053876
21	1	0	0.655514	6.303159	-0.614052
22	7	0	-0.239419	-0.281122	0.665825
23	6	0	-0.515742	-0.113097	2.027823
24	6	0	-1.477687	-0.373214	0.016279
25	6	0	-1.917152	-0.017508	2.234527
26	6	0	0.356015	-0.142736	3.121450
27	6	0	-2.532869	-0.185029	0.941897
28	6	0	-2.428303	0.130134	3.526885
29	6	0	-0.175115	-0.000522	4.398989

30	1	0	1.417307	-0.299921	2.991346
31	6	0	-3.863266	-0.260571	0.518665
32	6	0	-1.553884	0.152436	4.605170
33	1	0	-3.498330	0.209426	3.685692
34	1	0	0.493145	-0.024107	5.252731
35	6	0	-4.166104	-0.551157	-0.808392
36	1	0	-4.666892	-0.107941	1.232716
37	1	0	-1.937243	0.262309	5.612945
38	6	0	-3.100783	-0.793217	-1.698934
39	1	0	-3.318310	-1.063228	-2.726870
40	6	0	-1.769864	-0.718192	-1.306959
41	1	0	-0.987194	-0.951448	-2.014976
42	6	0	-5.613389	-0.633130	-1.274072
43	1	0	-6.238199	-0.413570	-0.400560
44	6	0	-5.935617	0.424782	-2.345114
45	1	0	-6.995456	0.392193	-2.616056
46	1	0	-5.705755	1.430913	-1.985732
47	1	0	-5.354537	0.255768	-3.256759
48	6	0	-5.988168	-2.044636	-1.761429
49	1	0	-5.410751	-2.325956	-2.647223
50	1	0	-5.795766	-2.791934	-0.987547
51	1	0	-7.048507	-2.093692	-2.027826
52	6	0	0.925411	2.100993	-1.549575
53	6	0	1.742871	-2.574633	0.029964
54	6	0	0.456707	-3.029225	0.691456
55	1	0	0.315935	-2.585398	1.677331
56	1	0	-0.425653	-2.786014	0.099158
57	1	0	0.480522	-4.113017	0.818354
58	6	0	0.424093	1.276007	-2.717426
59	1	0	0.787170	1.697404	-3.658754
60	1	0	0.770399	0.241020	-2.671717
61	1	0	-0.667157	1.261813	-2.765348
62	6	0	1.965298	2.381896	0.613783
63	6	0	2.631024	1.873136	1.876235
64	1	0	1.980120	1.975915	2.747477
65	1	0	2.920605	0.822909	1.796967
66	1	0	3.540489	2.445373	2.078351
67	6	0	3.343067	-0.996990	-0.945218
68	6	0	3.868849	0.352043	-1.390439
69	1	0	3.218126	0.832849	-2.120641
70	1	0	3.975023	1.052160	-0.561820
71	1	0	4.851050	0.226731	-1.849571

Compound 2a 2-RF-CN-TSa excited state

Method: cam-b3lyp/6-31G(d)
SCF Done: E(RCAM-B3LYP) = -1358.06569338 A.U. after 1 cycles
Lowest frequency = -25.8459

Zero-point correction= 0.610207
(Hartree/Particle)
Thermal correction to Energy= 0.642946
Thermal correction to Enthalpy= 0.643890
Thermal correction to Gibbs Free Energy= 0.545304
Sum of electronic and zero-point Energies= -1357.348407
Sum of electronic and thermal Energies= -1357.315669
Sum of electronic and thermal Enthalpies= -1357.314724
Sum of electronic and thermal Free Energies= -1357.413311

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.143555	-0.000576	-0.033973
2	6	0	5.126884	-4.299396	-1.043957
3	1	0	6.061583	-4.111095	-0.501847
4	1	0	4.756956	-5.280085	-0.730327
5	1	0	5.386923	-4.367537	-2.106882
6	6	0	4.104669	-3.224191	-0.787017
7	6	0	2.894889	-3.489174	-0.162494
8	1	0	2.679579	-4.510903	0.145086
9	6	0	2.152431	-1.139796	-0.286638
10	6	0	4.327744	-1.899357	-1.165290
11	1	0	5.263801	-1.648810	-1.661853
12	6	0	0.648544	3.467070	-1.838855
13	1	0	0.262730	3.821505	-2.792981
14	6	0	1.090089	4.394222	-0.902452
15	6	0	1.657904	3.895931	0.263933
16	1	0	2.077280	4.592466	0.987639
17	6	0	1.211593	1.578106	-0.386552
18	6	0	0.977186	5.875341	-1.150370
19	1	0	1.023788	6.106794	-2.218517
20	1	0	0.024414	6.267525	-0.774848
21	1	0	1.775615	6.427289	-0.645869
22	7	0	-0.203280	-0.254040	0.671909
23	6	0	-0.476889	-0.058671	2.036616
24	6	0	-1.437628	-0.453457	0.054722
25	6	0	-1.867788	-0.017816	2.265393
26	6	0	0.431488	-0.004967	3.084221
27	6	0	-2.495482	-0.277109	0.971235
28	6	0	-2.356888	0.157954	3.542433
29	6	0	-0.073602	0.162734	4.375108
30	1	0	1.490931	-0.118399	2.903681
31	6	0	-3.802003	-0.434966	0.564064
32	6	0	-1.442009	0.261232	4.599724
33	1	0	-3.423984	0.198314	3.734221
34	1	0	0.613917	0.208636	5.212451
35	6	0	-4.076562	-0.805943	-0.764597
36	1	0	-4.622253	-0.292369	1.261256
37	1	0	-1.811099	0.397054	5.610582
38	6	0	-3.010451	-1.031661	-1.642680
39	1	0	-3.215103	-1.354135	-2.658103
40	6	0	-1.686940	-0.864608	-1.251799
41	1	0	-0.871061	-1.075175	-1.928415
42	6	0	-5.510975	-0.980451	-1.221378
43	1	0	-6.152909	-0.755661	-0.361990
44	6	0	-5.867649	0.006471	-2.340169
45	1	0	-6.922780	-0.095573	-2.612106
46	1	0	-5.693409	1.040671	-2.029048
47	1	0	-5.271474	-0.180508	-3.239273
48	6	0	-5.795839	-2.425621	-1.649575
49	1	0	-5.199652	-2.706418	-2.523836
50	1	0	-5.568227	-3.131335	-0.845272
51	1	0	-6.851264	-2.539389	-1.915623
52	6	0	0.706245	2.093050	-1.606756
53	6	0	1.935936	-2.508722	0.090800
54	6	0	0.679147	-2.995797	0.773484
55	1	0	0.509499	-2.515588	1.741901

56	1	0	-0.218812	-2.832626	0.169736
57	1	0	0.746063	-4.071463	0.959877
58	6	0	0.283235	1.204285	-2.752221
59	1	0	0.582336	1.650474	-3.706142
60	1	0	0.741469	0.215623	-2.681716
61	1	0	-0.803183	1.071573	-2.791638
62	6	0	1.731292	2.528368	0.528004
63	6	0	2.463919	2.130055	1.787024
64	1	0	1.819308	2.174478	2.671244
65	1	0	2.864265	1.116856	1.712774
66	1	0	3.299475	2.813418	1.969409
67	6	0	3.412216	-0.883126	-0.939114
68	6	0	3.822064	0.490387	-1.418475
69	1	0	3.126158	0.900306	-2.155294
70	1	0	3.873053	1.219036	-0.605017
71	1	0	4.810633	0.443943	-1.884987

Compound 2a 2-RF-CN-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.19597045 A.U. after 1 cycles
Lowest frequency = -39.0870

Zero-point correction= 0.599954
(Hartree/Particle)
Thermal correction to Energy= 0.633275
Thermal correction to Enthalpy= 0.634220
Thermal correction to Gibbs Free Energy= 0.534403
Sum of electronic and zero-point Energies= -1358.596017
Sum of electronic and thermal Energies= -1358.562695
Sum of electronic and thermal Enthalpies= -1358.561751
Sum of electronic and thermal Free Energies= -1358.661568

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.137076	-0.018486	-0.006587
2	6	0	5.062242	-4.357199	-1.026070
3	1	0	4.573795	-5.309126	-1.244699
4	1	0	5.731822	-4.113512	-1.853948
5	1	0	5.683694	-4.504367	-0.135632
6	6	0	4.055178	-3.261899	-0.791526
7	6	0	2.787476	-3.542559	-0.291872
8	1	0	2.521443	-4.576162	-0.095570
9	6	0	2.155462	-1.167214	-0.285850
10	6	0	4.367954	-1.929324	-1.044791
11	1	0	5.348565	-1.688624	-1.442697
12	6	0	1.080362	3.563228	-1.585828
13	1	0	0.804616	4.010505	-2.537256
14	6	0	1.505185	4.386104	-0.546534
15	6	0	1.931668	3.763210	0.623005
16	1	0	2.333464	4.369805	1.430391
17	6	0	1.374423	1.549241	-0.239206
18	6	0	1.517854	5.888384	-0.687413
19	1	0	2.306851	6.340292	-0.081294
20	1	0	1.671226	6.191355	-1.726067
21	1	0	0.565946	6.319908	-0.358568

22	7	0	-0.245307	-0.337117	0.548548
23	6	0	-0.630244	-0.236044	1.890871
24	6	0	-1.426781	-0.428503	-0.199806
25	6	0	-2.044964	-0.180147	1.991962
26	6	0	0.155539	-0.295668	3.046547
27	6	0	-2.556058	-0.303625	0.648832
28	6	0	-2.657340	-0.101689	3.245452
29	6	0	-0.475490	-0.222218	4.283982
30	1	0	1.227299	-0.423965	2.992549
31	6	0	-3.847047	-0.388052	0.124475
32	6	0	-1.869196	-0.108611	4.388782
33	1	0	-3.738071	-0.053037	3.323884
34	1	0	0.125743	-0.269412	5.185265
35	6	0	-4.039789	-0.625762	-1.236192
36	1	0	-4.699631	-0.283846	0.787779
37	1	0	-2.331517	-0.052318	5.367404
38	6	0	-2.905435	-0.804868	-2.048139
39	1	0	-3.046779	-1.032099	-3.100179
40	6	0	-1.607581	-0.720610	-1.553296
41	1	0	-0.768736	-0.905978	-2.209192
42	6	0	-5.436029	-0.718708	-1.838039
43	1	0	-5.306936	-0.930214	-2.905859
44	6	0	-6.252598	-1.877625	-1.238112
45	1	0	-7.224835	-1.963779	-1.733140
46	1	0	-5.726938	-2.829220	-1.350158
47	1	0	-6.436649	-1.722696	-0.170803
48	6	0	-6.200958	0.612516	-1.724355
49	1	0	-6.377375	0.878957	-0.677922
50	1	0	-5.639861	1.429556	-2.184726
51	1	0	-7.174680	0.544597	-2.219405
52	6	0	1.018773	2.173755	-1.458244
53	6	0	1.841211	-2.550412	-0.034239
54	6	0	0.521448	-3.065283	0.505765
55	1	0	0.294455	-2.670471	1.496419
56	1	0	-0.319719	-2.816129	-0.141498
57	1	0	0.565039	-4.152885	0.586470
58	6	0	0.628108	1.392752	-2.696387
59	1	0	1.045433	1.868106	-3.588208
60	1	0	1.000814	0.366217	-2.672651
61	1	0	-0.455912	1.351810	-2.824676
62	6	0	1.885270	2.377128	0.788604
63	6	0	2.467818	1.825373	2.073932
64	1	0	1.749982	1.869812	2.896109
65	1	0	2.792763	0.787768	1.969118
66	1	0	3.342451	2.410004	2.371669
67	6	0	3.468330	-0.891408	-0.809395
68	6	0	3.990043	0.489351	-1.149450
69	1	0	3.385714	0.988352	-1.906871
70	1	0	4.010790	1.151651	-0.284076
71	1	0	5.008513	0.409714	-1.533650

Compound 2a 3-RF-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.15244754 A.U. after 1 cycles
Lowest frequency = -59.9356

Zero-point correction= 0.600073
(Hartree/Particle)

Thermal correction to Energy= 0.633623
Thermal correction to Enthalpy= 0.634567
Thermal correction to Gibbs Free Energy= 0.533270
Sum of electronic and zero-point Energies= -1358.552375
Sum of electronic and thermal Energies= -1358.518825
Sum of electronic and thermal Enthalpies= -1358.517881
Sum of electronic and thermal Free Energies= -1358.619178

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.918705	-1.619468	1.712494
2	6	0	-2.593497	-0.931541	0.643794
3	6	0	-1.598462	-0.548000	-0.281318
4	7	0	-0.303617	-0.888627	0.196188
5	6	0	-0.542159	-1.647910	1.378728
6	6	0	0.330509	-2.398244	2.165724
7	6	0	-0.159430	-3.050977	3.293524
8	6	0	-2.395860	-2.272029	2.851283
9	6	0	-3.949625	-0.743811	0.364908
10	6	0	-4.349911	-0.218211	-0.859258
11	6	0	-3.353101	0.061891	-1.811828
12	6	0	-1.999246	-0.112694	-1.547951
13	6	0	-5.824176	-0.005030	-1.171047
14	6	0	-6.148316	1.479669	-1.417498
15	6	0	-6.303094	-0.878487	-2.344793
16	1	0	1.359612	-2.523908	1.892325
17	1	0	0.524213	-3.641874	3.893077
18	1	0	-3.452156	-2.237599	3.094495
19	1	0	-4.696328	-1.039676	1.095225
20	1	0	-3.640590	0.402978	-2.800561
21	1	0	-1.289500	0.039745	-2.344361
22	1	0	-6.382962	-0.318448	-0.281689
23	1	0	-7.222215	1.620645	-1.573309
24	1	0	-5.842839	2.095745	-0.568158
25	1	0	-5.631171	1.855731	-2.305364
26	1	0	-7.378837	-0.755952	-2.503096
27	1	0	-6.104294	-1.936259	-2.155543
28	1	0	-5.798402	-0.605646	-3.276338
29	5	0	0.973398	-0.086443	-0.030020
30	6	0	2.298216	-0.752506	-0.723186
31	6	0	3.389556	-1.529756	-0.227098
32	6	0	2.383367	-0.418017	-2.106192
33	6	0	4.486267	-1.816649	-1.053134
34	6	0	3.487294	-0.740419	-2.893587
35	6	0	4.579233	-1.424096	-2.380550
36	1	0	5.303388	-2.390024	-0.625650
37	1	0	3.480179	-0.442236	-3.938591
38	6	0	1.031130	1.486136	0.429751
39	6	0	1.753799	1.700049	1.642717
40	6	0	0.490397	2.665083	-0.166913
41	6	0	1.949522	2.973302	2.175758
42	6	0	0.733272	3.925221	0.399027
43	6	0	1.466658	4.118657	1.558445
44	1	0	2.494263	3.060585	3.111450
45	1	0	0.306432	4.792338	-0.095713
46	6	0	1.244561	0.238185	-2.842797
47	1	0	0.663879	-0.511776	-3.390740

48	1	0	0.564164	0.759607	-2.181991
49	1	0	1.606886	0.970857	-3.568128
50	6	0	3.508929	-2.214274	1.123972
51	1	0	3.027480	-1.704633	1.945596
52	1	0	3.099269	-3.228612	1.062742
53	1	0	4.562577	-2.320543	1.390710
54	6	0	5.801882	-1.715820	-3.213299
55	1	0	6.503560	-0.874825	-3.186494
56	1	0	6.333223	-2.597256	-2.847072
57	1	0	5.539408	-1.887494	-4.260152
58	6	0	-0.365076	2.749247	-1.416925
59	1	0	0.242133	2.819764	-2.324209
60	1	0	-1.055835	1.921710	-1.523387
61	1	0	-0.972338	3.655255	-1.375413
62	6	0	2.356861	0.577739	2.451055
63	1	0	1.708550	-0.296565	2.506555
64	1	0	3.323824	0.281171	2.040137
65	1	0	2.525806	0.900979	3.480086
66	6	0	1.723740	5.493511	2.121626
67	1	0	1.666720	5.494087	3.213296
68	1	0	2.723501	5.848500	1.848198
69	1	0	1.001838	6.220658	1.743399
70	6	0	-1.509654	-2.977629	3.652588
71	1	0	-1.864395	-3.493176	4.537317

Compound 2a 3-RF-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1359.15226002 A.U. after 1 cycles
Lowest frequency = -59.7055

Zero-point correction= 0.600068
(Hartree/Particle)
Thermal correction to Energy= 0.633609
Thermal correction to Enthalpy= 0.634554
Thermal correction to Gibbs Free Energy= 0.533182
Sum of electronic and zero-point Energies= -1358.552192
Sum of electronic and thermal Energies= -1358.518651
Sum of electronic and thermal Enthalpies= -1358.517706
Sum of electronic and thermal Free Energies= -1358.619078

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.053729	-1.431745	1.578653
2	6	0	-2.627668	-0.799353	0.419389
3	6	0	-1.554295	-0.507624	-0.453076
4	7	0	-0.309561	-0.849097	0.142660
5	6	0	-0.658546	-1.520988	1.350668
6	6	0	0.129631	-2.242318	2.246235
7	6	0	-0.461632	-2.804064	3.374622
8	6	0	-2.632969	-1.992786	2.718520
9	6	0	-3.951920	-0.594835	0.031360
10	6	0	-4.244106	-0.140278	-1.253694
11	6	0	-3.173500	0.046470	-2.142413
12	6	0	-1.846070	-0.148931	-1.770068
13	6	0	-5.676574	0.098880	-1.710556

14	6	0	-6.520571	-1.188098	-1.675571
15	6	0	-6.352157	1.225704	-0.908220
16	1	0	1.170791	-2.415655	2.057481
17	1	0	0.157016	-3.373073	4.059823
18	1	0	-3.702357	-1.912539	2.880094
19	1	0	-4.751905	-0.824649	0.727352
20	1	0	-3.386762	0.330514	-3.168059
21	1	0	-1.076565	-0.070544	-2.520453
22	1	0	-5.625201	0.426853	-2.755159
23	1	0	-7.523801	-1.003049	-2.071349
24	1	0	-6.058815	-1.978833	-2.272051
25	1	0	-6.631303	-1.563005	-0.653779
26	1	0	-7.356481	1.426892	-1.293294
27	1	0	-5.773376	2.151010	-0.963740
28	1	0	-6.448107	0.956331	0.147849
29	5	0	1.001609	-0.091598	-0.037614
30	6	0	2.356485	-0.828493	-0.585414
31	6	0	3.384777	-1.598063	0.040435
32	6	0	2.556576	-0.582734	-1.975075
33	6	0	4.533872	-1.959633	-0.677906
34	6	0	3.708999	-0.977509	-2.652451
35	6	0	4.739512	-1.651787	-2.015033
36	1	0	5.299742	-2.523627	-0.153926
37	1	0	3.790320	-0.744905	-3.710874
38	6	0	1.065025	1.505782	0.325966
39	6	0	1.698502	1.780622	1.576164
40	6	0	0.600576	2.655481	-0.381480
41	6	0	1.881902	3.080383	2.045602
42	6	0	0.827419	3.943411	0.125790
43	6	0	1.472992	4.194269	1.325582
44	1	0	2.355973	3.215161	3.013578
45	1	0	0.460585	4.786211	-0.452108
46	6	0	1.494887	0.049357	-2.837132
47	1	0	0.937964	-0.721706	-3.380476
48	1	0	0.780229	0.626403	-2.264693
49	1	0	1.930297	0.725919	-3.576629
50	6	0	3.379706	-2.200503	1.435005
51	1	0	2.851613	-1.629036	2.184114
52	1	0	2.945969	-3.206122	1.402364
53	1	0	4.406056	-2.316379	1.789666
54	6	0	6.014683	-2.021101	-2.729854
55	1	0	6.737854	-1.199028	-2.690164
56	1	0	6.487691	-2.895201	-2.276377
57	1	0	5.830863	-2.242424	-3.784097
58	6	0	-0.148915	2.679255	-1.700381
59	1	0	0.532019	2.685667	-2.556679
60	1	0	-0.846113	1.858458	-1.816012
61	1	0	-0.737954	3.596126	-1.761634
62	6	0	2.213706	0.699019	2.493505
63	1	0	1.538962	-0.154511	2.558120
64	1	0	3.197846	0.353876	2.170741
65	1	0	2.320808	1.083837	3.509541
66	6	0	1.716150	5.596094	1.824862
67	1	0	1.560444	5.667160	2.904586
68	1	0	2.746071	5.910850	1.623735
69	1	0	1.051888	6.313485	1.338045
70	6	0	-1.830755	-2.668173	3.627466
71	1	0	-2.265338	-3.113059	4.514912

Compound Z-2b GS1

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1319.90432820 A.U. after 1 cycles
Lowest frequency = 21.2990

Zero-point correction= 0.572511
(Hartree/Particle)
Thermal correction to Energy= 0.605338
Thermal correction to Enthalpy= 0.606283
Thermal correction to Gibbs Free Energy= 0.507025
Sum of electronic and zero-point Energies= -1319.331817
Sum of electronic and thermal Energies= -1319.298990
Sum of electronic and thermal Enthalpies= -1319.298046
Sum of electronic and thermal Free Energies= -1319.397303

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.177427	0.038005	0.021389
2	6	0	3.712307	0.326221	-1.669237
3	1	0	3.006374	-0.086707	-2.396093
4	1	0	3.428108	1.366667	-1.499296
5	1	0	4.699767	0.317107	-2.134735
6	6	0	1.988631	2.005814	2.230251
7	1	0	2.230803	2.846186	2.883604
8	1	0	1.218599	1.413733	2.733657
9	1	0	2.876651	1.375978	2.147302
10	6	0	0.149088	1.320657	-2.519195
11	1	0	0.723469	0.402792	-2.652204
12	1	0	-0.893712	1.025641	-2.366853
13	1	0	0.198072	1.881404	-3.455025
14	6	0	1.075924	5.923037	-0.766923
15	1	0	0.876266	6.467029	0.159444
16	1	0	2.053381	6.254214	-1.135112
17	1	0	0.329665	6.223450	-1.506017
18	6	0	1.061017	4.430628	-0.543550
19	6	0	1.484019	3.878890	0.665245
20	1	0	1.798901	4.540775	1.466968
21	6	0	1.522015	2.499691	0.877267
22	6	0	1.094497	1.611779	-0.141689
23	6	0	0.648799	2.169496	-1.367326
24	6	0	0.651904	3.554649	-1.546661
25	1	0	0.319583	3.959228	-2.498598
26	6	0	2.640178	-1.445639	1.573395
27	6	0	3.867685	-1.995448	1.953617
28	1	0	3.925332	-2.578506	2.867145
29	6	0	5.006379	-1.810366	1.180857
30	6	0	4.927344	-1.056786	0.016224
31	1	0	5.813277	-0.912938	-0.593629
32	6	0	3.722999	-0.471061	-0.382388
33	6	0	2.551811	-0.662855	0.393246
34	6	0	1.442699	-1.729463	2.457648
35	1	0	0.840454	-2.548575	2.052509
36	1	0	1.768974	-2.025397	3.456966
37	1	0	0.779365	-0.870189	2.566317
38	7	0	-0.010033	-0.768474	-0.169728
39	6	0	-0.066323	-2.128431	-0.590750

40	6	0	-1.361608	-0.363432	0.033064
41	6	0	-1.410598	-2.554580	-0.654569
42	6	0	0.964270	-2.985009	-0.983132
43	6	0	-2.231720	-1.435361	-0.244254
44	6	0	-1.726406	-3.847597	-1.077707
45	6	0	0.631812	-4.271635	-1.398410
46	1	0	1.997453	-2.672631	-0.963533
47	6	0	-3.611985	-1.292764	-0.081906
48	6	0	-0.698429	-4.706596	-1.443199
49	1	0	-2.759964	-4.171968	-1.125715
50	1	0	1.425777	-4.946773	-1.697011
51	6	0	-4.143109	-0.086513	0.366322
52	1	0	-4.272495	-2.126336	-0.299110
53	1	0	-0.924438	-5.713924	-1.773533
54	6	0	-3.253624	0.964674	0.658242
55	1	0	-3.646179	1.908884	1.019749
56	6	0	-1.876552	0.844556	0.507655
57	1	0	-1.233388	1.677355	0.749742
58	6	0	-5.645636	0.081059	0.544336
59	1	0	-6.105951	-0.871247	0.256745
60	6	0	-6.026829	0.350339	2.011380
61	1	0	-7.113964	0.401012	2.124786
62	1	0	-5.651890	-0.439343	2.667222
63	1	0	-5.611934	1.299999	2.361885
64	6	0	-6.218289	1.166760	-0.384828
65	1	0	-5.810499	2.152521	-0.142200
66	1	0	-5.980506	0.956092	-1.430494
67	1	0	-7.306618	1.224121	-0.287025
68	1	0	5.950741	-2.248638	1.485155

Compound Z-2b GS2

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1319.90414102 A.U. after 1 cycles
Lowest frequency = 19.8828

Zero-point correction= 0.572546
(Hartree/Particle)
Thermal correction to Energy= 0.605332
Thermal correction to Enthalpy= 0.606276
Thermal correction to Gibbs Free Energy= 0.507070
Sum of electronic and zero-point Energies= -1319.331595
Sum of electronic and thermal Energies= -1319.298809
Sum of electronic and thermal Enthalpies= -1319.297865
Sum of electronic and thermal Free Energies= -1319.397071

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.196821	-0.075094	0.025359
2	6	0	3.706826	-0.177897	-1.723672
3	1	0	2.926163	-0.452243	-2.439543
4	1	0	3.604231	0.891572	-1.529029
5	1	0	4.668490	-0.341729	-2.213777
6	6	0	2.372342	1.683284	2.247148
7	1	0	2.765725	2.457511	2.908634
8	1	0	1.524218	1.218481	2.758591

9	1	0	3.139949	0.915302	2.132628
10	6	0	0.343601	1.413296	-2.466421
11	1	0	0.759639	0.418859	-2.634461
12	1	0	-0.728608	1.285082	-2.288749
13	1	0	0.457378	1.981277	-3.392175
14	6	0	2.069107	5.758530	-0.661890
15	1	0	1.982591	6.309481	0.277747
16	1	0	3.080679	5.928400	-1.047295
17	1	0	1.369185	6.194781	-1.378270
18	6	0	1.807943	4.285561	-0.462886
19	6	0	2.157592	3.646187	0.725976
20	1	0	2.596147	4.229387	1.530682
21	6	0	1.967495	2.276098	0.914150
22	6	0	1.375417	1.493558	-0.108776
23	6	0	1.003610	2.143025	-1.313662
24	6	0	1.235908	3.511353	-1.470085
25	1	0	0.956069	3.985355	-2.406729
26	6	0	2.424923	-1.814738	1.513813
27	6	0	3.551623	-2.568794	1.853811
28	1	0	3.531081	-3.172470	2.755463
29	6	0	4.688266	-2.559106	1.056313
30	6	0	4.710622	-1.778361	-0.092751
31	1	0	5.594744	-1.770758	-0.721842
32	6	0	3.612258	-0.992541	-0.451220
33	6	0	2.442518	-1.003380	0.349897
34	6	0	1.216444	-1.914186	2.422695
35	1	0	0.475944	-2.610574	2.017146
36	1	0	1.510000	-2.284345	3.407309
37	1	0	0.710123	-0.958381	2.565212
38	7	0	-0.112885	-0.667337	-0.149094
39	6	0	-0.405968	-1.989572	-0.592089
40	6	0	-1.372520	-0.045328	0.093893
41	6	0	-1.803447	-2.183586	-0.630455
42	6	0	0.457822	-2.997908	-1.024340
43	6	0	-2.417499	-0.951448	-0.181199
44	6	0	-2.340411	-3.396195	-1.068018
45	6	0	-0.094286	-4.201837	-1.453549
46	1	0	1.528878	-2.862964	-1.024837
47	6	0	-3.749549	-0.586594	0.014527
48	6	0	-1.479138	-4.407308	-1.473322
49	1	0	-3.414509	-3.542164	-1.096340
50	1	0	0.568833	-4.993657	-1.783172
51	6	0	-4.061530	0.685026	0.495896
52	1	0	-4.537271	-1.299995	-0.203652
53	1	0	-1.877870	-5.355413	-1.815363
54	6	0	-3.004028	1.563608	0.783530
55	1	0	-3.234958	2.551413	1.169224
56	6	0	-1.667059	1.219931	0.599905
57	1	0	-0.889959	1.929583	0.841260
58	6	0	-5.503967	1.119933	0.717586
59	1	0	-5.469550	2.144962	1.103901
60	6	0	-6.303822	1.151969	-0.597384
61	1	0	-7.316377	1.529364	-0.425216
62	1	0	-5.821062	1.795663	-1.336919
63	1	0	-6.391231	0.151926	-1.032511
64	6	0	-6.212584	0.254886	1.775541
65	1	0	-6.299096	-0.784617	1.445451
66	1	0	-5.663841	0.259480	2.720597
67	1	0	-7.223509	0.627922	1.965709
68	1	0	5.552820	-3.154466	1.329439

Compound E-2b GS1

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1319.90432873 A.U. after 1 cycles
Lowest frequency = 20.9114

Zero-point correction= 0.572485
(Hartree/Particle)
Thermal correction to Energy= 0.605318
Thermal correction to Enthalpy= 0.606262
Thermal correction to Gibbs Free Energy= 0.506982
Sum of electronic and zero-point Energies= -1319.331844
Sum of electronic and thermal Energies= -1319.299011
Sum of electronic and thermal Enthalpies= -1319.298066
Sum of electronic and thermal Free Energies= -1319.397347

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.940970	0.445629	-0.110898
2	6	0	3.352769	1.032308	-1.912855
3	1	0	2.677703	0.518476	-2.603628
4	1	0	2.945135	2.031616	-1.747241
5	1	0	4.314376	1.139714	-2.418337
6	6	0	1.557663	2.554761	2.019936
7	1	0	1.704012	3.434348	2.649841
8	1	0	0.890172	1.875978	2.559176
9	1	0	2.519373	2.047750	1.918548
10	6	0	-0.328988	1.498799	-2.642080
11	1	0	0.356690	0.659896	-2.769491
12	1	0	-1.317920	1.074996	-2.441540
13	1	0	-0.386086	2.028625	-3.595333
14	6	0	0.236608	4.744854	-0.776635
15	6	0	0.766725	4.310346	0.431972
16	1	0	1.020769	5.033642	1.199968
17	6	0	0.987279	2.952174	0.675108
18	6	0	0.645416	1.992079	-0.310559
19	6	0	0.091551	2.445158	-1.535773
20	6	0	-0.091801	3.813697	-1.752909
21	1	0	-0.500945	4.148254	-2.700810
22	6	0	2.656000	-0.799518	1.392064
23	6	0	3.960698	-1.173290	1.722579
24	1	0	4.128523	-1.728680	2.641089
25	6	0	5.048714	-0.862173	0.910166
26	6	0	4.799234	-0.146587	-0.260551
27	1	0	5.629300	0.099841	-0.916502
28	6	0	3.515007	0.269673	-0.615057
29	6	0	2.408692	-0.058046	0.208650
30	6	0	1.550624	-1.226547	2.337002
31	1	0	1.053467	-2.132366	1.976311
32	1	0	1.958694	-1.447995	3.325476
33	1	0	0.777682	-0.466646	2.459799
34	7	0	-0.142021	-0.509377	-0.220387
35	6	0	-0.043617	-1.876683	-0.609216
36	6	0	-1.524561	-0.270737	0.030960
37	6	0	-1.325140	-2.468640	-0.605919

38	6	0	1.069855	-2.608175	-1.027436
39	6	0	-2.263514	-1.449786	-0.185627
40	6	0	-1.492640	-3.801862	-0.987059
41	6	0	0.885305	-3.936808	-1.400285
42	1	0	2.055228	-2.168287	-1.058969
43	6	0	-3.643405	-1.475530	0.031121
44	6	0	-0.380379	-4.535449	-1.378006
45	1	0	-2.478331	-4.253712	-0.983335
46	1	0	1.745154	-4.515396	-1.718538
47	6	0	-4.303825	-0.332702	0.473737
48	1	0	-4.202197	-2.390332	-0.139728
49	1	0	-0.491035	-5.571614	-1.676392
50	6	0	-3.542554	0.828485	0.704785
51	1	0	-4.036180	1.726147	1.060916
52	6	0	-2.168099	0.876269	0.499790
53	1	0	-1.626013	1.788979	0.696821
54	6	0	-5.807822	-0.347654	0.708474
55	1	0	-6.155264	-1.358765	0.466757
56	6	0	-6.165872	-0.079538	2.181513
57	1	0	-7.245839	-0.161401	2.337246
58	1	0	-5.670663	-0.794003	2.843798
59	1	0	-5.861787	0.925647	2.488105
60	6	0	-6.545727	0.627195	-0.227110
61	1	0	-6.255520	1.663344	-0.029528
62	1	0	-6.322177	0.412823	-1.275161
63	1	0	-7.628339	0.552628	-0.086710
64	1	0	0.082812	5.803319	-0.956915
65	6	0	6.452591	-1.258047	1.297173
66	1	0	7.062542	-1.475785	0.417050
67	1	0	6.949891	-0.450745	1.846352
68	1	0	6.455328	-2.140964	1.940379

Compound E-2b GS2

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1319.90414446 A.U. after 1 cycles
Lowest frequency = 19.4776

Zero-point correction= 0.572508
(Hartree/Particle)
Thermal correction to Energy= 0.605326
Thermal correction to Enthalpy= 0.606270
Thermal correction to Gibbs Free Energy= 0.506972
Sum of electronic and zero-point Energies= -1319.331636
Sum of electronic and thermal Energies= -1319.298819
Sum of electronic and thermal Enthalpies= -1319.297875
Sum of electronic and thermal Free Energies= -1319.397172

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.993652	0.441601	-0.090294
2	6	0	3.421282	0.824715	-1.925803
3	1	0	2.690004	0.396024	-2.617527
4	1	0	3.114603	1.854068	-1.729637
5	1	0	4.381516	0.851726	-2.444404
6	6	0	1.858671	2.422658	2.077086

7	1	0	2.106275	3.266544	2.723932
8	1	0	1.134710	1.802654	2.614223
9	1	0	2.761018	1.822388	1.944097
10	6	0	-0.205585	1.682181	-2.570181
11	1	0	0.393096	0.785027	-2.734334
12	1	0	-1.226710	1.350317	-2.358164
13	1	0	-0.230075	2.241048	-3.508114
14	6	0	0.716732	4.805874	-0.639160
15	6	0	1.221434	4.289230	0.547747
16	1	0	1.560749	4.963225	1.327554
17	6	0	1.307738	2.909905	0.753903
18	6	0	0.853257	2.014761	-0.247162
19	6	0	0.327038	2.552731	-1.450039
20	6	0	0.279016	3.937891	-1.630676
21	1	0	-0.110630	4.336197	-2.561999
22	6	0	2.598090	-1.009581	1.348596
23	6	0	3.862855	-1.523814	1.643500
24	1	0	3.988727	-2.117097	2.544859
25	6	0	4.962655	-1.305209	0.816817
26	6	0	4.767760	-0.537703	-0.331080
27	1	0	5.607127	-0.360785	-0.997547
28	6	0	3.527120	0.016978	-0.649653
29	6	0	2.407706	-0.216540	0.188248
30	6	0	1.471275	-1.344242	2.305336
31	1	0	0.871124	-2.178713	1.929672
32	1	0	1.871836	-1.639837	3.277331
33	1	0	0.788666	-0.508970	2.468083
34	7	0	-0.182590	-0.395474	-0.201127
35	6	0	-0.231096	-1.755484	-0.624140
36	6	0	-1.528938	-0.023804	0.084288
37	6	0	-1.565519	-2.214901	-0.608600
38	6	0	0.794610	-2.584700	-1.082578
39	6	0	-2.389002	-1.117668	-0.144950
40	6	0	-1.874364	-3.513795	-1.018190
41	6	0	0.469433	-3.877703	-1.483677
42	1	0	1.818889	-2.246211	-1.123578
43	6	0	-3.758565	-1.012760	0.097654
44	6	0	-0.849746	-4.345784	-1.449805
45	1	0	-2.900585	-3.863775	-1.005072
46	1	0	1.260259	-4.531609	-1.833525
47	6	0	-4.292474	0.182224	0.580496
48	1	0	-4.401419	-1.867286	-0.085482
49	1	0	-1.070553	-5.357242	-1.770874
50	6	0	-3.414589	1.251788	0.821590
51	1	0	-3.817612	2.182498	1.207825
52	6	0	-2.043659	1.168579	0.591123
53	1	0	-1.410277	2.017996	0.798555
54	6	0	-5.782986	0.334781	0.852516
55	1	0	-5.933497	1.353259	1.228215
56	6	0	-6.619827	0.191197	-0.431642
57	1	0	-7.679453	0.369300	-0.224773
58	1	0	-6.296761	0.903890	-1.194525
59	1	0	-6.527914	-0.813803	-0.854252
60	6	0	-6.273546	-0.633619	1.943983
61	1	0	-6.169248	-1.675448	1.626589
62	1	0	-5.703163	-0.508301	2.867687
63	1	0	-7.330150	-0.459336	2.168703
64	1	0	0.667391	5.878741	-0.790937
65	6	0	6.324699	-1.853446	1.165657
66	1	0	6.893830	-2.108234	0.268307

67	1	0	6.911878	-1.116941	1.725505
68	1	0	6.247385	-2.749442	1.785737

Compound 2b 2-RF-CC-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1319.88671230 A.U. after 1 cycles
Lowest frequency = -60.7239

Zero-point correction= 0.572785
(Hartree/Particle)
Thermal correction to Energy= 0.604546
Thermal correction to Enthalpy= 0.605490
Thermal correction to Gibbs Free Energy= 0.509033
Sum of electronic and zero-point Energies= -1319.313927
Sum of electronic and thermal Energies= -1319.282166
Sum of electronic and thermal Enthalpies= -1319.281222
Sum of electronic and thermal Free Energies= -1319.377679

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.899676	0.351328	0.000043
2	6	0	0.592150	4.782654	0.000173
3	6	0	0.556814	4.076355	-1.192686
4	1	0	0.498490	4.611731	-2.135431
5	6	0	0.642687	1.943610	0.000084
6	6	0	0.556731	4.076279	1.192985
7	1	0	0.498341	4.611595	2.135760
8	6	0	4.551703	-0.442777	1.186301
9	1	0	5.073671	-0.567873	2.131596
10	6	0	5.279101	-0.473173	0.000172
11	6	0	4.551787	-0.442701	-1.186006
12	1	0	5.073822	-0.567736	-2.131273
13	6	0	2.439011	-0.120396	0.000083
14	6	0	6.784455	-0.572261	0.000222
15	1	0	7.150936	-1.098343	-0.884684
16	1	0	7.241192	0.423708	0.000274
17	1	0	7.150873	-1.098407	0.885117
18	7	0	-0.188106	-0.587974	-0.000025
19	6	0	-0.096679	-2.021840	-0.000070
20	6	0	-1.594563	-0.292021	-0.000065
21	6	0	-1.390022	-2.582342	-0.000135
22	6	0	1.023992	-2.853552	-0.000058
23	6	0	-2.335721	-1.487313	-0.000132
24	6	0	-1.571484	-3.966223	-0.000188
25	6	0	0.827230	-4.233076	-0.000112
26	1	0	2.024861	-2.454691	-0.000009
27	6	0	-3.731566	-1.467896	-0.000180
28	6	0	-0.454770	-4.791537	-0.000176
29	1	0	-2.570402	-4.387753	-0.000238
30	1	0	1.694922	-4.883036	-0.000103
31	6	0	-4.414429	-0.254621	-0.000163
32	1	0	-4.286200	-2.400885	-0.000232
33	1	0	-0.574715	-5.868822	-0.000217
34	6	0	-3.657044	0.929456	-0.000095
35	1	0	-4.165421	1.887491	-0.000079

36	6	0	-2.265354	0.931986	-0.000046
37	1	0	-1.735531	1.870137	0.000006
38	6	0	-5.936093	-0.219429	-0.000215
39	1	0	-6.276426	-1.261366	-0.000265
40	6	0	-6.496772	0.446845	1.269283
41	1	0	-7.589958	0.401678	1.277970
42	1	0	-6.127789	-0.048949	2.170583
43	1	0	-6.207386	1.500328	1.325836
44	6	0	-6.496682	0.446938	-1.269704
45	1	0	-6.207292	1.500425	-1.326160
46	1	0	-6.127636	-0.048791	-2.171014
47	1	0	-7.589868	0.401772	-1.278471
48	6	0	3.162819	-0.293164	1.206670
49	6	0	0.561644	2.678317	-1.210657
50	6	0	0.378384	2.026709	-2.565060
51	1	0	1.309595	1.991819	-3.134826
52	1	0	-0.012539	1.012699	-2.490381
53	1	0	-0.337616	2.603943	-3.155678
54	6	0	2.494844	-0.461036	2.556278
55	1	0	2.867644	-1.372405	3.032735
56	1	0	2.716747	0.366708	3.234526
57	1	0	1.414149	-0.561654	2.481985
58	6	0	3.162904	-0.293087	-1.206463
59	6	0	2.495025	-0.460875	-2.556129
60	1	0	1.414322	-0.561474	-2.481921
61	1	0	2.716995	0.366899	-3.234318
62	1	0	2.867840	-1.372227	-3.032606
63	6	0	0.561559	2.678240	1.210867
64	6	0	0.378202	2.026546	2.565215
65	1	0	-0.012693	1.012532	2.490444
66	1	0	1.309367	1.991642	3.135055
67	1	0	-0.337858	2.603728	3.155810
68	1	0	0.594747	5.867072	0.000208

Compound 2b 2-RF-CmesN-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1319.86689320 A.U. after 1 cycles
Lowest frequency = -39.4724

Zero-point correction= 0.572889
(Hartree/Particle)
Thermal correction to Energy= 0.604244
Thermal correction to Enthalpy= 0.605188
Thermal correction to Gibbs Free Energy= 0.510770
Sum of electronic and zero-point Energies= -1319.294004
Sum of electronic and thermal Energies= -1319.262649
Sum of electronic and thermal Enthalpies= -1319.261705
Sum of electronic and thermal Free Energies= -1319.356123

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.207007	-0.409732	-0.162782
2	6	0	3.208542	-3.971267	-1.828773
3	6	0	1.986725	-4.096358	-1.187544
4	1	0	1.529210	-5.075199	-1.099974

5	6	0	1.909971	-1.678644	-0.750086
6	6	0	3.794142	-2.720034	-1.940835
7	1	0	4.750164	-2.620907	-2.442265
8	6	0	1.756903	3.320086	-1.212130
9	1	0	1.479758	3.963554	-2.043031
10	6	0	2.467066	3.859401	-0.143200
11	6	0	2.876613	2.980391	0.855506
12	1	0	3.490771	3.353517	1.670855
13	6	0	1.753795	1.094819	-0.211047
14	6	0	2.792802	5.331258	-0.077881
15	1	0	3.723459	5.511150	0.465774
16	1	0	2.893296	5.763273	-1.076552
17	1	0	2.000611	5.884247	0.438915
18	7	0	-0.137009	-0.535319	0.540442
19	6	0	-0.333162	-0.582347	1.926134
20	6	0	-1.387800	-0.261357	-0.030290
21	6	0	-1.679651	-0.260813	2.240438
22	6	0	0.546688	-0.989618	2.934407
23	6	0	-2.354882	-0.055482	0.983382
24	6	0	-2.112120	-0.269440	3.569395
25	6	0	0.093192	-0.996723	4.249259
26	1	0	1.550068	-1.320587	2.706830
27	6	0	-3.685479	0.207809	0.644568
28	6	0	-1.219588	-0.623855	4.572195
29	1	0	-3.139034	-0.018111	3.811665
30	1	0	0.767811	-1.312792	5.037252
31	6	0	-4.080671	0.240551	-0.689609
32	1	0	-4.419994	0.371607	1.427242
33	1	0	-1.542950	-0.638625	5.606518
34	6	0	-3.113303	-0.025862	-1.679378
35	1	0	-3.411684	-0.047305	-2.722136
36	6	0	-1.783164	-0.283916	-1.371323
37	1	0	-1.085520	-0.523124	-2.161551
38	6	0	-5.528291	0.528767	-1.063146
39	1	0	-6.070270	0.687424	-0.123640
40	6	0	-5.663750	1.818153	-1.893386
41	1	0	-6.716182	2.041776	-2.093581
42	1	0	-5.227138	2.671561	-1.368647
43	1	0	-5.155063	1.724035	-2.857577
44	6	0	-6.192264	-0.661589	-1.778956
45	1	0	-5.710036	-0.867732	-2.739230
46	1	0	-6.130020	-1.569283	-1.173502
47	1	0	-7.248504	-0.454380	-1.976557
48	6	0	1.407388	1.969091	-1.268419
49	6	0	1.324070	-2.991104	-0.647772
50	6	0	0.000214	-3.314030	0.016611
51	1	0	-0.010882	-3.051859	1.074809
52	1	0	-0.838941	-2.799764	-0.452304
53	1	0	-0.186780	-4.386695	-0.058905
54	6	0	0.718183	1.495701	-2.531986
55	1	0	1.128490	2.016094	-3.401615
56	1	0	0.854989	0.425343	-2.702131
57	1	0	-0.355387	1.695983	-2.507971
58	6	0	2.546697	1.623437	0.835068
59	6	0	3.136266	0.762523	1.933715
60	1	0	2.544530	0.813595	2.850464
61	1	0	3.211198	-0.287573	1.642044
62	1	0	4.146290	1.103111	2.177046
63	6	0	3.180187	-1.579089	-1.421383
64	6	0	3.952851	-0.292989	-1.629038

65	1	0	3.394480	0.440545	-2.210439
66	1	0	4.216779	0.192135	-0.689458
67	1	0	4.878891	-0.508499	-2.164970
68	1	0	3.702610	-4.845443	-2.239522

Compound 2b 2-RF-CxylN-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1319.86835509 A.U. after 1 cycles
Lowest frequency = -41.0863

Zero-point correction= 0.572811
(Hartree/Particle)
Thermal correction to Energy= 0.604214
Thermal correction to Enthalpy= 0.605158
Thermal correction to Gibbs Free Energy= 0.510217
Sum of electronic and zero-point Energies= -1319.295544
Sum of electronic and thermal Energies= -1319.264141
Sum of electronic and thermal Enthalpies= -1319.263197
Sum of electronic and thermal Free Energies= -1319.358138

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.142900	0.225914	-0.125817
2	6	0	5.153855	-4.148365	0.071486
3	1	0	4.690070	-5.122465	0.240519
4	1	0	5.744059	-4.200431	-0.846121
5	1	0	5.850245	-3.968855	0.898256
6	6	0	4.123498	-3.051874	0.002177
7	6	0	2.914492	-3.154200	0.682974
8	1	0	2.710279	-4.056513	1.250198
9	6	0	2.183677	-0.934849	-0.079635
10	6	0	4.356796	-1.889027	-0.726625
11	1	0	5.290000	-1.791818	-1.272060
12	6	0	0.788440	3.021082	-2.843475
13	1	0	0.411885	3.108091	-3.858071
14	6	0	1.262419	4.146080	-2.184413
15	6	0	1.811902	4.000492	-0.918896
16	1	0	2.242611	4.860306	-0.414963
17	6	0	1.291606	1.616171	-0.912428
18	7	0	-0.174073	0.107882	0.629621
19	6	0	-0.451658	0.666801	1.883122
20	6	0	-1.408466	-0.253606	0.072422
21	6	0	-1.854807	0.737185	2.087313
22	6	0	0.427280	1.022829	2.911434
23	6	0	-2.467093	0.145563	0.924035
24	6	0	-2.365992	1.241196	3.286440
25	6	0	-0.103507	1.515641	4.098824
26	1	0	1.495524	0.895763	2.808304
27	6	0	-3.792591	-0.136552	0.580288
28	6	0	-1.487810	1.642659	4.284135
29	1	0	-3.437833	1.301440	3.441219
30	1	0	0.570446	1.792302	4.902087
31	6	0	-4.085167	-0.838607	-0.585375
32	1	0	-4.599343	0.179113	1.234842
33	1	0	-1.870840	2.031489	5.220467

34	6	0	-3.012567	-1.278206	-1.387082
35	1	0	-3.218973	-1.864216	-2.276371
36	6	0	-1.686707	-1.006228	-1.072745
37	1	0	-0.895517	-1.399253	-1.695467
38	6	0	-5.527340	-1.145959	-0.964675
39	1	0	-6.158483	-0.711592	-0.180723
40	6	0	-5.927543	-0.482146	-2.294878
41	1	0	-6.984917	-0.659687	-2.514342
42	1	0	-5.762459	0.597601	-2.260865
43	1	0	-5.343498	-0.882403	-3.129141
44	6	0	-5.811334	-2.658775	-0.994763
45	1	0	-5.224256	-3.158440	-1.771181
46	1	0	-5.563097	-3.124856	-0.037939
47	1	0	-6.868288	-2.850269	-1.204120
48	6	0	0.806909	1.763141	-2.234817
49	6	0	1.950746	-2.145807	0.665355
50	6	0	0.703031	-2.454067	1.469381
51	1	0	0.541251	-1.739950	2.277208
52	1	0	-0.198312	-2.456990	0.856084
53	1	0	0.799603	-3.443952	1.918870
54	6	0	0.356080	0.588935	-3.079180
55	1	0	0.684473	0.722591	-4.113520
56	1	0	0.772501	-0.357766	-2.727855
57	1	0	-0.731868	0.492069	-3.091819
58	6	0	1.845380	2.756949	-0.281928
59	6	0	2.554053	2.693593	1.055589
60	1	0	1.906603	3.017561	1.873522
61	1	0	2.909986	1.687556	1.288455
62	1	0	3.426919	3.352066	1.049143
63	6	0	3.435869	-0.844863	-0.785031
64	6	0	3.867848	0.335236	-1.630689
65	1	0	3.182901	0.529882	-2.455909
66	1	0	3.931301	1.259038	-1.055701
67	1	0	4.853869	0.138090	-2.054969
68	1	0	1.239388	5.117237	-2.666358

Compound 3 GS1

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.78422820 A.U. after 1 cycles
Lowest frequency = 18.4427

Zero-point correction= 0.631614
(Hartree/Particle)
Thermal correction to Energy= 0.669179
Thermal correction to Enthalpy= 0.670124
Thermal correction to Gibbs Free Energy= 0.558748
Sum of electronic and zero-point Energies= -1473.152614
Sum of electronic and thermal Energies= -1473.115049
Sum of electronic and thermal Enthalpies= -1473.114105
Sum of electronic and thermal Free Energies= -1473.225480

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.086419	1.457162	-0.290470
2	6	0	2.478667	0.118145	0.094856

3	6	0	1.294446	-0.639043	0.222557
4	7	0	0.162417	0.179836	-0.050718
5	6	0	0.682542	1.471777	-0.361462
6	6	0	0.020444	2.633088	-0.772975
7	6	0	0.771638	3.760780	-1.063221
8	6	0	2.175669	3.755405	-0.969628
9	6	0	2.844213	2.596568	-0.588393
10	6	0	3.724762	-0.456202	0.348001
11	6	0	3.811595	-1.791811	0.740294
12	6	0	2.618961	-2.520775	0.881621
13	6	0	1.364210	-1.967993	0.639043
14	6	0	5.154303	-2.453251	1.020781
15	6	0	6.043380	-2.506983	-0.234847
16	6	0	5.893936	-1.785833	2.194345
17	8	0	2.784388	4.938001	-1.284880
18	6	0	4.199718	5.002921	-1.218538
19	1	0	-1.054932	2.670144	-0.861399
20	1	0	0.288636	4.677940	-1.377055
21	1	0	3.923375	2.558116	-0.527321
22	1	0	4.622377	0.144546	0.244278
23	1	0	2.674294	-3.557699	1.197287
24	1	0	0.476159	-2.568371	0.768017
25	1	0	4.942211	-3.487484	1.314869
26	1	0	6.973857	-3.044333	-0.027721
27	1	0	5.532925	-3.013382	-1.057812
28	1	0	6.308842	-1.501755	-0.575803
29	1	0	6.822765	-2.318731	2.419486
30	1	0	5.277070	-1.779250	3.096393
31	1	0	6.154244	-0.748991	1.961251
32	1	0	4.465777	6.020547	-1.500404
33	1	0	4.668932	4.300734	-1.917647
34	1	0	4.565345	4.801845	-0.204722
35	5	0	-1.229045	-0.214333	-0.011177
36	6	0	-1.625375	-1.726590	-0.275256
37	6	0	-1.270351	-2.343414	-1.501442
38	6	0	-2.401067	-2.474402	0.645861
39	6	0	-1.693907	-3.645822	-1.777388
40	6	0	-2.781680	-3.782279	0.341248
41	6	0	-2.443271	-4.388935	-0.868161
42	1	0	-1.428086	-4.090899	-2.732134
43	1	0	-3.367011	-4.340014	1.066890
44	6	0	-2.343753	0.870921	0.294331
45	6	0	-3.443817	1.087193	-0.573098
46	6	0	-2.298764	1.603608	1.507569
47	6	0	-4.434304	2.009533	-0.231489
48	6	0	-3.324356	2.498254	1.822581
49	6	0	-4.398300	2.725318	0.964862
50	1	0	-5.262334	2.166867	-0.916894
51	1	0	-3.279630	3.033428	2.766980
52	6	0	-2.812430	-1.912545	1.990198
53	1	0	-1.944621	-1.618340	2.588082
54	1	0	-3.444600	-1.028648	1.883981
55	1	0	-3.365988	-2.657238	2.565453
56	6	0	-0.431112	-1.646509	-2.553534
57	1	0	-0.679220	-0.589975	-2.664740
58	1	0	0.633400	-1.699582	-2.305062
59	1	0	-0.565451	-2.123856	-3.526593
60	6	0	-2.856266	-5.809047	-1.169122
61	1	0	-2.901242	-5.991847	-2.245078
62	1	0	-2.142234	-6.523673	-0.744686

63	1	0	-3.836480	-6.038162	-0.743597
64	6	0	-1.165657	1.464678	2.504404
65	1	0	-0.819614	0.435893	2.614369
66	1	0	-0.300009	2.061612	2.201011
67	1	0	-1.478817	1.817344	3.489427
68	6	0	-3.573772	0.368833	-1.899488
69	1	0	-2.713316	0.557900	-2.548268
70	1	0	-3.647012	-0.712749	-1.769155
71	1	0	-4.463853	0.706250	-2.434085
72	6	0	-5.473794	3.727774	1.305624
73	1	0	-5.245356	4.709311	0.875422
74	1	0	-6.445812	3.419153	0.913057
75	1	0	-5.568957	3.859006	2.385898

Compound 3 GS2

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.78443155 A.U. after 1 cycles
Lowest frequency = 19.0168

Zero-point correction= 0.631665
(Hartree/Particle)
Thermal correction to Energy= 0.669208
Thermal correction to Enthalpy= 0.670152
Thermal correction to Gibbs Free Energy= 0.559203
Sum of electronic and zero-point Energies= -1473.152767
Sum of electronic and thermal Energies= -1473.115224
Sum of electronic and thermal Enthalpies= -1473.114280
Sum of electronic and thermal Free Energies= -1473.225229

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.807684	1.900394	-0.294323
2	6	0	2.440930	0.648746	0.060489
3	6	0	1.418035	-0.313297	0.181283
4	7	0	0.152432	0.288781	-0.066833
5	6	0	0.423748	1.659560	-0.354753
6	6	0	-0.443872	2.687790	-0.737267
7	6	0	0.085534	3.939066	-1.009556
8	6	0	1.467963	4.188693	-0.926169
9	6	0	2.341268	3.164848	-0.573900
10	6	0	3.774697	0.303465	0.294126
11	6	0	4.107861	-0.997847	0.658613
12	6	0	3.068313	-1.937586	0.794712
13	6	0	1.734152	-1.616435	0.571429
14	6	0	5.558041	-1.385710	0.911481
15	6	0	5.791420	-1.834812	2.365392
16	6	0	6.050749	-2.452447	-0.083206
17	8	0	1.846599	5.468584	-1.221176
18	6	0	3.226767	5.790388	-1.163443
19	1	0	-1.508874	2.529358	-0.816932
20	1	0	-0.560194	4.758351	-1.300702
21	1	0	3.409883	3.323232	-0.521231
22	1	0	4.554235	1.052941	0.197896
23	1	0	3.305408	-2.954191	1.089145
24	1	0	0.970493	-2.369763	0.694417

25	1	0	6.159399	-0.483893	0.747790
26	1	0	6.851160	-2.044537	2.539590
27	1	0	5.475720	-1.062881	3.071634
28	1	0	5.230787	-2.745791	2.594676
29	1	0	7.111867	-2.667892	0.075018
30	1	0	5.920701	-2.118401	-1.115612
31	1	0	5.499972	-3.390203	0.035471
32	1	0	3.299062	6.844722	-1.426056
33	1	0	3.809079	5.199476	-1.880179
34	1	0	3.633897	5.640423	-0.156618
35	5	0	-1.143204	-0.353995	-0.025386
36	6	0	-1.259732	-1.907847	-0.317979
37	6	0	-0.810619	-2.426215	-1.558851
38	6	0	-1.877141	-2.802061	0.592399
39	6	0	-0.992051	-3.778670	-1.858554
40	6	0	-2.015674	-4.151434	0.263582
41	6	0	-1.584066	-4.663205	-0.959986
42	1	0	-0.659202	-4.149530	-2.823942
43	1	0	-2.482492	-4.820249	0.981214
44	6	0	-2.433753	0.503142	0.311038
45	6	0	-3.564117	0.531437	-0.543938
46	6	0	-2.510537	1.207114	1.539558
47	6	0	-4.703254	1.248911	-0.175183
48	6	0	-3.679447	1.891477	1.881314
49	6	0	-4.786229	1.934478	1.036445
50	1	0	-5.553509	1.265486	-0.851160
51	1	0	-3.723331	2.406588	2.836840
52	6	0	-2.371955	-2.350242	1.950025
53	1	0	-1.567187	-1.913951	2.549289
54	1	0	-3.155614	-1.594748	1.864749
55	1	0	-2.775421	-3.194164	2.512985
56	6	0	-0.123850	-1.568289	-2.602567
57	1	0	-0.558221	-0.571148	-2.686953
58	1	0	0.936361	-1.435279	-2.365845
59	1	0	-0.184009	-2.041492	-3.585025
60	6	0	-1.733944	-6.128896	-1.287301
61	1	0	-1.755503	-6.296388	-2.366467
62	1	0	-0.897272	-6.708967	-0.882121
63	1	0	-2.651588	-6.541243	-0.860362
64	6	0	-1.360402	1.258499	2.525132
65	1	0	-0.829517	0.309117	2.609341
66	1	0	-0.623021	2.011178	2.229385
67	1	0	-1.722351	1.526517	3.520060
68	6	0	-3.574277	-0.171152	-1.885039
69	1	0	-2.770629	0.186599	-2.535612
70	1	0	-3.445613	-1.250136	-1.778300
71	1	0	-4.517179	0.007304	-2.405581
72	6	0	-6.023900	2.714638	1.406910
73	1	0	-5.984986	3.729807	0.996326
74	1	0	-6.926890	2.240006	1.015096
75	1	0	-6.129275	2.804566	2.490457

Compound 3 GS3

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.78366077   A.U. after   1 cycles
Lowest frequency = 18.1338

Zero-point correction=	0.631589
(Hartree/Particle)	
Thermal correction to Energy=	0.669184
Thermal correction to Enthalpy=	0.670128
Thermal correction to Gibbs Free Energy=	0.558525
Sum of electronic and zero-point Energies=	-1473.152072
Sum of electronic and thermal Energies=	-1473.114477
Sum of electronic and thermal Enthalpies=	-1473.113533
Sum of electronic and thermal Free Energies=	-1473.225135

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.947056	1.699290	-0.257403
2	6	0	2.513091	0.413670	0.096780
3	6	0	1.439460	-0.493362	0.216146
4	7	0	0.205295	0.173873	-0.032505
5	6	0	0.546506	1.530921	-0.319022
6	6	0	-0.260508	2.599719	-0.696032
7	6	0	0.330762	3.834197	-0.968018
8	6	0	1.720917	4.005446	-0.883446
9	6	0	2.535349	2.929037	-0.533141
10	6	0	3.825665	0.004638	0.330487
11	6	0	4.090891	-1.315212	0.695933
12	6	0	3.005380	-2.196556	0.829968
13	6	0	1.686649	-1.809230	0.605677
14	6	0	5.511128	-1.798748	0.956477
15	6	0	6.391171	-1.706312	-0.303231
16	6	0	6.162926	-1.064091	2.141945
17	8	0	2.369165	5.183444	-1.135092
18	6	0	1.598815	6.315902	-1.504964
19	1	0	-1.332440	2.498467	-0.775797
20	1	0	-0.308731	4.658852	-1.251433
21	1	0	3.607911	3.074438	-0.491904
22	1	0	4.633984	0.721599	0.232535
23	1	0	3.198783	-3.222917	1.125228
24	1	0	0.886475	-2.523552	0.728701
25	1	0	5.439957	-2.858136	1.228184
26	1	0	7.386386	-2.118623	-0.111026
27	1	0	5.947814	-2.258972	-1.135298
28	1	0	6.517715	-0.667660	-0.622943
29	1	0	7.155528	-1.473846	2.352223
30	1	0	5.556217	-1.158624	3.045976
31	1	0	6.282067	0.002757	1.930694
32	1	0	2.311972	7.126017	-1.650222
33	1	0	0.889731	6.597450	-0.717870
34	1	0	1.052316	6.145860	-2.439881
35	5	0	-1.120115	-0.401983	0.004327
36	6	0	-1.316655	-1.948404	-0.286890
37	6	0	-0.891357	-2.490362	-1.526139
38	6	0	-1.983997	-2.808562	0.621123
39	6	0	-1.143309	-3.831371	-1.826450
40	6	0	-2.192961	-4.148712	0.291821
41	6	0	-1.784748	-4.683025	-0.930122
42	1	0	-0.826935	-4.219602	-2.790562
43	1	0	-2.697229	-4.791569	1.007839
44	6	0	-2.368032	0.520411	0.333189
45	6	0	-3.488899	0.609279	-0.529691

46	6	0	-2.417828	1.223746	1.563424
47	6	0	-4.593048	1.382488	-0.166577
48	6	0	-3.552919	1.965581	1.899395
49	6	0	-4.650169	2.067168	1.047001
50	1	0	-5.436655	1.443733	-0.848360
51	1	0	-3.577636	2.478866	2.856628
52	6	0	-2.459120	-2.331103	1.976928
53	1	0	-1.634261	-1.939614	2.579762
54	1	0	-3.200146	-1.534048	1.888840
55	1	0	-2.910264	-3.152019	2.537705
56	6	0	-0.155098	-1.671200	-2.567195
57	1	0	-0.530397	-0.650250	-2.649522
58	1	0	0.910746	-1.600804	-2.328822
59	1	0	-0.241248	-2.137880	-3.550857
60	6	0	-2.011036	-6.138779	-1.257900
61	1	0	-2.036947	-6.305269	-2.337131
62	1	0	-1.208122	-6.762408	-0.849149
63	1	0	-2.951107	-6.501586	-0.834775
64	6	0	-1.272681	1.214438	2.555940
65	1	0	-0.794733	0.237749	2.644607
66	1	0	-0.493594	1.925062	2.263105
67	1	0	-1.625150	1.503558	3.548361
68	6	0	-3.524701	-0.088347	-1.872905
69	1	0	-2.696954	0.227091	-2.515067
70	1	0	-3.454956	-1.172943	-1.767936
71	1	0	-4.451995	0.141428	-2.401377
72	6	0	-5.850071	2.906724	1.412236
73	1	0	-5.759137	3.919916	1.004855
74	1	0	-6.773017	2.478153	1.013873
75	1	0	-5.957522	2.998898	2.495394

Compound 3 GS4

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.78384398 A.U. after 1 cycles
Lowest frequency = 19.3053

Zero-point correction= 0.631710
(Hartree/Particle)
Thermal correction to Energy= 0.669227
Thermal correction to Enthalpy= 0.670171
Thermal correction to Gibbs Free Energy= 0.559276
Sum of electronic and zero-point Energies= -1473.152134
Sum of electronic and thermal Energies= -1473.114617
Sum of electronic and thermal Enthalpies= -1473.113673
Sum of electronic and thermal Free Energies= -1473.224568

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.272574	2.335538	-0.262634
2	6	0	2.235412	1.304854	0.065337
3	6	0	1.524699	0.094165	0.179971
4	7	0	0.136177	0.317908	-0.045937
5	6	0	0.005165	1.714488	-0.313712
6	6	0	-1.114867	2.460747	-0.666428
7	6	0	-0.968329	3.824312	-0.924557

8	6	0	0.288421	4.444338	-0.850260
9	6	0	1.417648	3.693918	-0.524552
10	6	0	3.614832	1.346193	0.280691
11	6	0	4.305008	0.186347	0.621770
12	6	0	3.572578	-1.008594	0.752772
13	6	0	2.198953	-1.072567	0.546579
14	6	0	5.808884	0.218578	0.855460
15	6	0	6.177598	-0.162081	2.300843
16	6	0	6.568151	-0.656589	-0.158313
17	8	0	0.507273	5.773344	-1.089515
18	6	0	-0.598824	6.591229	-1.436237
19	1	0	-2.094187	2.011819	-0.737841
20	1	0	-1.848082	4.394710	-1.189074
21	1	0	2.382472	4.185061	-0.491251
22	1	0	4.149301	2.286459	0.188343
23	1	0	4.089097	-1.921292	1.029656
24	1	0	1.679367	-2.011605	0.664926
25	1	0	6.130618	1.254552	0.698357
26	1	0	7.255760	-0.067542	2.462023
27	1	0	5.667273	0.482867	3.020499
28	1	0	5.898260	-1.196235	2.523008
29	1	0	7.649017	-0.566628	-0.013314
30	1	0	6.336038	-0.361956	-1.184784
31	1	0	6.304689	-1.712572	-0.046849
32	1	0	-0.195479	7.593129	-1.575852
33	1	0	-1.350929	6.613930	-0.639110
34	1	0	-1.070434	6.260175	-2.368783
35	5	0	-0.923297	-0.665213	-0.007315
36	6	0	-0.600258	-2.184589	-0.325723
37	6	0	-0.036938	-2.536185	-1.578410
38	6	0	-0.931685	-3.230792	0.571657
39	6	0	0.165233	-3.880287	-1.901852
40	6	0	-0.689806	-4.559341	0.218877
41	6	0	-0.145259	-4.909746	-1.016449
42	1	0	0.578681	-4.127191	-2.875717
43	1	0	-0.942322	-5.343649	0.926923
44	6	0	-2.400855	-0.212497	0.349588
45	6	0	-3.500767	-0.488867	-0.500473
46	6	0	-2.661884	0.420397	1.591442
47	6	0	-4.792716	-0.127381	-0.114350
48	6	0	-3.973085	0.742283	1.950157
49	6	0	-5.054690	0.486279	1.110198
50	1	0	-5.619178	-0.340108	-0.786620
51	1	0	-4.151871	1.207367	2.915606
52	6	0	-1.517075	-2.957817	1.940897
53	1	0	-0.855934	-2.329130	2.544934
54	1	0	-2.478646	-2.444710	1.875939
55	1	0	-1.667590	-3.890456	2.488094
56	6	0	0.371360	-1.503806	-2.610134
57	1	0	-0.321364	-0.663189	-2.669111
58	1	0	1.357568	-1.088457	-2.380481
59	1	0	0.429346	-1.957689	-3.601814
60	6	0	0.118438	-6.353182	-1.369744
61	1	0	0.135121	-6.502409	-2.451669
62	1	0	1.087601	-6.682180	-0.978408
63	1	0	-0.643201	-7.013009	-0.946731
64	6	0	-1.563423	0.776502	2.572860
65	1	0	-0.792403	0.007941	2.644763
66	1	0	-1.062018	1.704703	2.281839
67	1	0	-1.978032	0.926045	3.572076

68	6	0	-3.324366	-1.144492	-1.853747
69	1	0	-2.655579	-0.567493	-2.499350
70	1	0	-2.900584	-2.146952	-1.765813
71	1	0	-4.283155	-1.226592	-2.369434
72	6	0	-6.458788	0.879108	1.500322
73	1	0	-6.712305	1.870628	1.108661
74	1	0	-7.194752	0.175359	1.103734
75	1	0	-6.575140	0.917466	2.585800

Compound 3 1-RF-C-TSaa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.71239452 A.U. after 1 cycles
Lowest frequency = -40.1649

Zero-point correction= 0.631600
(Hartree/Particle)
Thermal correction to Energy= 0.667619
Thermal correction to Enthalpy= 0.668563
Thermal correction to Gibbs Free Energy= 0.563178
Sum of electronic and zero-point Energies= -1473.080795
Sum of electronic and thermal Energies= -1473.044776
Sum of electronic and thermal Enthalpies= -1473.043832
Sum of electronic and thermal Free Energies= -1473.149216

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.556745	-0.198082	-0.207533
2	6	0	1.973494	1.052090	0.233746
3	6	0	0.651687	1.089051	-0.261862
4	7	0	0.288912	-0.214712	-0.780702
5	6	0	1.552439	-0.873753	-0.924204
6	6	0	1.937759	-1.822769	-1.866835
7	6	0	3.259792	-2.243050	-1.916276
8	6	0	4.228691	-1.687199	-1.064628
9	6	0	3.888210	-0.623161	-0.230986
10	6	0	2.554225	2.170050	0.833251
11	6	0	1.856687	3.373820	0.897823
12	6	0	0.586469	3.424350	0.301545
13	6	0	-0.017502	2.312319	-0.281990
14	6	0	2.479338	4.601217	1.547584
15	6	0	2.688626	5.747823	0.541927
16	6	0	1.669522	5.076409	2.767617
17	8	0	5.485048	-2.208214	-1.186098
18	6	0	6.522876	-1.653892	-0.392601
19	1	0	1.235606	-2.200342	-2.592453
20	1	0	3.580456	-2.983926	-2.638245
21	1	0	4.638053	-0.083070	0.330983
22	1	0	3.568015	2.111867	1.217482
23	1	0	0.049241	4.366210	0.267930
24	1	0	-0.975023	2.425497	-0.760688
25	1	0	3.469143	4.299424	1.909616
26	1	0	3.196924	6.591601	1.018485
27	1	0	3.292899	5.421033	-0.307992
28	1	0	1.734440	6.113332	0.151307
29	1	0	2.167343	5.917819	3.259297

30	1	0	1.553099	4.273629	3.500022
31	1	0	0.669011	5.407190	2.473444
32	1	0	7.415847	-2.233152	-0.622335
33	1	0	6.300513	-1.739958	0.677170
34	1	0	6.702674	-0.601521	-0.641329
35	5	0	-1.065736	-0.775066	-0.551817
36	6	0	-2.220778	0.313371	-0.711906
37	6	0	-2.734767	1.103166	0.336347
38	6	0	-2.739121	0.506446	-2.013727
39	6	0	-3.742625	2.036758	0.076009
40	6	0	-3.744888	1.447048	-2.237556
41	6	0	-4.266355	2.224461	-1.200977
42	1	0	-4.125781	2.636392	0.897841
43	1	0	-4.131024	1.576454	-3.245061
44	6	0	-1.422829	-2.222040	0.051664
45	6	0	-0.582578	-3.383011	0.145286
46	6	0	-2.563396	-2.281155	0.928981
47	6	0	-0.594898	-4.188948	1.279718
48	6	0	-2.545286	-3.111428	2.056640
49	6	0	-1.513150	-4.004801	2.313108
50	1	0	0.088509	-5.032938	1.321274
51	1	0	-3.399576	-3.082607	2.727298
52	6	0	-2.216590	-0.304050	-3.181702
53	1	0	-1.153371	-0.112290	-3.356487
54	1	0	-2.326797	-1.379325	-3.004682
55	1	0	-2.754714	-0.063009	-4.100653
56	6	0	-2.207097	1.016678	1.753911
57	1	0	-1.630313	0.109078	1.932707
58	1	0	-1.554796	1.866787	1.974389
59	1	0	-3.026516	1.040639	2.478331
60	6	0	-5.377656	3.214321	-1.456444
61	1	0	-5.423993	3.972901	-0.671874
62	1	0	-5.245219	3.724629	-2.414108
63	1	0	-6.351801	2.713749	-1.487617
64	6	0	-3.917187	-1.640382	0.663706
65	1	0	-4.150249	-0.812515	1.334541
66	1	0	-4.032664	-1.288953	-0.356000
67	1	0	-4.672127	-2.413799	0.836724
68	6	0	0.139256	-3.980887	-1.044226
69	1	0	-0.097110	-3.459804	-1.967180
70	1	0	1.220594	-4.034382	-0.923883
71	1	0	-0.228724	-5.005263	-1.163472
72	6	0	-1.453346	-4.813705	3.581543
73	1	0	-2.439143	-4.912191	4.041881
74	1	0	-1.056273	-5.815777	3.400463
75	1	0	-0.795852	-4.331773	4.313944

Compound 3 1-RF-C-TSab

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.71226508 A.U. after 1 cycles
Lowest frequency = -41.2846

Zero-point correction= 0.631543
(Hartree/Particle)
Thermal correction to Energy= 0.667579
Thermal correction to Enthalpy= 0.668523
Thermal correction to Gibbs Free Energy= 0.562919
Sum of electronic and zero-point Energies= -1473.080722

Sum of electronic and thermal Energies= -1473.044686
Sum of electronic and thermal Enthalpies= -1473.043742
Sum of electronic and thermal Free Energies= -1473.149347

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.435482	-0.484763	-0.291105
2	6	0	2.036157	0.833337	0.159864
3	6	0	0.719056	1.047824	-0.308605
4	7	0	0.172845	-0.197081	-0.811990
5	6	0	1.333979	-1.018509	-0.983844
6	6	0	1.567282	-2.008550	-1.933997
7	6	0	2.819560	-2.602488	-2.012497
8	6	0	3.872864	-2.183540	-1.183184
9	6	0	3.696815	-1.084514	-0.343769
10	6	0	2.776174	1.859539	0.742564
11	6	0	2.245863	3.148413	0.819205
12	6	0	0.984116	3.367752	0.250883
13	6	0	0.220959	2.347795	-0.319524
14	6	0	3.023521	4.296714	1.446779
15	6	0	3.284789	4.060656	2.945332
16	6	0	4.335517	4.588632	0.696048
17	8	0	5.044795	-2.868496	-1.331252
18	6	0	6.164214	-2.461149	-0.559872
19	1	0	0.804431	-2.287360	-2.642917
20	1	0	3.021572	-3.378602	-2.740375
21	1	0	4.524878	-0.650700	0.200212
22	1	0	3.780427	1.656293	1.099784
23	1	0	0.584931	4.377047	0.232650
24	1	0	-0.722730	2.590265	-0.777252
25	1	0	2.393393	5.189361	1.361194
26	1	0	3.787571	4.923973	3.391855
27	1	0	2.350489	3.892320	3.486661
28	1	0	3.922712	3.185705	3.102748
29	1	0	4.840523	5.459831	1.124328
30	1	0	4.148003	4.788561	-0.361812
31	1	0	5.025603	3.741810	0.758061
32	1	0	6.965597	-3.155627	-0.807234
33	1	0	5.954119	-2.518122	0.514306
34	1	0	6.479811	-1.442439	-0.813445
35	5	0	-1.237101	-0.571551	-0.544368
36	6	0	-2.238976	0.663050	-0.671146
37	6	0	-2.607996	1.511084	0.392140
38	6	0	-2.766903	0.929054	-1.956210
39	6	0	-3.488814	2.572902	0.163557
40	6	0	-3.643406	1.997106	-2.148479
41	6	0	-4.022710	2.833766	-1.096085
42	1	0	-3.761292	3.215956	0.996656
43	1	0	-4.040015	2.181306	-3.143331
44	6	0	-1.770126	-1.958127	0.071328
45	6	0	-1.090116	-3.220739	0.148332
46	6	0	-2.887200	-1.864718	0.975555
47	6	0	-1.184066	-4.019209	1.284293
48	6	0	-2.954130	-2.691303	2.104022
49	6	0	-2.045472	-3.715345	2.338072
50	1	0	-0.618375	-4.946745	1.311931
51	1	0	-3.780888	-2.548961	2.794405

52	6	0	-2.394244	0.060172	-3.139531
53	1	0	-1.320606	0.107449	-3.346551
54	1	0	-2.643020	-0.991193	-2.959284
55	1	0	-2.922324	0.375395	-4.041714
56	6	0	-2.052474	1.348677	1.792269
57	1	0	-1.575373	0.380526	1.944992
58	1	0	-1.303431	2.118366	2.000438
59	1	0	-2.842572	1.454143	2.541684
60	6	0	-4.997814	3.965241	-1.317511
61	1	0	-4.930865	4.710650	-0.521939
62	1	0	-4.814823	4.469055	-2.270359
63	1	0	-6.029798	3.597778	-1.338094
64	6	0	-4.148599	-1.047275	0.741965
65	1	0	-4.252213	-0.197277	1.417640
66	1	0	-4.239863	-0.680689	-0.274821
67	1	0	-4.996361	-1.712652	0.933401
68	6	0	-0.479147	-3.907856	-1.055042
69	1	0	-0.667692	-3.361557	-1.974448
70	1	0	0.588842	-4.099824	-0.959332
71	1	0	-0.978280	-4.876554	-1.161858
72	6	0	-2.065393	-4.526695	3.606208
73	1	0	-3.044421	-4.492143	4.089660
74	1	0	-1.811315	-5.572885	3.417667
75	1	0	-1.331993	-4.138765	4.322170

Compound 3 1-RF-C1-TSaa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.71191265 A.U. after 1 cycles
Lowest frequency = -41.6101

Zero-point correction= 0.631470
(Hartree/Particle)
Thermal correction to Energy= 0.667561
Thermal correction to Enthalpy= 0.668505
Thermal correction to Gibbs Free Energy= 0.562725
Sum of electronic and zero-point Energies= -1473.080443
Sum of electronic and thermal Energies= -1473.044352
Sum of electronic and thermal Enthalpies= -1473.043408
Sum of electronic and thermal Free Energies= -1473.149188

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.262679	0.811228	0.101500
2	6	0	1.320187	1.820504	0.538377
3	6	0	0.080728	1.509628	-0.054182
4	7	0	0.137718	0.181230	-0.643229
5	6	0	1.540155	-0.083347	-0.713367
6	6	0	2.238383	-0.846171	-1.641413
7	6	0	3.630317	-0.871156	-1.597174
8	6	0	4.360913	-0.108752	-0.670334
9	6	0	3.655820	0.763958	0.158027
10	6	0	1.535933	3.022448	1.220012
11	6	0	0.506221	3.958035	1.257352
12	6	0	-0.688450	3.700235	0.567551
13	6	0	-0.904987	2.498458	-0.094220

14	6	0	6.385780	-1.560005	-0.203459
15	1	0	1.719564	-1.374354	-2.425007
16	1	0	4.157996	-1.476367	-2.326424
17	1	0	4.197804	1.450983	0.800433
18	1	0	2.501784	3.222353	1.663993
19	1	0	-1.440075	4.479747	0.542084
20	1	0	-1.819519	2.366033	-0.646289
21	1	0	7.475776	-1.564010	-0.107103
22	1	0	6.114152	-2.316961	-0.945298
23	1	0	5.957490	-1.863596	0.755058
24	5	0	-1.014438	-0.746989	-0.534342
25	6	0	-2.415573	-0.009943	-0.725787
26	6	0	-3.178640	0.545168	0.320608
27	6	0	-2.899927	0.113388	-2.049074
28	6	0	-4.390863	1.182367	0.037137
29	6	0	-4.113197	0.755798	-2.295807
30	6	0	-4.880808	1.296948	-1.261426
31	1	0	-4.964575	1.605358	0.857904
32	1	0	-4.468414	0.836854	-3.319630
33	6	0	-0.994229	-2.269661	-0.015387
34	6	0	0.127082	-3.158880	0.108062
35	6	0	-2.131879	-2.689196	0.761891
36	6	0	0.259339	-3.999639	1.208931
37	6	0	-1.962904	-3.544433	1.858042
38	6	0	-0.744029	-4.133007	2.168511
39	1	0	1.145672	-4.624756	1.278002
40	1	0	-2.836473	-3.788432	2.456152
41	6	0	-2.114723	-0.451329	-3.214632
42	1	0	-1.135466	0.028782	-3.305907
43	1	0	-1.938406	-1.525896	-3.096187
44	1	0	-2.647369	-0.305067	-4.156467
45	6	0	-2.719017	0.521245	1.764037
46	1	0	-1.893692	-0.170933	1.930818
47	1	0	-2.381833	1.514076	2.076247
48	1	0	-3.537041	0.232571	2.430866
49	6	0	-6.206502	1.961633	-1.545634
50	1	0	-6.513156	2.608150	-0.720457
51	1	0	-6.161710	2.569139	-2.453493
52	1	0	-6.997107	1.217421	-1.692298
53	6	0	-3.588896	-2.431984	0.408499
54	1	0	-4.090792	-1.743751	1.089829
55	1	0	-3.726997	-2.063456	-0.602237
56	1	0	-4.106833	-3.393187	0.486199
57	6	0	1.071688	-3.467149	-1.035212
58	1	0	0.761351	-2.988242	-1.959098
59	1	0	2.111429	-3.216828	-0.828475
60	1	0	1.022295	-4.546445	-1.212759
61	6	0	-0.550685	-4.964062	3.408948
62	1	0	-1.500276	-5.352669	3.783946
63	1	0	0.118824	-5.808497	3.226343
64	1	0	-0.103532	-4.362652	4.208516
65	6	0	5.881044	-0.166613	-0.620481
66	1	0	6.198524	0.541294	0.153835
67	6	0	6.525914	0.282318	-1.944301
68	1	0	6.269781	-0.396425	-2.763069
69	1	0	6.192358	1.284299	-2.225339
70	1	0	7.616434	0.297425	-1.856009
71	8	0	0.574729	5.169303	1.887345
72	6	0	1.769546	5.499547	2.576398
73	1	0	2.627226	5.552689	1.895402

74	1	0	1.600159	6.481832	3.014974
75	1	0	1.986457	4.779960	3.374540

Compound 3 1-RF-N-TSaa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.68379062 A.U. after 1 cycles
Lowest frequency = -68.0060

Zero-point correction= 0.632083
(Hartree/Particle)
Thermal correction to Energy= 0.667429
Thermal correction to Enthalpy= 0.668373
Thermal correction to Gibbs Free Energy= 0.565528
Sum of electronic and zero-point Energies= -1473.051708
Sum of electronic and thermal Energies= -1473.016362
Sum of electronic and thermal Enthalpies= -1473.015417
Sum of electronic and thermal Free Energies= -1473.118263

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.089476	1.160902	-0.008937
2	6	0	6.000502	-1.513814	1.558765
3	1	0	5.923349	-2.259005	2.354116
4	1	0	6.167719	-2.055994	0.621169
5	1	0	6.885599	-0.900682	1.743818
6	6	0	4.754423	-0.675291	1.464906
7	6	0	3.504265	-1.173383	1.824918
8	1	0	3.438116	-2.145634	2.304317
9	6	0	2.345521	0.818724	0.936729
10	6	0	4.797749	0.673886	1.123138
11	1	0	5.759850	1.176561	1.070076
12	6	0	-0.302577	4.696710	-0.912557
13	1	0	-0.079662	5.748339	-0.752745
14	6	0	-1.568839	4.331637	-1.363318
15	6	0	-1.691712	3.032769	-1.851198
16	1	0	-2.580454	2.757926	-2.411624
17	6	0	0.481785	2.361499	-0.889970
18	6	0	-2.703395	5.317770	-1.434759
19	1	0	-3.360644	5.112181	-2.283006
20	1	0	-3.316174	5.261819	-0.527857
21	1	0	-2.339859	6.344543	-1.519774
22	6	0	0.733351	3.772753	-0.777181
23	6	0	2.328436	-0.451544	1.627297
24	6	0	1.111305	-1.025062	2.328580
25	1	0	0.328582	-0.288370	2.485612
26	1	0	0.677987	-1.884799	1.813025
27	1	0	1.434670	-1.372643	3.314449
28	6	0	2.117354	4.378954	-0.810550
29	1	0	2.149883	5.035982	-1.685620
30	1	0	2.362326	4.998094	0.054927
31	1	0	2.884466	3.628778	-0.955532
32	6	0	-0.693553	2.074423	-1.681474
33	6	0	-0.875408	0.820011	-2.515572
34	1	0	0.050774	0.271531	-2.661052
35	1	0	-1.623002	0.134052	-2.111490

36	1	0	-1.228151	1.132341	-3.503236
37	6	0	3.642082	1.439038	0.964910
38	6	0	3.854296	2.926628	1.125692
39	1	0	4.437047	3.390331	0.327079
40	1	0	2.919176	3.456967	1.254447
41	1	0	4.424475	3.063782	2.050052
42	7	0	0.175370	-0.051102	-0.098015
43	6	0	-1.136629	-0.145753	0.369705
44	6	0	0.491342	-1.294005	-0.663623
45	6	0	-1.655157	-1.438832	0.113747
46	6	0	-1.905431	0.796483	1.061245
47	6	0	-0.612163	-2.170203	-0.566550
48	6	0	-2.949200	-1.770646	0.533166
49	6	0	-3.184592	0.438355	1.463319
50	1	0	-1.521169	1.786081	1.275964
51	6	0	-0.547292	-3.468011	-1.098575
52	1	0	-3.345691	-2.762415	0.336460
53	1	0	-3.780188	1.172337	1.995719
54	6	0	0.624170	-3.869371	-1.729117
55	1	0	-1.400887	-4.127661	-1.017166
56	6	0	1.716304	-2.983858	-1.835863
57	1	0	2.605028	-3.338393	-2.343553
58	6	0	1.661188	-1.702339	-1.315502
59	1	0	2.513523	-1.041151	-1.410421
60	6	0	-3.730397	-0.838599	1.208467
61	6	0	-5.137782	-1.194496	1.668219
62	1	0	-5.319041	-2.229670	1.356047
63	6	0	-5.276578	-1.147986	3.200865
64	1	0	-6.275834	-1.470133	3.510073
65	1	0	-4.543379	-1.800251	3.681841
66	1	0	-5.121686	-0.134566	3.583068
67	6	0	-6.207442	-0.318534	0.990782
68	1	0	-6.094082	0.733235	1.270242
69	1	0	-6.136391	-0.382907	-0.097935
70	1	0	-7.212648	-0.634284	1.287059
71	6	0	-0.231941	-6.044425	-2.230801
72	1	0	0.135513	-6.941557	-2.727346
73	1	0	-0.497596	-6.288920	-1.195149
74	1	0	-1.125228	-5.683031	-2.754528
75	8	0	0.825603	-5.103816	-2.290972

Compound 3 2-RF-CC-TSaa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.76715093 A.U. after 1 cycles
Lowest frequency = -59.1160

Zero-point correction= 0.632093
(Hartree/Particle)
Thermal correction to Energy= 0.668482
Thermal correction to Enthalpy= 0.669426
Thermal correction to Gibbs Free Energy= 0.562255
Sum of electronic and zero-point Energies= -1473.135058
Sum of electronic and thermal Energies= -1473.098669
Sum of electronic and thermal Enthalpies= -1473.097725
Sum of electronic and thermal Free Energies= -1473.204896

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.979253	1.863751	-0.000041
2	6	0	-2.551849	0.535398	-0.000003
3	6	0	-1.484719	-0.382243	0.000014
4	7	0	-0.234168	0.322051	-0.000011
5	6	0	-0.582738	1.717384	-0.000046
6	6	0	0.227036	2.857313	-0.000082
7	6	0	-0.375170	4.106390	-0.000112
8	6	0	-1.773054	4.252075	-0.000106
9	6	0	-2.587456	3.123968	-0.000071
10	6	0	-3.877287	0.096453	0.000016
11	6	0	-4.163624	-1.265847	0.000052
12	6	0	-3.085005	-2.167431	0.000068
13	6	0	-1.757093	-1.751292	0.000050
14	6	0	-5.604145	-1.757385	0.000073
15	6	0	-5.938478	-2.561702	-1.269288
16	6	0	-5.938463	-2.561637	1.269479
17	8	0	-2.226809	5.540316	-0.000137
18	6	0	-3.628643	5.759224	-0.000133
19	1	0	1.302441	2.789171	-0.000088
20	1	0	0.228688	5.005449	-0.000140
21	1	0	-3.666154	3.201719	-0.000066
22	1	0	-4.687672	0.818756	0.000002
23	1	0	-3.281994	-3.233983	0.000096
24	1	0	-0.968737	-2.485825	0.000064
25	1	0	-6.242470	-0.866200	0.000054
26	1	0	-6.994541	-2.847943	-1.277985
27	1	0	-5.735762	-1.977983	-2.170676
28	1	0	-5.345161	-3.479058	-1.325721
29	1	0	-6.994526	-2.847877	1.278204
30	1	0	-5.735736	-1.977871	2.170835
31	1	0	-5.345145	-3.478989	1.325953
32	1	0	-3.762017	6.839911	-0.000160
33	1	0	-4.102409	5.337217	0.893835
34	1	0	-4.102423	5.337171	-0.894071
35	5	0	1.085456	-0.244421	0.000000
36	6	0	1.323187	-1.838565	0.000040
37	6	0	1.466276	-2.568965	1.206595
38	6	0	1.466269	-2.569028	-1.206477
39	6	0	1.878226	-3.904010	1.185851
40	6	0	1.878219	-3.904072	-1.185665
41	6	0	2.132455	-4.586233	0.000110
42	1	0	1.976585	-4.430692	2.131542
43	1	0	1.976572	-4.430803	-2.131329
44	6	0	2.405494	0.678621	-0.000028
45	6	0	3.039127	1.069203	1.206385
46	6	0	3.039122	1.069138	-1.206464
47	6	0	4.309647	1.650057	1.186063
48	6	0	4.309643	1.649994	-1.186178
49	6	0	4.989729	1.909704	-0.000066
50	1	0	4.765720	1.932964	2.131407
51	1	0	4.765712	1.932849	-2.131539
52	6	0	1.095608	-2.008121	-2.563486
53	1	0	0.579692	-2.773599	-3.148833
54	1	0	0.424625	-1.153131	-2.491834
55	1	0	1.974208	-1.704092	-3.136972
56	6	0	1.095622	-2.007987	2.563577
57	1	0	0.424645	-1.152997	2.491885

58	1	0	0.579704	-2.773432	3.148965
59	1	0	1.974227	-1.703935	3.137045
60	6	0	2.630618	-6.010297	0.000146
61	1	0	3.725911	-6.041131	0.000145
62	1	0	2.289810	-6.553396	0.885061
63	1	0	2.289807	-6.553442	-0.884740
64	6	0	2.355726	1.009455	-2.557420
65	1	0	2.812591	0.270432	-3.220396
66	1	0	1.292959	0.788882	-2.481334
67	1	0	2.445712	1.980836	-3.052053
68	6	0	2.355736	1.009591	2.557347
69	1	0	1.292967	0.789024	2.481276
70	1	0	2.812597	0.270596	3.220357
71	1	0	2.445733	1.980995	3.051933
72	6	0	6.386121	2.480826	-0.000084
73	1	0	6.566840	3.096083	0.884770
74	1	0	7.135210	1.681135	-0.000061
75	1	0	6.566838	3.096032	-0.884973

Compound 3 2-RF-CC-TSab

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.76697064 A.U. after 1 cycles
Lowest frequency = -59.2052

Zero-point correction= 0.632098
(Hartree/Particle)
Thermal correction to Energy= 0.668473
Thermal correction to Enthalpy= 0.669418
Thermal correction to Gibbs Free Energy= 0.562228
Sum of electronic and zero-point Energies= -1473.134873
Sum of electronic and thermal Energies= -1473.098497
Sum of electronic and thermal Enthalpies= -1473.097553
Sum of electronic and thermal Free Energies= -1473.204743

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.208736	1.445945	-0.000039
2	6	0	-2.566565	0.043803	-0.000002
3	6	0	-1.366532	-0.695176	0.000022
4	7	0	-0.242666	0.197538	-0.000001
5	6	0	-0.806706	1.520933	-0.000037
6	6	0	-0.186408	2.774228	-0.000068
7	6	0	-0.977839	3.912906	-0.000102
8	6	0	-2.381105	3.836959	-0.000105
9	6	0	-3.007625	2.594572	-0.000073
10	6	0	-3.806005	-0.594481	0.000013
11	6	0	-3.873836	-1.987772	0.000053
12	6	0	-2.668740	-2.706057	0.000076
13	6	0	-1.419698	-2.087791	0.000061
14	6	0	-5.208377	-2.720597	0.000070
15	6	0	-6.027953	-2.425669	1.269368
16	6	0	-6.027945	-2.425744	-1.269250
17	8	0	-3.032115	5.037607	-0.000139
18	6	0	-4.450914	5.032839	-0.000145
19	1	0	0.886153	2.876809	-0.000067

20	1	0	-0.522798	4.895698	-0.000126
21	1	0	-4.085135	2.501638	-0.000074
22	1	0	-4.713785	-0.000250	-0.000006
23	1	0	-2.705419	-3.790743	0.000107
24	1	0	-0.526179	-2.690170	0.000080
25	1	0	-4.980688	-3.792586	0.000102
26	1	0	-6.950979	-3.013204	1.278697
27	1	0	-5.459918	-2.668445	2.170821
28	1	0	-6.306217	-1.368982	1.325356
29	1	0	-6.950971	-3.013279	-1.278551
30	1	0	-5.459904	-2.668573	-2.170686
31	1	0	-6.306208	-1.369060	-1.325303
32	1	0	-4.752992	6.078979	-0.000175
33	1	0	-4.852169	4.541415	0.893851
34	1	0	-4.852162	4.541366	-0.894118
35	5	0	1.148425	-0.158297	0.000007
36	6	0	1.635546	-1.693556	0.000046
37	6	0	1.903795	-2.387928	1.206439
38	6	0	1.903794	-2.387989	-1.206312
39	6	0	2.566518	-3.617731	1.186254
40	6	0	2.566516	-3.617791	-1.186066
41	6	0	2.952779	-4.234828	0.000110
42	1	0	2.759474	-4.118528	2.131635
43	1	0	2.759471	-4.118636	-2.131421
44	6	0	2.306506	0.962794	-0.000022
45	6	0	2.862898	1.457003	1.206577
46	6	0	2.862894	1.456943	-1.206648
47	6	0	3.998076	2.271505	1.185737
48	6	0	3.998072	2.271446	-1.185852
49	6	0	4.612607	2.661697	-0.000068
50	1	0	4.395018	2.631383	2.131377
51	1	0	4.395011	2.631276	-2.131511
52	6	0	1.390596	-1.929864	-2.556288
53	1	0	0.860541	-2.755028	-3.040763
54	1	0	0.688328	-1.102389	-2.480186
55	1	0	2.199657	-1.632533	-3.228230
56	6	0	1.390599	-1.929735	2.556393
57	1	0	0.688328	-1.102266	2.480248
58	1	0	0.860546	-2.754876	3.040911
59	1	0	2.199660	-1.632367	3.228318
60	6	0	3.723020	-5.532082	0.000142
61	1	0	4.802714	-5.345293	0.000134
62	1	0	3.496594	-6.131969	0.885056
63	1	0	3.496589	-6.132017	-0.884739
64	6	0	2.230500	1.230752	-2.563903
65	1	0	2.737574	0.444581	-3.127802
66	1	0	1.175014	0.970610	-2.493207
67	1	0	2.297163	2.145823	-3.157842
68	6	0	2.230508	1.230880	2.563845
69	1	0	1.175023	0.970727	2.493165
70	1	0	2.737588	0.444742	3.127785
71	1	0	2.297167	2.145983	3.157736
72	6	0	5.869546	3.496085	-0.000091
73	1	0	5.925673	4.134858	0.884759
74	1	0	6.761306	2.859376	-0.000079
75	1	0	5.925668	4.134818	-0.884971

Compound 3 2-RF-CN-TSaa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.74746040 A.U. after 1 cycles
Lowest frequency = -37.8543

Zero-point correction= 0.632031
(Hartree/Particle)
Thermal correction to Energy= 0.668087
Thermal correction to Enthalpy= 0.669031
Thermal correction to Gibbs Free Energy= 0.563098
Sum of electronic and zero-point Energies= -1473.115429
Sum of electronic and thermal Energies= -1473.079374
Sum of electronic and thermal Enthalpies= -1473.078429
Sum of electronic and thermal Free Energies= -1473.184362

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.165379	1.098854	-0.783880
2	6	0	-2.414790	-0.197975	-0.208998
3	6	0	-1.147715	-0.807651	-0.027283
4	7	0	-0.128197	0.065443	-0.418403
5	6	0	-0.762769	1.212071	-0.922951
6	6	0	-0.220373	2.306968	-1.606298
7	6	0	-1.070901	3.301034	-2.061939
8	6	0	-2.463815	3.220873	-1.869185
9	6	0	-3.020145	2.110860	-1.244668
10	6	0	-3.585187	-0.901664	0.093706
11	6	0	-3.521974	-2.215092	0.548101
12	6	0	-2.253892	-2.820682	0.666411
13	6	0	-1.075173	-2.144445	0.379219
14	6	0	-4.793429	-2.983565	0.881258
15	6	0	-4.991240	-4.206026	-0.033474
16	6	0	-4.849904	-3.389576	2.365256
17	8	0	-3.178832	4.280827	-2.362287
18	6	0	-4.588047	4.261295	-2.214694
19	1	0	0.839155	2.379775	-1.806887
20	1	0	-0.682657	4.160010	-2.595520
21	1	0	-4.090297	2.005904	-1.126003
22	1	0	-4.552135	-0.426000	-0.040900
23	1	0	-2.187447	-3.857596	0.978442
24	1	0	-0.128557	-2.662181	0.446036
25	1	0	-5.631270	-2.300734	0.698012
26	1	0	-5.942633	-4.701944	0.182600
27	1	0	-4.990076	-3.913609	-1.086512
28	1	0	-4.194349	-4.942163	0.108683
29	1	0	-5.799764	-3.881186	2.597465
30	1	0	-4.748738	-2.517179	3.015637
31	1	0	-4.044982	-4.087026	2.616115
32	1	0	-4.948784	5.189073	-2.656718
33	1	0	-4.883058	4.225742	-1.159133
34	1	0	-5.038509	3.412078	-2.742630
35	5	0	1.332470	-0.028854	-0.001960
36	6	0	1.612222	0.569420	1.458069
37	6	0	1.911222	1.939112	1.649223
38	6	0	1.504178	-0.238555	2.614871
39	6	0	1.993034	2.472427	2.937534
40	6	0	1.593080	0.331460	3.886795
41	6	0	1.807657	1.693810	4.076431

42	1	0	2.228952	3.527486	3.049306
43	1	0	1.510528	-0.318009	4.754395
44	6	0	2.383530	-0.665389	-0.964581
45	6	0	2.023096	-1.183886	-2.259328
46	6	0	3.772132	-0.764117	-0.596671
47	6	0	2.995926	-1.750006	-3.083612
48	6	0	4.694935	-1.341189	-1.467081
49	6	0	4.333576	-1.845025	-2.713357
50	1	0	2.695505	-2.129511	-4.054904
51	1	0	5.734834	-1.397334	-1.161548
52	6	0	1.359653	-1.745491	2.551676
53	1	0	0.321067	-2.058389	2.681107
54	1	0	1.716771	-2.155919	1.604444
55	1	0	1.944067	-2.213548	3.348464
56	6	0	2.226066	2.877154	0.501892
57	1	0	2.560061	2.342013	-0.389946
58	1	0	1.360747	3.483309	0.224154
59	1	0	3.027923	3.563918	0.786265
60	6	0	1.852448	2.298001	5.458447
61	1	0	2.501460	3.176564	5.489957
62	1	0	0.854387	2.617721	5.778094
63	1	0	2.216352	1.579761	6.197303
64	6	0	4.356250	-0.271899	0.711392
65	1	0	4.205567	0.797383	0.859052
66	1	0	3.917791	-0.768821	1.576782
67	1	0	5.430759	-0.462973	0.725421
68	6	0	0.626516	-1.175262	-2.849548
69	1	0	-0.082103	-1.747997	-2.250663
70	1	0	0.221930	-0.168010	-2.950182
71	1	0	0.653742	-1.621606	-3.845261
72	6	0	5.350068	-2.492183	-3.617212
73	1	0	5.438738	-3.560971	-3.392303
74	1	0	5.065775	-2.401688	-4.667712
75	1	0	6.339799	-2.048750	-3.487107

Compound 3 2-RF-CN-TSab

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.74719292 A.U. after 1 cycles
Lowest frequency = -37.2857

Zero-point correction= 0.632058
(Hartree/Particle)
Thermal correction to Energy= 0.668094
Thermal correction to Enthalpy= 0.669039
Thermal correction to Gibbs Free Energy= 0.563076
Sum of electronic and zero-point Energies= -1473.115135
Sum of electronic and thermal Energies= -1473.079099
Sum of electronic and thermal Enthalpies= -1473.078154
Sum of electronic and thermal Free Energies= -1473.184117

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.166625	-0.012200	1.197441
2	6	0	2.357558	-0.349430	-0.190582
3	6	0	1.062968	-0.556076	-0.735467

4	7	0	0.084929	-0.317522	0.234915
5	6	0	0.771713	-0.030900	1.426096
6	6	0	0.281903	0.101814	2.730801
7	6	0	1.177206	0.331180	3.762975
8	6	0	2.563355	0.412512	3.528126
9	6	0	3.066888	0.223631	2.246364
10	6	0	3.495383	-0.555276	-0.973906
11	6	0	3.373429	-0.992901	-2.291838
12	6	0	2.082961	-1.245328	-2.793011
13	6	0	0.932114	-1.044429	-2.038000
14	6	0	4.595874	-1.222083	-3.171427
15	6	0	5.373574	0.081679	-3.427347
16	6	0	5.521736	-2.315403	-2.608125
17	8	0	3.326452	0.654281	4.640348
18	6	0	4.732106	0.735682	4.480338
19	1	0	-0.771504	0.004246	2.951922
20	1	0	0.829955	0.436739	4.783549
21	1	0	4.130544	0.236344	2.049321
22	1	0	4.477180	-0.386778	-0.542875
23	1	0	1.981081	-1.625786	-3.804622
24	1	0	-0.034317	-1.291078	-2.454646
25	1	0	4.226382	-1.576503	-4.140709
26	1	0	6.209173	-0.092033	-4.112553
27	1	0	4.726717	0.846567	-3.864171
28	1	0	5.784291	0.485816	-2.497176
29	1	0	6.355617	-2.507346	-3.290490
30	1	0	4.979420	-3.252534	-2.459565
31	1	0	5.944281	-2.019009	-1.643358
32	1	0	5.135128	0.943329	5.470658
33	1	0	5.014695	1.546623	3.798409
34	1	0	5.152710	-0.207504	4.111154
35	5	0	-1.383124	-0.022830	-0.035798
36	6	0	-1.656566	1.503624	-0.439703
37	6	0	-1.902896	2.493052	0.541359
38	6	0	-1.595719	1.928126	-1.788245
39	6	0	-1.980052	3.840875	0.183263
40	6	0	-1.677937	3.285479	-2.106952
41	6	0	-1.840471	4.268010	-1.134253
42	1	0	-2.175160	4.574922	0.960709
43	1	0	-1.632514	3.577506	-3.152898
44	6	0	-2.447275	-1.158178	0.087661
45	6	0	-2.092696	-2.505514	0.453821
46	6	0	-3.842891	-0.906137	-0.161286
47	6	0	-3.077660	-3.489104	0.547179
48	6	0	-4.777786	-1.933736	-0.050541
49	6	0	-4.422314	-3.233642	0.297955
50	1	0	-2.781279	-4.494501	0.828287
51	1	0	-5.822579	-1.710357	-0.241330
52	6	0	-1.511421	0.958958	-2.949870
53	1	0	-0.487670	0.853906	-3.316165
54	1	0	-1.875508	-0.036411	-2.685322
55	1	0	-2.122150	1.316350	-3.783389
56	6	0	-2.164570	2.157986	1.995563
57	1	0	-2.509090	1.129754	2.127370
58	1	0	-1.271596	2.293249	2.610155
59	1	0	-2.941001	2.813498	2.399202
60	6	0	-1.878912	5.732849	-1.494515
61	1	0	-2.499924	6.300090	-0.796861
62	1	0	-0.874225	6.169101	-1.466151
63	1	0	-2.272364	5.886611	-2.502334

64	6	0	-4.422063	0.438897	-0.548543
65	1	0	-4.231218	1.206582	0.201207
66	1	0	-4.013237	0.813997	-1.486764
67	1	0	-5.503321	0.349418	-0.667482
68	6	0	-0.690014	-2.988931	0.766283
69	1	0	-0.012092	-2.874271	-0.079941
70	1	0	-0.244304	-2.460619	1.609257
71	1	0	-0.723270	-4.049710	1.021347
72	6	0	-5.453102	-4.329179	0.377332
73	1	0	-5.583672	-4.805224	-0.600979
74	1	0	-5.155078	-5.107949	1.082523
75	1	0	-6.426883	-3.939915	0.682816

Compound 3 3-RF-TSaa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.70417047 A.U. after 1 cycles
Lowest frequency = -57.7376

Zero-point correction= 0.632153
(Hartree/Particle)
Thermal correction to Energy= 0.668427
Thermal correction to Enthalpy= 0.669371
Thermal correction to Gibbs Free Energy= 0.561882
Sum of electronic and zero-point Energies= -1473.072017
Sum of electronic and thermal Energies= -1473.035743
Sum of electronic and thermal Enthalpies= -1473.034799
Sum of electronic and thermal Free Energies= -1473.142289

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.144899	1.532629	-0.050091
2	6	0	2.514523	0.173516	-0.341469
3	6	0	1.326603	-0.499301	-0.705322
4	7	0	0.200478	0.354044	-0.579453
5	6	0	0.755777	1.636504	-0.275285
6	6	0	0.165411	2.900686	-0.231688
7	6	0	0.934621	4.006444	0.096409
8	6	0	2.306501	3.889833	0.377738
9	6	0	2.923192	2.648221	0.285661
10	6	0	3.758966	-0.455214	-0.439587
11	6	0	3.857313	-1.746402	-0.946795
12	6	0	2.678004	-2.366398	-1.400517
13	6	0	1.431727	-1.758489	-1.304523
14	6	0	5.207183	-2.440980	-1.054217
15	6	0	5.265970	-3.715830	-0.193108
16	6	0	5.592714	-2.741214	-2.514127
17	8	0	2.940889	5.058249	0.700193
18	6	0	4.329928	5.008668	0.980724
19	1	0	-0.864130	3.047442	-0.493977
20	1	0	0.492007	4.994756	0.122667
21	1	0	3.985845	2.528878	0.448962
22	1	0	4.658114	0.078732	-0.147601
23	1	0	2.734953	-3.343540	-1.868006
24	1	0	0.577798	-2.246990	-1.744977
25	1	0	5.953280	-1.743254	-0.656540

26	1	0	6.264148	-4.162732	-0.230622
27	1	0	5.028792	-3.497137	0.851010
28	1	0	4.552317	-4.465880	-0.547020
29	1	0	6.594364	-3.178589	-2.566850
30	1	0	5.585423	-1.830918	-3.118737
31	1	0	4.897226	-3.450982	-2.971764
32	1	0	4.623351	6.029333	1.221799
33	1	0	4.905087	4.663982	0.113124
34	1	0	4.545298	4.359114	1.837349
35	5	0	-1.189426	-0.070566	-0.122641
36	6	0	-2.519174	0.209175	-1.034534
37	6	0	-2.906528	-0.952915	-1.763081
38	6	0	-3.383799	1.334244	-1.198149
39	6	0	-4.088724	-1.022221	-2.498204
40	6	0	-4.571210	1.212736	-1.934599
41	6	0	-4.965637	0.049127	-2.579242
42	1	0	-4.318678	-1.947717	-3.019345
43	1	0	-5.209608	2.087853	-2.010994
44	6	0	-1.371528	-0.827960	1.320048
45	6	0	-1.876503	0.021384	2.351162
46	6	0	-1.113886	-2.174232	1.718587
47	6	0	-2.134791	-0.447086	3.638621
48	6	0	-1.409566	-2.600331	3.021783
49	6	0	-1.930826	-1.771060	4.001612
50	1	0	-2.501828	0.258614	4.378338
51	1	0	-1.201866	-3.635637	3.274627
52	6	0	-3.146136	2.762531	-0.739709
53	1	0	-2.592001	2.866003	0.181704
54	1	0	-2.617743	3.318974	-1.521835
55	1	0	-4.103436	3.267082	-0.592681
56	6	0	-2.019245	-2.166501	-1.863667
57	1	0	-1.301229	-2.227861	-1.056086
58	1	0	-2.601343	-3.091124	-1.843036
59	1	0	-1.457686	-2.149091	-2.804086
60	6	0	-6.276550	-0.046263	-3.318133
61	1	0	-6.199629	-0.710871	-4.182223
62	1	0	-7.063847	-0.444972	-2.668849
63	1	0	-6.608052	0.933061	-3.670922
64	6	0	-0.530794	-3.285490	0.866203
65	1	0	-1.304384	-3.819561	0.306543
66	1	0	0.228101	-2.944393	0.172660
67	1	0	-0.049406	-4.019981	1.514441
68	6	0	-2.165177	1.487774	2.142749
69	1	0	-1.404161	1.984766	1.541353
70	1	0	-3.140626	1.627872	1.672908
71	1	0	-2.188037	2.009076	3.101712
72	6	0	-2.256278	-2.274915	5.385045
73	1	0	-1.722641	-3.201575	5.607565
74	1	0	-1.993055	-1.539106	6.149475
75	1	0	-3.327920	-2.479132	5.485992

Compound 3 3-RF-TSab

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1473.70395894 A.U. after 1 cycles
Lowest frequency = -57.6183

Zero-point correction= 0.632172
(Hartree/Particle)

Thermal correction to Energy= 0.668431
Thermal correction to Enthalpy= 0.669375
Thermal correction to Gibbs Free Energy= 0.561887
Sum of electronic and zero-point Energies= -1473.071787
Sum of electronic and thermal Energies= -1473.035528
Sum of electronic and thermal Enthalpies= -1473.034584
Sum of electronic and thermal Free Energies= -1473.142072

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.174986	1.358116	0.009119
2	6	0	2.464343	0.021705	-0.439860
3	6	0	1.232043	-0.543338	-0.844345
4	7	0	0.157579	0.348119	-0.592731
5	6	0	0.789458	1.558547	-0.165704
6	6	0	0.270604	2.839441	0.030458
7	6	0	1.106025	3.860590	0.456682
8	6	0	2.474809	3.642110	0.686886
9	6	0	3.020152	2.387490	0.443155
10	6	0	3.669512	-0.653230	-0.638591
11	6	0	3.684583	-1.886636	-1.287279
12	6	0	2.465659	-2.387707	-1.772693
13	6	0	1.254065	-1.729770	-1.580092
14	6	0	4.979737	-2.653301	-1.517465
15	6	0	5.972471	-1.868559	-2.394113
16	6	0	5.633216	-3.084188	-0.191874
17	8	0	3.179257	4.732818	1.117738
18	6	0	4.569187	4.580051	1.353083
19	1	0	-0.754496	3.067884	-0.187233
20	1	0	0.718948	4.861764	0.602233
21	1	0	4.077942	2.195713	0.563467
22	1	0	4.597206	-0.194035	-0.312963
23	1	0	2.468418	-3.311268	-2.342936
24	1	0	0.366192	-2.121388	-2.049501
25	1	0	4.714541	-3.566311	-2.062883
26	1	0	6.864163	-2.468402	-2.600279
27	1	0	5.520194	-1.589814	-3.349091
28	1	0	6.298782	-0.949088	-1.899026
29	1	0	6.526226	-3.688563	-0.378361
30	1	0	4.942026	-3.674304	0.414949
31	1	0	5.936597	-2.215364	0.399961
32	1	0	4.923236	5.551027	1.696322
33	1	0	5.105859	4.304136	0.437550
34	1	0	4.766939	3.829295	2.127273
35	5	0	-1.239311	-0.057830	-0.140552
36	6	0	-2.578047	0.383609	-0.971512
37	6	0	-3.048891	-0.672073	-1.805145
38	6	0	-3.384860	1.562198	-0.984790
39	6	0	-4.254369	-0.601689	-2.501470
40	6	0	-4.598402	1.581113	-1.687508
41	6	0	-5.074159	0.515026	-2.437449
42	1	0	-4.549260	-1.452749	-3.109561
43	1	0	-5.190475	2.490584	-1.648095
44	6	0	-1.418470	-0.960011	1.216791
45	6	0	-1.845480	-0.203944	2.350764
46	6	0	-1.219984	-2.352622	1.459100
47	6	0	-2.084573	-0.795748	3.590202

48	6	0	-1.493557	-2.902176	2.720349
49	6	0	-1.936751	-2.159376	3.802520
50	1	0	-2.390516	-0.157433	4.414127
51	1	0	-1.332727	-3.967717	2.853294
52	6	0	-3.056145	2.918374	-0.385635
53	1	0	-2.470325	2.892559	0.521517
54	1	0	-2.521163	3.528339	-1.122053
55	1	0	-3.979604	3.452538	-0.152157
56	6	0	-2.232270	-1.911263	-2.065544
57	1	0	-1.489414	-2.091587	-1.299435
58	1	0	-2.862037	-2.802992	-2.114826
59	1	0	-1.705255	-1.824322	-3.021997
60	6	0	-6.409706	0.566161	-3.135464
61	1	0	-6.395324	-0.006629	-4.066039
62	1	0	-7.198150	0.142479	-2.503620
63	1	0	-6.696996	1.593098	-3.372755
64	6	0	-0.728859	-3.393538	0.470627
65	1	0	-1.550325	-3.823941	-0.109759
66	1	0	0.022349	-3.018876	-0.213909
67	1	0	-0.265859	-4.217151	1.017209
68	6	0	-2.068106	1.287916	2.308952
69	1	0	-1.297892	1.812085	1.743263
70	1	0	-3.046007	1.521777	1.883668
71	1	0	-2.044416	1.702926	3.318425
72	6	0	-2.240232	-2.793127	5.136672
73	1	0	-1.754302	-3.766304	5.235428
74	1	0	-1.905972	-2.160888	5.963508
75	1	0	-3.317593	-2.948200	5.261298

Compound 4 GS1

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.37269099 A.U. after 1 cycles
Lowest frequency = 11.1638

Zero-point correction= 0.603949
(Hartree/Particle)
Thermal correction to Energy= 0.642580
Thermal correction to Enthalpy= 0.643524
Thermal correction to Gibbs Free Energy= 0.528062
Sum of electronic and zero-point Energies= -1695.768742
Sum of electronic and thermal Energies= -1695.730111
Sum of electronic and thermal Enthalpies= -1695.729167
Sum of electronic and thermal Free Energies= -1695.844629

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.242463	0.011632	-0.113689
2	6	0	-1.887205	1.375257	0.215554
3	6	0	-0.479956	1.426091	0.285178
4	7	0	0.066828	0.135045	0.027661
5	6	0	-1.038590	-0.720232	-0.211263
6	6	0	-1.062793	-2.069552	-0.575936
7	6	0	-2.292439	-2.673909	-0.798433
8	6	0	-3.490513	-1.953105	-0.679956
9	6	0	-3.471422	-0.605621	-0.342861

10	6	0	-2.658551	2.510235	0.466386
11	6	0	-2.037782	3.713815	0.798961
12	6	0	-0.635141	3.736607	0.882454
13	6	0	0.154354	2.615857	0.640314
14	6	0	-2.845162	4.974516	1.077345
15	6	0	-3.638500	5.434360	-0.159177
16	6	0	-3.768115	4.810436	2.298447
17	1	0	-0.154353	-2.642661	-0.681234
18	1	0	-2.326192	-3.718691	-1.081380
19	1	0	-4.395663	-0.046887	-0.271994
20	1	0	-3.739904	2.447061	0.407476
21	1	0	-0.143314	4.665862	1.151316
22	1	0	1.228814	2.683474	0.722061
23	1	0	-2.124900	5.765180	1.316180
24	1	0	-4.156862	6.376355	0.043151
25	1	0	-2.979143	5.585601	-1.017470
26	1	0	-4.392819	4.694965	-0.444278
27	1	0	-4.286517	5.748305	2.518980
28	1	0	-3.200939	4.517635	3.185488
29	1	0	-4.529093	4.044634	2.121277
30	5	0	1.474285	-0.231042	0.014407
31	6	0	2.557429	0.858895	-0.361982
32	6	0	2.486307	1.522882	-1.612892
33	6	0	3.656964	1.147825	0.485455
34	6	0	3.487134	2.424268	-1.982577
35	6	0	4.620672	2.075657	0.087907
36	6	0	4.559266	2.724700	-1.145196
37	1	0	3.424678	2.905222	-2.954599
38	1	0	5.448310	2.290857	0.757748
39	6	0	1.895644	-1.712061	0.378685
40	6	0	2.699678	-2.497709	-0.485538
41	6	0	1.530416	-2.261841	1.633832
42	6	0	3.092716	-3.780249	-0.100331
43	6	0	1.968336	-3.539262	1.990417
44	6	0	2.741871	-4.322161	1.136123
45	1	0	3.698178	-4.369688	-0.782882
46	1	0	1.695047	-3.932546	2.965453
47	6	0	3.814659	0.502952	1.846358
48	1	0	2.947998	0.689514	2.487362
49	1	0	3.930970	-0.580066	1.770187
50	1	0	4.690951	0.901568	2.361026
51	6	0	1.354252	1.298121	-2.595329
52	1	0	1.041496	0.254302	-2.653025
53	1	0	0.471013	1.882506	-2.319542
54	1	0	1.652736	1.609608	-3.598432
55	6	0	5.607266	3.733478	-1.546673
56	1	0	5.678798	3.823735	-2.632802
57	1	0	5.367167	4.726324	-1.150226
58	1	0	6.592668	3.459754	-1.161714
59	6	0	0.670869	-1.516597	2.635634
60	1	0	0.891047	-0.448828	2.675795
61	1	0	-0.392150	-1.615598	2.394541
62	1	0	0.816432	-1.922863	3.638709
63	6	0	3.131627	-2.005498	-1.850844
64	1	0	2.275248	-1.737048	-2.476409
65	1	0	3.767364	-1.120562	-1.779587
66	1	0	3.689431	-2.780618	-2.379678
67	6	0	3.167638	-5.716846	1.524047
68	1	0	2.451800	-6.460682	1.156919
69	1	0	4.143339	-5.968272	1.101281

70	1	0	3.227048	-5.828594	2.608949
71	6	0	-4.792462	-2.668567	-0.889719
72	9	0	-5.110209	-3.462769	0.162827
73	9	0	-4.759120	-3.476522	-1.975709
74	9	0	-5.828887	-1.817953	-1.059177

Compound 4 GS2

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.37288854 A.U. after 1 cycles
Lowest frequency = 9.5904

Zero-point correction= 0.604032
(Hartree/Particle)
Thermal correction to Energy= 0.642620
Thermal correction to Enthalpy= 0.643564
Thermal correction to Gibbs Free Energy= 0.528288
Sum of electronic and zero-point Energies= -1695.768857
Sum of electronic and thermal Energies= -1695.730269
Sum of electronic and thermal Enthalpies= -1695.729325
Sum of electronic and thermal Free Energies= -1695.844601

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.253191	0.518847	-0.118801
2	6	0	-1.580737	1.762613	0.186297
3	6	0	-0.203127	1.478865	0.249546
4	7	0	0.019784	0.091500	0.011821
5	6	0	-1.258654	-0.480138	-0.208828
6	6	0	-1.605656	-1.790282	-0.551322
7	6	0	-2.945340	-2.087984	-0.759266
8	6	0	-3.936735	-1.101002	-0.648029
9	6	0	-3.595568	0.208191	-0.333249
10	6	0	-2.055506	3.055357	0.422213
11	6	0	-1.165729	4.079449	0.732200
12	6	0	0.205731	3.769188	0.810441
13	6	0	0.700189	2.490165	0.583154
14	6	0	-1.668610	5.492991	0.989310
15	6	0	-1.372172	5.958096	2.426591
16	6	0	-1.119993	6.495469	-0.042184
17	1	0	-0.860265	-2.564479	-0.650691
18	1	0	-3.228811	-3.098845	-1.024869
19	1	0	-4.359825	0.971793	-0.268128
20	1	0	-3.120007	3.260781	0.370363
21	1	0	0.913464	4.551608	1.061678
22	1	0	1.760171	2.299220	0.659231
23	1	0	-2.758046	5.466805	0.872378
24	1	0	-1.800723	6.948391	2.607209
25	1	0	-1.792981	5.265736	3.159938
26	1	0	-0.295536	6.024208	2.609236
27	1	0	-1.545671	7.489772	0.122558
28	1	0	-1.363009	6.185419	-1.061537
29	1	0	-0.031910	6.584060	0.029402
30	5	0	1.299880	-0.599134	-0.000356
31	6	0	2.607766	0.195384	-0.401410

32	6	0	2.685337	0.836519	-1.663859
33	6	0	3.752148	0.228015	0.435214
34	6	0	3.868616	1.467293	-2.054802
35	6	0	4.905280	0.893099	0.016219
36	6	0	4.988954	1.517545	-1.228242
37	1	0	3.913682	1.933089	-3.035131
38	1	0	5.766398	0.916119	0.677975
39	6	0	1.359556	-2.131385	0.389340
40	6	0	1.946395	-3.100346	-0.463532
41	6	0	0.884750	-2.556878	1.655991
42	6	0	2.027007	-4.432664	-0.055974
43	6	0	1.009787	-3.895452	2.034593
44	6	0	1.568157	-4.854258	1.191970
45	1	0	2.469162	-5.160792	-0.729941
46	1	0	0.659185	-4.195737	3.017933
47	6	0	3.764443	-0.413708	1.806641
48	1	0	2.971802	-0.017368	2.448057
49	1	0	3.621101	-1.494637	1.749105
50	1	0	4.714423	-0.225230	2.310314
51	6	0	1.523588	0.871365	-2.636651
52	1	0	0.970726	-0.068688	-2.673495
53	1	0	0.807519	1.654041	-2.367724
54	1	0	1.878739	1.085702	-3.646726
55	6	0	6.243342	2.240763	-1.653232
56	1	0	6.324624	2.292942	-2.741169
57	1	0	6.250064	3.268817	-1.274258
58	1	0	7.138639	1.746790	-1.267795
59	6	0	0.235495	-1.611479	2.647229
60	1	0	0.704367	-0.626589	2.667265
61	1	0	-0.822309	-1.457803	2.411833
62	1	0	0.287828	-2.023909	3.656963
63	6	0	2.469871	-2.748430	-1.840135
64	1	0	1.694824	-2.297621	-2.467000
65	1	0	3.296351	-2.036629	-1.789299
66	1	0	2.825056	-3.642450	-2.356066
67	6	0	1.653995	-6.303254	1.604215
68	1	0	0.779303	-6.862181	1.253491
69	1	0	2.538875	-6.786217	1.182705
70	1	0	1.693711	-6.407282	2.690782
71	6	0	-5.372950	-1.489694	-0.840859
72	9	0	-5.862278	-2.168917	0.226322
73	9	0	-5.540672	-2.299602	-1.912907
74	9	0	-6.178987	-0.420061	-1.021227

Compound 4 1-RF-C1-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.30075359 A.U. after 1 cycles
Lowest frequency = -39.7254

Zero-point correction= 0.603914
(Hartree/Particle)
Thermal correction to Energy= 0.640997
Thermal correction to Enthalpy= 0.641941
Thermal correction to Gibbs Free Energy= 0.532402
Sum of electronic and zero-point Energies= -1695.696839
Sum of electronic and thermal Energies= -1695.659757
Sum of electronic and thermal Enthalpies= -1695.658813
Sum of electronic and thermal Free Energies= -1695.768352

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.259261	0.464625	-0.091331
2	6	0	1.322511	1.519468	0.234436
3	6	0	0.071185	1.144759	-0.311107
4	7	0	0.123444	-0.231371	-0.742566
5	6	0	1.526063	-0.511052	-0.793187
6	6	0	2.211204	-1.380818	-1.632787
7	6	0	3.602806	-1.407232	-1.595215
8	6	0	4.345466	-0.548041	-0.767340
9	6	0	3.652370	0.418515	-0.039588
10	6	0	1.527395	2.786194	0.773610
11	6	0	0.496261	3.716611	0.708781
12	6	0	-0.701664	3.388070	0.064693
13	6	0	-0.920349	2.116299	-0.455607
14	1	0	1.683787	-1.993678	-2.345673
15	1	0	4.122165	-2.094927	-2.253767
16	1	0	4.201617	1.171918	0.515911
17	1	0	2.485437	3.059209	1.196994
18	1	0	-1.465735	4.145409	-0.058513
19	1	0	-1.835652	1.915891	-0.984526
20	5	0	-1.034997	-1.144461	-0.519742
21	6	0	-2.437487	-0.447797	-0.813742
22	6	0	-3.215541	0.235136	0.142614
23	6	0	-2.910442	-0.508687	-2.145858
24	6	0	-4.429991	0.816926	-0.234629
25	6	0	-4.126900	0.082532	-2.486415
26	6	0	-4.908788	0.750659	-1.540798
27	1	0	-5.015248	1.340567	0.516940
28	1	0	-4.473219	0.021241	-3.514523
29	6	0	-0.994126	-2.580686	0.190916
30	6	0	0.135994	-3.440550	0.409654
31	6	0	-2.114245	-2.894696	1.040106
32	6	0	0.297504	-4.118674	1.613151
33	6	0	-1.915658	-3.587142	2.241058
34	6	0	-0.685302	-4.119839	2.603846
35	1	0	1.187739	-4.726953	1.748794
36	1	0	-2.774620	-3.751160	2.885618
37	6	0	-2.109924	-1.217574	-3.218611
38	1	0	-1.136217	-0.741449	-3.371188
39	1	0	-1.921610	-2.263426	-2.953222
40	1	0	-2.637589	-1.208869	-4.174305
41	6	0	-2.773480	0.408185	1.581657
42	1	0	-1.920529	-0.219894	1.838911
43	1	0	-2.486728	1.445748	1.775934
44	1	0	-3.585910	0.165449	2.272979
45	6	0	-6.237552	1.357520	-1.922285
46	1	0	-6.552356	2.114040	-1.200246
47	1	0	-6.193230	1.827340	-2.908327
48	1	0	-7.021852	0.593595	-1.961876
49	6	0	-3.578275	-2.701448	0.677253
50	1	0	-4.081277	-1.937882	1.271765
51	1	0	-3.733577	-2.469641	-0.370823
52	1	0	-4.081690	-3.650676	0.886109
53	6	0	1.046900	-3.906935	-0.707131
54	1	0	0.725744	-3.538406	-1.676829

55	1	0	2.096549	-3.659703	-0.552933
56	1	0	0.969447	-4.998358	-0.749786
57	6	0	-0.459583	-4.768513	3.943318
58	1	0	-1.398580	-5.098762	4.393080
59	1	0	0.207091	-5.630982	3.864680
60	1	0	0.006382	-4.060760	4.638145
61	6	0	0.657894	5.075940	1.321232
62	9	0	0.075399	5.153065	2.544168
63	9	0	1.955873	5.414331	1.492332
64	9	0	0.089234	6.046855	0.569160
65	6	0	5.865454	-0.610591	-0.722110
66	1	0	6.193739	0.183045	-0.041383
67	6	0	6.362742	-1.947695	-0.142985
68	1	0	7.453176	-1.948069	-0.053850
69	1	0	5.939878	-2.130044	0.848103
70	1	0	6.080963	-2.786616	-0.786427
71	6	0	6.502381	-0.330014	-2.095099
72	1	0	6.235712	-1.100683	-2.824250
73	1	0	6.174657	0.633618	-2.492706
74	1	0	7.593374	-0.313207	-2.016074

Compound 4 1-RF-C1-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.30064915 A.U. after 1 cycles
Lowest frequency = -40.4996

Zero-point correction= 0.603909
(Hartree/Particle)
Thermal correction to Energy= 0.640986
Thermal correction to Enthalpy= 0.641931
Thermal correction to Gibbs Free Energy= 0.532208
Sum of electronic and zero-point Energies= -1695.696740
Sum of electronic and thermal Energies= -1695.659663
Sum of electronic and thermal Enthalpies= -1695.658719
Sum of electronic and thermal Free Energies= -1695.768441

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.283116	-0.118347	-0.246277
2	6	0	1.626408	1.112808	0.142707
3	6	0	0.300500	1.048539	-0.348529
4	7	0	0.017222	-0.290802	-0.805630
5	6	0	1.314924	-0.881141	-0.930979
6	6	0	1.744776	-1.859369	-1.815685
7	6	0	3.095752	-2.204894	-1.839559
8	6	0	4.048951	-1.562722	-1.036044
9	6	0	3.627914	-0.479597	-0.259939
10	6	0	2.138415	2.283596	0.693850
11	6	0	1.345595	3.425912	0.695952
12	6	0	0.077851	3.397177	0.104881
13	6	0	-0.447889	2.223952	-0.427385
14	1	0	1.062443	-2.316988	-2.513484
15	1	0	3.424107	-2.977376	-2.527580
16	1	0	4.350962	0.121040	0.281330
17	1	0	3.150854	2.319425	1.075126

18	1	0	-0.497614	4.311620	0.033058
19	1	0	-1.406923	2.252221	-0.914384
20	5	0	-1.308397	-0.922236	-0.544573
21	6	0	-2.525032	0.084490	-0.757029
22	6	0	-3.084374	0.897649	0.249013
23	6	0	-3.054996	0.174016	-2.065909
24	6	0	-4.147707	1.752701	-0.057727
25	6	0	-4.116321	1.037668	-2.335766
26	6	0	-4.683420	1.837563	-1.340449
27	1	0	-4.564940	2.373011	0.731397
28	1	0	-4.510409	1.088579	-3.347115
29	6	0	-1.567772	-2.350206	0.136079
30	6	0	-0.656102	-3.450612	0.286361
31	6	0	-2.693951	-2.424953	1.030817
32	6	0	-0.604242	-4.180968	1.468830
33	6	0	-2.609526	-3.177886	2.208603
34	6	0	-1.519445	-3.986276	2.504173
35	1	0	0.128269	-4.979371	1.551983
36	1	0	-3.455885	-3.160198	2.889440
37	6	0	-2.484497	-0.666029	-3.189713
38	1	0	-1.434037	-0.422312	-3.377339
39	1	0	-2.532739	-1.734958	-2.955635
40	1	0	-3.034115	-0.506004	-4.119318
41	6	0	-2.553708	0.921671	1.668191
42	1	0	-1.858081	0.107540	1.871936
43	1	0	-2.027983	1.859794	1.868430
44	1	0	-3.370103	0.850857	2.393027
45	6	0	-5.851836	2.743606	-1.645934
46	1	0	-5.960974	3.522691	-0.888417
47	1	0	-5.736131	3.229751	-2.618224
48	1	0	-6.790185	2.178922	-1.675341
49	6	0	-4.088679	-1.893199	0.740270
50	1	0	-4.378342	-1.051942	1.371031
51	1	0	-4.230156	-1.602862	-0.295158
52	1	0	-4.786899	-2.708195	0.955589
53	6	0	0.076975	-4.081230	-0.879683
54	1	0	-0.192016	-3.623278	-1.826851
55	1	0	1.160880	-4.082920	-0.770923
56	1	0	-0.248947	-5.125031	-0.936947
57	6	0	-1.392511	-4.706270	3.819996
58	1	0	-2.362551	-4.826203	4.307542
59	1	0	-0.944812	-5.695439	3.695043
60	1	0	-0.748315	-4.142878	4.504413
61	6	0	1.840249	4.694193	1.324973
62	9	0	1.350190	4.862361	2.578923
63	9	0	3.187920	4.725847	1.432279
64	9	0	1.470857	5.791125	0.623730
65	6	0	5.509202	-1.990357	-1.079759
66	1	0	5.572812	-2.827836	-1.783807
67	6	0	6.427950	-0.874765	-1.610113
68	1	0	7.457748	-1.233699	-1.696873
69	1	0	6.102894	-0.530264	-2.594900
70	1	0	6.434575	-0.010657	-0.939398
71	6	0	5.992476	-2.502006	0.289433
72	1	0	5.965939	-1.706874	1.040418
73	1	0	5.364549	-3.320791	0.649505
74	1	0	7.022560	-2.864871	0.224439

Compound 4 1-RF-C-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.30031334 A.U. after 1 cycles
Lowest frequency = -39.4213

Zero-point correction= 0.603969
(Hartree/Particle)
Thermal correction to Energy= 0.641009
Thermal correction to Enthalpy= 0.641953
Thermal correction to Gibbs Free Energy= 0.532754
Sum of electronic and zero-point Energies= -1695.696345
Sum of electronic and thermal Energies= -1695.659304
Sum of electronic and thermal Enthalpies= -1695.658360
Sum of electronic and thermal Free Energies= -1695.767560

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.093632	0.743301	-0.006720
2	6	0	1.096489	1.719777	0.375362
3	6	0	-0.128402	1.292533	-0.179412
4	7	0	0.009056	-0.060752	-0.685907
5	6	0	1.418102	-0.247406	-0.753105
6	6	0	2.145181	-1.040949	-1.633265
7	6	0	3.534951	-0.994650	-1.603926
8	6	0	4.203577	-0.125452	-0.733709
9	6	0	3.484548	0.776966	0.044844
10	6	0	1.226411	2.973763	0.972982
11	6	0	0.153439	3.860855	0.976953
12	6	0	-1.024146	3.463216	0.322524
13	6	0	-1.177604	2.207541	-0.260693
14	6	0	0.278891	5.232483	1.624153
15	6	0	0.124426	6.373281	0.602232
16	6	0	-0.703341	5.402765	2.797369
17	1	0	1.647157	-1.646653	-2.372032
18	1	0	4.106748	-1.608550	-2.288250
19	1	0	4.002283	1.530224	0.624482
20	1	0	2.177867	3.272169	1.401801
21	1	0	-1.850881	4.160841	0.242126
22	1	0	-2.089237	1.978440	-0.785066
23	1	0	1.293151	5.296516	2.034713
24	1	0	0.285538	7.343636	1.081248
25	1	0	0.844297	6.272180	-0.213687
26	1	0	-0.877845	6.382593	0.163978
27	1	0	-0.552893	6.367951	3.290216
28	1	0	-0.568045	4.614899	3.542582
29	1	0	-1.741246	5.362811	2.453530
30	5	0	-1.088055	-1.058474	-0.522694
31	6	0	-2.530925	-0.440983	-0.797637
32	6	0	-3.365021	0.137721	0.180237
33	6	0	-2.984112	-0.465857	-2.137717
34	6	0	-4.612569	0.652943	-0.185171
35	6	0	-4.234887	0.056968	-2.465994
36	6	0	-5.071487	0.620529	-1.499815
37	1	0	-5.241488	1.095059	0.583344
38	1	0	-4.564795	0.023766	-3.500774
39	6	0	-0.953567	-2.524286	0.113373
40	6	0	0.228870	-3.321678	0.291408

41	6	0	-2.048951	-2.948265	0.946428
42	6	0	0.436965	-4.041630	1.462679
43	6	0	-1.803248	-3.680490	2.115014
44	6	0	-0.540482	-4.149070	2.453370
45	1	0	1.363738	-4.598811	1.569772
46	1	0	-2.648299	-3.928096	2.751234
47	6	0	-2.125335	-1.062433	-3.233536
48	1	0	-1.187234	-0.510785	-3.350923
49	1	0	-1.865112	-2.104132	-3.017079
50	1	0	-2.643735	-1.044244	-4.194148
51	6	0	-2.950986	0.268926	1.631878
52	1	0	-2.089678	-0.350753	1.881965
53	1	0	-2.686534	1.304341	1.865096
54	1	0	-3.770528	-0.013005	2.299383
55	6	0	-6.435461	1.152104	-1.869330
56	1	0	-6.810426	1.847017	-1.114759
57	1	0	-6.413649	1.673640	-2.829824
58	1	0	-7.163869	0.338619	-1.958497
59	6	0	-3.522865	-2.833948	0.590824
60	1	0	-4.074615	-2.137646	1.223495
61	1	0	-3.694748	-2.559361	-0.444218
62	1	0	-3.961379	-3.824266	0.749382
63	6	0	1.160330	-3.684242	-0.847569
64	1	0	0.815575	-3.291238	-1.799474
65	1	0	2.195999	-3.389190	-0.682704
66	1	0	1.142759	-4.775037	-0.940521
67	6	0	-0.269017	-4.841421	3.762056
68	1	0	-1.185021	-5.241228	4.202632
69	1	0	0.442752	-5.662085	3.642140
70	1	0	0.164206	-4.139923	4.483863
71	6	0	5.702602	-0.152966	-0.671808
72	9	0	6.155186	-1.129308	0.153846
73	9	0	6.222250	1.008161	-0.214896
74	9	0	6.260344	-0.390157	-1.881824

Compound 4 1-RF-C-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.30016101 A.U. after 2 cycles
Lowest frequency = -39.6645

Zero-point correction= 0.603888
(Hartree/Particle)
Thermal correction to Energy= 0.640964
Thermal correction to Enthalpy= 0.641908
Thermal correction to Gibbs Free Energy= 0.532257
Sum of electronic and zero-point Energies= -1695.696273
Sum of electronic and thermal Energies= -1695.659197
Sum of electronic and thermal Enthalpies= -1695.658253
Sum of electronic and thermal Free Energies= -1695.767904

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.100371	0.480909	-0.075436
2	6	0	1.249448	1.589323	0.303480
3	6	0	-0.031493	1.321560	-0.229491

4	7	0	-0.084367	-0.047326	-0.710631
5	6	0	1.286486	-0.420834	-0.795778
6	6	0	1.886435	-1.316367	-1.673718
7	6	0	3.270343	-1.456431	-1.664903
8	6	0	4.063129	-0.672838	-0.818294
9	6	0	3.483689	0.328812	-0.044351
10	6	0	1.558205	2.820836	0.876470
11	6	0	0.611434	3.845703	0.878573
12	6	0	-0.615477	3.599360	0.247232
13	6	0	-0.947667	2.366375	-0.314919
14	6	0	0.908118	5.206372	1.492917
15	6	0	1.146251	5.108679	3.010646
16	6	0	2.081433	5.915747	0.792858
17	1	0	1.299763	-1.859966	-2.395492
18	1	0	3.743612	-2.151078	-2.347229
19	1	0	4.106993	1.014374	0.515113
20	1	0	2.550290	2.986380	1.282995
21	1	0	-1.337148	4.406596	0.171463
22	1	0	-1.890391	2.255510	-0.822411
23	1	0	0.015384	5.823504	1.340391
24	1	0	1.293925	6.102610	3.443514
25	1	0	0.297054	4.640152	3.514320
26	1	0	2.036311	4.512950	3.234214
27	1	0	2.228861	6.917529	1.207249
28	1	0	1.899582	6.013884	-0.280209
29	1	0	3.016211	5.362585	0.923712
30	5	0	-1.301329	-0.885839	-0.510602
31	6	0	-2.652535	-0.080702	-0.764006
32	6	0	-3.374746	0.618008	0.224139
33	6	0	-3.136944	-0.057285	-2.093131
34	6	0	-4.548422	1.295937	-0.119970
35	6	0	-4.311567	0.629170	-2.400337
36	6	0	-5.039237	1.312744	-1.423264
37	1	0	-5.091599	1.828988	0.656201
38	1	0	-4.667850	0.630965	-3.426884
39	6	0	-1.356093	-2.348676	0.144528
40	6	0	-0.289302	-3.295974	0.318250
41	6	0	-2.486697	-2.611819	0.996873
42	6	0	-0.163922	-4.025193	1.495680
43	6	0	-2.325866	-3.358820	2.170732
44	6	0	-1.133307	-3.990149	2.499199
45	1	0	0.681164	-4.700554	1.598383
46	1	0	-3.187714	-3.483570	2.820234
47	6	0	-2.394355	-0.777551	-3.199457
48	1	0	-1.391797	-0.362494	-3.343449
49	1	0	-2.275852	-1.843205	-2.975695
50	1	0	-2.926909	-0.696594	-4.149029
51	6	0	-2.910708	0.706903	1.663796
52	1	0	-2.127121	-0.013466	1.899165
53	1	0	-2.513640	1.703089	1.879436
54	1	0	-3.741461	0.534053	2.354302
55	6	0	-6.325497	2.023443	-1.769711
56	1	0	-6.589178	2.763242	-1.010762
57	1	0	-6.251057	2.536611	-2.732127
58	1	0	-7.158606	1.315797	-1.843270
59	6	0	-3.936743	-2.301527	0.660280
60	1	0	-4.377965	-1.528200	1.290253
61	1	0	-4.085995	-2.018566	-0.376034
62	1	0	-4.504001	-3.220404	0.839280
63	6	0	0.571314	-3.791465	-0.826263

64	1	0	0.266802	-3.369519	-1.779486
65	1	0	1.638664	-3.630817	-0.678614
66	1	0	0.411605	-4.871905	-0.902743
67	6	0	-0.939989	-4.699509	3.812649
68	1	0	-1.895415	-4.972496	4.266184
69	1	0	-0.342348	-5.606919	3.694902
70	1	0	-0.411592	-4.053476	4.522739
71	6	0	5.545796	-0.899928	-0.775800
72	9	0	5.877361	-1.907198	0.069885
73	9	0	6.223728	0.191987	-0.357005
74	9	0	6.046390	-1.239675	-1.986216

Compound 4 1-RF-N-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.27472634 A.U. after 1 cycles
Lowest frequency = -68.2255

Zero-point correction= 0.604502
(Hartree/Particle)
Thermal correction to Energy= 0.640916
Thermal correction to Enthalpy= 0.641860
Thermal correction to Gibbs Free Energy= 0.534609
Sum of electronic and zero-point Energies= -1695.670225
Sum of electronic and thermal Energies= -1695.633810
Sum of electronic and thermal Enthalpies= -1695.632866
Sum of electronic and thermal Free Energies= -1695.740118

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.772443	1.626644	-0.010846
2	6	0	3.814835	4.581198	1.947519
3	1	0	4.334158	4.167329	2.815000
4	1	0	4.460326	4.421703	1.076398
5	1	0	3.714350	5.660124	2.086010
6	6	0	2.478704	3.922079	1.737395
7	6	0	2.238075	2.606695	2.129363
8	1	0	2.986805	2.082139	2.715522
9	6	0	0.041066	2.570764	1.001416
10	6	0	1.379473	4.623626	1.248070
11	1	0	1.438699	5.704963	1.157997
12	6	0	-4.388682	2.147380	-1.377956
13	1	0	-5.200751	2.868257	-1.335442
14	6	0	-4.650847	0.855163	-1.825579
15	6	0	-3.537163	0.086707	-2.158175
16	1	0	-3.675955	-0.836894	-2.712294
17	6	0	-1.994816	1.666985	-1.051896
18	6	0	-6.053457	0.360793	-2.054584
19	1	0	-6.102643	-0.327864	-2.901341
20	1	0	-6.415883	-0.181181	-1.173701
21	1	0	-6.746171	1.185255	-2.238303
22	6	0	-3.096018	2.590435	-1.097930
23	6	0	1.048131	1.946038	1.830767
24	6	0	0.849157	0.637023	2.572148
25	1	0	-0.191808	0.329894	2.616199
26	1	0	1.437367	-0.188495	2.165359

27	1	0	1.186672	0.790215	3.601531
28	6	0	-2.928082	4.091113	-1.146865
29	1	0	-3.381223	4.426532	-2.085160
30	1	0	-3.435884	4.630002	-0.344382
31	1	0	-1.885534	4.380825	-1.183010
32	6	0	-2.238566	0.479277	-1.840562
33	6	0	-1.150854	-0.331101	-2.521048
34	1	0	-0.203817	0.198119	-2.578207
35	1	0	-0.978102	-1.304522	-2.057009
36	1	0	-1.477699	-0.521376	-3.547555
37	6	0	0.157756	4.004202	0.985530
38	6	0	-1.028899	4.939593	0.988165
39	1	0	-1.047128	5.650798	0.159834
40	1	0	-1.968026	4.402803	1.033742
41	1	0	-0.958703	5.530398	1.907069
42	7	0	-0.184501	0.217422	0.026833
43	6	0	-0.829188	-0.942039	0.475951
44	6	0	1.091439	-0.159199	-0.378025
45	6	0	0.035572	-2.055205	0.365677
46	6	0	-2.104912	-1.090892	1.027851
47	6	0	1.268501	-1.556105	-0.198459
48	6	0	-0.388776	-3.319351	0.790767
49	6	0	-2.498612	-2.356203	1.441001
50	1	0	-2.776670	-0.247355	1.127753
51	6	0	2.468917	-2.163792	-0.570095
52	1	0	0.276665	-4.172891	0.704739
53	1	0	-3.489626	-2.472310	1.866447
54	6	0	3.475384	-1.381490	-1.122413
55	1	0	2.616376	-3.228343	-0.440142
56	6	0	3.288739	0.000966	-1.311358
57	1	0	4.083720	0.586490	-1.756894
58	6	0	2.104643	0.621421	-0.949086
59	1	0	1.975370	1.685057	-1.102972
60	6	0	-1.660243	-3.486418	1.330156
61	6	0	-2.129289	-4.857721	1.797210
62	1	0	-1.305746	-5.554954	1.604747
63	6	0	-2.411073	-4.888293	3.310462
64	1	0	-2.682227	-5.898106	3.633217
65	1	0	-1.534051	-4.571983	3.880596
66	1	0	-3.238190	-4.222449	3.574425
67	6	0	-3.347183	-5.355884	0.998026
68	1	0	-4.217052	-4.711312	1.156356
69	1	0	-3.134895	-5.371893	-0.073922
70	1	0	-3.624367	-6.368593	1.306251
71	6	0	4.792400	-1.985844	-1.501549
72	9	0	5.190646	-1.606740	-2.741092
73	9	0	4.768442	-3.337366	-1.491177
74	9	0	5.789642	-1.610015	-0.659268

Compound 4 1-RF-N-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.27444925 A.U. after 1 cycles
Lowest frequency = -68.0616

Zero-point correction= 0.604475
(Hartree/Particle)
Thermal correction to Energy= 0.640899
Thermal correction to Enthalpy= 0.641843

Thermal correction to Gibbs Free Energy= 0.534327
Sum of electronic and zero-point Energies= -1695.669975
Sum of electronic and thermal Energies= -1695.633550
Sum of electronic and thermal Enthalpies= -1695.632606
Sum of electronic and thermal Free Energies= -1695.740122

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.530275	-1.060775	0.021564
2	6	0	-1.144584	-5.888614	1.789863
3	1	0	-1.817617	-5.795677	2.645394
4	1	0	-1.768583	-6.029767	0.900112
5	1	0	-0.546591	-6.794037	1.916127
6	6	0	-0.277919	-4.668636	1.633821
7	6	0	-0.702238	-3.407592	2.047988
8	1	0	-1.624999	-3.317224	2.613404
9	6	0	1.240797	-2.302802	0.996993
10	6	0	1.035056	-4.750642	1.176191
11	1	0	1.499988	-5.727477	1.073510
12	6	0	4.987536	0.233013	-1.242291
13	1	0	6.043759	-0.015087	-1.180900
14	6	0	4.612453	1.502736	-1.673270
15	6	0	3.274620	1.655270	-2.031502
16	1	0	2.968770	2.544792	-2.574243
17	6	0	2.647312	-0.490855	-0.982348
18	6	0	5.615096	2.609272	-1.858955
19	1	0	5.348989	3.254604	-2.699439
20	1	0	5.656414	3.241244	-0.964562
21	1	0	6.620614	2.217383	-2.028369
22	6	0	4.056123	-0.777305	-1.002438
23	6	0	0.037299	-2.253371	1.797911
24	6	0	-0.428350	-1.026860	2.560530
25	1	0	0.338447	-0.261656	2.640075
26	1	0	-1.330738	-0.572037	2.146037
27	1	0	-0.673386	-1.348450	3.577196
28	6	0	4.625280	-2.175402	-1.063296
29	1	0	5.208181	-2.236826	-1.987764
30	1	0	5.307061	-2.422478	-0.246975
31	1	0	3.848109	-2.925807	-1.134028
32	6	0	2.312978	0.686039	-1.753817
33	6	0	0.984968	0.896925	-2.457222
34	1	0	0.405953	-0.017759	-2.548458
35	1	0	0.359673	1.659239	-1.987471
36	1	0	1.202627	1.244611	-3.471340
37	6	0	1.821169	-3.618482	0.963169
38	6	0	3.309567	-3.876503	1.000775
39	1	0	3.687219	-4.474368	0.168778
40	1	0	3.878085	-2.958815	1.083216
41	1	0	3.503652	-4.450307	1.912631
42	7	0	0.343086	-0.100635	0.056359
43	6	0	0.351740	1.214626	0.538626
44	6	0	-0.949746	-0.363309	-0.383580
45	6	0	-0.936548	1.788316	0.414142
46	6	0	1.390253	1.935907	1.130113
47	6	0	-1.772238	0.777651	-0.194024
48	6	0	-1.175076	3.089515	0.864339
49	6	0	1.123798	3.228117	1.567980

50	1	0	2.380040	1.511189	1.242457
51	6	0	-3.108334	0.753285	-0.596239
52	1	0	-2.166848	3.518169	0.763440
53	1	0	1.926067	3.798079	2.025819
54	6	0	-3.611137	-0.398443	-1.188894
55	1	0	-3.745846	1.617423	-0.459155
56	6	0	-2.786972	-1.522091	-1.387224
57	1	0	-3.198787	-2.403108	-1.864267
58	6	0	-1.458605	-1.516322	-0.994830
59	1	0	-0.836947	-2.387527	-1.156768
60	6	0	-0.144850	3.827591	1.444924
61	6	0	-0.371102	5.248188	1.946670
62	1	0	0.584481	5.594793	2.356716
63	6	0	-0.755484	6.208911	0.806817
64	1	0	-0.848585	7.233904	1.178563
65	1	0	-0.003413	6.200598	0.013849
66	1	0	-1.714102	5.929647	0.359468
67	6	0	-1.404403	5.301902	3.086524
68	1	0	-2.392837	4.984569	2.741123
69	1	0	-1.114565	4.647375	3.912322
70	1	0	-1.499955	6.320375	3.475168
71	6	0	-5.048346	-0.480665	-1.602465
72	9	0	-5.191522	-0.974778	-2.857076
73	9	0	-5.667381	0.720857	-1.578706
74	9	0	-5.767542	-1.302466	-0.794649

Compound 4 2-RF-CC-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.35487040 A.U. after 1 cycles
Lowest frequency = -59.4467

Zero-point correction= 0.604365
(Hartree/Particle)
Thermal correction to Energy= 0.641855
Thermal correction to Enthalpy= 0.642799
Thermal correction to Gibbs Free Energy= 0.530647
Sum of electronic and zero-point Energies= -1695.750506
Sum of electronic and thermal Energies= -1695.713015
Sum of electronic and thermal Enthalpies= -1695.712071
Sum of electronic and thermal Free Energies= -1695.824223

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.379256	0.261559	-0.012565
2	6	0	1.850905	1.607396	-0.009720
3	6	0	0.448805	1.504338	-0.006712
4	7	0	0.058935	0.120467	-0.008205
5	6	0	1.281574	-0.623468	-0.012736
6	6	0	1.500023	-2.003350	-0.020391
7	6	0	2.808514	-2.470702	-0.025587
8	6	0	3.897762	-1.589409	-0.024290
9	6	0	3.688407	-0.216567	-0.017528
10	6	0	2.483177	2.852092	-0.009126
11	6	0	1.725059	4.019193	-0.005718
12	6	0	0.324189	3.896800	-0.002760

13	6	0	-0.324780	2.666194	-0.003145
14	6	0	2.399050	5.383763	-0.005288
15	6	0	2.065248	6.190711	-1.273091
16	6	0	2.070895	6.187148	1.266240
17	1	0	0.683906	-2.706172	-0.024625
18	1	0	2.986594	-3.538882	-0.038680
19	1	0	4.528372	0.465770	-0.021316
20	1	0	3.566916	2.909936	-0.011385
21	1	0	-0.287996	4.791987	-0.000084
22	1	0	-1.401617	2.630567	-0.000784
23	1	0	3.479941	5.202453	-0.007957
24	1	0	2.612127	7.138177	-1.281343
25	1	0	2.331711	5.635648	-2.175941
26	1	0	0.997584	6.423119	-1.326753
27	1	0	2.617737	7.134634	1.274672
28	1	0	2.341450	5.629597	2.166335
29	1	0	1.003466	6.419310	1.325346
30	5	0	-1.283354	-0.406759	-0.003535
31	6	0	-2.569981	0.559544	0.003929
32	6	0	-3.183355	0.969292	1.214489
33	6	0	-3.195217	0.973052	-1.199274
34	6	0	-4.430801	1.598148	1.200794
35	6	0	-4.442413	1.601916	-1.171339
36	6	0	-5.106020	1.886096	0.018470
37	1	0	-4.871652	1.895521	2.148794
38	1	0	-4.892539	1.902322	-2.114005
39	6	0	-1.569340	-1.991083	-0.004663
40	6	0	-1.730902	-2.717608	1.202101
41	6	0	-1.743225	-2.713764	-1.211992
42	6	0	-2.191840	-4.036351	1.181129
43	6	0	-2.203967	-4.032579	-1.190601
44	6	0	-2.478041	-4.706427	-0.004380
45	1	0	-2.303218	-4.561132	2.126332
46	1	0	-2.324954	-4.554338	-2.136302
47	6	0	-2.526334	0.881640	-2.555538
48	1	0	-2.614440	1.842828	-3.069501
49	1	0	-1.464096	0.654834	-2.486126
50	1	0	-2.994612	0.132224	-3.198208
51	6	0	-2.501130	0.873839	2.563809
52	1	0	-1.440305	0.644202	2.483531
53	1	0	-2.581442	1.834456	3.080136
54	1	0	-2.965118	0.124699	3.209931
55	6	0	-6.479207	2.510563	0.026200
56	1	0	-7.258057	1.739942	0.029247
57	1	0	-6.631761	3.130996	0.912657
58	1	0	-6.640765	3.133120	-0.857164
59	6	0	-1.352348	-2.168193	-2.569796
60	1	0	-2.222039	-1.867802	-3.158655
61	1	0	-0.678829	-1.315203	-2.500811
62	1	0	-0.831910	-2.942300	-3.139687
63	6	0	-1.326853	-2.176186	2.557691
64	1	0	-0.651817	-1.324705	2.484784
65	1	0	-2.190649	-1.874965	3.154725
66	1	0	-0.803392	-2.952858	3.121241
67	6	0	-3.028651	-6.110820	-0.003772
68	1	0	-2.703599	-6.667647	0.878384
69	1	0	-4.124238	-6.100040	0.002283
70	1	0	-2.713336	-6.664611	-0.891356
71	6	0	5.288961	-2.152106	0.009562
72	9	0	5.451038	-3.156339	-0.883479

73	9	0	5.595038	-2.671292	1.223843
74	9	0	6.229733	-1.221612	-0.263588

Compound 4 2-RF-CC-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.35471899 A.U. after 1 cycles
Lowest frequency = -59.4540

Zero-point correction= 0.604425
(Hartree/Particle)
Thermal correction to Energy= 0.641867
Thermal correction to Enthalpy= 0.642811
Thermal correction to Gibbs Free Energy= 0.531317
Sum of electronic and zero-point Energies= -1695.750294
Sum of electronic and thermal Energies= -1695.712852
Sum of electronic and thermal Enthalpies= -1695.711908
Sum of electronic and thermal Free Energies= -1695.823402

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.324307	-0.082245	-0.013233
2	6	0	2.019539	1.331710	-0.010000
3	6	0	0.616941	1.454976	-0.006640
4	7	0	0.011002	0.150687	-0.008305
5	6	0	1.098852	-0.779237	-0.013269
6	6	0	1.092737	-2.176157	-0.021510
7	6	0	2.309071	-2.848029	-0.027217
8	6	0	3.525645	-2.153343	-0.026212
9	6	0	3.539347	-0.764508	-0.018975
10	6	0	2.845058	2.454804	-0.009151
11	6	0	2.282786	3.731044	-0.005152
12	6	0	0.883379	3.834064	-0.001975
13	6	0	0.040964	2.724142	-0.002591
14	6	0	3.148791	4.983055	-0.004326
15	6	0	4.016966	5.081309	1.263119
16	6	0	4.010042	5.087616	-1.275993
17	1	0	0.173984	-2.738362	-0.026067
18	1	0	2.313341	-3.930891	-0.041232
19	1	0	4.478163	-0.226110	-0.023643
20	1	0	3.922248	2.327347	-0.011603
21	1	0	0.431593	4.820741	0.001104
22	1	0	-1.027149	2.864914	-0.000020
23	1	0	2.465819	5.840017	-0.000328
24	1	0	4.579163	6.019748	1.273333
25	1	0	3.403156	5.041802	2.166392
26	1	0	4.739369	4.261272	1.314392
27	1	0	4.572382	6.025988	-1.284517
28	1	0	3.391275	5.052828	-2.176075
29	1	0	4.731936	4.267678	-1.335395
30	5	0	-1.397457	-0.158061	-0.003505
31	6	0	-2.511903	1.003722	0.004185
32	6	0	-3.044227	1.514193	1.214903
33	6	0	-3.055507	1.519780	-1.199130
34	6	0	-4.149472	2.368812	1.200813
35	6	0	-4.160501	2.374356	-1.170781

36	6	0	-4.755258	2.783410	0.018779
37	1	0	-4.528982	2.740210	2.149048
38	1	0	-4.548805	2.750193	-2.113693
39	6	0	-1.934979	-1.674661	-0.004881
40	6	0	-2.221034	-2.361942	1.201697
41	6	0	-2.231837	-2.356049	-1.212198
42	6	0	-2.924119	-3.568966	1.181127
43	6	0	-2.934725	-3.563177	-1.191313
44	6	0	-3.335824	-4.170029	-0.004749
45	1	0	-3.129179	-4.065540	2.126042
46	1	0	-3.148197	-4.055138	-2.136781
47	6	0	-2.438991	1.273847	-2.560188
48	1	0	-2.481657	2.190146	-3.154247
49	1	0	-1.391128	0.982204	-2.497072
50	1	0	-2.973239	0.503422	-3.120475
51	6	0	-2.415115	1.262040	2.569039
52	1	0	-1.368100	0.969994	2.494942
53	1	0	-2.451606	2.175827	3.167363
54	1	0	-2.944647	0.489582	3.131000
55	6	0	-5.981767	3.661625	0.026536
56	1	0	-6.895028	3.056300	0.029128
57	1	0	-6.011545	4.299519	0.913215
58	1	0	-6.019540	4.303996	-0.856601
59	6	0	-1.710323	-1.912807	-2.563995
60	1	0	-2.513060	-1.593294	-3.233158
61	1	0	-0.984922	-1.105025	-2.492480
62	1	0	-1.205657	-2.752621	-3.050289
63	6	0	-1.688031	-1.925037	2.551059
64	1	0	-0.962366	-1.117715	2.477104
65	1	0	-2.484980	-1.607553	3.228074
66	1	0	-1.180299	-2.767422	3.029609
67	6	0	-4.147963	-5.441220	-0.004209
68	1	0	-3.937044	-6.050547	0.877932
69	1	0	-5.220699	-5.218348	0.001808
70	1	0	-3.945933	-6.045622	-0.891800
71	6	0	4.809325	-2.930462	0.011004
72	9	0	4.796173	-3.972656	-0.852352
73	9	0	5.046846	-3.456536	1.237670
74	9	0	5.882376	-2.170124	-0.299404

Compound 4 2-RF-CN-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.33800773 A.U. after 1 cycles
Lowest frequency = -37.1346

Zero-point correction= 0.604461
(Hartree/Particle)
Thermal correction to Energy= 0.641564
Thermal correction to Enthalpy= 0.642508
Thermal correction to Gibbs Free Energy= 0.532379
Sum of electronic and zero-point Energies= -1695.733547
Sum of electronic and thermal Energies= -1695.696444
Sum of electronic and thermal Enthalpies= -1695.695499
Sum of electronic and thermal Free Energies= -1695.805628

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	2.209075	-0.300662	-0.210880
2	6	0	1.995486	1.124005	-0.186395
3	6	0	0.596770	1.318396	-0.276859
4	7	0	-0.065120	0.081021	-0.307133
5	6	0	0.924566	-0.898941	-0.315316
6	6	0	0.808618	-2.280472	-0.515019
7	6	0	1.960828	-3.050790	-0.531635
8	6	0	3.229150	-2.466492	-0.369173
9	6	0	3.357980	-1.090858	-0.221753
10	6	0	2.861907	2.221247	-0.167215
11	6	0	2.359944	3.514979	-0.267422
12	6	0	0.967883	3.682021	-0.416087
13	6	0	0.084641	2.610023	-0.431262
14	6	0	3.296920	4.714765	-0.245292
15	6	0	3.260302	5.504456	-1.566355
16	6	0	3.024545	5.635738	0.957869
17	1	0	-0.150786	-2.746824	-0.684879
18	1	0	1.886049	-4.118779	-0.695671
19	1	0	4.339569	-0.642180	-0.137636
20	1	0	3.933220	2.063375	-0.090260
21	1	0	0.563434	4.681064	-0.538288
22	1	0	-0.970423	2.784113	-0.587352
23	1	0	4.312516	4.319056	-0.130073
24	1	0	3.989620	6.319971	-1.549243
25	1	0	3.490562	4.859000	-2.417628
26	1	0	2.274188	5.945857	-1.739302
27	1	0	3.751089	6.453245	0.991611
28	1	0	3.088294	5.083633	1.898793
29	1	0	2.026678	6.080807	0.899114
30	5	0	-1.547986	-0.143076	-0.013262
31	6	0	-1.864290	-0.217686	1.554475
32	6	0	-1.798564	-1.442791	2.259908
33	6	0	-2.153315	0.947799	2.303403
34	6	0	-1.913240	-1.464377	3.651585
35	6	0	-2.261825	0.885360	3.694385
36	6	0	-2.114355	-0.306683	4.398088
37	1	0	-1.862533	-2.422315	4.162368
38	1	0	-2.488731	1.797871	4.239364
39	6	0	-2.568987	-0.270352	-1.182831
40	6	0	-2.173271	-0.185218	-2.565963
41	6	0	-3.970930	-0.480792	-0.926945
42	6	0	-3.127171	-0.302248	-3.576472
43	6	0	-4.873164	-0.589445	-1.983234
44	6	0	-4.479521	-0.500895	-3.315525
45	1	0	-2.799550	-0.237829	-4.608935
46	1	0	-5.922206	-0.751419	-1.757572
47	6	0	-2.430557	2.290425	1.658189
48	1	0	-1.555310	2.943487	1.687797
49	1	0	-2.741023	2.192443	0.615472
50	1	0	-3.237597	2.802732	2.188813
51	6	0	-1.678747	-2.784600	1.566087
52	1	0	-2.002258	-2.742310	0.523597
53	1	0	-0.653812	-3.162314	1.585913
54	1	0	-2.307071	-3.524783	2.068695
55	6	0	-2.185854	-0.344887	5.904691
56	1	0	-2.574947	-1.301180	6.262525
57	1	0	-1.192075	-0.211127	6.346098
58	1	0	-2.825543	0.450344	6.294996

59	6	0	-4.588836	-0.604697	0.450313
60	1	0	-4.178248	-1.439700	1.017843
61	1	0	-4.436145	0.287569	1.057389
62	1	0	-5.664311	-0.763071	0.354147
63	6	0	-0.755915	0.025469	-3.061165
64	1	0	-0.326160	0.963961	-2.710323
65	1	0	-0.083062	-0.774872	-2.752056
66	1	0	-0.755241	0.051030	-4.152099
67	6	0	-5.484869	-0.590918	-4.433219
68	1	0	-5.885266	0.401357	-4.669414
69	1	0	-5.033796	-0.986765	-5.345540
70	1	0	-6.329722	-1.226940	-4.160239
71	6	0	4.435781	-3.353977	-0.344705
72	9	0	4.400034	-4.291323	-1.323689
73	9	0	4.544616	-4.037635	0.823134
74	9	0	5.589846	-2.666784	-0.497380

Compound 4 2-RF-CN-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.33778030 A.U. after 2 cycles
Lowest frequency = -36.5623

Zero-point correction= 0.604499
(Hartree/Particle)
Thermal correction to Energy= 0.641590
Thermal correction to Enthalpy= 0.642534
Thermal correction to Gibbs Free Energy= 0.532313
Sum of electronic and zero-point Energies= -1695.733281
Sum of electronic and thermal Energies= -1695.696190
Sum of electronic and thermal Enthalpies= -1695.695246
Sum of electronic and thermal Free Energies= -1695.805467

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.131651	-0.347024	-0.212461
2	6	0	1.974101	1.084764	-0.271680
3	6	0	0.581749	1.327589	-0.371500
4	7	0	-0.126808	0.116535	-0.326426
5	6	0	0.824643	-0.899702	-0.278976
6	6	0	0.654573	-2.285000	-0.396428
7	6	0	1.776156	-3.099269	-0.369580
8	6	0	3.066632	-2.556377	-0.244481
9	6	0	3.248850	-1.180211	-0.178821
10	6	0	2.883457	2.142950	-0.317849
11	6	0	2.430153	3.449789	-0.492226
12	6	0	1.047842	3.660361	-0.647713
13	6	0	0.119910	2.624924	-0.600377
14	6	0	3.395776	4.626718	-0.542372
15	6	0	4.142211	4.813929	0.791016
16	6	0	4.383154	4.518519	-1.718390
17	1	0	-0.322871	-2.723037	-0.536249
18	1	0	1.659332	-4.171355	-0.469953
19	1	0	4.247450	-0.765885	-0.123382
20	1	0	3.945670	1.938086	-0.233886
21	1	0	0.690823	4.669781	-0.825851

22	1	0	-0.927666	2.832428	-0.765369
23	1	0	2.790605	5.525739	-0.706555
24	1	0	4.780536	5.702030	0.756284
25	1	0	3.442038	4.928996	1.622174
26	1	0	4.781213	3.953523	1.011032
27	1	0	5.020257	5.406547	-1.771231
28	1	0	3.854343	4.420947	-2.669819
29	1	0	5.036806	3.648004	-1.609607
30	5	0	-1.615323	-0.031055	-0.013995
31	6	0	-1.924181	0.000800	1.556521
32	6	0	-1.902083	-1.182549	2.332457
33	6	0	-2.162137	1.218718	2.236821
34	6	0	-2.008327	-1.118189	3.723450
35	6	0	-2.264029	1.241983	3.629529
36	6	0	-2.158935	0.088265	4.401456
37	1	0	-1.991948	-2.045863	4.289372
38	1	0	-2.451381	2.193068	4.120962
39	6	0	-2.647580	-0.188691	-1.169918
40	6	0	-2.257224	-0.202304	-2.557034
41	6	0	-4.055019	-0.329135	-0.896611
42	6	0	-3.220887	-0.343802	-3.555152
43	6	0	-4.966984	-0.466863	-1.941018
44	6	0	-4.578184	-0.474411	-3.277693
45	1	0	-2.897184	-0.354339	-4.590807
46	1	0	-6.020092	-0.574365	-1.702140
47	6	0	-2.390756	2.531382	1.515349
48	1	0	-1.490413	3.149967	1.502975
49	1	0	-2.711485	2.385297	0.481447
50	1	0	-3.173711	3.105087	2.018526
51	6	0	-1.839474	-2.566397	1.718124
52	1	0	-2.166030	-2.572220	0.675734
53	1	0	-0.830379	-2.983260	1.757517
54	1	0	-2.494491	-3.250062	2.264797
55	6	0	-2.222026	0.141130	5.907993
56	1	0	-2.645539	-0.776651	6.323031
57	1	0	-1.220943	0.261536	6.336550
58	1	0	-2.827853	0.982213	6.253661
59	6	0	-4.668836	-0.345215	0.487911
60	1	0	-4.288309	-1.160368	1.103282
61	1	0	-4.476891	0.575098	1.039349
62	1	0	-5.750341	-0.465840	0.405594
63	6	0	-0.835980	-0.075113	-3.069223
64	1	0	-0.369189	0.865272	-2.775508
65	1	0	-0.191957	-0.881063	-2.716331
66	1	0	-0.840972	-0.113365	-4.159775
67	6	0	-5.593053	-0.593370	-4.384024
68	1	0	-5.965252	0.396552	-4.670792
69	1	0	-5.160154	-1.050817	-5.276073
70	1	0	-6.454815	-1.188039	-4.073163
71	6	0	4.238576	-3.486413	-0.169190
72	9	0	4.159181	-4.483060	-1.084881
73	9	0	4.331071	-4.096569	1.040041
74	9	0	5.416708	-2.855351	-0.372750

Compound 4 3-RF-TSa

Method: b3lyp/6-311g(d,p)

SCF Done: E(RB3LYP) = -1696.29360417   A.U. after   1 cycles
Lowest frequency = -57.9164

Zero-point correction=   0.604619
(Hartree/Particle)
Thermal correction to Energy=   0.641933
Thermal correction to Enthalpy=   0.642877
Thermal correction to Gibbs Free Energy=   0.531197
Sum of electronic and zero-point Energies=   -1695.688985
Sum of electronic and thermal Energies=   -1695.651672
Sum of electronic and thermal Enthalpies=   -1695.650727
Sum of electronic and thermal Free Energies=   -1695.762407

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.253080	-0.549808	-0.187388
2	6	0	-2.210821	0.873989	-0.383955
3	6	0	-0.867651	1.200259	-0.668554
4	7	0	-0.037197	0.047808	-0.577271
5	6	0	-0.934596	-1.031842	-0.384530
6	6	0	-0.715423	-2.410350	-0.408090
7	6	0	-1.776644	-3.274939	-0.180539
8	6	0	-3.068679	-2.790473	0.067978
9	6	0	-3.312236	-1.423772	0.050883
10	6	0	-3.222229	1.835101	-0.458872
11	6	0	-2.928842	3.131305	-0.867615
12	6	0	-1.604181	3.415916	-1.248171
13	6	0	-0.585515	2.473381	-1.172801
14	6	0	-4.019724	4.189109	-0.949307
15	6	0	-3.747546	5.366195	0.004845
16	6	0	-4.242707	4.683360	-2.390130
17	1	0	0.245686	-2.818622	-0.650509
18	1	0	-1.606531	-4.343820	-0.220209
19	1	0	-4.315106	-1.045478	0.202262
20	1	0	-4.246326	1.560023	-0.227148
21	1	0	-1.362034	4.397555	-1.640735
22	1	0	0.388260	2.728349	-1.556108
23	1	0	-4.948940	3.709697	-0.620880
24	1	0	-4.574863	6.081732	-0.019199
25	1	0	-3.626251	5.019687	1.034117
26	1	0	-2.836187	5.902254	-0.276693
27	1	0	-5.075814	5.391378	-2.429574
28	1	0	-4.469931	3.851832	-3.061749
29	1	0	-3.356235	5.193676	-2.778332
30	5	0	1.421110	0.012041	-0.112561
31	6	0	2.607791	-0.591102	-1.062078
32	6	0	3.113335	-1.905888	-1.302055
33	6	0	3.310244	0.451210	-1.734386
34	6	0	4.280337	-2.086270	-2.058904
35	6	0	4.457421	0.221355	-2.491407
36	6	0	4.987847	-1.049969	-2.650789
37	1	0	4.640700	-3.101365	-2.195569
38	1	0	4.941055	1.070953	-2.965860
39	6	0	1.799607	0.589643	1.371915
40	6	0	2.025287	-0.431586	2.344399
41	6	0	1.941814	1.925986	1.854695
42	6	0	2.395366	-0.138618	3.656086

43	6	0	2.336057	2.165921	3.179009
44	6	0	2.582543	1.162264	4.101779
45	1	0	2.532633	-0.964651	4.347830
46	1	0	2.437226	3.198955	3.497058
47	6	0	2.812770	1.873011	-1.743950
48	1	0	2.261370	2.077082	-2.668102
49	1	0	2.152770	2.089686	-0.913561
50	1	0	3.638477	2.586397	-1.686656
51	6	0	2.486942	-3.234195	-0.911920
52	1	0	1.928994	-3.230530	0.013004
53	1	0	1.824257	-3.581042	-1.712623
54	1	0	3.266530	-3.991364	-0.806191
55	6	0	6.264860	-1.292381	-3.414628
56	1	0	7.138233	-1.171681	-2.764341
57	1	0	6.298968	-2.304432	-3.824248
58	1	0	6.374627	-0.586621	-4.241644
59	6	0	1.717241	3.209413	1.077885
60	1	0	2.611396	3.517392	0.528169
61	1	0	0.884814	3.154899	0.386786
62	1	0	1.486329	4.015569	1.776297
63	6	0	1.878235	-1.902953	2.045029
64	1	0	1.016900	-2.120466	1.413967
65	1	0	2.779348	-2.292716	1.567705
66	1	0	1.730535	-2.464631	2.969316
67	6	0	3.025008	1.463038	5.511300
68	1	0	2.537168	0.801260	6.231721
69	1	0	4.105874	1.322268	5.620887
70	1	0	2.797469	2.494419	5.789109
71	6	0	-4.170513	-3.762110	0.364962
72	9	0	-4.095002	-4.246190	1.630327
73	9	0	-4.132478	-4.841180	-0.453076
74	9	0	-5.397016	-3.209041	0.236218

Compound 4 3-RF-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1696.29340032 A.U. after 1 cycles
Lowest frequency = -57.9087

Zero-point correction= 0.604587
(Hartree/Particle)
Thermal correction to Energy= 0.641916
Thermal correction to Enthalpy= 0.642861
Thermal correction to Gibbs Free Energy= 0.531018
Sum of electronic and zero-point Energies= -1695.688813
Sum of electronic and thermal Energies= -1695.651484
Sum of electronic and thermal Enthalpies= -1695.650540
Sum of electronic and thermal Free Energies= -1695.762382

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.194198	0.519321	-0.203823
2	6	0	2.156125	-0.890434	-0.488411
3	6	0	0.809677	-1.203716	-0.781576
4	7	0	-0.023403	-0.062199	-0.609855
5	6	0	0.872440	1.007009	-0.359073

6	6	0	0.648289	2.383404	-0.295168
7	6	0	1.708412	3.236578	-0.023207
8	6	0	3.004127	2.743052	0.183738
9	6	0	3.252109	1.380879	0.079349
10	6	0	3.170786	-1.837107	-0.631194
11	6	0	2.876684	-3.109655	-1.116572
12	6	0	1.551903	-3.374341	-1.499776
13	6	0	0.527354	-2.442431	-1.359887
14	6	0	3.955265	-4.171022	-1.282791
15	6	0	5.044313	-3.740014	-2.281789
16	6	0	4.571586	-4.575791	0.068567
17	1	0	-0.316326	2.802089	-0.503410
18	1	0	1.533993	4.305133	0.005403
19	1	0	4.257658	0.998083	0.198239
20	1	0	4.192763	-1.562567	-0.392318
21	1	0	1.318071	-4.335408	-1.946499
22	1	0	-0.448380	-2.678990	-1.749825
23	1	0	3.464471	-5.058831	-1.697695
24	1	0	5.768405	-4.545919	-2.434059
25	1	0	4.611171	-3.482953	-3.251604
26	1	0	5.593250	-2.865873	-1.919376
27	1	0	5.296741	-5.384217	-0.064219
28	1	0	3.803318	-4.917689	0.766506
29	1	0	5.093203	-3.734046	0.533687
30	5	0	-1.477276	-0.063935	-0.130577
31	6	0	-2.676511	0.590239	-1.029172
32	6	0	-3.188957	1.915199	-1.183348
33	6	0	-3.382251	-0.411916	-1.756783
34	6	0	-4.364509	2.136773	-1.915533
35	6	0	-4.538097	-0.140834	-2.486569
36	6	0	-5.074644	1.135617	-2.562316
37	1	0	-4.729820	3.156831	-1.986185
38	1	0	-5.023656	-0.961775	-3.007234
39	6	0	-1.838407	-0.734968	1.318683
40	6	0	-2.058657	0.223375	2.354282
41	6	0	-1.970355	-2.099189	1.719646
42	6	0	-2.415064	-0.151317	3.648874
43	6	0	-2.350800	-2.421845	3.030321
44	6	0	-2.592762	-1.477953	4.015342
45	1	0	-2.549057	0.630006	4.391342
46	1	0	-2.444459	-3.472952	3.285243
47	6	0	-2.879621	-1.828242	-1.858823
48	1	0	-2.334694	-1.971828	-2.798071
49	1	0	-2.212453	-2.093523	-1.048527
50	1	0	-3.702239	-2.547220	-1.840103
51	6	0	-2.562467	3.219448	-0.719443
52	1	0	-1.996742	3.161722	0.198980
53	1	0	-1.907414	3.615617	-1.503358
54	1	0	-3.342854	3.966697	-0.561889
55	6	0	-6.360566	1.419092	-3.296498
56	1	0	-7.226253	1.261066	-2.643930
57	1	0	-6.399987	2.452555	-3.648119
58	1	0	-6.479567	0.760830	-4.160554
59	6	0	-1.747729	-3.331513	0.863484
60	1	0	-2.646488	-3.610789	0.305975
61	1	0	-0.923555	-3.229862	0.167852
62	1	0	-1.504635	-4.177347	1.508833
63	6	0	-1.920141	1.711063	2.144718
64	1	0	-1.066435	1.970783	1.519279
65	1	0	-2.827688	2.125806	1.701834

66	1	0	-1.764423	2.215281	3.100298
67	6	0	-3.021213	-1.867101	5.407451
68	1	0	-2.538697	-1.240963	6.162424
69	1	0	-4.103375	-1.749790	5.531165
70	1	0	-2.776411	-2.909326	5.623284
71	6	0	4.105139	3.698774	0.531015
72	9	0	4.037184	4.105686	1.823660
73	9	0	4.058145	4.824905	-0.220397
74	9	0	5.332320	3.158500	0.360758

Compound 5 GS1

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1394.92187425 A.U. after 1 cycles
Lowest frequency = 20.8026

Zero-point correction= 0.562450
(Hartree/Particle)
Thermal correction to Energy= 0.595260
Thermal correction to Enthalpy= 0.596204
Thermal correction to Gibbs Free Energy= 0.497380
Sum of electronic and zero-point Energies= -1394.359425
Sum of electronic and thermal Energies= -1394.326614
Sum of electronic and thermal Enthalpies= -1394.325670
Sum of electronic and thermal Free Energies= -1394.424494

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.584410	0.227458	-0.048021
2	6	0	2.671926	1.331917	-1.986681
3	1	0	2.090498	0.582761	-2.530270
4	1	0	2.062888	2.237651	-1.940960
5	1	0	3.560242	1.553178	-2.581864
6	6	0	0.803122	2.926047	1.408301
7	1	0	0.576341	3.876237	1.896485
8	1	0	0.625308	2.132507	2.137754
9	1	0	1.873178	2.911011	1.186850
10	6	0	-1.143792	0.271199	-2.564099
11	1	0	-0.254756	-0.359529	-2.607914
12	1	0	-1.959547	-0.350234	-2.184138
13	1	0	-1.398665	0.552969	-3.587909
14	6	0	-2.127024	5.141863	-1.988918
15	1	0	-3.085402	5.280449	-1.476257
16	1	0	-1.526039	6.035273	-1.801169
17	1	0	-2.333436	5.088476	-3.060108
18	6	0	-1.431727	3.896152	-1.498404
19	6	0	-0.662951	3.912588	-0.334284
20	1	0	-0.549494	4.845925	0.209964
21	6	0	-0.027364	2.770452	0.149530
22	6	0	-0.179119	1.527632	-0.523758
23	6	0	-0.950273	1.511641	-1.714776
24	6	0	-1.546983	2.687790	-2.177890
25	1	0	-2.118405	2.653492	-3.101064
26	6	0	2.598339	-0.172881	1.551076
27	6	0	3.948452	-0.039161	1.881108
28	1	0	4.286519	-0.384825	2.853873

29	6	0	4.875433	0.512939	0.998659
30	6	0	4.412403	0.939691	-0.245719
31	1	0	5.119240	1.354664	-0.958623
32	6	0	3.066457	0.850879	-0.605234
33	6	0	2.127097	0.287478	0.295022
34	6	0	1.689667	-0.821955	2.576314
35	1	0	1.415288	-1.837677	2.278250
36	1	0	2.192202	-0.885447	3.543582
37	1	0	0.756945	-0.273630	2.725144
38	6	0	6.326211	0.664680	1.384893
39	1	0	6.980679	0.595249	0.512801
40	1	0	6.506811	1.639516	1.851561
41	1	0	6.630708	-0.101430	2.101718
42	7	0	-0.101464	-1.065940	0.032781
43	6	0	0.467209	-2.268257	-0.491114
44	6	0	-1.480619	-1.338355	0.234056
45	6	0	-0.559588	-3.211807	-0.710819
46	6	0	1.785603	-2.574288	-0.840680
47	6	0	-1.787226	-2.613788	-0.250788
48	6	0	-2.467716	-0.580907	0.940477
49	6	0	-0.275556	-4.462633	-1.266771
50	6	0	2.051722	-3.827834	-1.384296
51	1	0	2.590507	-1.872753	-0.688630
52	6	0	-3.104502	-3.122327	-0.216396
53	6	0	-3.807071	-1.104978	0.942318
54	6	0	-2.218205	0.589981	1.697490
55	6	0	1.035985	-4.767883	-1.599697
56	1	0	-1.069645	-5.182160	-1.432577
57	1	0	3.074502	-4.076764	-1.643900
58	6	0	-4.097393	-2.360566	0.334341
59	1	0	-3.318599	-4.102929	-0.626013
60	6	0	-4.827721	-0.380657	1.607444
61	6	0	-3.227945	1.251105	2.357359
62	1	0	-1.212729	0.970266	1.771048
63	1	0	1.277799	-5.734332	-2.026767
64	1	0	-5.120221	-2.720364	0.357551
65	6	0	-4.553721	0.777522	2.293984
66	1	0	-5.837951	-0.775811	1.581870
67	1	0	-2.998936	2.140322	2.933561
68	1	0	-5.346405	1.312557	2.804498

Compound 5 1-RF-C-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1394.85345131 A.U. after 1 cycles
Lowest frequency = -26.3568

Zero-point correction= 0.562008
(Hartree/Particle)
Thermal correction to Energy= 0.593378
Thermal correction to Enthalpy= 0.594322
Thermal correction to Gibbs Free Energy= 0.500661
Sum of electronic and zero-point Energies= -1394.291443
Sum of electronic and thermal Energies= -1394.260073
Sum of electronic and thermal Enthalpies= -1394.259129
Sum of electronic and thermal Free Energies= -1394.352790

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.562984	0.366060	0.394355
2	6	0	-1.448969	5.065526	-2.373955
3	1	0	-0.698033	5.825795	-2.600923
4	1	0	-1.727447	4.586746	-3.319545
5	1	0	-2.340983	5.566822	-1.989890
6	6	0	-0.925616	4.044200	-1.398868
7	6	0	0.435272	3.816907	-1.233177
8	1	0	1.144371	4.472799	-1.730456
9	6	0	0.043983	1.871550	0.218859
10	6	0	-1.774565	3.346206	-0.540890
11	1	0	-2.818848	3.638055	-0.469549
12	6	0	3.868030	-0.447782	2.236810
13	1	0	4.165585	-0.616021	3.268344
14	6	0	4.830089	-0.518683	1.227811
15	6	0	4.410630	-0.298776	-0.082048
16	1	0	5.140508	-0.350247	-0.886008
17	6	0	2.112769	0.063039	0.624496
18	6	0	6.278977	-0.792697	1.552770
19	1	0	6.813448	-1.189761	0.686806
20	1	0	6.793013	0.123472	1.864121
21	1	0	6.375640	-1.512109	2.370064
22	6	0	2.530721	-0.164564	1.956088
23	6	0	0.940712	2.810126	-0.400753
24	6	0	2.428228	2.937844	-0.113779
25	1	0	2.727725	2.439342	0.802131
26	1	0	3.063939	2.573461	-0.921195
27	1	0	2.642806	4.004259	0.001822
28	6	0	1.538501	-0.119430	3.099451
29	1	0	2.048789	-0.134037	4.064693
30	1	0	0.920466	0.783231	3.063887
31	1	0	0.862385	-0.980340	3.070692
32	6	0	3.080037	-0.012107	-0.400281
33	6	0	2.743145	0.189794	-1.864581
34	1	0	2.757743	-0.762314	-2.401222
35	1	0	1.757758	0.632301	-2.013749
36	1	0	3.478515	0.841689	-2.345210
37	6	0	-1.308579	2.337377	0.296421
38	6	0	-2.210650	1.985201	1.454121
39	1	0	-3.197654	1.634364	1.151189
40	1	0	-1.766099	1.257884	2.122659
41	1	0	-2.356432	2.899868	2.040128
42	7	0	-0.245430	-0.862386	0.128150
43	6	0	0.313992	-1.814640	-0.812924
44	6	0	-1.652988	-0.950636	-0.133555
45	6	0	-0.623875	-2.055968	-1.843384
46	6	0	1.497155	-2.541164	-0.761425
47	6	0	-1.884488	-1.485505	-1.401224
48	6	0	-2.710496	-0.935748	0.814282
49	6	0	-0.314990	-2.913983	-2.898320
50	6	0	1.782274	-3.419796	-1.809207
51	1	0	2.176910	-2.450987	0.071270
52	6	0	-3.197637	-1.621141	-1.901798
53	6	0	-4.047032	-1.080786	0.308524
54	6	0	-2.514051	-0.958641	2.219558
55	1	0	-1.033767	-3.094597	-3.689850
56	1	0	2.697628	-3.999562	-1.770755
57	6	0	-4.257211	-1.349475	-1.073395

58	1	0	-3.363070	-1.970619	-2.914616
59	6	0	-5.126329	-1.063062	1.228936
60	6	0	-3.581537	-1.010033	3.082460
61	1	0	-1.501513	-0.957217	2.603187
62	1	0	-5.275453	-1.440047	-1.435928
63	6	0	-4.904128	-1.021017	2.584725
64	1	0	-6.137951	-1.130186	0.842047
65	1	0	-3.410108	-1.046966	4.152422
66	1	0	-5.739905	-1.035132	3.274995
67	6	0	0.906243	-3.581662	-2.885565
68	1	0	1.157412	-4.266380	-3.687495

Compound 5 1-RF-C1-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1394.84760961 A.U. after 1 cycles
Lowest frequency = -38.1445

Zero-point correction= 0.561813
(Hartree/Particle)
Thermal correction to Energy= 0.593227
Thermal correction to Enthalpy= 0.594171
Thermal correction to Gibbs Free Energy= 0.500203
Sum of electronic and zero-point Energies= -1394.285796
Sum of electronic and thermal Energies= -1394.254383
Sum of electronic and thermal Enthalpies= -1394.253438
Sum of electronic and thermal Free Energies= -1394.347406

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.280489	-2.877341	-3.007488
2	1	0	3.978230	-3.786793	-3.531687
3	1	0	4.277524	-2.060727	-3.738260
4	1	0	5.311239	-3.002584	-2.666338
5	6	0	3.353466	-2.563618	-1.863452
6	6	0	2.056756	-3.059204	-1.810356
7	1	0	1.739500	-3.791288	-2.547671
8	6	0	1.495481	-1.675966	0.147558
9	6	0	3.782230	-1.845383	-0.747357
10	1	0	4.840781	-1.630671	-0.628115
11	6	0	-3.013700	-2.112741	1.902472
12	1	0	-3.392969	-2.428736	2.870735
13	6	0	-3.837844	-2.215515	0.777479
14	6	0	-3.319914	-1.797908	-0.443349
15	1	0	-3.944650	-1.858102	-1.330638
16	6	0	-1.191444	-1.203733	0.563051
17	6	0	-5.233699	-2.780320	0.890295
18	1	0	-5.820527	-2.572695	-0.006934
19	1	0	-5.210289	-3.866999	1.026599
20	1	0	-5.766428	-2.359415	1.747770
21	6	0	-1.714026	-1.619001	1.813894
22	6	0	1.151155	-2.700795	-0.804384
23	6	0	-0.075960	-3.595984	-0.736493
24	1	0	-0.582188	-3.556513	0.222047
25	1	0	-0.810756	-3.392818	-1.516103
26	1	0	0.272405	-4.622435	-0.887307

27	6	0	-0.871140	-1.538094	3.070034
28	1	0	-1.416979	-1.919737	3.935185
29	1	0	0.049990	-2.122887	2.974445
30	1	0	-0.578351	-0.506132	3.289682
31	6	0	-2.020315	-1.294548	-0.569832
32	6	0	-1.573595	-0.864391	-1.951252
33	1	0	-2.114181	0.030608	-2.269926
34	1	0	-0.507913	-0.639763	-1.999844
35	1	0	-1.783686	-1.645001	-2.688995
36	6	0	2.911291	-1.467974	0.269800
37	6	0	3.582252	-1.109567	1.578087
38	1	0	4.212154	-0.222674	1.516049
39	1	0	2.872462	-0.986703	2.389006
40	1	0	4.227034	-1.953007	1.849280
41	5	0	0.312001	-0.687651	0.582465
42	7	0	0.462929	0.789016	0.828186
43	6	0	1.680297	1.453145	1.164302
44	6	0	-0.153811	1.698683	-0.121809
45	6	0	1.991234	2.437096	0.202975
46	6	0	2.362602	1.416103	2.372659
47	6	0	0.825935	2.545739	-0.653268
48	6	0	-1.528726	1.971398	-0.382358
49	6	0	3.113080	3.251105	0.363809
50	6	0	3.461936	2.256966	2.545609
51	1	0	2.030228	0.774614	3.178163
52	6	0	0.530139	3.450969	-1.694675
53	6	0	-1.818148	2.895596	-1.448436
54	6	0	-2.608347	1.526454	0.424162
55	1	0	3.359490	4.007460	-0.372931
56	6	0	3.860163	3.136580	1.533511
57	1	0	3.999631	2.242710	3.486838
58	6	0	-0.764005	3.569475	-2.126340
59	1	0	1.319359	4.053412	-2.130147
60	6	0	-3.171868	3.195959	-1.745005
61	6	0	-3.903726	1.888390	0.140857
62	1	0	-2.401126	0.910372	1.285536
63	1	0	4.718893	3.779726	1.689270
64	1	0	-1.016853	4.248315	-2.933452
65	6	0	-4.196523	2.699372	-0.976103
66	1	0	-3.381692	3.864280	-2.573749
67	1	0	-4.706293	1.546613	0.784113
68	1	0	-5.224848	2.957036	-1.203833

Compound 5 1-RF-N-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1394.83132896 A.U. after 1 cycles
Lowest frequency = -70.7751

Zero-point correction= 0.562881
(Hartree/Particle)
Thermal correction to Energy= 0.593709
Thermal correction to Enthalpy= 0.594653
Thermal correction to Gibbs Free Energy= 0.502863
Sum of electronic and zero-point Energies= -1394.268448
Sum of electronic and thermal Energies= -1394.237620
Sum of electronic and thermal Enthalpies= -1394.236676
Sum of electronic and thermal Free Energies= -1394.328466

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.467365	0.877667	-0.189991
2	6	0	-4.939238	2.640060	-1.185488
3	1	0	-5.482498	2.163647	-2.005130
4	1	0	-5.357495	2.252582	-0.249722
5	1	0	-5.138605	3.713797	-1.215244
6	6	0	-3.465845	2.346110	-1.254223
7	6	0	-2.976831	1.161268	-1.798077
8	1	0	-3.659942	0.488864	-2.308665
9	6	0	-0.682795	1.637376	-1.017248
10	6	0	-2.506956	3.285832	-0.882185
11	1	0	-2.815780	4.310241	-0.691389
12	6	0	4.021779	2.195785	0.771704
13	1	0	4.630835	3.090637	0.675235
14	6	0	4.633260	0.991801	1.106946
15	6	0	3.780759	-0.034362	1.506614
16	1	0	4.200379	-0.920785	1.972989
17	6	0	1.781797	1.170856	0.695086
18	6	0	6.130047	0.841208	1.147081
19	1	0	6.443902	0.171519	1.951414
20	1	0	6.496199	0.413026	0.207147
21	1	0	6.628182	1.803706	1.284247
22	6	0	2.636427	2.325407	0.664139
23	6	0	-1.627693	0.817354	-1.742875
24	6	0	-1.236536	-0.349412	-2.630003
25	1	0	-0.173764	-0.373473	-2.851812
26	1	0	-1.529623	-1.320766	-2.227152
27	1	0	-1.763542	-0.225655	-3.580890
28	6	0	2.140756	3.747064	0.782159
29	1	0	2.650878	4.192350	1.641833
30	1	0	2.371612	4.377640	-0.078849
31	1	0	1.079585	3.787217	0.991834
32	6	0	2.397273	0.043298	1.361279
33	6	0	1.632939	-1.052885	2.080068
34	1	0	0.612259	-0.767895	2.319094
35	1	0	1.610901	-1.997836	1.532804
36	1	0	2.145005	-1.244819	3.027542
37	6	0	-1.144398	2.991618	-0.861715
38	6	0	-0.245054	4.202888	-0.959925
39	1	0	-0.258570	4.851491	-0.081467
40	1	0	0.774775	3.931494	-1.201031
41	1	0	-0.617719	4.801585	-1.797127
42	7	0	0.269821	-0.635409	-0.284938
43	6	0	1.146879	-1.461075	-0.997543
44	6	0	-0.757081	-1.451011	0.202167
45	6	0	0.664965	-2.792156	-0.990612
46	6	0	2.306417	-1.121771	-1.704827
47	6	0	-0.547757	-2.777760	-0.216908
48	6	0	-1.837603	-1.125978	1.082898
49	6	0	1.362130	-3.793904	-1.678266
50	6	0	2.981809	-2.131713	-2.377401
51	1	0	2.677338	-0.104739	-1.725159
52	6	0	-1.445175	-3.808429	0.144738
53	6	0	-2.735593	-2.193155	1.428647
54	6	0	-2.056265	0.145660	1.668822
55	1	0	0.999624	-4.816198	-1.676850

56	1	0	3.885998	-1.888313	-2.924194
57	6	0	-2.523143	-3.514632	0.933066
58	1	0	-1.273955	-4.821326	-0.202950
59	6	0	-3.821340	-1.917222	2.295737
60	6	0	-3.111579	0.371729	2.523965
61	1	0	-1.385645	0.964163	1.444132
62	1	0	-3.226242	-4.289960	1.217018
63	6	0	-4.013021	-0.665888	2.833188
64	1	0	-4.500604	-2.726880	2.542255
65	1	0	-3.247259	1.354810	2.960415
66	1	0	-4.846682	-0.479282	3.500921
67	6	0	2.519094	-3.458814	-2.365097
68	1	0	3.070311	-4.222187	-2.902194

Compound 5 2-RF-CC-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1394.89561417 A.U. after 1 cycles
Lowest frequency = -49.6764

Zero-point correction= 0.562815
(Hartree/Particle)
Thermal correction to Energy= 0.594378
Thermal correction to Enthalpy= 0.595323
Thermal correction to Gibbs Free Energy= 0.500880
Sum of electronic and zero-point Energies= -1394.332799
Sum of electronic and thermal Energies= -1394.301236
Sum of electronic and thermal Enthalpies= -1394.300292
Sum of electronic and thermal Free Energies= -1394.394734

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.498375	-0.219301	0.293369
2	6	0	1.866458	-5.556126	-0.931684
3	1	0	2.612829	-5.532443	-1.729635
4	1	0	2.312581	-6.046793	-0.063266
5	1	0	1.040719	-6.188573	-1.276369
6	6	0	1.378019	-4.169725	-0.592330
7	6	0	1.297176	-3.171149	-1.557834
8	1	0	1.648870	-3.380104	-2.564484
9	6	0	0.331852	-1.571553	0.019841
10	6	0	1.007872	-3.823254	0.702064
11	1	0	1.133451	-4.548447	1.502194
12	6	0	-4.278724	-1.222410	0.824674
13	1	0	-4.913620	-1.597015	1.623560
14	6	0	-4.807882	-1.089289	-0.456146
15	6	0	-3.998489	-0.482077	-1.409605
16	1	0	-4.406693	-0.270404	-2.394631
17	6	0	-2.097526	-0.366023	0.125653
18	6	0	-6.206145	-1.551082	-0.783840
19	1	0	-6.645044	-0.957372	-1.589387
20	1	0	-6.205758	-2.596682	-1.111524
21	1	0	-6.864154	-1.483295	0.086123
22	6	0	-2.964692	-0.862599	1.131204
23	6	0	0.797962	-1.896494	-1.280866
24	6	0	0.837145	-0.908735	-2.427317

25	1	0	-0.060909	-0.970568	-3.046155
26	1	0	0.947543	0.121588	-2.091135
27	1	0	1.690139	-1.127794	-3.073568
28	6	0	-2.592228	-0.913763	2.599562
29	1	0	-3.417398	-0.517982	3.198494
30	1	0	-2.407692	-1.931995	2.948062
31	1	0	-1.714055	-0.311669	2.830295
32	6	0	-2.683023	-0.095200	-1.138316
33	6	0	-2.007772	0.727622	-2.217687
34	1	0	-2.571055	1.654868	-2.362159
35	1	0	-0.989635	1.014987	-1.975358
36	1	0	-1.995160	0.205357	-3.178177
37	6	0	0.511897	-2.557445	1.021885
38	6	0	0.316869	-2.289205	2.501148
39	1	0	0.121728	-1.241770	2.723636
40	1	0	-0.498894	-2.881533	2.921368
41	1	0	1.223093	-2.568906	3.047798
42	7	0	0.097595	1.083464	0.525383
43	6	0	-0.693030	2.286214	0.507674
44	6	0	1.437998	1.515704	0.194377
45	6	0	0.060672	3.341794	-0.034366
46	6	0	-1.991226	2.508978	0.960090
47	6	0	1.393866	2.833831	-0.263868
48	6	0	2.697964	0.859551	0.343321
49	6	0	-0.494306	4.614244	-0.185597
50	6	0	-2.531437	3.785755	0.816435
51	1	0	-2.576546	1.726982	1.415567
52	6	0	2.532107	3.474878	-0.799231
53	6	0	3.842857	1.512671	-0.236766
54	6	0	2.928330	-0.313137	1.103589
55	1	0	0.090551	5.424599	-0.605908
56	1	0	-3.538726	3.970707	1.171662
57	6	0	3.720851	2.800005	-0.830132
58	1	0	2.454017	4.485266	-1.183769
59	6	0	5.112108	0.887716	-0.144326
60	6	0	4.180543	-0.871199	1.204836
61	1	0	2.108408	-0.759342	1.635887
62	1	0	4.605888	3.258908	-1.257044
63	6	0	5.282263	-0.285893	0.548289
64	1	0	5.960245	1.376453	-0.612334
65	1	0	4.320577	-1.765729	1.800859
66	1	0	6.262382	-0.743868	0.618107
67	6	0	-1.800099	4.828179	0.236794
68	1	0	-2.248348	5.810121	0.137591

Compound 5 2-RF-CN-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1394.89186903 A.U. after 1 cycles
Lowest frequency = -30.0516

Zero-point correction= 0.562758
(Hartree/Particle)
Thermal correction to Energy= 0.594241
Thermal correction to Enthalpy= 0.595186
Thermal correction to Gibbs Free Energy= 0.500493
Sum of electronic and zero-point Energies= -1394.329111
Sum of electronic and thermal Energies= -1394.297628
Sum of electronic and thermal Enthalpies= -1394.296683

Sum of electronic and thermal Free Energies= -1394.391376

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.703226	0.233994	0.009527
2	6	0	6.165990	-2.097956	0.132867
3	1	0	6.343939	-2.664996	1.048950
4	1	0	6.303942	-2.784149	-0.710208
5	1	0	6.932271	-1.323778	0.050987
6	6	0	4.781142	-1.505385	0.111433
7	6	0	3.731329	-2.099018	0.805075
8	1	0	3.929733	-2.995740	1.383187
9	6	0	2.131798	-0.397687	0.038522
10	6	0	4.497871	-0.363501	-0.632226
11	1	0	5.299681	0.110634	-1.189235
12	6	0	-0.844539	2.808900	-2.535220
13	1	0	-1.285152	2.794721	-3.528519
14	6	0	-0.793326	4.008834	-1.832721
15	6	0	-0.137927	3.995604	-0.605427
16	1	0	-0.014936	4.927447	-0.059725
17	6	0	0.261419	1.588072	-0.732650
18	6	0	-1.405248	5.272302	-2.385583
19	1	0	-2.449296	5.372014	-2.068489
20	1	0	-0.872733	6.160537	-2.036811
21	1	0	-1.395057	5.276559	-3.478299
22	6	0	-0.325664	1.618314	-2.020317
23	6	0	2.431540	-1.591521	0.787485
24	6	0	1.432294	-2.400149	1.593385
25	1	0	1.036134	-1.846544	2.445120
26	1	0	0.577910	-2.723497	1.000100
27	1	0	1.924073	-3.293783	1.982119
28	6	0	-0.364539	0.413866	-2.934646
29	1	0	-0.235748	0.727409	-3.974003
30	1	0	0.426098	-0.302915	-2.710261
31	1	0	-1.314952	-0.119815	-2.871794
32	6	0	0.394403	2.827020	-0.055610
33	6	0	1.166149	2.986879	1.239372
34	1	0	0.504591	3.006432	2.107783
35	1	0	1.891744	2.186599	1.394380
36	1	0	1.720178	3.929531	1.228164
37	6	0	3.221816	0.193970	-0.691794
38	6	0	3.105962	1.423659	-1.568654
39	1	0	2.352697	1.309644	-2.347547
40	1	0	2.834627	2.315168	-1.002751
41	1	0	4.064116	1.615891	-2.054762
42	7	0	-0.420638	-0.390043	0.837567
43	6	0	-0.723907	0.123346	2.111988
44	6	0	-1.619668	-0.924761	0.339469
45	6	0	-2.116296	0.020358	2.357471
46	6	0	0.139147	0.595897	3.105124
47	6	0	-2.682222	-0.640872	1.211633
48	6	0	-1.800291	-1.825443	-0.754190
49	6	0	-2.647059	0.448234	3.579065
50	6	0	-0.407730	1.004974	4.316435
51	1	0	1.209853	0.628867	2.952209
52	6	0	-3.996425	-1.067975	0.915201
53	6	0	-3.145337	-2.237931	-1.042093

54	6	0	-0.743641	-2.413189	-1.493011
55	1	0	-3.711747	0.373138	3.771382
56	1	0	0.251663	1.363773	5.098819
57	6	0	-4.224042	-1.812121	-0.211068
58	1	0	-4.813258	-0.809285	1.579849
59	6	0	-3.364711	-3.129541	-2.121372
60	6	0	-0.992382	-3.307345	-2.509359
61	1	0	0.280982	-2.161973	-1.248726
62	1	0	-5.227254	-2.139904	-0.460441
63	6	0	-2.317646	-3.651976	-2.844744
64	1	0	-4.384958	-3.418643	-2.351846
65	1	0	-0.165081	-3.750474	-3.052161
66	1	0	-2.507254	-4.345498	-3.656212
67	6	0	-1.790367	0.947598	4.550034
68	1	0	-2.185816	1.274226	5.504898

Compound 5 3-RF-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1394.85115264 A.U. after 1 cycles
Lowest frequency = -28.5754

Zero-point correction= 0.563071
(Hartree/Particle)
Thermal correction to Energy= 0.594343
Thermal correction to Enthalpy= 0.595287
Thermal correction to Gibbs Free Energy= 0.501102
Sum of electronic and zero-point Energies= -1394.288082
Sum of electronic and thermal Energies= -1394.256810
Sum of electronic and thermal Enthalpies= -1394.255865
Sum of electronic and thermal Free Energies= -1394.350050

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.713845	-0.149340	0.182642
2	6	0	1.928233	-3.173645	4.649379
3	1	0	1.186088	-3.656278	5.292314
4	1	0	2.547906	-3.967476	4.219312
5	1	0	2.570105	-2.555214	5.280072
6	6	0	1.267477	-2.355885	3.568151
7	6	0	0.288173	-2.901689	2.742338
8	1	0	-0.012078	-3.935396	2.887276
9	6	0	0.023176	-0.807032	1.470883
10	6	0	1.598122	-1.031928	3.340595
11	1	0	2.343647	-0.558376	3.973661
12	6	0	-3.774714	2.129324	0.834319
13	1	0	-3.922571	3.035570	1.414273
14	6	0	-4.811862	1.658346	0.037346
15	6	0	-4.595990	0.447023	-0.599876
16	1	0	-5.408817	-0.001386	-1.164714
17	6	0	-2.273532	0.285238	0.183530
18	6	0	-6.108401	2.415045	-0.102994
19	1	0	-6.022203	3.200135	-0.862312
20	1	0	-6.925335	1.755594	-0.404366
21	1	0	-6.390673	2.900418	0.834835
22	6	0	-2.548078	1.472534	0.938615

23	6	0	-0.330997	-2.170125	1.732486
24	6	0	-1.372743	-2.914925	0.933517
25	1	0	-2.346629	-2.430496	0.999127
26	1	0	-1.096960	-2.996607	-0.120393
27	1	0	-1.485043	-3.932295	1.312196
28	6	0	-1.572595	2.093367	1.915428
29	1	0	-1.118277	1.345671	2.563437
30	1	0	-0.770712	2.643622	1.420013
31	1	0	-2.096164	2.808174	2.552752
32	6	0	-3.383692	-0.252430	-0.529214
33	6	0	-3.480822	-1.636869	-1.147766
34	1	0	-3.937180	-1.584254	-2.140528
35	1	0	-2.544694	-2.165958	-1.239001
36	1	0	-4.144206	-2.253851	-0.531639
37	6	0	1.013818	-0.257577	2.326675
38	6	0	1.520780	1.168713	2.314194
39	1	0	1.054032	1.802511	1.577176
40	1	0	1.357366	1.628282	3.294621
41	1	0	2.597060	1.187480	2.124925
42	7	0	0.113730	0.064736	-1.089548
43	6	0	0.133699	-1.024943	-2.027268
44	6	0	1.483016	0.443492	-1.002993
45	6	0	1.461564	-1.492635	-2.198419
46	6	0	-0.883010	-1.511949	-2.839763
47	6	0	2.322399	-0.531907	-1.541140
48	6	0	1.977679	1.744748	-0.724505
49	6	0	1.728931	-2.558551	-3.059352
50	6	0	-0.600411	-2.567135	-3.707160
51	1	0	-1.850985	-1.039682	-2.850742
52	6	0	3.724378	-0.354426	-1.543097
53	6	0	3.401308	1.917559	-0.727124
54	6	0	1.149588	2.886006	-0.572719
55	1	0	2.743447	-2.919049	-3.188320
56	1	0	-1.386307	-2.943988	-4.352026
57	6	0	4.247990	0.830218	-1.091119
58	1	0	4.374225	-1.137069	-1.918006
59	6	0	3.925247	3.202907	-0.437953
60	6	0	1.695852	4.125454	-0.334860
61	1	0	0.078155	2.770413	-0.683314
62	1	0	5.321582	0.984328	-1.078045
63	6	0	3.096294	4.281227	-0.234197
64	1	0	5.002679	3.329226	-0.409228
65	1	0	1.050399	4.991296	-0.238431
66	1	0	3.515957	5.259774	-0.030401
67	6	0	0.684473	-3.113837	-3.790639
68	1	0	0.877197	-3.933857	-4.472683

Compound 6 GS1

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1512.89656157 A.U. after 1 cycles
Lowest frequency = 18.0104

Zero-point correction= 0.646092
(Hartree/Particle)
Thermal correction to Energy= 0.683488
Thermal correction to Enthalpy= 0.684432
Thermal correction to Gibbs Free Energy= 0.574979
Sum of electronic and zero-point Energies= -1512.250470

Sum of electronic and thermal Energies= -1512.213074
Sum of electronic and thermal Enthalpies= -1512.212130
Sum of electronic and thermal Free Energies= -1512.321583

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.541046	0.738964	-0.032470
2	6	0	0.201611	2.990671	2.005840
3	1	0	-0.286885	2.106165	2.422935
4	1	0	1.276753	2.858480	2.147070
5	1	0	-0.112954	3.850491	2.600900
6	6	0	3.049689	2.236087	-0.989641
7	1	0	4.066674	2.501582	-1.286016
8	1	0	2.576049	1.749071	-1.845336
9	1	0	2.498906	3.163638	-0.815265
10	6	0	0.928835	-0.907386	2.507610
11	1	0	-0.035721	-0.409012	2.401757
12	1	0	0.829406	-1.897623	2.054166
13	1	0	1.109086	-1.054151	3.574667
14	6	0	5.727559	0.463236	2.848109
15	1	0	6.376002	-0.298628	2.401333
16	1	0	6.265014	1.413920	2.803565
17	1	0	5.588001	0.199220	3.898702
18	6	0	4.409120	0.540180	2.118917
19	6	0	4.275962	1.291689	0.950941
20	1	0	5.133532	1.845405	0.579208
21	6	0	3.073998	1.362434	0.249011
22	6	0	1.941364	0.627378	0.693751
23	6	0	2.071193	-0.126960	1.888375
24	6	0	3.288820	-0.146943	2.574666
25	1	0	3.358328	-0.718563	3.495754
26	6	0	-0.446184	2.433515	-1.742923
27	6	0	-0.888756	3.712078	-2.088016
28	1	0	-1.171649	3.908071	-3.118375
29	6	0	-0.988610	4.739164	-1.151018
30	6	0	-0.626244	4.454236	0.165210
31	1	0	-0.714711	5.232481	0.917930
32	6	0	-0.151770	3.198128	0.547247
33	6	0	-0.052559	2.156092	-0.408883
34	6	0	-0.413697	1.385947	-2.838178
35	1	0	-1.222857	0.660210	-2.718525
36	1	0	-0.531796	1.855295	-3.816932
37	1	0	0.519332	0.818451	-2.855437
38	6	0	-1.451178	6.118586	-1.551414
39	1	0	-1.964585	6.621773	-0.728655
40	1	0	-0.601594	6.747863	-1.839374
41	1	0	-2.131865	6.079274	-2.405018
42	7	0	-0.259173	-0.453587	-0.321730
43	6	0	-1.661113	-0.520264	-0.047605
44	6	0	0.164839	-1.794408	-0.518983
45	6	0	-2.058336	-1.869436	0.033509
46	6	0	-2.596153	0.489923	0.194624
47	6	0	-0.896924	-2.669050	-0.264271
48	6	0	1.399909	-2.294914	-1.039613
49	6	0	-3.378926	-2.211283	0.341175
50	6	0	-3.905334	0.126078	0.489553
51	1	0	-2.330034	1.534175	0.146528

52	6	0	-0.736871	-4.070184	-0.343367
53	6	0	1.550154	-3.724478	-1.089118
54	6	0	2.444624	-1.504505	-1.578373
55	6	0	-4.322926	-1.216012	0.570213
56	1	0	-3.669042	-3.255683	0.399626
57	1	0	-4.625790	0.918557	0.660854
58	6	0	0.476955	-4.581787	-0.710127
59	1	0	-1.569023	-4.725322	-0.111910
60	6	0	2.764328	-4.271708	-1.573978
61	6	0	3.597893	-2.070854	-2.069590
62	1	0	2.333743	-0.433430	-1.616668
63	1	0	0.630855	-5.654104	-0.761805
64	6	0	3.774217	-3.468869	-2.046641
65	1	0	2.872820	-5.351300	-1.584928
66	1	0	4.373610	-1.435212	-2.481186
67	1	0	4.692153	-3.906654	-2.422133
68	6	0	-5.766035	-1.574078	0.896483
69	1	0	-5.825983	-2.668575	0.904065
70	6	0	-6.181569	-1.082115	2.294748
71	1	0	-7.198963	-1.407520	2.532227
72	1	0	-5.510645	-1.471040	3.064796
73	1	0	-6.160020	0.010065	2.354376
74	6	0	-6.742567	-1.068516	-0.181006
75	1	0	-6.744853	0.024251	-0.233244
76	1	0	-6.470234	-1.448500	-1.168797
77	1	0	-7.763980	-1.392859	0.040183

Compound 6 GS2

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1512.89633195 A.U. after 1 cycles
Lowest frequency = 18.6608

Zero-point correction= 0.646035
(Hartree/Particle)
Thermal correction to Energy= 0.683459
Thermal correction to Enthalpy= 0.684404
Thermal correction to Gibbs Free Energy= 0.574624
Sum of electronic and zero-point Energies= -1512.250297
Sum of electronic and thermal Energies= -1512.212873
Sum of electronic and thermal Enthalpies= -1512.211928
Sum of electronic and thermal Free Energies= -1512.321708

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.682680	0.691870	-0.020839
2	6	0	0.829461	2.920678	2.064138
3	1	0	0.172005	2.145198	2.465633
4	1	0	1.855487	2.569010	2.194691
5	1	0	0.698556	3.813007	2.679743
6	6	0	3.443082	1.647762	-0.978402
7	1	0	4.490932	1.697767	-1.281916
8	1	0	2.870791	1.286969	-1.836287
9	1	0	3.102189	2.667507	-0.783301
10	6	0	0.734450	-1.048422	2.486855
11	1	0	-0.108779	-0.363108	2.391277

12	1	0	0.434425	-1.992582	2.023501
13	1	0	0.884159	-1.241086	3.551353
14	6	0	5.714899	-0.711809	2.804694
15	1	0	6.187943	-1.583357	2.338671
16	1	0	6.438181	0.106966	2.771286
17	1	0	5.529590	-0.960712	3.851895
18	6	0	4.437120	-0.348741	2.089571
19	6	0	4.456597	0.434687	0.935208
20	1	0	5.408521	0.804131	0.564304
21	6	0	3.291703	0.766680	0.245910
22	6	0	2.033252	0.275987	0.689292
23	6	0	2.010213	-0.510508	1.869919
24	6	0	3.200947	-0.795675	2.544470
25	1	0	3.155173	-1.385884	3.455277
26	6	0	0.066685	2.591571	-1.689757
27	6	0	-0.099430	3.941467	-2.005668
28	1	0	-0.338494	4.214220	-3.029652
29	6	0	0.021044	4.946529	-1.047405
30	6	0	0.319914	4.564069	0.259967
31	1	0	0.398613	5.327296	1.028976
32	6	0	0.522158	3.228576	0.612885
33	6	0	0.397956	2.209550	-0.364696
34	6	0	-0.125447	1.583749	-2.805730
35	1	0	-1.069847	1.043561	-2.695418
36	1	0	-0.143377	2.087541	-3.774285
37	1	0	0.666102	0.831998	-2.839984
38	6	0	-0.143747	6.400425	-1.416395
39	1	0	-0.536623	6.982484	-0.579397
40	1	0	0.817613	6.843686	-1.699271
41	1	0	-0.821303	6.522698	-2.264631
42	7	0	-0.351556	-0.299819	-0.323653
43	6	0	-1.735536	-0.074480	-0.040157
44	6	0	-0.219745	-1.696984	-0.543025
45	6	0	-2.407046	-1.313265	0.026760
46	6	0	-2.436638	1.103633	0.220596
47	6	0	-1.439218	-2.333728	-0.290921
48	6	0	0.880276	-2.437022	-1.080705
49	6	0	-3.766241	-1.379058	0.339422
50	6	0	-3.793488	1.013972	0.520685
51	1	0	-1.960017	2.070570	0.184366
52	6	0	-1.576335	-3.735886	-0.389458
53	6	0	0.728145	-3.865615	-1.149549
54	6	0	2.063747	-1.874571	-1.618893
55	6	0	-4.481318	-0.209121	0.588331
56	1	0	-4.258532	-2.344836	0.384718
57	1	0	-4.340281	1.932442	0.708767
58	6	0	-0.498383	-4.484928	-0.772626
59	1	0	-2.525853	-4.205862	-0.159654
60	6	0	1.798556	-4.647486	-1.651330
61	6	0	3.070253	-2.662300	-2.127180
62	1	0	2.178431	-0.803495	-1.643483
63	1	0	-0.572544	-5.564867	-0.839197
64	6	0	2.950961	-4.066560	-2.122690
65	1	0	1.679172	-5.725682	-1.676580
66	1	0	3.959068	-2.197027	-2.537911
67	1	0	3.755091	-4.681025	-2.511362
68	6	0	-5.966431	-0.238651	0.923969
69	1	0	-6.276560	0.801143	1.078364
70	6	0	-6.808420	-0.800772	-0.235747
71	1	0	-7.875612	-0.750714	0.000971

72	1	0	-6.636373	-0.237997	-1.156589
73	1	0	-6.560682	-1.847825	-0.434199
74	6	0	-6.248033	-0.999924	2.231935
75	1	0	-5.976542	-2.056064	2.142738
76	1	0	-5.677883	-0.578821	3.063757
77	1	0	-7.311023	-0.950830	2.486931

Compound 6 1-RF-C1-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1512.82223343 A.U. after 1 cycles
Lowest frequency = -36.2257

Zero-point correction= 0.645504
(Hartree/Particle)
Thermal correction to Energy= 0.681475
Thermal correction to Enthalpy= 0.682419
Thermal correction to Gibbs Free Energy= 0.577778
Sum of electronic and zero-point Energies= -1512.176729
Sum of electronic and thermal Energies= -1512.140759
Sum of electronic and thermal Enthalpies= -1512.139815
Sum of electronic and thermal Free Energies= -1512.244455

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.456762	4.891836	3.041951
2	1	0	0.716042	5.620153	3.379894
3	1	0	1.681869	4.235137	3.889887
4	1	0	2.377021	5.426368	2.793185
5	6	0	0.950397	4.088703	1.873480
6	6	0	-0.406685	3.942080	1.614862
7	1	0	-1.121134	4.519775	2.194586
8	6	0	0.001596	2.276855	-0.152376
9	6	0	1.817727	3.536814	0.931156
10	1	0	2.869557	3.808957	0.953537
11	6	0	-3.922708	0.488900	-2.386647
12	1	0	-4.248022	0.514226	-3.423369
13	6	0	-4.871936	0.311554	-1.375214
14	6	0	-4.418278	0.280679	-0.061368
15	1	0	-5.135498	0.133579	0.741866
16	6	0	-2.115629	0.614853	-0.755878
17	6	0	-6.339161	0.178311	-1.706410
18	1	0	-6.909052	-0.185141	-0.848726
19	1	0	-6.766382	1.142232	-2.003600
20	1	0	-6.499315	-0.514928	-2.537103
21	6	0	-2.567857	0.639151	-2.099387
22	6	0	-0.897034	3.122434	0.591120
23	6	0	-2.363061	3.360485	0.265195
24	1	0	-2.644192	3.011447	-0.722606
25	1	0	-3.050180	2.919397	0.987930
26	1	0	-2.522339	4.442836	0.293992
27	6	0	-1.591107	0.832903	-3.241028
28	1	0	-2.108370	0.851716	-4.202381
29	1	0	-1.039336	1.773900	-3.142557
30	1	0	-0.851562	0.026219	-3.276225
31	6	0	-3.065066	0.425757	0.264533

32	6	0	-2.693568	0.366146	1.731278
33	1	0	-2.840915	-0.642814	2.125224
34	1	0	-1.655334	0.642749	1.915865
35	1	0	-3.326934	1.036163	2.320991
36	6	0	1.368197	2.714489	-0.097310
37	6	0	2.328035	2.569787	-1.258091
38	1	0	3.254245	2.058910	-0.996867
39	1	0	1.876244	2.073524	-2.110223
40	1	0	2.591032	3.581759	-1.585751
41	5	0	-0.553596	0.827246	-0.550353
42	7	0	0.256139	-0.439727	-0.559180
43	6	0	1.677174	-0.517128	-0.670586
44	6	0	-0.046306	-1.442795	0.447058
45	6	0	2.229729	-1.173220	0.445318
46	6	0	2.461371	-0.292783	-1.794052
47	6	0	1.109228	-1.714738	1.189860
48	6	0	-1.191417	-2.276908	0.607937
49	6	0	3.602022	-1.418173	0.514530
50	6	0	3.824032	-0.574646	-1.729786
51	1	0	2.021487	0.062215	-2.716954
52	6	0	1.076457	-2.561839	2.318044
53	6	0	-1.214014	-3.135845	1.763962
54	6	0	-2.219182	-2.434679	-0.357992
55	1	0	4.025660	-1.921019	1.378117
56	6	0	4.421659	-1.098412	-0.569767
57	1	0	4.430387	-0.403508	-2.612510
58	6	0	-0.089856	-3.206427	2.633468
59	1	0	1.971409	-2.708381	2.912245
60	6	0	-2.333810	-3.981969	1.966210
61	6	0	-3.258273	-3.311088	-0.154278
62	1	0	-2.167994	-1.869700	-1.275938
63	1	0	-0.146008	-3.852954	3.502414
64	6	0	-3.340821	-4.065549	1.035274
65	1	0	-2.359439	-4.597890	2.859253
66	1	0	-4.020059	-3.422433	-0.917177
67	1	0	-4.178997	-4.734498	1.195570
68	6	0	5.916262	-1.384778	-0.515319
69	1	0	6.120486	-1.808541	0.474598
70	6	0	6.345996	-2.431173	-1.559485
71	1	0	7.408681	-2.668667	-1.452121
72	1	0	5.776373	-3.356910	-1.447058
73	1	0	6.189707	-2.064990	-2.578375
74	6	0	6.751860	-0.098258	-0.644697
75	1	0	7.818456	-0.317399	-0.536710
76	1	0	6.606109	0.372053	-1.621731
77	1	0	6.474903	0.630337	0.121462

Compound 6 1-RF-C-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1512.82806070 A.U. after 1 cycles
Lowest frequency = -26.8767

Zero-point correction= 0.645792
(Hartree/Particle)
Thermal correction to Energy= 0.681661
Thermal correction to Enthalpy= 0.682605
Thermal correction to Gibbs Free Energy= 0.578737
Sum of electronic and zero-point Energies= -1512.182269

Sum of electronic and thermal Energies= -1512.146400
Sum of electronic and thermal Enthalpies= -1512.145456
Sum of electronic and thermal Free Energies= -1512.249324

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.280863	-1.100314	-0.334582
2	6	0	-3.409466	-2.520581	4.356202
3	1	0	-3.089099	-3.431558	4.867006
4	1	0	-3.135104	-1.672814	4.994125
5	1	0	-4.499985	-2.531880	4.284227
6	6	0	-2.767137	-2.391022	3.000291
7	6	0	-1.582282	-3.044241	2.683376
8	1	0	-1.169639	-3.760637	3.388240
9	6	0	-1.386403	-1.874544	0.529430
10	6	0	-3.379651	-1.690442	1.962003
11	1	0	-4.403397	-1.346241	2.081504
12	6	0	2.293474	-2.996653	-2.516371
13	1	0	2.315676	-3.397821	-3.526063
14	6	0	3.418405	-3.134299	-1.701513
15	6	0	3.352719	-2.606272	-0.414258
16	1	0	4.216304	-2.699278	0.239454
17	6	0	1.075309	-1.827752	-0.758013
18	6	0	4.649307	-3.859282	-2.190680
19	1	0	5.539215	-3.552454	-1.636396
20	1	0	4.543430	-4.942879	-2.067501
21	1	0	4.828805	-3.669788	-3.252123
22	6	0	1.137044	-2.357078	-2.067783
23	6	0	-0.920227	-2.865328	1.461940
24	6	0	0.162156	-3.898249	1.191827
25	1	0	0.385638	-4.012502	0.136372
26	1	0	1.097272	-3.701624	1.716986
27	1	0	-0.211348	-4.858628	1.559018
28	6	0	-0.040125	-2.230690	-3.012253
29	1	0	0.103196	-2.843484	-3.904581
30	1	0	-0.974821	-2.546818	-2.538553
31	1	0	-0.173884	-1.194863	-3.341237
32	6	0	2.211267	-1.960039	0.068755
33	6	0	2.267743	-1.411671	1.480949
34	1	0	2.897044	-0.519126	1.525298
35	1	0	1.285423	-1.136718	1.866187
36	1	0	2.701894	-2.146625	2.165124
37	6	0	-2.750541	-1.489590	0.737306
38	6	0	-3.661399	-1.122400	-0.408775
39	1	0	-4.217388	-0.198020	-0.249421
40	1	0	-3.137037	-1.061508	-1.354768
41	1	0	-4.395424	-1.930023	-0.509990
42	7	0	-0.273650	0.367385	-0.611060
43	6	0	0.925937	1.092997	-0.234532
44	6	0	-1.312569	1.319712	-0.345513
45	6	0	0.576801	2.164114	0.615186
46	6	0	2.239846	0.957225	-0.665276
47	6	0	-0.868351	2.295052	0.548525
48	6	0	-2.471424	1.574717	-1.125973
49	6	0	1.558070	3.003594	1.142667
50	6	0	3.203496	1.824467	-0.149824
51	1	0	2.518846	0.214747	-1.396599

52	6	0	-1.736449	3.312723	1.000400
53	6	0	-3.352901	2.614188	-0.672163
54	6	0	-2.713349	0.992069	-2.397213
55	6	0	2.894312	2.831091	0.779269
56	1	0	1.278774	3.822253	1.798522
57	1	0	4.223829	1.718536	-0.502263
58	6	0	-2.986626	3.417202	0.444542
59	1	0	-1.403464	4.022103	1.749561
60	6	0	-4.522927	2.888690	-1.425837
61	6	0	-3.822928	1.332099	-3.132055
62	1	0	-1.992620	0.286731	-2.791482
63	6	0	3.971695	3.752364	1.335083
64	1	0	-3.674406	4.186264	0.779198
65	6	0	-4.760799	2.259373	-2.624485
66	1	0	-5.209631	3.644628	-1.058949
67	1	0	-3.979421	0.890664	-4.109932
68	1	0	3.471108	4.446811	2.019708
69	6	0	5.023186	2.980461	2.152546
70	6	0	4.637804	4.595528	0.232638
71	1	0	-5.646617	2.500825	-3.200886
72	1	0	5.749365	3.668231	2.596429
73	1	0	4.555073	2.411697	2.959935
74	1	0	5.574443	2.275443	1.523259
75	1	0	5.175202	3.963953	-0.480838
76	1	0	3.895486	5.171274	-0.325651
77	1	0	5.359021	5.295794	0.664891

Compound 6 1-RF-N-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1512.80568247 A.U. after 1 cycles
Lowest frequency = -70.7549

Zero-point correction= 0.646580
(Hartree/Particle)
Thermal correction to Energy= 0.681940
Thermal correction to Enthalpy= 0.682884
Thermal correction to Gibbs Free Energy= 0.580718
Sum of electronic and zero-point Energies= -1512.159102
Sum of electronic and thermal Energies= -1512.123743
Sum of electronic and thermal Enthalpies= -1512.122799
Sum of electronic and thermal Free Energies= -1512.224964

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.557408	1.145425	0.236998
2	6	0	5.709361	-0.508833	2.253907
3	1	0	5.730147	-1.347992	2.953389
4	1	0	6.093570	-0.875057	1.295264
5	1	0	6.398803	0.258890	2.612881
6	6	0	4.316662	0.031890	2.080472
7	6	0	3.191635	-0.778085	2.210581
8	1	0	3.307232	-1.793555	2.577909
9	6	0	1.697955	0.995446	1.360486
10	6	0	4.069780	1.389927	1.891493
11	1	0	4.880362	2.100014	2.032719

12	6	0	-1.533157	4.325282	-0.668130
13	1	0	-1.621034	5.370987	-0.385618
14	6	0	-2.562079	3.728780	-1.390320
15	6	0	-2.263909	2.500576	-1.975126
16	1	0	-2.943883	2.085964	-2.713419
17	6	0	-0.187523	2.260522	-0.656917
18	6	0	-3.878091	4.420547	-1.623382
19	1	0	-4.285374	4.185087	-2.609576
20	1	0	-4.616742	4.096613	-0.881512
21	1	0	-3.783327	5.505543	-1.538453
22	6	0	-0.336537	3.664117	-0.388180
23	6	0	1.907729	-0.322302	1.918286
24	6	0	0.791148	-1.233718	2.391357
25	1	0	-0.161524	-0.720869	2.484284
26	1	0	0.651319	-2.114755	1.762108
27	1	0	1.064917	-1.592839	3.388040
28	6	0	0.811166	4.585981	-0.050684
29	1	0	0.809033	5.384686	-0.798781
30	1	0	0.728117	5.070969	0.924083
31	1	0	1.767145	4.084512	-0.130178
32	6	0	-1.103132	1.790896	-1.674252
33	6	0	-0.836989	0.613205	-2.593366
34	1	0	0.213988	0.341762	-2.637001
35	1	0	-1.415420	-0.277081	-2.337052
36	1	0	-1.136588	0.908996	-3.603096
37	6	0	2.790975	1.887322	1.644762
38	6	0	2.616187	3.349747	1.985946
39	1	0	3.157804	4.036827	1.332372
40	1	0	1.572313	3.632616	2.032455
41	1	0	3.024721	3.487021	2.992154
42	7	0	-0.045889	-0.221376	-0.083621
43	6	0	-1.357491	-0.563261	0.267706
44	6	0	0.526828	-1.353113	-0.672551
45	6	0	-1.609385	-1.912821	-0.065566
46	6	0	-2.335063	0.198834	0.917406
47	6	0	-0.403324	-2.409687	-0.672230
48	6	0	1.800651	-1.502640	-1.307940
49	6	0	-2.850946	-2.490419	0.232845
50	6	0	-3.555097	-0.398585	1.198623
51	1	0	-2.156896	1.231425	1.190740
52	6	0	-0.074162	-3.672139	-1.216793
53	6	0	2.108254	-2.798565	-1.847171
54	6	0	2.749949	-0.465172	-1.482925
55	6	0	-3.837512	-1.741717	0.863784
56	1	0	-3.043793	-3.527528	-0.024563
57	1	0	-4.315302	0.194771	1.695255
58	6	0	1.160636	-3.863303	-1.772318
59	1	0	-0.799772	-4.477795	-1.191528
60	6	0	3.359370	-2.993722	-2.482272
61	6	0	3.948195	-0.687172	-2.124113
62	1	0	2.538665	0.526627	-1.106216
63	6	0	-5.189787	-2.360799	1.190493
64	1	0	1.434246	-4.825948	-2.190172
65	6	0	4.264758	-1.967524	-2.619360
66	1	0	3.587354	-3.978818	-2.876429
67	1	0	4.650218	0.129779	-2.247117
68	1	0	-5.154335	-3.398781	0.839743
69	6	0	-5.459101	-2.398673	2.705838
70	6	0	-6.341058	-1.664089	0.442459
71	1	0	5.213434	-2.137855	-3.116050

72	1	0	-6.404824	-2.906598	2.918891
73	1	0	-4.661320	-2.927042	3.233787
74	1	0	-5.523210	-1.389453	3.123508
75	1	0	-6.443768	-0.620730	0.755537
76	1	0	-6.170455	-1.672420	-0.637012
77	1	0	-7.293024	-2.165871	0.641914

Compound 6 2-RF-CC-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1512.87041146 A.U. after 1 cycles
Lowest frequency = -49.9071

Zero-point correction= 0.646505
(Hartree/Particle)
Thermal correction to Energy= 0.682624
Thermal correction to Enthalpy= 0.683568
Thermal correction to Gibbs Free Energy= 0.578617
Sum of electronic and zero-point Energies= -1512.223906
Sum of electronic and thermal Energies= -1512.187788
Sum of electronic and thermal Enthalpies= -1512.186843
Sum of electronic and thermal Free Energies= -1512.291794

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.510779	0.646560	0.286343
2	6	0	-6.231891	1.908438	-0.822576
3	1	0	-6.669166	1.304040	-1.621255
4	1	0	-6.876684	1.828768	0.055966
5	1	0	-6.257080	2.952836	-1.153113
6	6	0	-4.820446	1.475048	-0.512858
7	6	0	-3.984617	0.962130	-1.499926
8	1	0	-4.378421	0.816057	-2.502106
9	6	0	-2.097571	0.771928	0.043378
10	6	0	-4.301007	1.548045	0.774644
11	1	0	-4.946661	1.863330	1.590515
12	6	0	0.910404	4.287987	0.842615
13	1	0	0.995350	5.010588	1.650249
14	6	0	1.309231	4.654596	-0.439982
15	6	0	1.304929	3.656668	-1.407739
16	1	0	1.699138	3.875525	-2.396918
17	6	0	0.304601	2.030928	0.122252
18	6	0	1.756684	6.060443	-0.754999
19	1	0	2.473640	6.076745	-1.579439
20	1	0	0.905783	6.684867	-1.049477
21	1	0	2.223763	6.535387	0.111468
22	6	0	0.430591	3.010607	1.139313
23	6	0	-2.657567	0.605379	-1.250078
24	6	0	-1.905887	-0.000832	-2.416034
25	1	0	-1.450167	0.765269	-3.047553
26	1	0	-1.123751	-0.689693	-2.099508
27	1	0	-2.596728	-0.567879	-3.044197
28	6	0	0.188969	2.721173	2.607298
29	1	0	0.992047	3.163793	3.203292
30	1	0	-0.747639	3.150841	2.968350
31	1	0	0.179801	1.654073	2.827504

32	6	0	0.845725	2.362407	-1.146754
33	6	0	1.088731	1.348685	-2.247378
34	1	0	2.165519	1.269981	-2.426733
35	1	0	0.738050	0.350193	-2.006395
36	1	0	0.626665	1.654379	-3.189993
37	6	0	-2.982266	1.193421	1.067236
38	6	0	-2.627131	1.162406	2.540772
39	1	0	-1.655506	0.713060	2.736932
40	1	0	-2.635043	2.159643	2.986240
41	1	0	-3.369382	0.569103	3.084486
42	7	0	0.201199	-0.600644	0.489433
43	6	0	1.639111	-0.661794	0.448974
44	6	0	-0.234998	-1.938138	0.152152
45	6	0	2.049125	-1.883558	-0.105352
46	6	0	2.592247	0.252873	0.890319
47	6	0	0.855751	-2.668188	-0.325368
48	6	0	-1.501662	-2.579496	0.309641
49	6	0	3.404201	-2.175483	-0.277266
50	6	0	3.938663	-0.058573	0.723547
51	1	0	2.314344	1.184223	1.356464
52	6	0	0.705204	-3.962138	-0.869571
53	6	0	-1.646398	-3.885722	-0.279468
54	6	0	-2.580458	-2.088210	1.085008
55	6	0	4.369959	-1.258623	0.130314
56	1	0	3.706891	-3.123984	-0.709342
57	1	0	4.674151	0.656054	1.076274
58	6	0	-0.536858	-4.533370	-0.890657
59	1	0	1.566598	-4.485137	-1.268770
60	6	0	-2.893709	-4.552192	-0.178821
61	6	0	-3.763634	-2.779735	1.193210
62	1	0	-2.458664	-1.166117	1.622943
63	6	0	5.851140	-1.564383	-0.042880
64	1	0	-0.685904	-5.516345	-1.323940
65	6	0	-3.938633	-4.010848	0.529065
66	1	0	-2.996932	-5.522428	-0.653444
67	1	0	-4.565328	-2.375546	1.800656
68	1	0	5.916993	-2.550303	-0.517316
69	6	0	6.540216	-0.556413	-0.980453
70	6	0	6.584009	-1.655236	1.307879
71	1	0	-4.881865	-4.539861	0.604716
72	1	0	7.586792	-0.832062	-1.141441
73	1	0	6.043829	-0.519986	-1.953419
74	1	0	6.523103	0.453113	-0.559375
75	1	0	6.573261	-0.694744	1.831391
76	1	0	6.116367	-2.396091	1.961092
77	1	0	7.629795	-1.941351	1.160697

Compound 6 2-RF-CN-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1512.86630674 A.U. after 1 cycles
Lowest frequency = -27.8850

Zero-point correction= 0.646514
(Hartree/Particle)
Thermal correction to Energy= 0.682508
Thermal correction to Enthalpy= 0.683452
Thermal correction to Gibbs Free Energy= 0.578471
Sum of electronic and zero-point Energies= -1512.219792

Sum of electronic and thermal Energies= -1512.183799
Sum of electronic and thermal Enthalpies= -1512.182855
Sum of electronic and thermal Free Energies= -1512.287836

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.916303	-0.481789	0.220712
2	6	0	4.410287	-4.555369	-2.328168
3	1	0	3.914879	-5.043209	-3.170303
4	1	0	5.322973	-4.085846	-2.711892
5	1	0	4.714615	-5.323541	-1.613773
6	6	0	3.517294	-3.527366	-1.683751
7	6	0	2.544950	-2.855157	-2.417635
8	1	0	2.425449	-3.096880	-3.468848
9	6	0	1.840042	-1.539031	-0.465348
10	6	0	3.659236	-3.189570	-0.341142
11	1	0	4.418582	-3.693802	0.248005
12	6	0	1.422907	1.459768	3.608458
13	1	0	1.975640	2.323846	3.967428
14	6	0	0.579351	0.782523	4.483467
15	6	0	-0.034956	-0.370449	4.004486
16	1	0	-0.644541	-0.966018	4.679017
17	6	0	0.912437	-0.066925	1.772396
18	6	0	0.355045	1.266528	5.894826
19	1	0	-0.495481	1.955734	5.941126
20	1	0	0.139242	0.436994	6.572696
21	1	0	1.228077	1.800639	6.277828
22	6	0	1.607799	1.054639	2.284213
23	6	0	1.717173	-1.880096	-1.859861
24	6	0	0.739333	-1.254473	-2.836714
25	1	0	-0.298996	-1.476985	-2.589358
26	1	0	0.828481	-0.169832	-2.883189
27	1	0	0.930734	-1.647069	-3.837137
28	6	0	2.628151	1.827315	1.477990
29	1	0	3.445324	2.157703	2.124750
30	1	0	3.066552	1.227521	0.679708
31	1	0	2.198490	2.718646	1.016588
32	6	0	0.123385	-0.809008	2.687743
33	6	0	-0.526664	-2.133441	2.339405
34	1	0	-1.583189	-2.015294	2.090522
35	1	0	-0.041661	-2.627368	1.495654
36	1	0	-0.464927	-2.814061	3.192984
37	6	0	2.864701	-2.225071	0.276516
38	6	0	3.182840	-1.979694	1.736986
39	1	0	3.425194	-0.936814	1.939384
40	1	0	2.352610	-2.238473	2.394440
41	1	0	4.042033	-2.585945	2.029520
42	7	0	-0.194583	0.192292	-0.583697
43	6	0	-1.508509	-0.310370	-0.526245
44	6	0	-0.318864	1.567461	-0.836176
45	6	0	-2.440124	0.749888	-0.622669
46	6	0	-1.956477	-1.633525	-0.482741
47	6	0	-1.669533	1.950757	-0.808546
48	6	0	0.684111	2.478666	-1.287240
49	6	0	-3.813766	0.482155	-0.614166
50	6	0	-3.324998	-1.871980	-0.487555
51	1	0	-1.262546	-2.463842	-0.463886

52	6	0	-2.044464	3.296307	-1.024181
53	6	0	0.281423	3.842102	-1.490010
54	6	0	2.003641	2.106571	-1.645241
55	6	0	-4.273231	-0.828807	-0.537505
56	1	0	-4.525862	1.298544	-0.686119
57	1	0	-3.667472	-2.900921	-0.464096
58	6	0	-1.081658	4.225268	-1.314369
59	1	0	-3.088100	3.584485	-0.963052
60	6	0	1.249911	4.775944	-1.934785
61	6	0	2.906821	3.034288	-2.112211
62	1	0	2.306479	1.070451	-1.558930
63	6	0	-5.766446	-1.126817	-0.535092
64	1	0	-1.349429	5.264237	-1.472331
65	6	0	2.535194	4.388588	-2.235989
66	1	0	0.947946	5.810459	-2.062199
67	1	0	3.907255	2.721134	-2.388826
68	1	0	-6.280599	-0.160014	-0.584451
69	6	0	-6.198174	-1.938454	-1.770036
70	6	0	-6.215050	-1.818217	0.765216
71	1	0	3.255828	5.116948	-2.590391
72	1	0	-7.283036	-2.081957	-1.778922
73	1	0	-5.913644	-1.429636	-2.694402
74	1	0	-5.732846	-2.928653	-1.777776
75	1	0	-5.749512	-2.802599	0.872267
76	1	0	-5.942751	-1.223839	1.640957
77	1	0	-7.299955	-1.961514	0.773393

Compound 6 3-RF-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1512.82578971 A.U. after 1 cycles
Lowest frequency = -25.0527

Zero-point correction= 0.646733
(Hartree/Particle)
Thermal correction to Energy= 0.682553
Thermal correction to Enthalpy= 0.683497
Thermal correction to Gibbs Free Energy= 0.578837
Sum of electronic and zero-point Energies= -1512.179057
Sum of electronic and thermal Energies= -1512.143237
Sum of electronic and thermal Enthalpies= -1512.142293
Sum of electronic and thermal Free Energies= -1512.246952

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.792480	0.616182	0.248963
2	6	0	1.231051	-2.076064	5.600938
3	1	0	1.491795	-1.357939	6.384081
4	1	0	0.255886	-2.499829	5.863048
5	1	0	1.963403	-2.885517	5.627582
6	6	0	1.188998	-1.417132	4.245037
7	6	0	0.452286	-0.256158	4.025366
8	1	0	-0.094708	0.189122	4.851359
9	6	0	1.072210	-0.170425	1.641430
10	6	0	1.872628	-1.928686	3.156493
11	1	0	2.476788	-2.822615	3.285904

12	6	0	3.471671	3.142069	-0.949220
13	1	0	4.529522	3.057044	-1.179954
14	6	0	2.818695	4.344228	-1.197009
15	6	0	1.495702	4.419800	-0.792551
16	1	0	0.969917	5.365757	-0.890272
17	6	0	1.426992	2.068009	-0.086792
18	6	0	3.522881	5.507416	-1.848561
19	1	0	3.529095	5.399402	-2.938813
20	1	0	3.030326	6.454054	-1.615447
21	1	0	4.564289	5.576237	-1.523609
22	6	0	2.826874	2.036324	-0.394157
23	6	0	0.390667	0.366041	2.781356
24	6	0	-0.450894	1.617571	2.720072
25	1	0	0.138076	2.478600	2.405107
26	1	0	-1.295842	1.507514	2.036450
27	1	0	-0.865193	1.844342	3.703966
28	6	0	3.719787	0.843824	-0.126695
29	1	0	3.560570	0.435325	0.869968
30	1	0	3.576589	0.038230	-0.848958
31	1	0	4.766433	1.145327	-0.196579
32	6	0	0.801330	3.339390	-0.231412
33	6	0	-0.563025	3.744938	0.299899
34	1	0	-1.114141	4.318106	-0.451372
35	1	0	-1.190739	2.928578	0.622525
36	1	0	-0.425251	4.409238	1.160177
37	6	0	1.830139	-1.346984	1.880222
38	6	0	2.695855	-2.076740	0.875588
39	1	0	2.719439	-1.626918	-0.104094
40	1	0	3.727060	-2.124582	1.241000
41	1	0	2.349438	-3.106022	0.752718
42	7	0	-0.115259	-0.051776	-0.788235
43	6	0	-1.520120	0.240980	-0.680726
44	6	0	-0.092841	-1.464100	-0.962565
45	6	0	-2.248239	-0.949200	-0.443766
46	6	0	-2.207083	1.421365	-0.936986
47	6	0	-1.319751	-2.043196	-0.636800
48	6	0	0.887573	-2.206881	-1.671567
49	6	0	-3.636473	-0.912148	-0.297016
50	6	0	-3.593622	1.436625	-0.801545
51	1	0	-1.687756	2.292403	-1.300541
52	6	0	-1.503935	-3.441162	-0.731265
53	6	0	0.694782	-3.625070	-1.762600
54	6	0	1.958207	-1.614211	-2.388439
55	6	0	-4.325919	0.290820	-0.443966
56	1	0	-4.186936	-1.828962	-0.110319
57	1	0	-4.119710	2.360719	-1.015425
58	6	0	-0.489842	-4.216039	-1.234310
59	1	0	-2.443478	-3.890494	-0.429921
60	6	0	1.665324	-4.394894	-2.452304
61	6	0	2.856803	-2.390923	-3.081613
62	1	0	2.035204	-0.533866	-2.410149
63	6	0	-5.839322	0.339469	-0.285491
64	1	0	-0.608419	-5.291645	-1.308988
65	6	0	2.728859	-3.797776	-3.087787
66	1	0	1.537485	-5.471655	-2.496199
67	1	0	3.659755	-1.921744	-3.639072
68	1	0	-6.162400	-0.676011	-0.028964
69	6	0	-6.264071	1.262262	0.871221
70	6	0	-6.549661	0.729348	-1.594434
71	1	0	3.451847	-4.401930	-3.623989

72	1	0	-7.348735	1.231690	1.012276
73	1	0	-5.789715	0.962456	1.809041
74	1	0	-5.983460	2.300944	0.672471
75	1	0	-6.288281	1.746069	-1.902182
76	1	0	-6.274799	0.053852	-2.408277
77	1	0	-7.636047	0.690098	-1.470000

Compound 7 GS1

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.47332637 A.U. after 1 cycles
Lowest frequency = 19.1800

Zero-point correction= 0.594429
(Hartree/Particle)
Thermal correction to Energy= 0.630056
Thermal correction to Enthalpy= 0.631000
Thermal correction to Gibbs Free Energy= 0.525404
Sum of electronic and zero-point Energies= -1508.878897
Sum of electronic and thermal Energies= -1508.843270
Sum of electronic and thermal Enthalpies= -1508.842326
Sum of electronic and thermal Free Energies= -1508.947922

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.795978	2.357189	-0.170693
2	6	0	-0.495651	2.894733	0.144053
3	6	0	0.345054	1.819782	0.450611
4	7	0	-0.349200	0.594885	0.267891
5	6	0	-1.701342	0.953789	-0.047360
6	6	0	-2.823846	0.167222	-0.293496
7	6	0	-4.026019	0.787188	-0.636561
8	6	0	-4.117212	2.182777	-0.753396
9	6	0	-2.994000	2.973436	-0.522326
10	6	0	-0.041203	4.230589	0.195529
11	6	0	1.244679	4.481105	0.587140
12	6	0	2.097719	3.424941	1.019738
13	6	0	1.644733	2.059956	0.999296
14	8	0	-5.260807	2.855344	-1.088084
15	6	0	-6.439622	2.106423	-1.336789
16	6	0	3.388220	3.713154	1.530118
17	6	0	4.188230	2.726963	2.054652
18	6	0	3.713963	1.400902	2.106438
19	6	0	2.479305	1.080634	1.591619
20	1	0	-2.792729	-0.908108	-0.216224
21	1	0	-4.892016	0.163232	-0.810005
22	1	0	-3.079118	4.048811	-0.619785
23	1	0	-0.708184	5.040693	-0.076548
24	1	0	1.624290	5.496507	0.618409
25	1	0	-7.209583	2.836612	-1.581779
26	1	0	-6.751757	1.537359	-0.453403
27	1	0	-6.312648	1.420311	-2.182281
28	1	0	3.726508	4.744073	1.518618
29	1	0	5.168707	2.968729	2.448992
30	1	0	4.322902	0.626654	2.559084
31	1	0	2.138451	0.060370	1.653078

32	5	0	0.184698	-0.744588	0.025796
33	6	0	-0.716217	-1.994264	0.390236
34	6	0	-1.003877	-3.006236	-0.559570
35	6	0	-1.200837	-2.162107	1.712612
36	6	0	-1.746172	-4.127501	-0.183565
37	6	0	-1.915896	-3.312071	2.053067
38	6	0	-2.206298	-4.306696	1.120491
39	1	0	-1.966454	-4.885043	-0.930434
40	1	0	-2.259037	-3.431583	3.076843
41	6	0	1.602770	-0.956507	-0.642945
42	6	0	1.936562	-0.278492	-1.843442
43	6	0	2.530447	-1.910396	-0.142276
44	6	0	3.151500	-0.543291	-2.482600
45	6	0	3.741330	-2.123134	-0.798472
46	6	0	4.076316	-1.448644	-1.973199
47	1	0	3.376668	-0.023250	-3.409360
48	1	0	4.442690	-2.842205	-0.384588
49	6	0	2.272532	-2.724552	1.110134
50	1	0	1.892435	-2.121750	1.938414
51	1	0	1.535039	-3.511181	0.932936
52	1	0	3.194843	-3.201055	1.449075
53	6	0	1.017463	0.719939	-2.518706
54	1	0	-0.037758	0.458974	-2.428447
55	1	0	1.137047	1.721483	-2.095738
56	1	0	1.251728	0.786087	-3.583373
57	6	0	5.403036	-1.682294	-2.652380
58	1	0	5.365325	-1.405568	-3.708253
59	1	0	6.191716	-1.083351	-2.183596
60	1	0	5.707540	-2.729915	-2.584852
61	6	0	-0.559756	-2.905669	-2.004461
62	1	0	-0.825013	-1.942134	-2.447229
63	1	0	0.522604	-3.015567	-2.103501
64	1	0	-1.033908	-3.684739	-2.605018
65	6	0	-0.974021	-1.131441	2.800771
66	1	0	0.060319	-0.783626	2.847040
67	1	0	-1.597989	-0.246768	2.646439
68	1	0	-1.225615	-1.548168	3.778144
69	6	0	-3.017614	-5.520801	1.501749
70	1	0	-4.088819	-5.335894	1.363557
71	1	0	-2.754332	-6.385438	0.887995
72	1	0	-2.866295	-5.788336	2.550144

Compound 7 GS2

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.47401553 A.U. after 1 cycles
Lowest frequency = 20.0676

Zero-point correction= 0.594468
(Hartree/Particle)
Thermal correction to Energy= 0.630070
Thermal correction to Enthalpy= 0.631014
Thermal correction to Gibbs Free Energy= 0.525529
Sum of electronic and zero-point Energies= -1508.879548
Sum of electronic and thermal Energies= -1508.843945
Sum of electronic and thermal Enthalpies= -1508.843001
Sum of electronic and thermal Free Energies= -1508.948487

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.458238	-1.587640	0.158915
2	6	0	-1.403881	-2.506575	-0.185393
3	6	0	-0.262563	-1.751388	-0.479845
4	7	0	-0.528816	-0.375328	-0.264018
5	6	0	-1.920274	-0.291890	0.065559
6	6	0	-2.730454	0.813335	0.351882
7	6	0	-4.054605	0.597265	0.698386
8	6	0	-4.595251	-0.699157	0.784866
9	6	0	-3.796070	-1.804156	0.517834
10	6	0	-1.401125	-3.916513	-0.271624
11	6	0	-0.265797	-4.556422	-0.684647
12	6	0	0.879588	-3.819726	-1.104589
13	6	0	0.888724	-2.382562	-1.049289
14	8	0	-5.914442	-0.757340	1.139054
15	6	0	-6.523896	-2.033457	1.245902
16	6	0	2.006729	-4.494575	-1.636189
17	6	0	3.079291	-3.805199	-2.148459
18	6	0	3.055840	-2.396363	-2.165617
19	6	0	1.991374	-1.709203	-1.629860
20	1	0	-2.355134	1.823086	0.298307
21	1	0	-4.708859	1.433785	0.910908
22	1	0	-4.181681	-2.812734	0.579853
23	1	0	-2.290298	-4.478460	-0.008724
24	1	0	-0.232271	-5.638889	-0.742521
25	1	0	-7.557928	-1.848079	1.532717
26	1	0	-6.040973	-2.647983	2.014814
27	1	0	-6.505251	-2.570429	0.290206
28	1	0	1.995861	-5.579513	-1.651026
29	1	0	3.928460	-4.339322	-2.559419
30	1	0	3.879435	-1.847678	-2.608121
31	1	0	1.996342	-0.632380	-1.665448
32	5	0	0.405808	0.721989	-0.008497
33	6	0	-0.051632	2.197057	-0.352330
34	6	0	0.004761	3.236765	0.609574
35	6	0	-0.468851	2.525646	-1.667585
36	6	0	-0.347076	4.539680	0.252028
37	6	0	-0.784828	3.846975	-1.989608
38	6	0	-0.737724	4.870959	-1.044936
39	1	0	-0.310738	5.318828	1.008150
40	1	0	-1.081142	4.081331	-3.008110
41	6	0	1.818318	0.459144	0.652787
42	6	0	1.921705	-0.311421	1.839426
43	6	0	3.000417	1.075510	0.158992
44	6	0	3.159561	-0.459789	2.472017
45	6	0	4.217953	0.878425	0.807794
46	6	0	4.323560	0.111633	1.968759
47	1	0	3.209940	-1.040647	3.388576
48	1	0	5.111006	1.342875	0.399150
49	6	0	3.012480	1.951710	-1.078035
50	1	0	2.453357	1.519476	-1.911290
51	1	0	2.569767	2.931113	-0.880756
52	1	0	4.037481	2.110862	-1.419587
53	6	0	0.733589	-0.975562	2.506391
54	1	0	-0.180527	-0.384297	2.438227
55	1	0	0.518623	-1.950317	2.059354
56	1	0	0.941515	-1.141429	3.565622

57	6	0	5.657490	-0.102869	2.640036
58	1	0	5.536694	-0.368715	3.692464
59	1	0	6.210593	-0.916043	2.156979
60	1	0	6.281753	0.792607	2.583761
61	6	0	0.405281	2.983855	2.048672
62	1	0	-0.147969	2.148851	2.486254
63	1	0	1.467552	2.744744	2.137235
64	1	0	0.206390	3.865850	2.660936
65	6	0	-0.589242	1.489946	-2.768028
66	1	0	0.278818	0.829665	-2.826756
67	1	0	-1.463241	0.850131	-2.617877
68	1	0	-0.698655	1.977554	-3.738844
69	6	0	-1.127215	6.283609	-1.405536
70	1	0	-2.200694	6.444200	-1.255497
71	1	0	-0.598930	7.013343	-0.787473
72	1	0	-0.908737	6.502402	-2.453386

Compound 7 1-RF-C1-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.40020834 A.U. after 1 cycles
Lowest frequency = -35.4088

Zero-point correction= 0.593979
(Hartree/Particle)
Thermal correction to Energy= 0.628091
Thermal correction to Enthalpy= 0.629035
Thermal correction to Gibbs Free Energy= 0.529086
Sum of electronic and zero-point Energies= -1508.806229
Sum of electronic and thermal Energies= -1508.772118
Sum of electronic and thermal Enthalpies= -1508.771173
Sum of electronic and thermal Free Energies= -1508.871122

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.065917	4.656877	-3.046289
2	1	0	-1.382836	5.391637	-3.478647
3	1	0	-2.333165	3.950530	-3.840418
4	1	0	-2.982778	5.172025	-2.748909
5	6	0	-1.437287	3.932141	-1.885898
6	6	0	-0.058981	3.837974	-1.737611
7	1	0	0.584784	4.403858	-2.405172
8	6	0	-0.262561	2.259276	0.140947
9	6	0	-2.203708	3.407439	-0.845887
10	1	0	-3.262050	3.648093	-0.791804
11	6	0	3.891765	0.698476	2.118968
12	1	0	4.302758	0.786665	3.121254
13	6	0	4.757076	0.494915	1.039475
14	6	0	4.194952	0.383375	-0.227263
15	1	0	4.845871	0.214587	-1.081106
16	6	0	1.949859	0.690225	0.645784
17	6	0	6.250588	0.419577	1.249156
18	1	0	6.757596	0.032038	0.363008
19	1	0	6.669724	1.408411	1.464793
20	1	0	6.502832	-0.228356	2.093482
21	6	0	2.513364	0.796584	1.942444

22	6	0	0.542205	3.088592	-0.719348
23	6	0	2.022054	3.384122	-0.532870
24	1	0	2.396746	3.094653	0.443048
25	1	0	2.659424	2.925432	-1.289496
26	1	0	2.143473	4.467547	-0.628513
27	6	0	1.631175	1.021954	3.153145
28	1	0	2.227403	1.109137	4.063658
29	1	0	1.039737	1.938520	3.054601
30	1	0	0.926621	0.195708	3.293797
31	6	0	2.815092	0.474378	-0.442022
32	6	0	2.322355	0.328008	-1.866347
33	1	0	2.459357	-0.697885	-2.218129
34	1	0	1.266040	0.574814	-1.975040
35	1	0	2.887609	0.976850	-2.542561
36	6	0	-1.642386	2.654856	0.181383
37	6	0	-2.495019	2.546876	1.426460
38	1	0	-3.423308	1.997062	1.274261
39	1	0	-1.956322	2.111131	2.261098
40	1	0	-2.762298	3.567322	1.722880
41	5	0	0.369945	0.849313	0.564599
42	7	0	-0.396830	-0.435144	0.710946
43	6	0	-1.802268	-0.538732	0.948177
44	6	0	-0.152941	-1.482056	-0.262676
45	6	0	-2.427976	-1.272013	-0.074447
46	6	0	-2.493666	-0.280645	2.127132
47	6	0	-1.360674	-1.825552	-0.884150
48	6	0	0.999502	-2.292393	-0.484611
49	6	0	-3.793913	-1.568123	-0.024145
50	6	0	-3.843083	-0.597826	2.202104
51	1	0	-1.988048	0.132011	2.990214
52	6	0	-1.400842	-2.731607	-1.965413
53	6	0	0.946915	-3.211431	-1.592370
54	6	0	2.113127	-2.370619	0.391603
55	1	0	-4.256392	-2.141054	-0.816357
56	6	0	-4.506556	-1.196710	1.116720
57	1	0	-4.410208	-0.414422	3.106181
58	6	0	-0.247386	-3.360116	-2.351799
59	1	0	-2.339368	-2.933614	-2.469516
60	6	0	2.070882	-4.036020	-1.851741
61	6	0	3.157884	-3.227628	0.139622
62	1	0	2.125278	-1.759555	1.280883
63	1	0	-0.247823	-4.050564	-3.188149
64	6	0	3.158933	-4.041788	-1.012700
65	1	0	2.036822	-4.698045	-2.710874
66	1	0	3.987398	-3.277026	0.835444
67	1	0	4.000713	-4.694952	-1.213973
68	8	0	-5.838492	-1.432349	1.307039
69	6	0	-6.563826	-2.077896	0.272142
70	1	0	-6.188360	-3.091079	0.087680
71	1	0	-7.593523	-2.136183	0.621483
72	1	0	-6.530111	-1.504012	-0.661105

Compound 7 1-RF-C-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.40550434 A.U. after 1 cycles
Lowest frequency = -26.9008

Zero-point correction= 0.594132
(Hartree/Particle)
Thermal correction to Energy= 0.628218
Thermal correction to Enthalpy= 0.629162
Thermal correction to Gibbs Free Energy= 0.529371
Sum of electronic and zero-point Energies= -1508.811373
Sum of electronic and thermal Energies= -1508.777286
Sum of electronic and thermal Enthalpies= -1508.776342
Sum of electronic and thermal Free Energies= -1508.876133

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.352943	-0.954553	-0.312813
2	6	0	-2.038845	-3.548897	4.310671
3	1	0	-1.381980	-4.239746	4.844250
4	1	0	-2.167004	-2.663247	4.943259
5	1	0	-3.020653	-4.017959	4.207760
6	6	0	-1.466963	-3.163734	2.971803
7	6	0	-0.107604	-3.257352	2.699274
8	1	0	0.545228	-3.731177	3.427041
9	6	0	-0.352253	-2.119505	0.533062
10	6	0	-2.283199	-2.788460	1.905619
11	1	0	-3.360074	-2.906754	1.990532
12	6	0	3.564048	-1.597601	-2.376786
13	1	0	3.790155	-1.956767	-3.377184
14	6	0	4.611664	-1.242466	-1.525224
15	6	0	4.282690	-0.784790	-0.251559
16	1	0	5.080378	-0.499563	0.429635
17	6	0	1.903638	-1.044253	-0.680167
18	6	0	6.050319	-1.381266	-1.962258
19	1	0	6.707479	-0.728617	-1.383113
20	1	0	6.405827	-2.408833	-1.826952
21	1	0	6.172004	-1.132876	-3.019767
22	6	0	2.230364	-1.504573	-1.976697
23	6	0	0.456973	-2.819247	1.494449
24	6	0	1.882109	-3.300106	1.272662
25	1	0	2.166868	-3.314464	0.225897
26	1	0	2.629516	-2.724104	1.818996
27	1	0	1.937110	-4.326483	1.647084
28	6	0	1.144547	-1.892600	-2.958649
29	1	0	1.565544	-2.387066	-3.836477
30	1	0	0.417584	-2.576107	-2.508752
31	1	0	0.593930	-1.012770	-3.307617
32	6	0	2.958381	-0.679389	0.183337
33	6	0	2.727070	-0.151493	1.585551
34	1	0	2.926529	0.922157	1.633107
35	1	0	1.705434	-0.309331	1.932332
36	1	0	3.401083	-0.635890	2.298210
37	6	0	-1.757642	-2.343658	0.696455
38	6	0	-2.702397	-2.393154	-0.479540
39	1	0	-3.596829	-1.782966	-0.350364
40	1	0	-2.221317	-2.123086	-1.411830
41	1	0	-3.031055	-3.433148	-0.587335
42	7	0	-0.246084	0.378355	-0.619356
43	6	0	0.527930	1.542529	-0.219365
44	6	0	-1.594276	0.809785	-0.400563
45	6	0	-0.263908	2.373648	0.596014

46	6	0	1.792410	1.970446	-0.613375
47	6	0	-1.628041	1.888382	0.485505
48	6	0	-2.728715	0.550800	-1.215140
49	6	0	0.242903	3.556926	1.142418
50	6	0	2.290452	3.158487	-0.090374
51	1	0	2.380631	1.412181	-1.324784
52	6	0	-2.856347	2.452491	0.893740
53	6	0	-3.978103	1.129231	-0.805602
54	6	0	-2.663650	-0.087983	-2.480745
55	6	0	1.543550	3.934172	0.810656
56	1	0	-0.387890	4.181236	1.760646
57	1	0	3.266028	3.523103	-0.387483
58	6	0	-4.017250	2.020297	0.303790
59	1	0	-2.875493	3.240984	1.637734
60	6	0	-5.130777	0.883505	-1.594993
61	6	0	-3.789441	-0.248818	-3.251172
62	1	0	-1.701512	-0.428976	-2.841877
63	1	0	-4.973931	2.433194	0.605041
64	6	0	-5.044942	0.204030	-2.786828
65	1	0	-6.082100	1.285156	-1.261401
66	1	0	-3.715336	-0.721720	-4.224034
67	1	0	-5.931497	0.048553	-3.391035
68	8	0	2.163442	5.064537	1.265567
69	6	0	1.453116	5.908008	2.157634
70	1	0	2.133460	6.721482	2.405104
71	1	0	0.551863	6.322418	1.690663
72	1	0	1.173499	5.378818	3.076122

Compound 7 1-RF-C-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.40531075 A.U. after 1 cycles
Lowest frequency = -26.7899

Zero-point correction= 0.594108
(Hartree/Particle)
Thermal correction to Energy= 0.628207
Thermal correction to Enthalpy= 0.629151
Thermal correction to Gibbs Free Energy= 0.529346
Sum of electronic and zero-point Energies= -1508.811203
Sum of electronic and thermal Energies= -1508.777104
Sum of electronic and thermal Enthalpies= -1508.776160
Sum of electronic and thermal Free Energies= -1508.875965

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.141450	-0.949416	0.358709
2	6	0	2.604006	-3.579580	-4.043693
3	1	0	2.060182	-4.411701	-4.496788
4	1	0	2.590726	-2.750150	-4.759785
5	1	0	3.647076	-3.879620	-3.915155
6	6	0	1.984466	-3.159372	-2.736982
7	6	0	0.656625	-3.433076	-2.431956
8	1	0	0.081995	-4.068638	-3.099933
9	6	0	0.730945	-2.068818	-0.387063
10	6	0	2.736683	-2.562397	-1.726462

11	1	0	3.818538	-2.521117	-1.820007
12	6	0	-3.236221	-1.870439	2.496579
13	1	0	-3.413729	-2.167248	3.526802
14	6	0	-4.318808	-1.752866	1.623107
15	6	0	-4.052132	-1.369056	0.310944
16	1	0	-4.878353	-1.269571	-0.388577
17	6	0	-1.663845	-1.234972	0.745718
18	6	0	-5.723964	-2.063996	2.080165
19	1	0	-6.467053	-1.579411	1.442730
20	1	0	-5.918576	-3.141838	2.049911
21	1	0	-5.891900	-1.733388	3.108496
22	6	0	-1.928021	-1.618565	2.080732
23	6	0	0.035345	-2.972025	-1.264337
24	6	0	-1.300388	-3.638347	-0.975247
25	1	0	-1.575048	-3.600714	0.073758
26	1	0	-2.128559	-3.231346	-1.556174
27	1	0	-1.202810	-4.690940	-1.256576
28	6	0	-0.803393	-1.752187	3.086256
29	1	0	-1.153128	-2.219795	4.008953
30	1	0	0.018205	-2.360758	2.695579
31	1	0	-0.388954	-0.773169	3.348494
32	6	0	-2.754825	-1.109015	-0.140196
33	6	0	-2.592433	-0.681507	-1.585505
34	1	0	-2.932402	0.347876	-1.726277
35	1	0	-1.557910	-0.731580	-1.926181
36	1	0	-3.193214	-1.312962	-2.246698
37	6	0	2.153416	-2.089545	-0.554872
38	6	0	3.100019	-1.879007	0.601641
39	1	0	3.884191	-1.148572	0.400238
40	1	0	2.586271	-1.603960	1.514774
41	1	0	3.592100	-2.838677	0.796637
42	7	0	0.247728	0.478488	0.541263
43	6	0	-0.692872	1.476996	0.056280
44	6	0	1.516104	1.091189	0.273090
45	6	0	-0.030719	2.341646	-0.846979
46	6	0	-1.999768	1.745005	0.424777
47	6	0	1.391556	2.076206	-0.707656
48	6	0	2.672045	1.081870	1.098316
49	6	0	-0.710825	3.371307	-1.483847
50	6	0	-2.682489	2.796927	-0.198917
51	1	0	-2.499461	1.171021	1.189474
52	6	0	2.520562	2.783002	-1.174409
53	6	0	3.820533	1.805715	0.628893
54	6	0	2.699219	0.552070	2.414609
55	6	0	-2.057344	3.584070	-1.173525
56	1	0	-0.218450	4.048895	-2.170638
57	1	0	-3.699946	3.000470	0.105502
58	6	0	3.730112	2.588800	-0.556177
59	1	0	2.421348	3.495609	-1.985342
60	6	0	4.992929	1.809489	1.427693
61	6	0	3.832209	0.633289	3.186849
62	1	0	1.799275	0.098929	2.811105
63	1	0	4.614017	3.115000	-0.900032
64	6	0	5.005645	1.231717	2.674767
65	1	0	5.873432	2.320876	1.052504
66	1	0	3.826820	0.240290	4.197348
67	1	0	5.902347	1.267094	3.282974
68	8	0	-2.660174	4.616343	-1.837903
69	6	0	-4.010733	4.922227	-1.529521
70	1	0	-4.281618	5.756929	-2.174376

71	1	0	-4.674487	4.075118	-1.738187
72	1	0	-4.128218	5.223446	-0.482153

Compound 7 1-RF-N-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.38285669 A.U. after 1 cycles
Lowest frequency = -70.3696

Zero-point correction= 0.594996
(Hartree/Particle)
Thermal correction to Energy= 0.628534
Thermal correction to Enthalpy= 0.629478
Thermal correction to Gibbs Free Energy= 0.531635
Sum of electronic and zero-point Energies= -1508.787860
Sum of electronic and thermal Energies= -1508.754323
Sum of electronic and thermal Enthalpies= -1508.753379
Sum of electronic and thermal Free Energies= -1508.851222

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.312675	1.162747	-0.230518
2	6	0	-5.689032	-0.096555	-1.927210
3	1	0	-5.811052	-0.896934	-2.660993
4	1	0	-6.024841	-0.487971	-0.960377
5	1	0	-6.354612	0.726397	-2.198022
6	6	0	-4.257158	0.354238	-1.833834
7	6	0	-3.195731	-0.512200	-2.081369
8	1	0	-3.399000	-1.500803	-2.482423
9	6	0	-1.539921	1.129944	-1.268765
10	6	0	-3.915243	1.685286	-1.605078
11	1	0	-4.689045	2.446836	-1.654976
12	6	0	2.025266	4.173397	0.646761
13	1	0	2.155255	5.224432	0.402889
14	6	0	3.067150	3.485585	1.261125
15	6	0	2.739101	2.250693	1.815330
16	1	0	3.445608	1.763818	2.481029
17	6	0	0.560229	2.191748	0.650883
18	6	0	4.436949	4.088125	1.419763
19	1	0	4.898715	3.790343	2.364257
20	1	0	5.098569	3.749547	0.614479
21	1	0	4.404128	5.179310	1.379661
22	6	0	0.773051	3.595821	0.432255
23	6	0	-1.868718	-0.145697	-1.865638
24	6	0	-0.846806	-1.097136	-2.458684
25	1	0	0.126265	-0.636598	-2.600707
26	1	0	-0.715637	-2.012564	-1.878568
27	1	0	-1.213021	-1.393581	-3.446247
28	6	0	-0.339056	4.596877	0.226133
29	1	0	-0.233450	5.355374	1.007901
30	1	0	-0.299011	5.124991	-0.728746
31	1	0	-1.315114	4.147126	0.355595
32	6	0	1.518331	1.623667	1.574652
33	6	0	1.248707	0.421777	2.460708
34	1	0	0.188892	0.210977	2.573174
35	1	0	1.749986	-0.487873	2.122844

36	1	0	1.640125	0.651691	3.456081
37	6	0	-2.594115	2.095637	-1.432425
38	6	0	-2.354472	3.559856	-1.722044
39	1	0	-2.806851	4.245349	-1.002288
40	1	0	-1.300976	3.783667	-1.830990
41	1	0	-2.822227	3.767885	-2.689605
42	7	0	0.233552	-0.247693	-0.017889
43	6	0	1.498338	-0.640156	-0.481251
44	6	0	-0.353827	-1.374174	0.559718
45	6	0	1.699665	-2.012891	-0.229447
46	6	0	2.466464	0.102180	-1.170583
47	6	0	0.516568	-2.476113	0.442439
48	6	0	-1.584561	-1.491427	1.282107
49	6	0	2.880746	-2.654790	-0.640986
50	6	0	3.626218	-0.536519	-1.570433
51	1	0	2.326732	1.154291	-1.384640
52	6	0	0.159439	-3.745566	0.952668
53	6	0	-1.921442	-2.795101	1.783409
54	6	0	-2.461169	-0.417546	1.575100
55	6	0	3.841188	-1.906724	-1.308115
56	1	0	3.021902	-3.708400	-0.440450
57	1	0	4.402715	0.003139	-2.098577
58	6	0	-1.040222	-3.901655	1.589513
59	1	0	0.836315	-4.585220	0.837083
60	6	0	-3.131585	-2.958132	2.501093
61	6	0	-3.619991	-0.610130	2.293997
62	1	0	-2.224569	0.579640	1.228910
63	1	0	-1.334404	-4.868658	1.982579
64	6	0	-3.968172	-1.895594	2.752725
65	1	0	-3.383039	-3.948753	2.866102
66	1	0	-4.265959	0.234204	2.506597
67	1	0	-4.885920	-2.042410	3.311199
68	8	0	5.036732	-2.397757	-1.763820
69	6	0	5.320221	-3.769061	-1.547846
70	1	0	4.586503	-4.416340	-2.043241
71	1	0	6.303485	-3.944439	-1.982315
72	1	0	5.349729	-4.012292	-0.478863

Compound 7 1-RF-N-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.38164857 A.U. after 1 cycles
Lowest frequency = -70.7339

Zero-point correction= 0.594868
(Hartree/Particle)
Thermal correction to Energy= 0.628463
Thermal correction to Enthalpy= 0.629408
Thermal correction to Gibbs Free Energy= 0.531265
Sum of electronic and zero-point Energies= -1508.786780
Sum of electronic and thermal Energies= -1508.753185
Sum of electronic and thermal Enthalpies= -1508.752241
Sum of electronic and thermal Free Energies= -1508.850384

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	-0.215790	1.126576	-0.208612
2	6	0	-5.636317	0.417163	-2.062928
3	1	0	-5.817553	-0.370319	-2.798387
4	1	0	-6.036627	0.065968	-1.105245
5	1	0	-6.208024	1.301558	-2.353830
6	6	0	-4.169612	0.722255	-1.929655
7	6	0	-3.193826	-0.245790	-2.151155
8	1	0	-3.483486	-1.208986	-2.560823
9	6	0	-1.405766	1.221498	-1.285844
10	6	0	-3.702580	2.012675	-1.688055
11	1	0	-4.394368	2.847931	-1.758852
12	6	0	2.372874	3.891639	0.781422
13	1	0	2.613405	4.926131	0.551102
14	6	0	3.316540	3.104619	1.433935
15	6	0	2.848799	1.904023	1.962191
16	1	0	3.476731	1.348048	2.652108
17	6	0	0.723753	2.061110	0.710575
18	6	0	4.729091	3.573601	1.657359
19	1	0	5.120489	3.223742	2.615665
20	1	0	5.390140	3.183606	0.875105
21	1	0	4.800248	4.663428	1.632139
22	6	0	1.081214	3.437954	0.509953
23	6	0	-1.843312	-0.013755	-1.897311
24	6	0	-0.904680	-1.060509	-2.466643
25	1	0	0.116543	-0.704673	-2.563954
26	1	0	-0.894870	-1.992158	-1.897693
27	1	0	-1.261367	-1.303763	-3.472177
28	6	0	0.081933	4.542235	0.259395
29	1	0	0.229526	5.290558	1.044102
30	1	0	0.211461	5.059364	-0.693540
31	1	0	-0.937708	4.190207	0.349411
32	6	0	1.584350	1.398426	1.666442
33	6	0	1.167067	0.222282	2.529558
34	1	0	0.088514	0.113999	2.601617
35	1	0	1.590409	-0.729265	2.200625
36	1	0	1.541818	0.405904	3.540812
37	6	0	-2.352463	2.288602	-1.477889
38	6	0	-1.957918	3.720017	-1.763537
39	1	0	-2.361813	4.452041	-1.060966
40	1	0	-0.884369	3.836819	-1.839633
41	1	0	-2.371733	3.967474	-2.746303
42	7	0	0.180964	-0.330825	0.011341
43	6	0	1.417035	-0.843972	-0.414267
44	6	0	-0.534666	-1.398012	0.558560
45	6	0	1.469768	-2.237181	-0.168647
46	6	0	2.474813	-0.203424	-1.058231
47	6	0	0.221773	-2.581329	0.459755
48	6	0	-1.794528	-1.395329	1.239130
49	6	0	2.589494	-2.981240	-0.545103
50	6	0	3.588994	-0.952465	-1.428476
51	1	0	2.450835	0.858800	-1.266422
52	6	0	-0.276956	-3.811559	0.944462
53	6	0	-2.277859	-2.661787	1.715782
54	6	0	-2.566914	-0.239861	1.514962
55	6	0	3.650488	-2.335161	-1.171890
56	1	0	2.656602	-4.048131	-0.369215
57	1	0	4.410665	-0.449402	-1.919642
58	6	0	-1.507402	-3.850411	1.539836
59	1	0	0.317154	-4.713033	0.841782
60	6	0	-3.521944	-2.705823	2.391971

61	6	0	-3.762371	-0.318588	2.193922
62	1	0	-2.218843	0.730659	1.187494
63	1	0	-1.910543	-4.785412	1.913013
64	6	0	-4.254176	-1.565593	2.627256
65	1	0	-3.884600	-3.668258	2.738257
66	1	0	-4.326062	0.585435	2.394757
67	1	0	-5.200245	-1.622323	3.154019
68	8	0	4.716283	-3.130596	-1.509820
69	6	0	5.825375	-2.536596	-2.161184
70	1	0	6.297661	-1.766263	-1.539706
71	1	0	6.537949	-3.342712	-2.331478
72	1	0	5.543587	-2.097596	-3.125804

Compound 7 2-RF-CC-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.44811874 A.U. after 1 cycles
Lowest frequency = -50.1610

Zero-point correction= 0.594900
(Hartree/Particle)
Thermal correction to Energy= 0.629208
Thermal correction to Enthalpy= 0.630152
Thermal correction to Gibbs Free Energy= 0.529472
Sum of electronic and zero-point Energies= -1508.853219
Sum of electronic and thermal Energies= -1508.818911
Sum of electronic and thermal Enthalpies= -1508.817967
Sum of electronic and thermal Free Energies= -1508.918647

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.329659	0.655111	0.295473
2	6	0	-6.075651	1.613968	-0.980812
3	1	0	-6.461516	0.974340	-1.778558
4	1	0	-6.738406	1.517836	-0.117404
5	1	0	-6.143923	2.649751	-1.331747
6	6	0	-4.653025	1.257203	-0.627500
7	6	0	-3.767250	0.769722	-1.583379
8	1	0	-4.126868	0.587115	-2.592401
9	6	0	-1.914096	0.700057	0.010653
10	6	0	-4.171559	1.378724	0.671034
11	1	0	-4.853003	1.676126	1.464200
12	6	0	0.902419	4.368158	0.826857
13	1	0	0.933058	5.105840	1.624688
14	6	0	1.314773	4.734449	-0.451524
15	6	0	1.382990	3.723035	-1.402818
16	1	0	1.791654	3.945780	-2.385227
17	6	0	0.423281	2.074067	0.128278
18	6	0	1.702214	6.155356	-0.778230
19	1	0	2.438004	6.193769	-1.585141
20	1	0	0.830060	6.733617	-1.103271
21	1	0	2.124359	6.665059	0.091523
22	6	0	0.477627	3.073488	1.132426
23	6	0	-2.431246	0.483756	-1.293289
24	6	0	-1.620215	-0.103520	-2.428758
25	1	0	-1.184352	0.673978	-3.060339

26	1	0	-0.814929	-0.748859	-2.080219
27	1	0	-2.265925	-0.712523	-3.065618
28	6	0	0.216983	2.793502	2.599102
29	1	0	0.989489	3.275472	3.204976
30	1	0	-0.743143	3.190153	2.935403
31	1	0	0.245662	1.729890	2.833770
32	6	0	0.979858	2.412207	-1.132268
33	6	0	1.299510	1.394619	-2.209533
34	1	0	2.382974	1.367310	-2.362055
35	1	0	0.993180	0.383799	-1.959428
36	1	0	0.846035	1.661778	-3.167919
37	6	0	-2.844932	1.095702	1.003434
38	6	0	-2.526655	1.111395	2.485529
39	1	0	-1.542535	0.707491	2.715386
40	1	0	-2.586682	2.116981	2.907638
41	1	0	-3.257400	0.499719	3.024382
42	7	0	0.435889	-0.551811	0.538254
43	6	0	1.877046	-0.544214	0.534012
44	6	0	0.074333	-1.913135	0.216863
45	6	0	2.359686	-1.753050	0.017613
46	6	0	2.776130	0.425551	0.979758
47	6	0	1.212229	-2.598648	-0.216612
48	6	0	-1.163770	-2.613202	0.352345
49	6	0	3.730880	-1.999244	-0.120908
50	6	0	4.135760	0.182125	0.854331
51	1	0	2.443857	1.351709	1.419617
52	6	0	1.138971	-3.908204	-0.739142
53	6	0	-1.229016	-3.935366	-0.214838
54	6	0	-2.285997	-2.161339	1.089043
55	6	0	4.621006	-1.013330	0.294869
56	1	0	4.074783	-2.943675	-0.519989
57	1	0	4.858715	0.911706	1.197387
58	6	0	-0.072884	-4.539549	-0.782938
59	1	0	2.034833	-4.396399	-1.105535
60	6	0	-2.445054	-4.659797	-0.135055
61	6	0	-3.437138	-2.907509	1.178667
62	1	0	-2.223707	-1.224898	1.612175
63	1	0	-0.162374	-5.536235	-1.201007
64	6	0	-3.534204	-4.157262	0.533828
65	1	0	-2.488204	-5.642300	-0.593447
66	1	0	-4.273853	-2.531963	1.756528
67	1	0	-4.452621	-4.730093	0.594193
68	8	0	5.981128	-1.114426	0.225591
69	6	0	6.540646	-2.298996	-0.319339
70	1	0	7.620286	-2.161212	-0.287455
71	1	0	6.272092	-3.181266	0.273261
72	1	0	6.226543	-2.451585	-1.358445

Compound 7 2-RF-CC-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.44770082 A.U. after 1 cycles
Lowest frequency = -48.8430

Zero-point correction= 0.594980
(Hartree/Particle)
Thermal correction to Energy= 0.629247
Thermal correction to Enthalpy= 0.630192
Thermal correction to Gibbs Free Energy= 0.529699

Sum of electronic and zero-point Energies= -1508.852721
Sum of electronic and thermal Energies= -1508.818453
Sum of electronic and thermal Enthalpies= -1508.817509
Sum of electronic and thermal Free Energies= -1508.918002

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.211268	0.643372	0.278353
2	6	0	-5.680928	2.743345	-0.838816
3	1	0	-6.203573	2.205929	-1.634049
4	1	0	-6.330011	2.765697	0.039922
5	1	0	-5.550772	3.777913	-1.175586
6	6	0	-4.349422	2.106796	-0.526002
7	6	0	-3.602095	1.464870	-1.508508
8	1	0	-4.015588	1.369831	-2.508893
9	6	0	-1.760846	1.008938	0.034983
10	6	0	-3.821250	2.114757	0.759955
11	1	0	-4.410065	2.531972	1.573084
12	6	0	1.759892	4.024838	0.806348
13	1	0	1.956912	4.731753	1.608318
14	6	0	2.208413	4.315533	-0.479174
15	6	0	2.047928	3.322833	-1.439206
16	1	0	2.469612	3.470329	-2.430297
17	6	0	0.808760	1.884007	0.103595
18	6	0	2.867294	5.632810	-0.805756
19	1	0	3.582979	5.529946	-1.625102
20	1	0	2.123576	6.376413	-1.113313
21	1	0	3.396465	6.040999	0.059040
22	6	0	1.087986	2.839486	1.113007
23	6	0	-2.342652	0.916142	-1.256336
24	6	0	-1.691862	0.195752	-2.417921
25	1	0	-1.120800	0.879377	-3.050355
26	1	0	-1.026824	-0.604847	-2.096643
27	1	0	-2.460744	-0.259253	-3.046512
28	6	0	0.807707	2.601849	2.583469
29	1	0	1.672534	2.915602	3.174945
30	1	0	-0.047731	3.177126	2.943338
31	1	0	0.629929	1.551249	2.811037
32	6	0	1.393627	2.117721	-1.167983
33	6	0	1.475041	1.069475	-2.259991
34	1	0	2.526140	0.821241	-2.437399
35	1	0	0.972210	0.140490	-2.010975
36	1	0	1.066808	1.435917	-3.205806
37	6	0	-2.569739	1.569481	1.054871
38	6	0	-2.218979	1.502858	2.528215
39	1	0	-1.328558	0.910174	2.728919
40	1	0	-2.069666	2.495017	2.959945
41	1	0	-3.042748	1.039943	3.081054
42	7	0	0.301415	-0.694573	0.491279
43	6	0	1.715138	-0.976780	0.452445
44	6	0	-0.333242	-1.953066	0.168306
45	6	0	1.932022	-2.254321	-0.094582
46	6	0	2.796196	-0.221295	0.884894
47	6	0	0.630125	-2.846386	-0.305304
48	6	0	-1.682722	-2.391910	0.333538
49	6	0	3.215932	-2.758882	-0.268935
50	6	0	4.087663	-0.727834	0.722261

51	1	0	2.668303	0.745489	1.344079
52	6	0	0.282106	-4.106662	-0.836983
53	6	0	-2.027733	-3.665723	-0.243077
54	6	0	-2.670582	-1.733723	1.106289
55	6	0	4.302997	-1.983002	0.134761
56	1	0	3.397794	-3.741759	-0.685784
57	1	0	4.920523	-0.131750	1.068728
58	6	0	-1.032779	-4.481325	-0.850492
59	1	0	1.052846	-4.758235	-1.232238
60	6	0	-3.362235	-4.131925	-0.133662
61	6	0	-3.945324	-2.234670	1.223736
62	1	0	-2.406642	-0.836314	1.634958
63	1	0	-1.331967	-5.433743	-1.274156
64	6	0	-4.309136	-3.430316	0.571460
65	1	0	-3.614829	-5.078953	-0.599040
66	1	0	-4.673502	-1.706988	1.829009
67	1	0	-5.322069	-3.807742	0.654009
68	8	0	5.535077	-2.539754	-0.063770
69	6	0	6.682996	-1.811828	0.344827
70	1	0	7.537472	-2.435555	0.086735
71	1	0	6.763046	-0.854472	-0.182714
72	1	0	6.682979	-1.630678	1.425780

Compound 7 2-RF-CN-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.44354040 A.U. after 1 cycles
Lowest frequency = -28.5294

Zero-point correction= 0.594879
(Hartree/Particle)
Thermal correction to Energy= 0.629070
Thermal correction to Enthalpy= 0.630014
Thermal correction to Gibbs Free Energy= 0.529227
Sum of electronic and zero-point Energies= -1508.848661
Sum of electronic and thermal Energies= -1508.814470
Sum of electronic and thermal Enthalpies= -1508.813526
Sum of electronic and thermal Free Energies= -1508.914313

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.899283	-0.310656	0.179986
2	6	0	5.703329	-2.450495	-2.584754
3	1	0	5.441035	-2.959370	-3.514711
4	1	0	6.390537	-1.635803	-2.839159
5	1	0	6.249705	-3.151157	-1.949422
6	6	0	4.481087	-1.913216	-1.886902
7	6	0	3.346706	-1.542379	-2.602073
8	1	0	3.348043	-1.662956	-3.680597
9	6	0	2.163807	-0.853428	-0.560860
10	6	0	4.458981	-1.735798	-0.506734
11	1	0	5.337023	-2.008124	0.070199
12	6	0	0.576224	1.187947	3.806235
13	1	0	0.761658	2.134758	4.306442
14	6	0	0.025367	0.134706	4.529717
15	6	0	-0.108440	-1.083550	3.870992

16	1	0	-0.468975	-1.947992	4.422402
17	6	0	0.707157	-0.147509	1.766185
18	6	0	-0.391736	0.301540	5.970143
19	1	0	-1.436525	0.624255	6.039808
20	1	0	-0.303110	-0.636619	6.523488
21	1	0	0.216018	1.054656	6.477734
22	6	0	0.925672	1.067266	2.459007
23	6	0	2.206386	-1.018723	-1.991586
24	6	0	1.090217	-0.658051	-2.954077
25	1	0	0.200308	-1.271864	-2.812487
26	1	0	0.775760	0.380734	-2.861683
27	1	0	1.436086	-0.811304	-3.978064
28	6	0	1.602119	2.263401	1.826609
29	1	0	2.223412	2.777373	2.564884
30	1	0	2.249352	1.982225	0.995119
31	1	0	0.881309	2.989915	1.446246
32	6	0	0.229447	-1.245847	2.525253
33	6	0	0.123298	-2.653184	1.972038
34	1	0	-0.897340	-2.896143	1.669413
35	1	0	0.771094	-2.811849	1.108199
36	1	0	0.419051	-3.376966	2.736469
37	6	0	3.351962	-1.218650	0.164157
38	6	0	3.524560	-1.080315	1.662700
39	1	0	3.355322	-0.060949	2.008227
40	1	0	2.837427	-1.715569	2.222147
41	1	0	4.541572	-1.363545	1.939873
42	7	0	-0.362379	0.017162	-0.616672
43	6	0	-1.398774	-0.936232	-0.706274
44	6	0	-0.985787	1.268796	-0.701961
45	6	0	-2.654395	-0.290393	-0.731190
46	6	0	-1.322834	-2.324672	-0.862196
47	6	0	-2.383454	1.121614	-0.716455
48	6	0	-0.388504	2.539473	-0.965826
49	6	0	-3.842203	-1.028680	-0.848510
50	6	0	-2.498028	-3.046975	-0.985546
51	1	0	-0.371154	-2.837949	-0.904337
52	6	0	-3.229213	2.252053	-0.787515
53	6	0	-1.267355	3.673422	-1.023919
54	6	0	0.980326	2.732457	-1.276191
55	6	0	-3.755893	-2.410978	-0.963194
56	1	0	-4.795400	-0.517773	-0.869826
57	1	0	-2.477202	-4.121816	-1.117023
58	6	0	-2.678137	3.500393	-0.894533
59	1	0	-4.306113	2.126246	-0.760357
60	6	0	-0.710136	4.950240	-1.281963
61	6	0	1.479993	3.983077	-1.561202
62	1	0	1.646493	1.878910	-1.298539
63	1	0	-3.311456	4.379578	-0.939641
64	6	0	0.631930	5.108855	-1.540672
65	1	0	-1.374143	5.808407	-1.299844
66	1	0	2.529646	4.101664	-1.805363
67	1	0	1.034418	6.093201	-1.751622
68	8	0	-4.829172	-3.251972	-1.087747
69	6	0	-6.127978	-2.683972	-1.082283
70	1	0	-6.272286	-1.997367	-1.925010
71	1	0	-6.820443	-3.519044	-1.178530
72	1	0	-6.331716	-2.151999	-0.145409

Compound 7 2-RF-CN-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.44247192 A.U. after 1 cycles
Lowest frequency = -28.3566

Zero-point correction= 0.594805
(Hartree/Particle)
Thermal correction to Energy= 0.629023
Thermal correction to Enthalpy= 0.629967
Thermal correction to Gibbs Free Energy= 0.529122
Sum of electronic and zero-point Energies= -1508.847667
Sum of electronic and thermal Energies= -1508.813449
Sum of electronic and thermal Enthalpies= -1508.812505
Sum of electronic and thermal Free Energies= -1508.913350

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.806926	-0.365514	0.216641
2	6	0	5.291893	-3.356634	-2.283223
3	1	0	4.975692	-3.879307	-3.188422
4	1	0	6.094839	-2.666811	-2.566241
5	1	0	5.718959	-4.087735	-1.593085
6	6	0	4.148091	-2.606606	-1.651707
7	6	0	3.088392	-2.129514	-2.416647
8	1	0	3.087964	-2.322953	-3.484526
9	6	0	1.987174	-1.140601	-0.454485
10	6	0	4.130820	-2.334964	-0.286878
11	1	0	4.952128	-2.689351	0.327828
12	6	0	0.665264	1.418638	3.722877
13	1	0	0.983558	2.360958	4.160771
14	6	0	-0.045806	0.513111	4.504273
15	6	0	-0.351572	-0.715935	3.928090
16	1	0	-0.844210	-1.475652	4.529314
17	6	0	0.620754	-0.063872	1.783107
18	6	0	-0.451980	0.842647	5.919533
19	1	0	-1.439728	1.316316	5.942355
20	1	0	-0.507179	-0.055659	6.539400
21	1	0	0.252215	1.535583	6.386549
22	6	0	1.009515	1.151560	2.395541
23	6	0	2.025633	-1.409335	-1.869477
24	6	0	0.985152	-0.963150	-2.879706
25	1	0	0.011219	-1.422404	-2.709237
26	1	0	0.831046	0.115264	-2.874021
27	1	0	1.312837	-1.247053	-3.881580
28	6	0	1.864840	2.185908	1.697803
29	1	0	2.546405	2.654138	2.412951
30	1	0	2.473402	1.753041	0.903025
31	1	0	1.265292	2.981679	1.251377
32	6	0	-0.024914	-1.022157	2.604874
33	6	0	-0.333352	-2.434184	2.147465
34	1	0	-1.375447	-2.543235	1.840131
35	1	0	0.292852	-2.747631	1.310405
36	1	0	-0.157180	-3.137476	2.966111
37	6	0	3.099371	-1.621616	0.321714
38	6	0	3.267286	-1.408791	1.812038
39	1	0	3.245467	-0.354530	2.086305
40	1	0	2.485045	-1.896884	2.393883

41	1	0	4.226767	-1.818592	2.132718
42	7	0	-0.378383	0.090224	-0.631533
43	6	0	-1.547026	-0.701465	-0.676379
44	6	0	-0.805746	1.413396	-0.813432
45	6	0	-2.693724	0.127911	-0.765504
46	6	0	-1.683393	-2.085666	-0.735294
47	6	0	-2.208020	1.481132	-0.841330
48	6	0	-0.019455	2.557083	-1.151641
49	6	0	-3.967770	-0.430828	-0.850159
50	6	0	-2.960404	-2.638931	-0.827031
51	1	0	-0.821373	-2.739758	-0.725075
52	6	0	-2.871534	2.717673	-1.004946
53	6	0	-0.714447	3.804489	-1.302948
54	6	0	1.365722	2.517504	-1.446878
55	6	0	-4.100486	-1.817512	-0.868515
56	1	0	-4.859087	0.180436	-0.923879
57	1	0	-3.056130	-3.714747	-0.880376
58	6	0	-2.135597	3.857600	-1.187770
59	1	0	-3.955103	2.756691	-0.988702
60	6	0	0.034115	4.960626	-1.636353
61	6	0	2.053257	3.654442	-1.806238
62	1	0	1.893576	1.573213	-1.397133
63	1	0	-2.627034	4.817192	-1.304676
64	6	0	1.386691	4.894616	-1.879078
65	1	0	-0.490476	5.906427	-1.725109
66	1	0	3.110943	3.595105	-2.036898
67	1	0	1.936867	5.789152	-2.148502
68	8	0	-5.384045	-2.290289	-0.954010
69	6	0	-5.588868	-3.692079	-0.995621
70	1	0	-5.208650	-4.184744	-0.092767
71	1	0	-6.667276	-3.834057	-1.052031
72	1	0	-5.121043	-4.145291	-1.877731

Compound 7 3-RF-TSa

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.40327759 A.U. after 1 cycles
Lowest frequency = -25.7394

Zero-point correction= 0.595111
(Hartree/Particle)
Thermal correction to Energy= 0.629126
Thermal correction to Enthalpy= 0.630070
Thermal correction to Gibbs Free Energy= 0.529627
Sum of electronic and zero-point Energies= -1508.808167
Sum of electronic and thermal Energies= -1508.774152
Sum of electronic and thermal Enthalpies= -1508.773208
Sum of electronic and thermal Free Energies= -1508.873651

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.891392	-0.193988	0.240826
2	6	0	0.682269	1.823703	5.676576
3	1	0	0.051205	1.388819	6.457449
4	1	0	1.712026	1.514463	5.884274
5	1	0	0.635636	2.910497	5.771291

6	6	0	0.246414	1.372180	4.305198
7	6	0	0.080964	0.022684	4.004542
8	1	0	0.260898	-0.718773	4.777594
9	6	0	-0.553573	0.496880	1.670621
10	6	0	-0.008848	2.267612	3.281976
11	1	0	0.088043	3.332336	3.476568
12	6	0	-4.615811	-0.414735	-0.799890
13	1	0	-5.395300	0.326538	-0.949744
14	6	0	-4.876443	-1.744610	-1.111316
15	6	0	-3.875059	-2.653612	-0.811692
16	1	0	-4.064383	-3.712741	-0.964208
17	6	0	-2.310426	-0.907979	-0.078240
18	6	0	-6.187680	-2.171777	-1.721019
19	1	0	-6.186333	-2.009446	-2.804520
20	1	0	-6.381650	-3.232701	-1.548279
21	1	0	-7.024042	-1.601195	-1.308813
22	6	0	-3.392689	0.010035	-0.280930
23	6	0	-0.313699	-0.419861	2.744783
24	6	0	-0.447859	-1.915509	2.592872
25	1	0	-1.458308	-2.196874	2.297633
26	1	0	0.251874	-2.314385	1.854929
27	1	0	-0.230770	-2.413729	3.539310
28	6	0	-3.321082	1.481389	0.065921
29	1	0	-2.904812	1.642138	1.059275
30	1	0	-2.725723	2.054880	-0.646684
31	1	0	-4.323980	1.911862	0.054734
32	6	0	-2.628402	-2.279633	-0.290864
33	6	0	-1.792723	-3.480564	0.118652
34	1	0	-1.755084	-4.217068	-0.689303
35	1	0	-0.778691	-3.255514	0.411275
36	1	0	-2.274542	-3.975129	0.969231
37	6	0	-0.393957	1.870582	1.992382
38	6	0	-0.651395	3.044163	1.071531
39	1	0	-0.990320	2.772176	0.084685
40	1	0	-1.410268	3.700115	1.510950
41	1	0	0.257668	3.638806	0.951032
42	7	0	0.181386	-0.167399	-0.853012
43	6	0	1.093930	-1.283939	-0.837761
44	6	0	1.047823	0.951686	-0.982600
45	6	0	2.413813	-0.832550	-0.615352
46	6	0	0.878097	-2.614520	-1.184247
47	6	0	2.375706	0.610434	-0.719366
48	6	0	0.732655	2.191934	-1.598131
49	6	0	3.487412	-1.729372	-0.562657
50	6	0	1.942115	-3.505475	-1.141404
51	1	0	-0.083596	-2.941005	-1.543790
52	6	0	3.396664	1.585754	-0.783902
53	6	0	1.773228	3.176705	-1.658565
54	6	0	-0.496229	2.453283	-2.255854
55	6	0	3.235641	-3.080528	-0.791070
56	1	0	4.491119	-1.361067	-0.398753
57	1	0	1.806126	-4.544035	-1.416818
58	6	0	3.082533	2.856176	-1.194466
59	1	0	4.418559	1.325880	-0.531087
60	6	0	1.482585	4.429510	-2.255211
61	6	0	-0.727541	3.667039	-2.859775
62	1	0	-1.237652	1.665030	-2.305139
63	1	0	3.850130	3.620945	-1.244287
64	6	0	0.259009	4.677645	-2.832304
65	1	0	2.259358	5.187096	-2.275070

66	1	0	-1.665771	3.845489	-3.373087
67	1	0	0.060905	5.636466	-3.297764
68	8	0	4.185275	-4.062777	-0.765029
69	6	0	5.521057	-3.698223	-0.455765
70	1	0	6.092755	-4.624956	-0.463274
71	1	0	5.936143	-3.013238	-1.204379
72	1	0	5.592848	-3.236756	0.535922

Compound 7 3-RF-TSb

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1509.40276505 A.U. after 1 cycles
Lowest frequency = -25.4911

Zero-point correction= 0.595108
(Hartree/Particle)
Thermal correction to Energy= 0.629121
Thermal correction to Enthalpy= 0.630065
Thermal correction to Gibbs Free Energy= 0.529691
Sum of electronic and zero-point Energies= -1508.807657
Sum of electronic and thermal Energies= -1508.773644
Sum of electronic and thermal Enthalpies= -1508.772700
Sum of electronic and thermal Free Energies= -1508.873074

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.799623	-0.313248	0.250944
2	6	0	0.147017	2.215780	5.616616
3	1	0	-0.385469	1.678234	6.406894
4	1	0	1.215404	2.157504	5.849745
5	1	0	-0.147195	3.266180	5.665323
6	6	0	-0.144528	1.625437	4.259807
7	6	0	-0.006428	0.261153	4.017744
8	1	0	0.307866	-0.391777	4.826839
9	6	0	-0.662461	0.492386	1.653338
10	6	0	-0.558617	2.402329	3.192540
11	1	0	-0.699316	3.469654	3.340519
12	6	0	-4.357960	-1.387519	-0.840056
13	1	0	-5.277164	-0.842455	-1.033755
14	6	0	-4.312294	-2.752791	-1.099673
15	6	0	-3.143458	-3.406972	-0.746190
16	1	0	-3.091729	-4.486765	-0.857292
17	6	0	-2.019684	-1.333178	-0.060471
18	6	0	-5.481985	-3.480881	-1.712302
19	1	0	-5.487469	-3.365093	-2.801758
20	1	0	-5.444119	-4.550884	-1.496121
21	1	0	-6.433371	-3.091844	-1.340214
22	6	0	-3.271492	-0.684430	-0.319222
23	6	0	-0.260646	-0.306670	2.772181
24	6	0	-0.063329	-1.800635	2.685018
25	1	0	-0.979229	-2.306635	2.380825
26	1	0	0.728809	-2.065844	1.981031
27	1	0	0.227384	-2.201864	3.657447
28	6	0	-3.533267	0.778679	-0.034135
29	1	0	-3.186432	1.065216	0.957554
30	1	0	-3.061135	1.441418	-0.761510

31	1	0	-4.605659	0.976690	-0.078998
32	6	0	-2.023079	-2.747873	-0.221537
33	6	0	-0.953051	-3.717320	0.250887
34	1	0	-0.731590	-4.454848	-0.526258
35	1	0	-0.022935	-3.260372	0.552149
36	1	0	-1.335138	-4.276517	1.112030
37	6	0	-0.812691	1.879707	1.915351
38	6	0	-1.291437	2.931178	0.937171
39	1	0	-1.541007	2.551410	-0.040789
40	1	0	-2.182723	3.428041	1.334584
41	1	0	-0.526867	3.700445	0.802236
42	7	0	0.270470	-0.098409	-0.822248
43	6	0	1.408847	-0.982317	-0.743902
44	6	0	0.871533	1.180204	-0.990281
45	6	0	2.591629	-0.233314	-0.511089
46	6	0	1.508043	-2.332582	-1.032827
47	6	0	2.232075	1.159689	-0.682715
48	6	0	0.305187	2.289578	-1.671797
49	6	0	3.824661	-0.864978	-0.396553
50	6	0	2.748118	-2.970502	-0.926144
51	1	0	0.655888	-2.882603	-1.396275
52	6	0	3.011040	2.334670	-0.775449
53	6	0	1.100701	3.479419	-1.760999
54	6	0	-0.932645	2.239338	-2.362021
55	6	0	3.895930	-2.249389	-0.568613
56	1	0	4.740659	-0.311378	-0.229816
57	1	0	2.810512	-4.023624	-1.163664
58	6	0	2.433518	3.482584	-1.255827
59	1	0	4.056879	2.320517	-0.490138
60	6	0	0.554417	4.607463	-2.424014
61	6	0	-1.412032	3.342370	-3.028846
62	1	0	-1.478076	1.303646	-2.384220
63	1	0	3.012070	4.397136	-1.329081
64	6	0	-0.676680	4.548614	-3.034251
65	1	0	1.142249	5.518648	-2.467038
66	1	0	-2.351963	3.283397	-3.566110
67	1	0	-1.070752	5.417068	-3.549783
68	8	0	5.139953	-2.799362	-0.429354
69	6	0	5.294337	-4.191936	-0.652266
70	1	0	6.346059	-4.407568	-0.469955
71	1	0	4.680418	-4.781881	0.038173
72	1	0	5.044614	-4.466997	-1.683583

Compound 8 GS1

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1732.06260351 A.U. after 1 cycles
Lowest frequency = 7.7978

Zero-point correction= 0.566817
(Hartree/Particle)
Thermal correction to Energy= 0.603487
Thermal correction to Enthalpy= 0.604431
Thermal correction to Gibbs Free Energy= 0.494559
Sum of electronic and zero-point Energies= -1731.495786
Sum of electronic and thermal Energies= -1731.459117
Sum of electronic and thermal Enthalpies= -1731.458173
Sum of electronic and thermal Free Energies= -1731.568044

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.810114	0.719357	-0.026936
2	6	0	0.764748	3.000038	2.003983
3	1	0	0.168291	2.183192	2.418460
4	1	0	1.814244	2.736915	2.154518
5	1	0	0.553559	3.892960	2.595693
6	6	0	3.517432	1.870433	-0.906242
7	1	0	4.567363	1.986815	-1.182871
8	1	0	2.991977	1.470259	-1.776381
9	1	0	3.107047	2.867149	-0.726322
10	6	0	0.905933	-0.994169	2.500768
11	1	0	0.026491	-0.355845	2.402896
12	1	0	0.668642	-1.946206	2.017814
13	1	0	1.048058	-1.195745	3.564378
14	6	0	5.837295	-0.296178	2.961318
15	1	0	6.382406	-1.138346	2.520792
16	1	0	6.502883	0.570297	2.936577
17	1	0	5.639268	-0.544890	4.006150
18	6	0	4.559054	-0.031545	2.205453
19	6	0	4.556557	0.744552	1.045981
20	1	0	5.489990	1.179791	0.700633
21	6	0	3.392146	0.987524	0.319907
22	6	0	2.159797	0.408813	0.730469
23	6	0	2.158096	-0.371416	1.916117
24	6	0	3.345380	-0.565040	2.627343
25	1	0	3.315561	-1.151090	3.541325
26	6	0	0.083297	2.525942	-1.752374
27	6	0	-0.183935	3.851106	-2.101137
28	1	0	-0.426720	4.081949	-3.134383
29	6	0	-0.159275	4.883038	-1.164394
30	6	0	0.150026	4.554669	0.155464
31	1	0	0.156488	5.338661	0.907211
32	6	0	0.452937	3.248182	0.542114
33	6	0	0.422411	2.200683	-0.413789
34	6	0	-0.005632	1.484122	-2.850307
35	1	0	-0.915149	0.883799	-2.758514
36	1	0	-0.026922	1.965787	-3.829836
37	1	0	0.835340	0.787485	-2.844719
38	6	0	-0.434905	6.310275	-1.568462
39	1	0	-0.887348	6.876116	-0.750797
40	1	0	0.492494	6.823312	-1.846518
41	1	0	-1.105503	6.359047	-2.429378
42	7	0	-0.145551	-0.355060	-0.340952
43	6	0	-1.538134	-0.232171	-0.079524
44	6	0	0.094831	-1.737379	-0.564307
45	6	0	-2.120835	-1.517767	-0.036683
46	6	0	-2.319923	0.898714	0.182716
47	6	0	-1.079351	-2.463645	-0.342408
48	6	0	1.259248	-2.391764	-1.077879
49	6	0	-3.476925	-1.682102	0.250324
50	6	0	-3.668590	0.723404	0.458214
51	1	0	-1.903769	1.893292	0.164800
52	6	0	-1.115234	-3.871399	-0.454095
53	6	0	1.209848	-3.826502	-1.161069
54	6	0	2.413987	-1.741966	-1.577511
55	6	0	-4.247856	-0.554896	0.494822

56	1	0	-3.921816	-2.668020	0.286224
57	1	0	-4.284206	1.592553	0.654705
58	6	0	0.021930	-4.536000	-0.818828
59	1	0	-2.033425	-4.409824	-0.249262
60	6	0	2.344561	-4.526316	-1.641532
61	6	0	3.486306	-2.452239	-2.065352
62	1	0	2.455840	-0.665412	-1.587217
63	1	0	0.027362	-5.617599	-0.896108
64	6	0	3.465020	-3.861017	-2.077301
65	1	0	2.302111	-5.609775	-1.678995
66	1	0	4.351255	-1.921825	-2.446809
67	1	0	4.319836	-4.413630	-2.450094
68	6	0	-5.717948	-0.675784	0.768218
69	9	0	-6.095649	0.057064	1.842856
70	9	0	-6.465943	-0.232534	-0.272358
71	9	0	-6.098089	-1.950724	1.004755

Compound 8 1-RF-C-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1731.99420888 A.U. after 1 cycles
Lowest frequency = -26.3633

Zero-point correction= 0.566548
(Hartree/Particle)
Thermal correction to Energy= 0.601655
Thermal correction to Enthalpy= 0.602599
Thermal correction to Gibbs Free Energy= 0.498913
Sum of electronic and zero-point Energies= -1731.427661
Sum of electronic and thermal Energies= -1731.392554
Sum of electronic and thermal Enthalpies= -1731.391610
Sum of electronic and thermal Free Energies= -1731.495296

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.608445	1.155561	-0.296121
2	6	0	3.668070	1.600005	4.618737
3	1	0	3.488460	2.511186	5.193769
4	1	0	3.208463	0.769900	5.166932
5	1	0	4.744876	1.414908	4.594092
6	6	0	3.092007	1.698278	3.231048
7	6	0	2.066574	2.584136	2.922764
8	1	0	1.752135	3.307950	3.669312
9	6	0	1.785133	1.641446	0.670156
10	6	0	3.626063	0.978297	2.162499
11	1	0	4.562006	0.442486	2.295003
12	6	0	-1.479262	3.637158	-2.405291
13	1	0	-1.380623	4.109530	-3.378878
14	6	0	-2.602464	3.912416	-1.622865
15	6	0	-2.694835	3.287515	-0.381565
16	1	0	-3.560691	3.483980	0.245475
17	6	0	-0.574602	2.143295	-0.705439
18	6	0	-3.661760	4.878321	-2.096551
19	1	0	-4.611842	4.710505	-1.584610
20	1	0	-3.363245	5.914765	-1.904141
21	1	0	-3.834643	4.785270	-3.171832

22	6	0	-0.476492	2.770520	-1.969298
23	6	0	1.454424	2.627695	1.663708
24	6	0	0.596918	3.862040	1.436878
25	1	0	0.451689	4.091432	0.386567
26	1	0	-0.383205	3.808203	1.911561
27	1	0	1.123012	4.706047	1.892381
28	6	0	0.706848	2.506085	-2.876833
29	1	0	0.718470	3.198463	-3.720961
30	1	0	1.657134	2.615172	-2.344749
31	1	0	0.674415	1.490232	-3.284626
32	6	0	-1.709645	2.414102	0.088381
33	6	0	-1.932805	1.783344	1.449099
34	1	0	-2.735413	1.042238	1.409258
35	1	0	-1.043844	1.282520	1.833798
36	1	0	-2.232854	2.538032	2.181760
37	6	0	3.042546	0.993785	0.900022
38	6	0	3.934614	0.557677	-0.236483
39	1	0	4.313995	-0.459255	-0.132035
40	1	0	3.458305	0.661491	-1.203997
41	1	0	4.801153	1.228720	-0.242244
42	7	0	0.352581	-0.267586	-0.696256
43	6	0	-0.970494	-0.778143	-0.424140
44	6	0	1.187351	-1.412253	-0.465580
45	6	0	-0.867160	-1.953250	0.356588
46	6	0	-2.209836	-0.364118	-0.900094
47	6	0	0.530134	-2.346872	0.334482
48	6	0	2.322243	-1.819569	-1.216010
49	6	0	-2.008330	-2.621773	0.790347
50	6	0	-3.346070	-1.056306	-0.487876
51	1	0	-2.301773	0.459466	-1.590025
52	6	0	1.172653	-3.536745	0.740230
53	6	0	2.974623	-3.032438	-0.808902
54	6	0	2.734154	-1.202739	-2.425529
55	1	0	-1.935302	-3.517810	1.393141
56	1	0	-4.315789	-0.755830	-0.864178
57	6	0	2.410291	-3.830236	0.226565
58	1	0	0.677649	-4.222444	1.418323
59	6	0	4.114338	-3.465394	-1.533977
60	6	0	3.801718	-1.690133	-3.139331
61	1	0	2.176564	-0.349815	-2.791666
62	1	0	2.928727	-4.734368	0.526396
63	6	0	4.526198	-2.808368	-2.668870
64	1	0	4.631787	-4.358914	-1.200588
65	1	0	4.088984	-1.217908	-4.071984
66	1	0	5.383090	-3.168698	-3.226492
67	6	0	-3.253058	-2.150497	0.379578
68	6	0	-4.509133	-2.808871	0.868861
69	9	0	-4.298815	-4.076542	1.288902
70	9	0	-5.467086	-2.858844	-0.085080
71	9	0	-5.051624	-2.140458	1.918155

Compound 8 1-RF-C1-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1731.98809746 A.U. after 1 cycles
Lowest frequency = -34.6072

Zero-point correction= 0.566304
(Hartree/Particle)

Thermal correction to Energy= 0.601468
Thermal correction to Enthalpy= 0.602412
Thermal correction to Gibbs Free Energy= 0.498432
Sum of electronic and zero-point Energies= -1731.421793
Sum of electronic and thermal Energies= -1731.386629
Sum of electronic and thermal Enthalpies= -1731.385685
Sum of electronic and thermal Free Energies= -1731.489665

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.236412	4.806537	3.153911
2	1	0	0.483619	5.489168	3.554345
3	1	0	1.516389	4.117350	3.958549
4	1	0	2.127472	5.385933	2.899775
5	6	0	0.715574	4.043143	1.965691
6	6	0	-0.644519	3.870989	1.740762
7	1	0	-1.355769	4.402502	2.366623
8	6	0	-0.245191	2.297638	-0.108957
9	6	0	1.569169	3.560047	0.973012
10	1	0	2.612523	3.863334	0.975639
11	6	0	-4.143682	0.454891	-2.354087
12	1	0	-4.478636	0.498210	-3.387031
13	6	0	-5.077869	0.220093	-1.340513
14	6	0	-4.611711	0.167709	-0.031595
15	1	0	-5.316803	-0.023900	0.772903
16	6	0	-2.327281	0.594582	-0.734793
17	6	0	-6.543082	0.050608	-1.663327
18	1	0	-7.092651	-0.360850	-0.814170
19	1	0	-7.003603	1.010154	-1.922292
20	1	0	-6.688880	-0.617564	-2.516762
21	6	0	-2.791852	0.640913	-2.073695
22	6	0	-1.144186	3.084529	0.695507
23	6	0	-2.623621	3.295669	0.417850
24	1	0	-2.924352	2.969592	-0.571931
25	1	0	-3.278925	2.818058	1.146833
26	1	0	-2.806602	4.372615	0.483789
27	6	0	-1.832377	0.896277	-3.217903
28	1	0	-2.360083	0.933207	-4.172891
29	1	0	-1.303342	1.847315	-3.094669
30	1	0	-1.074244	0.109169	-3.287862
31	6	0	-3.261139	0.346578	0.287856
32	6	0	-2.876397	0.254802	1.749559
33	1	0	-2.990450	-0.769315	2.114089
34	1	0	-1.845835	0.557765	1.936159
35	1	0	-3.525731	0.886348	2.363569
36	6	0	1.110297	2.772731	-0.077358
37	6	0	2.028229	2.717106	-1.279468
38	1	0	2.997153	2.265414	-1.067708
39	1	0	1.574874	2.215888	-2.127948
40	1	0	2.211079	3.751957	-1.589558
41	5	0	-0.772047	0.852356	-0.541918
42	7	0	0.082277	-0.393256	-0.597898
43	6	0	1.496204	-0.413368	-0.741703
44	6	0	-0.160549	-1.421264	0.399242
45	6	0	2.099562	-1.069464	0.351924
46	6	0	2.239456	-0.125920	-1.879603
47	6	0	1.019555	-1.665979	1.110968

48	6	0	-1.273754	-2.295649	0.570613
49	6	0	3.480336	-1.250612	0.393466
50	6	0	3.613247	-0.342570	-1.855815
51	1	0	1.759227	0.223487	-2.783474
52	6	0	1.044587	-2.534726	2.223179
53	6	0	-1.238761	-3.174797	1.710450
54	6	0	-2.318398	-2.468687	-0.373704
55	1	0	3.956480	-1.747465	1.228804
56	6	0	4.234332	-0.857846	-0.710451
57	1	0	4.206958	-0.137178	-2.737424
58	6	0	-0.091642	-3.223550	2.552074
59	1	0	1.958091	-2.662173	2.792766
60	6	0	-2.324152	-4.061614	1.923357
61	6	0	-3.322714	-3.383031	-0.161399
62	1	0	-2.308640	-1.885222	-1.281473
63	1	0	-0.105249	-3.888038	3.408895
64	6	0	-3.350370	-4.161281	1.014976
65	1	0	-2.307557	-4.694700	2.804345
66	1	0	-4.099140	-3.506093	-0.907414
67	1	0	-4.161549	-4.860940	1.182344
68	6	0	5.728857	-0.995271	-0.690336
69	9	0	6.335575	0.178709	-0.380757
70	9	0	6.154367	-1.899296	0.219307
71	9	0	6.224840	-1.373668	-1.890781

Compound 8 1-RF-N-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1731.97331079 A.U. after 1 cycles
Lowest frequency = -70.0116

Zero-point correction= 0.567407
(Hartree/Particle)
Thermal correction to Energy= 0.602010
Thermal correction to Enthalpy= 0.602955
Thermal correction to Gibbs Free Energy= 0.500591
Sum of electronic and zero-point Energies= -1731.405904
Sum of electronic and thermal Energies= -1731.371300
Sum of electronic and thermal Enthalpies= -1731.370356
Sum of electronic and thermal Free Energies= -1731.472720

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.837668	1.153345	-0.237004
2	6	0	-5.726780	-1.113483	-2.306098
3	1	0	-5.640905	-1.943987	-3.010873
4	1	0	-6.071061	-1.530390	-1.353010
5	1	0	-6.500937	-0.431928	-2.665912
6	6	0	-4.410892	-0.410270	-2.117541
7	6	0	-3.195720	-1.081358	-2.231062
8	1	0	-3.185565	-2.103827	-2.596878
9	6	0	-1.934188	0.860658	-1.372792
10	6	0	-4.329671	0.967847	-1.931457
11	1	0	-5.217481	1.575706	-2.084140
12	6	0	0.868263	4.551871	0.647119
13	1	0	0.839949	5.597730	0.353517

14	6	0	1.955043	4.082044	1.378436
15	6	0	1.793170	2.835015	1.978164
16	1	0	2.510956	2.508847	2.724917
17	6	0	-0.236924	2.349657	0.655066
18	6	0	3.184785	4.918435	1.606486
19	1	0	3.605345	4.749823	2.600695
20	1	0	3.961935	4.660729	0.878205
21	1	0	2.973095	5.984320	1.496163
22	6	0	-0.246666	3.758953	0.372632
23	6	0	-1.979234	-0.475516	-1.925816
24	6	0	-0.756469	-1.249957	-2.380865
25	1	0	0.126508	-0.624888	-2.476865
26	1	0	-0.514595	-2.100496	-1.740713
27	1	0	-0.976306	-1.651605	-3.374337
28	6	0	-1.490614	4.542545	0.027425
29	1	0	-1.582293	5.337493	0.773915
30	1	0	-1.458559	5.032419	-0.947852
31	1	0	-2.383795	3.935988	0.104370
32	6	0	0.720707	1.997094	1.681663
33	6	0	0.580576	0.808112	2.614187
34	1	0	-0.431313	0.414196	2.646633
35	1	0	1.265745	-0.010502	2.382697
36	1	0	0.825509	1.151144	3.623551
37	6	0	-3.122286	1.615243	-1.672849
38	6	0	-3.120170	3.087604	-2.014028
39	1	0	-3.745665	3.704752	-1.365690
40	1	0	-2.117177	3.492987	-2.052045
41	1	0	-3.533702	3.175203	-3.023676
42	7	0	-0.079869	-0.136146	0.102259
43	6	0	1.258893	-0.324151	-0.232965
44	6	0	-0.525483	-1.322889	0.698605
45	6	0	1.663869	-1.635078	0.118317
46	6	0	2.143591	0.548729	-0.881247
47	6	0	0.518582	-2.264508	0.717715
48	6	0	-1.781769	-1.613031	1.319768
49	6	0	2.964366	-2.067334	-0.157590
50	6	0	3.427590	0.104976	-1.145886
51	1	0	1.842869	1.548539	-1.166409
52	6	0	0.334072	-3.552670	1.270882
53	6	0	-1.942123	-2.930790	1.868861
54	6	0	-2.847396	-0.691783	1.471605
55	1	0	3.286625	-3.066792	0.104892
56	1	0	4.128030	0.764037	-1.644162
57	6	0	-0.876379	-3.879161	1.815304
58	1	0	1.148334	-4.268663	1.260644
59	6	0	-3.169162	-3.265144	2.492547
60	6	0	-4.018956	-1.046643	2.102047
61	1	0	-2.748979	0.313774	1.085482
62	1	0	-1.041632	-4.863027	2.240197
63	6	0	-4.189345	-2.350166	2.608345
64	1	0	-3.285472	-4.266169	2.894844
65	1	0	-4.813498	-0.316789	2.207833
66	1	0	-5.117479	-2.625210	3.096615
67	6	0	3.839917	-1.193452	-0.785509
68	6	0	5.252186	-1.600734	-1.076269
69	9	0	5.594196	-1.367939	-2.367744
70	9	0	6.147658	-0.911050	-0.323870
71	9	0	5.476662	-2.912247	-0.839788

Compound 8 2-RF-CC-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1732.03573310 A.U. after 1 cycles
Lowest frequency = -50.0481

Zero-point correction= 0.567276
(Hartree/Particle)
Thermal correction to Energy= 0.602620
Thermal correction to Enthalpy= 0.603565
Thermal correction to Gibbs Free Energy= 0.498764
Sum of electronic and zero-point Energies= -1731.468457
Sum of electronic and thermal Energies= -1731.433113
Sum of electronic and thermal Enthalpies= -1731.432169
Sum of electronic and thermal Free Energies= -1731.536969

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.743235	0.658319	0.291859
2	6	0	-6.541423	1.309273	-0.928222
3	1	0	-6.898200	0.656432	-1.728658
4	1	0	-7.190693	1.169865	-0.060560
5	1	0	-6.668684	2.342730	-1.269240
6	6	0	-5.098604	1.028319	-0.589351
7	6	0	-4.197192	0.590898	-1.554732
8	1	0	-4.556076	0.391497	-2.560731
9	6	0	-2.328334	0.617884	0.021269
10	6	0	-4.611943	1.172770	0.704983
11	1	0	-5.300733	1.431224	1.505305
12	6	0	0.312667	4.422739	0.827542
13	1	0	0.314234	5.158258	1.627798
14	6	0	0.698135	4.812624	-0.452355
15	6	0	0.806388	3.809063	-1.408143
16	1	0	1.196380	4.054360	-2.392621
17	6	0	-0.061837	2.111175	0.123810
18	6	0	1.016661	6.251026	-0.776048
19	1	0	1.745313	6.326645	-1.586640
20	1	0	0.116224	6.787992	-1.094484
21	1	0	1.418730	6.777214	0.093262
22	6	0	-0.048499	3.108757	1.131554
23	6	0	-2.844964	0.376782	-1.278512
24	6	0	-2.014913	-0.161543	-2.424351
25	1	0	-1.629596	0.640597	-3.057897
26	1	0	-1.171494	-0.763065	-2.087646
27	1	0	-2.632705	-0.803251	-3.056604
28	6	0	-0.287195	2.813493	2.598956
29	1	0	0.461769	3.334094	3.202246
30	1	0	-1.264911	3.159621	2.939983
31	1	0	-0.203133	1.752542	2.832886
32	6	0	0.467439	2.479671	-1.140289
33	6	0	0.823669	1.484609	-2.227203
34	1	0	1.904800	1.512042	-2.395140
35	1	0	0.569810	0.458194	-1.981430
36	1	0	0.345090	1.733926	-3.177956
37	6	0	-3.269156	0.960808	1.024381
38	6	0	-2.938620	0.990204	2.503572
39	1	0	-1.932560	0.638537	2.724606

40	1	0	-3.048262	1.990143	2.928899
41	1	0	-3.631022	0.339637	3.047341
42	7	0	0.086187	-0.515055	0.523537
43	6	0	1.517894	-0.433106	0.502249
44	6	0	-0.212930	-1.893046	0.196009
45	6	0	2.054266	-1.616948	-0.034034
46	6	0	2.363372	0.579721	0.951989
47	6	0	0.948961	-2.518388	-0.259370
48	6	0	-1.413658	-2.652642	0.344914
49	6	0	3.430941	-1.777081	-0.186334
50	6	0	3.735744	0.410332	0.810163
51	1	0	1.982475	1.478519	1.407767
52	6	0	0.935594	-3.826758	-0.789773
53	6	0	-1.420804	-3.972385	-0.230945
54	6	0	-2.545398	-2.260397	1.100278
55	1	0	3.845062	-2.687974	-0.598527
56	1	0	4.404928	1.182551	1.168034
57	6	0	-0.244601	-4.515572	-0.819822
58	1	0	1.849612	-4.267401	-1.170565
59	6	0	-2.597988	-4.756836	-0.138857
60	6	0	-3.656348	-3.063791	1.201408
61	1	0	-2.522115	-1.325135	1.628694
62	1	0	-0.291109	-5.512994	-1.242681
63	6	0	-3.700364	-4.312680	0.549374
64	1	0	-2.599368	-5.737345	-0.603137
65	1	0	-4.502164	-2.734337	1.793788
66	1	0	-4.588144	-4.930789	0.619223
67	6	0	4.268122	-0.750464	0.232701
68	6	0	5.754410	-0.859342	0.050501
69	9	0	6.186377	-0.136245	-1.011969
70	9	0	6.156909	-2.132257	-0.158547
71	9	0	6.433654	-0.397671	1.125710

Compound 8 2-RF-CN-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1732.03327168 A.U. after 1 cycles
Lowest frequency = -27.4288

Zero-point correction= 0.567331
(Hartree/Particle)
Thermal correction to Energy= 0.602560
Thermal correction to Enthalpy= 0.603504
Thermal correction to Gibbs Free Energy= 0.498703
Sum of electronic and zero-point Energies= -1731.465941
Sum of electronic and thermal Energies= -1731.430712
Sum of electronic and thermal Enthalpies= -1731.429768
Sum of electronic and thermal Free Energies= -1731.534569

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.101922	-0.475478	0.217850
2	6	0	4.538624	-4.533302	-2.423072
3	1	0	4.021772	-5.023007	-3.251041
4	1	0	5.439487	-4.062059	-2.831765
5	1	0	4.863671	-5.299714	-1.716123

6	6	0	3.661616	-3.506131	-1.756436
7	6	0	2.674384	-2.830496	-2.467584
8	1	0	2.532727	-3.068607	-3.516783
9	6	0	2.012407	-1.521294	-0.495846
10	6	0	3.833696	-3.172001	-0.416295
11	1	0	4.605700	-3.678233	0.154206
12	6	0	1.666349	1.470071	3.592091
13	1	0	2.222311	2.336555	3.939883
14	6	0	0.841126	0.791177	4.483238
15	6	0	0.223842	-0.365690	4.017583
16	1	0	-0.370087	-0.963151	4.704137
17	6	0	1.128190	-0.060977	1.768003
18	6	0	0.639753	1.276794	5.897313
19	1	0	-0.216114	1.958126	5.957708
20	1	0	0.444317	0.447252	6.581172
21	1	0	1.514976	1.819885	6.262000
22	6	0	1.829133	1.063810	2.265379
23	6	0	1.859658	-1.857176	-1.889168
24	6	0	0.862434	-1.226787	-2.843205
25	1	0	-0.170257	-1.464344	-2.585548
26	1	0	0.940592	-0.140959	-2.877363
27	1	0	1.042496	-1.603743	-3.851462
28	6	0	2.833100	1.838590	1.440767
29	1	0	3.661008	2.170181	2.072940
30	1	0	3.258666	1.239646	0.634917
31	1	0	2.394026	2.729745	0.987919
32	6	0	0.360085	-0.805752	2.699023
33	6	0	-0.286850	-2.136104	2.367143
34	1	0	-1.353529	-2.030436	2.158862
35	1	0	0.174470	-2.622106	1.505811
36	1	0	-0.187449	-2.819264	3.214973
37	6	0	3.054007	-2.208971	0.221631
38	6	0	3.404680	-1.966508	1.674876
39	1	0	3.647597	-0.923278	1.874587
40	1	0	2.590778	-2.230608	2.350424
41	1	0	4.272522	-2.570234	1.945865
42	7	0	-0.041371	0.193702	-0.555131
43	6	0	-1.341840	-0.319191	-0.479365
44	6	0	-0.178748	1.568527	-0.814873
45	6	0	-2.286319	0.735048	-0.568624
46	6	0	-1.769690	-1.650804	-0.424399
47	6	0	-1.530468	1.941589	-0.769737
48	6	0	0.811133	2.485381	-1.283230
49	6	0	-3.654771	0.458927	-0.539526
50	6	0	-3.131100	-1.909919	-0.410897
51	1	0	-1.063649	-2.470065	-0.416052
52	6	0	-1.921900	3.282974	-0.983620
53	6	0	0.393310	3.844171	-1.484378
54	6	0	2.127702	2.122720	-1.660041
55	1	0	-4.384258	1.255886	-0.604859
56	1	0	-3.479663	-2.935071	-0.387379
57	6	0	-0.970378	4.217320	-1.290016
58	1	0	-2.966867	3.562155	-0.908746
59	6	0	1.346089	4.784837	-1.947765
60	6	0	3.014811	3.056535	-2.145223
61	1	0	2.441391	1.089906	-1.574584
62	1	0	-1.248369	5.253526	-1.447432
63	6	0	2.629466	4.406849	-2.268134
64	1	0	1.033261	5.816055	-2.074355
65	1	0	4.013351	2.751145	-2.436577

66	1	0	3.337971	5.139760	-2.637020
67	6	0	-4.070082	-0.863042	-0.452040
68	6	0	-5.528445	-1.203994	-0.388878
69	9	0	-6.322372	-0.153393	-0.691481
70	9	0	-5.854645	-2.206193	-1.241344
71	9	0	-5.898857	-1.627808	0.846178

Compound 8 3-RF-TS

Method: b3lyp/6-311g(d,p)
SCF Done: E(RB3LYP) = -1731.99165001 A.U. after 1 cycles
Lowest frequency = -23.8076

Zero-point correction= 0.567568
(Hartree/Particle)
Thermal correction to Energy= 0.602598
Thermal correction to Enthalpy= 0.603542
Thermal correction to Gibbs Free Energy= 0.499247
Sum of electronic and zero-point Energies= -1731.424082
Sum of electronic and thermal Energies= -1731.389052
Sum of electronic and thermal Enthalpies= -1731.388108
Sum of electronic and thermal Free Energies= -1731.492403

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.000209	0.585985	0.283865
2	6	0	1.252638	-2.299285	5.541480
3	1	0	1.529188	-1.620768	6.353785
4	1	0	0.255586	-2.689200	5.771638
5	1	0	1.949024	-3.140163	5.551343
6	6	0	1.262728	-1.592238	4.209633
7	6	0	0.592793	-0.385796	4.024023
8	1	0	0.063158	0.060848	4.860361
9	6	0	1.238657	-0.255002	1.649417
10	6	0	1.931576	-2.101565	3.110689
11	1	0	2.488126	-3.028910	3.215532
12	6	0	3.781911	2.997815	-0.896852
13	1	0	4.833717	2.868372	-1.134175
14	6	0	3.179871	4.227510	-1.136467
15	6	0	1.865755	4.361281	-0.715988
16	1	0	1.383796	5.331452	-0.800034
17	6	0	1.698715	2.010086	-0.025973
18	6	0	3.927243	5.360676	-1.792295
19	1	0	3.890884	5.271679	-2.883653
20	1	0	3.497008	6.329204	-1.527983
21	1	0	4.980829	5.364819	-1.501780
22	6	0	3.094235	1.918583	-0.340010
23	6	0	0.576856	0.280467	2.801630
24	6	0	-0.192662	1.578845	2.777863
25	1	0	0.441753	2.412857	2.479276
26	1	0	-1.048525	1.534658	2.100074
27	1	0	-0.587077	1.803976	3.770056
28	6	0	3.939471	0.690475	-0.077204
29	1	0	3.742005	0.265689	0.905394
30	1	0	3.789705	-0.093674	-0.821636
31	1	0	4.996592	0.959418	-0.113825

32	6	0	1.130030	3.310845	-0.152555
33	6	0	-0.201055	3.776197	0.413828
34	1	0	-0.731676	4.401807	-0.309669
35	1	0	-0.868432	2.988056	0.727695
36	1	0	-0.011036	4.405939	1.289873
37	6	0	1.934408	-1.475567	1.855161
38	6	0	2.781558	-2.208514	0.837216
39	1	0	2.829234	-1.733074	-0.129406
40	1	0	3.807489	-2.301576	1.208680
41	1	0	2.401566	-3.221749	0.684261
42	7	0	0.047935	-0.014677	-0.762599
43	6	0	-1.331643	0.351557	-0.672333
44	6	0	0.000240	-1.421147	-0.981317
45	6	0	-2.130215	-0.806437	-0.485887
46	6	0	-1.940052	1.581434	-0.899909
47	6	0	-1.260246	-1.943566	-0.693868
48	6	0	0.950841	-2.192419	-1.700678
49	6	0	-3.513491	-0.699229	-0.357905
50	6	0	-3.323115	1.678922	-0.788122
51	1	0	-1.361995	2.428306	-1.228437
52	6	0	-1.518360	-3.326091	-0.831785
53	6	0	0.684498	-3.594806	-1.835563
54	6	0	2.057323	-1.635265	-2.390480
55	1	0	-4.128327	-1.578086	-0.212266
56	1	0	-3.809189	2.626540	-0.982911
57	6	0	-0.537439	-4.137907	-1.341041
58	1	0	-2.485617	-3.732636	-0.559391
59	6	0	1.621106	-4.394386	-2.538086
60	6	0	2.920425	-2.437465	-3.099443
61	1	0	2.191705	-0.560377	-2.379656
62	1	0	-0.710754	-5.203008	-1.449264
63	6	0	2.720020	-3.834886	-3.146965
64	1	0	1.437979	-5.461108	-2.615041
65	1	0	3.751548	-1.995069	-3.636952
66	1	0	3.415873	-4.460053	-3.694689
67	6	0	-4.102387	0.555822	-0.480092
68	6	0	-5.583255	0.717396	-0.299758
69	9	0	-5.895148	1.162178	0.943153
70	9	0	-6.108843	1.614362	-1.166279
71	9	0	-6.254298	-0.443139	-0.472488

Compound 2a n-Hexane

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : n-Hexane
SCF Done: E(RCAM-B3LYP) = -1358.10338799 a.u.
Lowest frequency = 20.3334

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.938283	0.255300	-0.063468
2	6	0	3.317164	0.884628	-1.877083
3	1	0	2.720070	0.325925	-2.606748
4	1	0	2.808261	1.835680	-1.703234
5	1	0	4.282102	1.097397	-2.344467
6	6	0	1.478186	2.262785	2.177871
7	1	0	1.686904	3.120118	2.823046
8	1	0	0.767546	1.621317	2.711225
9	1	0	2.403449	1.693364	2.061865
10	6	0	-0.325091	1.406845	-2.532172
11	1	0	0.413701	0.626636	-2.731032
12	1	0	-1.276893	0.903380	-2.333231
13	1	0	-0.446191	1.989675	-3.449154
14	6	0	-0.071468	6.056878	-0.700805
15	1	0	-0.292097	6.551787	0.249259
16	1	0	0.821192	6.537264	-1.118490
17	1	0	-0.898671	6.254165	-1.388587
18	6	0	0.147355	4.578737	-0.513148
19	6	0	0.674725	4.075028	0.671220
20	1	0	0.903440	4.761196	1.483408
21	6	0	0.925392	2.715794	0.847248
22	6	0	0.619469	1.800487	-0.182198
23	6	0	0.066527	2.305462	-1.380578
24	6	0	-0.147177	3.674244	-1.527611
25	1	0	-0.562367	4.043700	-2.462595
26	6	0	2.667974	-1.016607	1.381772
27	6	0	3.971997	-1.396799	1.690771
28	1	0	4.149760	-1.979370	2.591958
29	6	0	5.049430	-1.060454	0.878148
30	6	0	4.789178	-0.317253	-0.268206
31	1	0	5.613655	-0.050736	-0.925438
32	6	0	3.502133	0.102562	-0.598239
33	6	0	2.410850	-0.245844	0.225487
34	6	0	1.566339	-1.470034	2.313407
35	1	0	1.027503	-2.328134	1.898148
36	1	0	1.981545	-1.777272	3.276961
37	1	0	0.825516	-0.690163	2.505586
38	6	0	6.453912	-1.463927	1.242339
39	1	0	7.081223	-1.573639	0.353210
40	1	0	6.926346	-0.710538	1.883651
41	1	0	6.468423	-2.411059	1.789230
42	7	0	-0.124992	-0.704642	-0.218864
43	6	0	-0.006193	-2.050466	-0.658630
44	6	0	-1.507931	-0.497544	0.036667
45	6	0	-1.271703	-2.660372	-0.681816
46	6	0	1.118330	-2.747701	-1.098676

47	6	0	-2.226901	-1.671802	-0.226398
48	6	0	-1.420683	-3.977150	-1.110875
49	6	0	0.954724	-4.060822	-1.520213
50	1	0	2.097486	-2.289997	-1.114840
51	6	0	-3.603384	-1.728945	-0.017973
52	6	0	-0.299451	-4.678164	-1.524856
53	1	0	-2.402190	-4.441534	-1.125583
54	1	0	1.825148	-4.614725	-1.857983
55	6	0	-4.280256	-0.617053	0.464507
56	1	0	-4.147174	-2.646665	-0.227136
57	1	0	-0.394423	-5.705325	-1.862264
58	6	0	-3.539420	0.543205	0.742033
59	1	0	-4.050864	1.418825	1.131396
60	6	0	-2.168662	0.620334	0.545155
61	1	0	-1.639138	1.532319	0.783259
62	6	0	-5.780107	-0.660395	0.693810
63	1	0	-6.118794	-1.665186	0.412241
64	6	0	-6.138263	-0.449099	2.169545
65	1	0	-7.218748	-0.541606	2.322061
66	1	0	-5.638488	-1.184241	2.807342
67	1	0	-5.839130	0.547660	2.511008
68	6	0	-6.520437	0.343483	-0.197783
69	1	0	-6.234399	1.372785	0.043714
70	1	0	-6.296068	0.174363	-1.255173
71	1	0	-7.603457	0.258378	-0.059546

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=n-hexane)

Excited State 1: Singlet-A 4.2783 eV 289.79 nm f=0.3186
<S**2>=0.000
119 ->124 -0.10058
122 ->124 0.16949
123 ->124 0.64227

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1358.19002814 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1358.03303577 a.u.

Excited State 1: Singlet-A 4.2767 eV 289.91 nm f=0.2498
<S**2>=0.000
122 ->124 0.19452
123 ->124 0.63593

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1357.97171210 a.u.

Lowest frequency = 19.8580

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.032813	0.291551	-0.058904
2	6	0	3.856180	0.951116	-0.870270
3	1	0	3.209659	0.862833	-1.749921
4	1	0	3.674015	1.949480	-0.461330
5	1	0	4.897841	0.911207	-1.202213
6	6	0	2.005725	2.313922	1.948941
7	1	0	2.099388	3.156412	2.640501
8	1	0	1.420500	1.527991	2.438345
9	1	0	3.004615	1.894432	1.796041
10	6	0	-0.194584	1.498486	-2.609224
11	1	0	0.573492	0.766885	-2.884351
12	1	0	-1.101406	0.932344	-2.368619
13	1	0	-0.418241	2.100588	-3.494466
14	6	0	0.346573	6.133834	-0.812772
15	1	0	-0.506255	6.490152	-0.221481
16	1	0	1.224240	6.697156	-0.479526
17	1	0	0.152197	6.399608	-1.856072
18	6	0	0.549392	4.650207	-0.653820
19	6	0	1.179003	4.123647	0.472463
20	1	0	1.533538	4.805611	1.243236
21	6	0	1.357784	2.757421	0.659445
22	6	0	0.891472	1.823764	-0.315769
23	6	0	0.262467	2.372147	-1.469113
24	6	0	0.103127	3.747760	-1.612208
25	1	0	-0.369708	4.128641	-2.515562
26	6	0	2.123137	-1.568577	1.447477
27	6	0	3.243956	-2.260884	1.897937
28	1	0	3.106067	-3.075108	2.606923
29	6	0	4.531874	-1.932736	1.491430
30	6	0	4.667402	-0.865186	0.606090
31	1	0	5.663222	-0.589889	0.263473
32	6	0	3.577041	-0.146634	0.128138
33	6	0	2.250208	-0.483556	0.535248
34	6	0	0.785518	-1.973258	2.012111
35	1	0	0.161598	-2.496787	1.278931
36	1	0	0.911562	-2.646690	2.864625
37	1	0	0.214999	-1.101529	2.352115
38	6	0	5.731408	-2.707606	1.969293
39	1	0	6.081084	-3.418325	1.210109
40	1	0	6.572480	-2.045074	2.198339
41	1	0	5.500529	-3.282388	2.871044
42	7	0	-0.189359	-0.567324	-0.445715
43	6	0	-0.206748	-1.611244	-1.361557
44	6	0	-1.459993	-0.444716	0.061771
45	6	0	-1.502180	-2.173660	-1.445871
46	6	0	0.862737	-2.107703	-2.099939
47	6	0	-2.327692	-1.404952	-0.517024
48	6	0	-1.734604	-3.235881	-2.291989
49	6	0	0.606513	-3.178978	-2.957882
50	1	0	1.853024	-1.684262	-1.992447
51	6	0	-3.652522	-1.441292	-0.147796
52	6	0	-0.664915	-3.733368	-3.054045
53	1	0	-2.718948	-3.685995	-2.372431

54	1	0	1.416250	-3.589042	-3.551534
55	6	0	-4.138641	-0.522414	0.804364
56	1	0	-4.332081	-2.168946	-0.582025
57	1	0	-0.835025	-4.570291	-3.722982
58	6	0	-3.263833	0.422360	1.356057
59	1	0	-3.642499	1.135444	2.080713
60	6	0	-1.924554	0.486592	0.996098
61	1	0	-1.259234	1.237096	1.402777
62	6	0	-5.597627	-0.558981	1.211454
63	1	0	-6.068292	-1.378315	0.655349
64	6	0	-5.759126	-0.859777	2.707121
65	1	0	-6.819622	-0.942624	2.964561
66	1	0	-5.266627	-1.797436	2.980518
67	1	0	-5.328775	-0.062465	3.321578
68	6	0	-6.322688	0.738114	0.829401
69	1	0	-5.912139	1.596535	1.370682
70	1	0	-6.234757	0.943343	-0.241394
71	1	0	-7.386114	0.665098	1.077674

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1358.06563674 a.u.

Excited State 1: Singlet-A 2.9187 eV 424.80 nm f=0.0397
<S**2>=0.000
115 ->124 -0.11169
123 ->124 0.68276

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,
NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1358.17156600 a.u.

Results

Absorb Energy =	0.157 a.u.	4.272 eV	290.226 nm
Emission Energy =	0.106 a.u.	2.882 eV	430.130 nm
Stokes Shift =	0.051 a.u.	1.389 eV	139.903 nm

Compound 2a THF

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : TetraHydroFuran
SCF Done: E(RCAM-B3LYP) = -1358.10645336 a.u.
Lowest frequency = 20.6874

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	0.940160	0.260451	-0.062873
2	6	0	3.323363	0.869981	-1.883050
3	1	0	2.760477	0.285972	-2.620232
4	1	0	2.779871	1.804831	-1.727619
5	1	0	4.290501	1.110614	-2.331811
6	6	0	1.446709	2.274545	2.184600
7	1	0	1.675824	3.134918	2.818564
8	1	0	0.717953	1.659140	2.724339
9	1	0	2.356926	1.679574	2.078923
10	6	0	-0.307397	1.402022	-2.541200
11	1	0	0.446683	0.636971	-2.742134
12	1	0	-1.249359	0.879835	-2.343559
13	1	0	-0.439944	1.984817	-3.456488
14	6	0	-0.097235	6.056894	-0.713124
15	1	0	-0.332902	6.550355	0.233994
16	1	0	0.797880	6.542663	-1.119067
17	1	0	-0.916068	6.248152	-1.412381
18	6	0	0.129043	4.580256	-0.522120
19	6	0	0.650682	4.080833	0.666981
20	1	0	0.869147	4.769218	1.480065
21	6	0	0.907344	2.722737	0.846847
22	6	0	0.615369	1.804380	-0.184069
23	6	0	0.068062	2.304877	-1.387340
24	6	0	-0.152980	3.672369	-1.537862
25	1	0	-0.563099	4.038355	-2.476383
26	6	0	2.667483	-1.003024	1.391157
27	6	0	3.970636	-1.383428	1.704576
28	1	0	4.146432	-1.960198	2.609822
29	6	0	5.050231	-1.053174	0.891306
30	6	0	4.792364	-0.316784	-0.260351
31	1	0	5.618010	-0.055668	-0.918226
32	6	0	3.505754	0.102123	-0.595287
33	6	0	2.412880	-0.238667	0.229618
34	6	0	1.563438	-1.447271	2.324609
35	1	0	1.013303	-2.297800	1.908471
36	1	0	1.977962	-1.762419	3.285766
37	1	0	0.832652	-0.659018	2.521459
38	6	0	6.453722	-1.456174	1.260034
39	1	0	7.081413	-1.573896	0.372292
40	1	0	6.926575	-0.697890	1.895176
41	1	0	6.465712	-2.398122	1.815709
42	7	0	-0.120806	-0.703058	-0.219588
43	6	0	0.001902	-2.047039	-0.662467
44	6	0	-1.503939	-0.500489	0.036635
45	6	0	-1.262093	-2.660933	-0.687517
46	6	0	1.128502	-2.739964	-1.104960
47	6	0	-2.220272	-1.675986	-0.229665
48	6	0	-1.407573	-3.977470	-1.120171
49	6	0	0.968936	-4.052738	-1.530178
50	1	0	2.105934	-2.278655	-1.121992
51	6	0	-3.597090	-1.737759	-0.021237
52	6	0	-0.283817	-4.674102	-1.536084
53	1	0	-2.387546	-4.444929	-1.136332
54	1	0	1.840717	-4.602980	-1.870349
55	6	0	-4.276712	-0.628744	0.465029
56	1	0	-4.138450	-2.656248	-0.232966
57	1	0	-0.375694	-5.700567	-1.876300
58	6	0	-3.538466	0.532815	0.746672
59	1	0	-4.051815	1.405551	1.139905

60	6	0	-2.167660	0.613920	0.549581
61	1	0	-1.639988	1.525625	0.792820
62	6	0	-5.776466	-0.676870	0.694946
63	1	0	-6.112907	-1.680678	0.408127
64	6	0	-6.133901	-0.473909	2.172098
65	1	0	-7.214180	-0.569230	2.323622
66	1	0	-5.633626	-1.212529	2.805729
67	1	0	-5.836433	0.521644	2.518619
68	6	0	-6.519551	0.330690	-0.190242
69	1	0	-6.236003	1.359272	0.057358
70	1	0	-6.296709	0.167544	-1.249044
71	1	0	-7.601996	0.241411	-0.050965

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=THF)

Excited State 1: Singlet-A 4.2884 eV 289.11 nm f=0.3216
<S**2>=0.000
122 ->124 0.15901
123 ->124 0.64448

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1358.19336547 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1358.03543583 a.u.

Excited State 1: Singlet-A 4.2888 eV 289.09 nm f=0.2490
<S**2>=0.000
120 ->124 0.10135
122 ->124 0.18133
123 ->124 0.63905

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1357.97357701 a.u.
Lowest frequency = 18.7046

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.026261	0.292121	-0.059426
2	6	0	3.845974	0.962148	-0.890535
3	1	0	3.194206	0.861394	-1.765150
4	1	0	3.658707	1.961205	-0.485154
5	1	0	4.885842	0.927870	-1.228551
6	6	0	1.983778	2.326037	1.950818

7	1	0	2.072678	3.168810	2.642598
8	1	0	1.399009	1.538108	2.437895
9	1	0	2.984827	1.911182	1.798171
10	6	0	-0.191991	1.487561	-2.611433
11	1	0	0.583564	0.761055	-2.879223
12	1	0	-1.093769	0.913514	-2.370223
13	1	0	-0.418786	2.084125	-3.499636
14	6	0	0.304106	6.133125	-0.820545
15	1	0	-0.554617	6.482106	-0.233578
16	1	0	1.174799	6.704262	-0.482497
17	1	0	0.112042	6.396175	-1.864885
18	6	0	0.518459	4.651124	-0.659089
19	6	0	1.148696	4.130710	0.470738
20	1	0	1.494732	4.816500	1.242025
21	6	0	1.336692	2.765535	0.659670
22	6	0	0.878998	1.827438	-0.314421
23	6	0	0.253029	2.368728	-1.472588
24	6	0	0.083166	3.743771	-1.618478
25	1	0	-0.389749	4.119609	-2.523918
26	6	0	2.138327	-1.547846	1.454465
27	6	0	3.264821	-2.233874	1.903542
28	1	0	3.133724	-3.043957	2.618575
29	6	0	4.549507	-1.904219	1.486751
30	6	0	4.676248	-0.841576	0.592933
31	1	0	5.669112	-0.565455	0.242328
32	6	0	3.579606	-0.130696	0.116516
33	6	0	2.256981	-0.470875	0.531958
34	6	0	0.804066	-1.951255	2.027524
35	1	0	0.178569	-2.479934	1.299255
36	1	0	0.934078	-2.618763	2.884098
37	1	0	0.232804	-1.077545	2.361166
38	6	0	5.754808	-2.671755	1.962873
39	1	0	6.101799	-3.386374	1.206234
40	1	0	6.595411	-2.005045	2.181012
41	1	0	5.531284	-3.241288	2.869701
42	7	0	-0.182908	-0.569712	-0.439072
43	6	0	-0.193969	-1.623854	-1.347660
44	6	0	-1.459151	-0.448188	0.063434
45	6	0	-1.486711	-2.191136	-1.429768
46	6	0	0.877154	-2.117029	-2.085316
47	6	0	-2.319270	-1.416017	-0.511755
48	6	0	-1.714426	-3.260902	-2.268096
49	6	0	0.627090	-3.197446	-2.934301
50	1	0	1.864007	-1.682305	-1.989538
51	6	0	-3.645755	-1.456693	-0.148308
52	6	0	-0.641475	-3.759919	-3.024798
53	1	0	-2.697225	-3.714042	-2.347197
54	1	0	1.438140	-3.605951	-3.527182
55	6	0	-4.139790	-0.533971	0.796301
56	1	0	-4.318954	-2.191178	-0.580264
57	1	0	-0.807405	-4.602528	-3.687401
58	6	0	-3.270756	0.415531	1.349081
59	1	0	-3.653682	1.128171	2.071881
60	6	0	-1.929362	0.481989	0.995075
61	1	0	-1.267593	1.231042	1.410716
62	6	0	-5.600335	-0.574941	1.197103
63	1	0	-6.065855	-1.395442	0.639165
64	6	0	-5.766578	-0.875836	2.692286
65	1	0	-6.828124	-0.961437	2.944320
66	1	0	-5.273387	-1.812892	2.966852

67	1	0	-5.340873	-0.077134	3.308294
68	6	0	-6.327174	0.720321	0.812239
69	1	0	-5.921726	1.579839	1.355814
70	1	0	-6.235856	0.924824	-0.258514
71	1	0	-7.391256	0.642907	1.056153

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1) SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1358.07622186 a.u.

Excited State 1: Singlet-A 2.8157 eV 440.33 nm f=0.0440 <S**2>=0.000
115 ->124 0.11172
123 ->124 -0.68242

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1358.17319586 a.u.

Results

Absorb Energy =	0.158 a.u.	4.297 eV	288.504 nm
Emission Energy =	0.097 a.u.	2.639 eV	469.851 nm
Stokes Shift =	0.061 a.u.	1.659 eV	181.347 nm

Compound 2° acetonitrile

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : Acetonitrile
SCF Done: E(RCAM-B3LYP) = -1358.10775073 a.u.
Lowest frequency = 20.7042

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.940702	0.261285	-0.062435
2	6	0	3.328187	0.862547	-1.882105
3	1	0	2.770878	0.274225	-2.620053
4	1	0	2.780281	1.795715	-1.731964
5	1	0	4.296454	1.105526	-2.327053
6	6	0	1.436671	2.278171	2.186998
7	1	0	1.675309	3.139461	2.816122
8	1	0	0.699316	1.675158	2.729051
9	1	0	2.339491	1.671177	2.086486
10	6	0	-0.299217	1.399984	-2.544878
11	1	0	0.459431	0.639615	-2.746604
12	1	0	-1.238030	0.872039	-2.347437
13	1	0	-0.435474	1.982670	-3.459629

14	6	0	-0.095514	6.057312	-0.721326
15	1	0	-0.329392	6.552602	0.225218
16	1	0	0.799404	6.541607	-1.129432
17	1	0	-0.914881	6.247515	-1.420204
18	6	0	0.130254	4.580908	-0.527785
19	6	0	0.648407	4.082827	0.663532
20	1	0	0.864230	4.772134	1.476506
21	6	0	0.904138	2.724686	0.845936
22	6	0	0.615738	1.805073	-0.184948
23	6	0	0.071762	2.304221	-1.390516
24	6	0	-0.149017	3.671601	-1.543359
25	1	0	-0.556280	4.036528	-2.483515
26	6	0	2.664238	-1.001729	1.395748
27	6	0	3.966379	-1.383499	1.712142
28	1	0	4.139918	-1.958781	2.618741
29	6	0	5.048031	-1.055843	0.900117
30	6	0	4.793041	-0.321243	-0.253467
31	1	0	5.620129	-0.062756	-0.910531
32	6	0	3.507332	0.098569	-0.591556
33	6	0	2.412631	-0.238898	0.232343
34	6	0	1.557749	-1.441555	2.328531
35	1	0	0.999084	-2.284757	1.908887
36	1	0	1.971047	-1.765546	3.287205
37	1	0	0.834692	-0.647468	2.530852
38	6	0	6.450346	-1.460129	1.271979
39	1	0	7.080174	-1.576824	0.385677
40	1	0	6.921773	-0.702800	1.909300
41	1	0	6.460194	-2.402517	1.826899
42	7	0	-0.120463	-0.702325	-0.220529
43	6	0	0.002172	-2.044967	-0.666716
44	6	0	-1.503278	-0.500253	0.036511
45	6	0	-1.261996	-2.658861	-0.693474
46	6	0	1.128833	-2.736825	-1.111167
47	6	0	-2.220145	-1.674833	-0.233135
48	6	0	-1.407538	-3.974572	-1.129321
49	6	0	0.969376	-4.048687	-1.539578
50	1	0	2.106022	-2.274981	-1.128144
51	6	0	-3.597183	-1.736891	-0.024690
52	6	0	-0.283540	-4.670197	-1.546761
53	1	0	-2.387365	-4.442223	-1.146755
54	1	0	1.840995	-4.598036	-1.881554
55	6	0	-4.276248	-0.629027	0.465397
56	1	0	-4.138973	-2.654450	-0.239149
57	1	0	-0.375348	-5.695831	-1.889406
58	6	0	-3.537367	0.531420	0.751126
59	1	0	-4.050123	1.402748	1.148197
60	6	0	-2.166482	0.612589	0.553841
61	1	0	-1.638099	1.522734	0.801390
62	6	0	-5.775869	-0.677731	0.696445
63	1	0	-6.113304	-1.679046	0.402564
64	6	0	-6.131019	-0.485380	2.175624
65	1	0	-7.211218	-0.580577	2.327501
66	1	0	-5.631296	-1.229801	2.802993
67	1	0	-5.831814	0.507223	2.529072
68	6	0	-6.519487	0.337111	-0.179940
69	1	0	-6.235802	1.363700	0.075700
70	1	0	-6.298328	0.181986	-1.240369
71	1	0	-7.601684	0.246494	-0.039990

Step2

 Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=acetonitrile)

 Excited State   1:   Singlet-A   4.2939 eV 288.74 nm f=0.3127
<S**2>=0.000
     122 ->124   0.15401
     123 ->124   0.64561

Step3

 Method: cam-b3lyp/6-31+G(d,p)
SCRF(Solvent=acetonitrile,NonEquilibrium=Save)
 SCF Done: E(RCAM-B3LYP) = -1358.19479223 a.u.

Step4

 Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
 SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Read)

 After PCM corrections, the energy is -1358.03634565 a.u.

 Excited State   1:   Singlet-A   4.2954 eV 288.64 nm f=0.2490
<S**2>=0.000
     120 ->124   0.10014
     122 ->124   0.17195
     123 ->124   0.64129

Step5

 Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

 Total Energy, E(TD-HF/TD-DFT) = -1357.97447012 a.u.
 Lowest frequency = 18.3067

                          Standard orientation:

 Center   Atomic   Atomic   Coordinates (Angstroms)
 Number   Number   Type   X   Y   Z
 ----
      1   5   0   1.023809   0.294008   -0.058371
      2   6   0   3.840369   0.974027   -0.899096
      3   1   0   3.185967   0.867503   -1.771141
      4   1   0   3.650118   1.972888   -0.494364
      5   1   0   4.879205   0.943651   -1.240510
      6   6   0   1.964924   2.335989   1.953502
      7   1   0   2.048448   3.179326   2.645198
      8   1   0   1.381911   1.545750   2.439095
      9   1   0   2.968318   1.926069   1.802312
     10   6   0   -0.185602   1.479492   -2.615551
     11   1   0   0.597254   0.758744   -2.877874
     12   1   0   -1.083227   0.897963   -2.376594
     13   1   0   -0.413943   2.072493   -3.505719
     14   6   0   0.269121   6.131315   -0.826077
     15   1   0   -0.594645   6.474086   -0.242935
     16   1   0   1.133930   6.708841   -0.483900
     17   1   0   0.079516   6.392478   -1.871291
     18   6   0   0.493209   4.650867   -0.662901
     19   6   0   1.122630   4.135460   0.470125

20	1	0	1.460652	4.824142	1.242366
21	6	0	1.318939	2.771487	0.660525
22	6	0	0.870250	1.829905	-0.314000
23	6	0	0.247281	2.365816	-1.476167
24	6	0	0.068623	3.739927	-1.623987
25	1	0	-0.402940	4.111923	-2.531701
26	6	0	2.149060	-1.533287	1.460109
27	6	0	3.279125	-2.215644	1.906991
28	1	0	3.152783	-3.023612	2.625265
29	6	0	4.561409	-1.884743	1.483186
30	6	0	4.682200	-0.824077	0.585623
31	1	0	5.673032	-0.546871	0.230189
32	6	0	3.581676	-0.117408	0.111418
33	6	0	2.261699	-0.460560	0.532020
34	6	0	0.817418	-1.935875	2.039535
35	1	0	0.190559	-2.469001	1.315630
36	1	0	0.950767	-2.598660	2.899234
37	1	0	0.245819	-1.060770	2.369067
38	6	0	5.770472	-2.648394	1.956253
39	1	0	6.114672	-3.365142	1.200398
40	1	0	6.611207	-1.979538	2.167016
41	1	0	5.552470	-3.215073	2.866153
42	7	0	-0.178558	-0.572260	-0.434517
43	6	0	-0.185139	-1.630552	-1.339843
44	6	0	-1.457357	-0.453389	0.065725
45	6	0	-1.475899	-2.202007	-1.421353
46	6	0	0.887735	-2.121003	-2.076686
47	6	0	-2.312987	-1.425101	-0.508766
48	6	0	-1.699290	-3.276111	-2.255477
49	6	0	0.642436	-3.206128	-2.921283
50	1	0	1.872086	-1.679260	-1.986188
51	6	0	-3.640601	-1.468367	-0.149348
52	6	0	-0.623851	-3.774418	-3.009226
53	1	0	-2.680470	-3.732664	-2.333703
54	1	0	1.454853	-3.612836	-3.513526
55	6	0	-4.139515	-0.544754	0.791868
56	1	0	-4.310394	-2.205618	-0.581596
57	1	0	-0.786306	-4.620256	-3.668487
58	6	0	-3.273917	0.406608	1.346921
59	1	0	-3.659810	1.118019	2.069381
60	6	0	-1.931433	0.475205	0.996574
61	1	0	-1.271695	1.223285	1.417385
62	6	0	-5.601270	-0.587939	1.187820
63	1	0	-6.063649	-1.408908	0.628300
64	6	0	-5.771849	-0.888962	2.682490
65	1	0	-6.834216	-0.975315	2.930759
66	1	0	-5.279227	-1.826051	2.958074
67	1	0	-5.348613	-0.089933	3.299830
68	6	0	-6.328325	0.706548	0.800755
69	1	0	-5.925567	1.566521	1.345708
70	1	0	-6.234241	0.910565	-0.269894
71	1	0	-7.393004	0.627470	1.041461

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1358.08027162 a.u.

```
 Excited State   1:      Singlet-A      2.7801 eV  445.98 nm  f=0.0457
<S**2>=0.000
     115 ->124         0.11103
     123 ->124         0.68225

Step7

  Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=acetonitrile,
NonEquilibrium=Read)

 SCF Done: E(RCAM-B3LYP) = -1358.17363401 a.u.

                              Results
 ------------------------------------------------------------------------
     Absorb Energy     =  | 0.158 a.u. | 4.312 eV | 287.563 nm
 --------------------------|------------|----------|---------------
     Emission Energy   =  | 0.093 a.u. | 2.541 eV | 488.027 nm
 --------------------------|------------|----------|---------------
     Stokes Shift      =  | 0.065 a.u. | 1.771 eV | 200.464 nm
 ------------------------------------------------------------------------

Compound Z-2b n-hexane

Step1

 Method: cam-b3lyp/6-31G(d)
 Solvent : n-Hexane
 SCF Done: E(RCAM-B3LYP) = -1318.81006533 a.u.
 Lowest frequency =  20.9622

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          5           0        1.176474    0.058784    0.022789
      2          6           0        3.677597    0.346881   -1.702102
      3          1           0        3.015207   -0.128369   -2.434240
      4          1           0        3.318495    1.368625   -1.556649
      5          1           0        4.672304    0.398938   -2.152307
      6          6           0        1.891721    2.033194    2.247139
      7          1           0        2.179238    2.872885    2.885099
      8          1           0        1.089918    1.493695    2.763616
      9          1           0        2.745256    1.354629    2.177141
     10          6           0        0.155913    1.306699   -2.511863
     11          1           0        0.787772    0.428463   -2.664444
     12          1           0       -0.863127    0.942535   -2.344514
     13          1           0        0.152274    1.878036   -3.443924
     14          6           0        0.941696    5.925485   -0.756184
     15          1           0        0.725350    6.464579    0.170601
     16          1           0        1.911985    6.282497   -1.121048
     17          1           0        0.190471    6.208353   -1.498949
     18          6           0        0.962140    4.436150   -0.534053
     19          6           0        1.379056    3.896568    0.678375
     20          1           0        1.665734    4.566443    1.485751
     21          6           0        1.446767    2.521105    0.888724
     22          6           0        1.061320    1.628444   -0.134342
     23          6           0        0.620182    2.172212   -1.361817
     24          6           0        0.589551    3.553526   -1.541775
     25          1           0        0.258218    3.951276   -2.498336
```

26	6	0	2.668919	-1.382690	1.567424
27	6	0	3.901314	-1.916977	1.941719
28	1	0	3.972089	-2.490703	2.861758
29	6	0	5.028182	-1.731311	1.155577
30	6	0	4.930044	-0.993766	-0.014770
31	1	0	5.808202	-0.847748	-0.637584
32	6	0	3.717665	-0.426408	-0.405336
33	6	0	2.562773	-0.617520	0.383671
34	6	0	1.480062	-1.665376	2.458276
35	1	0	0.856457	-2.463107	2.041188
36	1	0	1.812179	-1.990924	3.447712
37	1	0	0.834730	-0.794512	2.595750
38	7	0	0.010014	-0.764911	-0.163515
39	6	0	-0.022372	-2.125656	-0.571597
40	6	0	-1.345523	-0.382925	0.031827
41	6	0	-1.351898	-2.575437	-0.633766
42	6	0	1.022836	-2.966362	-0.952221
43	6	0	-2.193805	-1.465875	-0.237057
44	6	0	-1.646586	-3.874140	-1.041787
45	6	0	0.713851	-4.259653	-1.353231
46	1	0	2.051187	-2.633390	-0.939044
47	6	0	-3.573591	-1.348223	-0.083086
48	6	0	-0.606021	-4.717972	-1.395663
49	1	0	-2.676787	-4.214510	-1.086587
50	1	0	1.521029	-4.924570	-1.644475
51	6	0	-4.125137	-0.150260	0.350481
52	1	0	-4.218672	-2.196784	-0.296360
53	1	0	-0.814763	-5.733807	-1.715678
54	6	0	-3.257231	0.916281	0.635463
55	1	0	-3.670358	1.857145	0.987529
56	6	0	-1.881084	0.819514	0.492103
57	1	0	-1.251818	1.664733	0.733869
58	6	0	-5.626258	-0.003721	0.521291
59	1	0	-6.076140	-0.964616	0.242248
60	6	0	-6.009428	0.279654	1.978568
61	1	0	-7.097899	0.324407	2.090250
62	1	0	-5.628626	-0.498689	2.646532
63	1	0	-5.601496	1.238437	2.316026
64	6	0	-6.203368	1.065558	-0.413782
65	1	0	-5.801385	2.056565	-0.177326
66	1	0	-5.963167	0.848883	-1.458938
67	1	0	-7.292924	1.117094	-0.316369
68	1	0	5.980873	-2.158021	1.455131

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=n-hexane)

Excited State 1: Singlet-A 4.2779 eV 289.83 nm f=0.3063 <S**2>=0.000

118	->120	0.19135
119	->120	0.63522

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1318.89397871 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1318.73738373 a.u.

Excited State 1: Singlet-A 4.2698 eV 290.37 nm f=0.2375
<S**2>=0.000
118 ->120 0.21993
119 ->120 0.62776

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1318.67906564 a.u.
Lowest frequency = 17.3371

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.244845	-0.045926	0.089977
2	6	0	4.183526	-0.010151	-0.542601
3	1	0	3.586164	-0.043432	-1.459938
4	1	0	4.181482	1.035148	-0.219160
5	1	0	5.214020	-0.279914	-0.791995
6	6	0	2.463527	1.918333	2.018508
7	1	0	2.673075	2.783814	2.653953
8	1	0	1.705687	1.301346	2.513178
9	1	0	3.369918	1.306758	1.977572
10	6	0	0.451347	1.147122	-2.632808
11	1	0	1.073444	0.258541	-2.787932
12	1	0	-0.564894	0.792268	-2.427667
13	1	0	0.413364	1.700141	-3.575621
14	6	0	1.774925	5.731644	-1.137161
15	1	0	0.969013	6.292959	-0.648025
16	1	0	2.720337	6.144764	-0.770946
17	1	0	1.710107	5.938014	-2.209571
18	6	0	1.671134	4.255981	-0.855752
19	6	0	2.107623	3.718737	0.353619
20	1	0	2.537024	4.384626	1.099929
21	6	0	2.001610	2.364625	0.652136
22	6	0	1.427076	1.456877	-0.288580
23	6	0	0.996488	2.012916	-1.525907
24	6	0	1.121646	3.375801	-1.780684
25	1	0	0.794501	3.760279	-2.744926
26	6	0	1.839124	-1.945422	1.809230
27	6	0	2.766122	-2.803493	2.394390
28	1	0	2.425301	-3.514606	3.143085
29	6	0	4.110711	-2.752103	2.057007
30	6	0	4.528483	-1.819483	1.116366
31	1	0	5.577467	-1.775776	0.833629
32	6	0	3.632649	-0.945294	0.506895
33	6	0	2.242905	-0.986345	0.835366
34	6	0	0.413539	-2.030315	2.291291
35	1	0	-0.255135	-2.483088	1.550586
36	1	0	0.346788	-2.639181	3.197405

37	1	0	0.010054	-1.037866	2.521992
38	7	0	-0.097431	-0.682557	-0.328328
39	6	0	-0.266888	-1.775960	-1.168194
40	6	0	-1.345980	-0.274607	0.072443
41	6	0	-1.640915	-2.081347	-1.310603
42	6	0	0.724674	-2.530694	-1.786610
43	6	0	-2.351233	-1.092927	-0.502055
44	6	0	-2.028892	-3.145256	-2.095510
45	6	0	0.312316	-3.599356	-2.584939
46	1	0	1.771416	-2.301289	-1.633873
47	6	0	-3.676362	-0.840122	-0.232112
48	6	0	-1.035895	-3.902481	-2.738094
49	1	0	-3.076452	-3.401322	-2.218307
50	1	0	1.058483	-4.206881	-3.085308
51	6	0	-4.025703	0.231669	0.614456
52	1	0	-4.460373	-1.455030	-0.664466
53	1	0	-1.328682	-4.743339	-3.357816
54	6	0	-3.014958	1.031561	1.163074
55	1	0	-3.286753	1.862485	1.805462
56	6	0	-1.670776	0.804089	0.901517
57	1	0	-0.894601	1.441886	1.304074
58	6	0	-5.484445	0.513358	0.911452
59	1	0	-6.074350	-0.245402	0.383879
60	6	0	-5.791945	0.382904	2.408769
61	1	0	-6.861242	0.529710	2.589930
62	1	0	-5.513282	-0.604326	2.788504
63	1	0	-5.249465	1.133214	2.992920
64	6	0	-5.912559	1.887302	0.379318
65	1	0	-5.372470	2.694262	0.884779
66	1	0	-5.721319	1.976343	-0.693968
67	1	0	-6.982167	2.043550	0.550554
68	1	0	4.824087	-3.426500	2.521153

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1318.77084669 a.u.

Excited State 1: Singlet-A 2.8686 eV 432.21 nm f=0.0374
<S**2>=0.000
111 ->120 -0.11159
119 ->120 0.68297

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,
NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1318.87477663 a.u.

Results

Absorb Energy =	0.157 a.u.	4.261 eV	290.963 nm
Emission Energy =	0.104 a.u.	2.828 eV	438.404 nm
Stokes Shift =	0.053 a.u.	1.433 eV	147.441 nm

Compound Z-2b THF

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : TetraHydroFuran
SCF Done: E(RCAM-B3LYP) = -1318.81313146 a.u.
Lowest frequency = 20.7561

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.178833	0.064538	0.025353
2	6	0	3.679303	0.332069	-1.708893
3	1	0	3.041350	-0.171388	-2.443999
4	1	0	3.289310	1.344849	-1.581883
5	1	0	4.678684	0.406345	-2.145172
6	6	0	1.856000	2.052130	2.255265
7	1	0	2.169427	2.892208	2.880259
8	1	0	1.035951	1.547344	2.778462
9	1	0	2.687078	1.345285	2.197400
10	6	0	0.173245	1.298187	-2.518772
11	1	0	0.821225	0.431582	-2.670697
12	1	0	-0.839547	0.915986	-2.353402
13	1	0	0.160863	1.869925	-3.450392
14	6	0	0.912324	5.928805	-0.770493
15	1	0	0.677216	6.468354	0.151377
16	1	0	1.885786	6.292155	-1.120219
17	1	0	0.171624	6.203195	-1.526750
18	6	0	0.941107	4.440235	-0.543831
19	6	0	1.351906	3.906813	0.673780
20	1	0	1.627338	4.580919	1.481518
21	6	0	1.426373	2.532011	0.889137
22	6	0	1.056383	1.633551	-0.134728
23	6	0	0.620961	2.170955	-1.367432
24	6	0	0.582083	3.551721	-1.552026
25	1	0	0.256008	3.944414	-2.512428
26	6	0	2.672828	-1.364503	1.578978
27	6	0	3.905321	-1.896361	1.957289
28	1	0	3.976569	-2.462403	2.882018
29	6	0	5.032411	-1.717017	1.169025
30	6	0	4.933773	-0.989109	-0.007629
31	1	0	5.811616	-0.848643	-0.632135
32	6	0	3.720765	-0.424893	-0.402653
33	6	0	2.566495	-0.608159	0.389145
34	6	0	1.483697	-1.637753	2.472593
35	1	0	0.848129	-2.424928	2.053478
36	1	0	1.815256	-1.973279	3.458742
37	1	0	0.850810	-0.758873	2.617486
38	7	0	0.015188	-0.764137	-0.161827
39	6	0	-0.011756	-2.124088	-0.571742
40	6	0	-1.341611	-0.387446	0.033182
41	6	0	-1.339803	-2.579179	-0.635392
42	6	0	1.036739	-2.960441	-0.954033
43	6	0	-2.186252	-1.473001	-0.238082
44	6	0	-1.629893	-3.878817	-1.045329
45	6	0	0.732931	-4.254647	-1.357262

46	1	0	2.063591	-2.622883	-0.942415
47	6	0	-3.567157	-1.360883	-0.085566
48	6	0	-0.585584	-4.718306	-1.400193
49	1	0	-2.658706	-4.223126	-1.090885
50	1	0	1.542544	-4.915773	-1.650306
51	6	0	-4.123280	-0.165203	0.349663
52	1	0	-4.208850	-2.211346	-0.301231
53	1	0	-0.790307	-5.734426	-1.721743
54	6	0	-3.259001	0.903991	0.638279
55	1	0	-3.675527	1.842425	0.992748
56	6	0	-1.882067	0.812125	0.495975
57	1	0	-1.255810	1.658249	0.742336
58	6	0	-5.625272	-0.023948	0.518476
59	1	0	-6.071432	-0.985718	0.237377
60	6	0	-6.011467	0.256676	1.975539
61	1	0	-7.100279	0.297699	2.084314
62	1	0	-5.630564	-0.522045	2.643258
63	1	0	-5.607331	1.216500	2.314743
64	6	0	-6.204068	1.045280	-0.415707
65	1	0	-5.805310	2.037118	-0.177061
66	1	0	-5.963208	0.830217	-1.461203
67	1	0	-7.293749	1.092803	-0.318749
68	1	0	5.985158	-2.141251	1.471807

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=THF)

Excited State 1: Singlet-A 4.2909 eV 288.95 nm f=0.3104
<S**2>=0.000
118 ->120 0.18040
119 ->120 0.63740

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1318.89732152 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1318.73970347 a.u.

Excited State 1: Singlet-A 4.2844 eV 289.38 nm f=0.2373
<S**2>=0.000
117 ->120 0.10114
118 ->120 0.20598
119 ->120 0.63126

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1318.68095586 a.u.
Lowest frequency = 18.9788

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.241092	-0.040765	0.084310
2	6	0	4.179901	0.011537	-0.568914
3	1	0	3.575122	-0.033815	-1.480929
4	1	0	4.170541	1.058172	-0.249413
5	1	0	5.210876	-0.250216	-0.824609
6	6	0	2.445085	1.937785	2.014880
7	1	0	2.645145	2.803991	2.652317
8	1	0	1.692260	1.312084	2.506637
9	1	0	3.358504	1.336634	1.971215
10	6	0	0.437740	1.143655	-2.632203
11	1	0	1.067571	0.260034	-2.784133
12	1	0	-0.574271	0.779067	-2.422815
13	1	0	0.392005	1.693681	-3.576422
14	6	0	1.711189	5.746210	-1.139945
15	1	0	0.899229	6.297224	-0.649270
16	1	0	2.651590	6.170730	-0.773991
17	1	0	1.641827	5.952035	-2.212093
18	6	0	1.625007	4.269152	-0.858596
19	6	0	2.069551	3.736633	0.350929
20	1	0	2.491325	4.407653	1.097044
21	6	0	1.978441	2.380990	0.649188
22	6	0	1.411625	1.467408	-0.289907
23	6	0	0.975510	2.017332	-1.528077
24	6	0	1.084535	3.382481	-1.783253
25	1	0	0.750954	3.763231	-2.746781
26	6	0	1.865371	-1.921495	1.812335
27	6	0	2.801528	-2.771617	2.397056
28	1	0	2.469762	-3.479515	3.152886
29	6	0	4.143630	-2.715533	2.049179
30	6	0	4.550100	-1.786538	1.098859
31	1	0	5.596865	-1.739291	0.808306
32	6	0	3.644110	-0.921780	0.489811
33	6	0	2.257524	-0.969695	0.827110
34	6	0	0.443391	-2.006935	2.304364
35	1	0	-0.228230	-2.465959	1.570126
36	1	0	0.383368	-2.609338	3.215248
37	1	0	0.039012	-1.013102	2.527736
38	7	0	-0.087908	-0.686358	-0.324944
39	6	0	-0.252156	-1.790824	-1.156013
40	6	0	-1.341995	-0.282269	0.073061
41	6	0	-1.624094	-2.105609	-1.292269
42	6	0	0.742439	-2.538963	-1.776897
43	6	0	-2.340558	-1.112312	-0.493966
44	6	0	-2.007811	-3.178190	-2.067961
45	6	0	0.335258	-3.617997	-2.564615
46	1	0	1.788424	-2.295206	-1.640216
47	6	0	-3.667776	-0.866989	-0.226527
48	6	0	-1.011415	-3.933632	-2.707664
49	1	0	-3.053906	-3.440940	-2.186923
50	1	0	1.083643	-4.221328	-3.066675
51	6	0	-4.024344	0.209684	0.611261
52	1	0	-4.446764	-1.491812	-0.652987
53	1	0	-1.300536	-4.781088	-3.319832
54	6	0	-3.019297	1.018790	1.156787
55	1	0	-3.295963	1.850282	1.796289

56	6	0	-1.672989	0.796431	0.898551
57	1	0	-0.901314	1.436441	1.306866
58	6	0	-5.485174	0.483929	0.904615
59	1	0	-6.069328	-0.281423	0.381018
60	6	0	-5.793554	0.361321	2.402440
61	1	0	-6.864209	0.502526	2.579817
62	1	0	-5.510087	-0.622336	2.788099
63	1	0	-5.256842	1.119054	2.982449
64	6	0	-5.920069	1.852282	0.363620
65	1	0	-5.385377	2.665260	0.865342
66	1	0	-5.728692	1.934848	-0.710255
67	1	0	-6.990855	2.002272	0.532854
68	1	0	4.864025	-3.382973	2.512732

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1) SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1318.78179141 a.u.

Excited State 1: Singlet-A 2.7598 eV 449.24 nm f=0.0416 <S**2>=0.000
111 ->120 -0.11114
119 ->120 0.68264

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1318.87631384 a.u.

Results

Absorb Energy =	0.158 a.u.	4.289 eV	289.074 nm
Emission Energy =	0.095 a.u.	2.572 eV	482.037 nm
Stokes Shift =	0.063 a.u.	1.717 eV	192.963 nm

Compound Z-2b ACN

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : Acetonitrile
SCF Done: E(RCAM-B3LYP) = -1318.81442492 a.u.
Lowest frequency = 21.2116

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.179502	0.064556	0.025944
2	6	0	3.682683	0.319537	-1.708927
3	1	0	3.060269	-0.199052	-2.446894
4	1	0	3.275181	1.326674	-1.592792
5	1	0	4.685141	0.406680	-2.135540

6	6	0	1.844708	2.057400	2.257123
7	1	0	2.165901	2.897608	2.877919
8	1	0	1.018341	1.564317	2.781539
9	1	0	2.668125	1.341242	2.204759
10	6	0	0.183995	1.292576	-2.523104
11	1	0	0.840219	0.432356	-2.676523
12	1	0	-0.824988	0.900693	-2.357146
13	1	0	0.165304	1.865085	-3.454081
14	6	0	0.911537	5.927684	-0.780307
15	1	0	0.677113	6.468925	0.140679
16	1	0	1.884829	6.290261	-1.131285
17	1	0	0.170691	6.200290	-1.537024
18	6	0	0.940687	4.439553	-0.550700
19	6	0	1.347392	3.908593	0.669469
20	1	0	1.619079	4.584339	1.477071
21	6	0	1.421894	2.534027	0.887715
22	6	0	1.056813	1.633409	-0.136029
23	6	0	0.625330	2.168305	-1.371429
24	6	0	0.585879	3.548771	-1.558745
25	1	0	0.263192	3.939507	-2.521064
26	6	0	2.670074	-1.360336	1.585785
27	6	0	3.901893	-1.890607	1.968939
28	1	0	3.971389	-2.452801	2.896123
29	6	0	5.030886	-1.714007	1.182419
30	6	0	4.934617	-0.991111	0.002353
31	1	0	5.813727	-0.853308	-0.620932
32	6	0	3.722145	-0.428883	-0.397748
33	6	0	2.566341	-0.608301	0.392780
34	6	0	1.478950	-1.629396	2.478142
35	1	0	0.838836	-2.411594	2.056606
36	1	0	1.808151	-1.969640	3.463399
37	1	0	0.851403	-0.747003	2.625295
38	7	0	0.015640	-0.764173	-0.162006
39	6	0	-0.011172	-2.123209	-0.574096
40	6	0	-1.340940	-0.387727	0.033489
41	6	0	-1.339302	-2.578429	-0.638742
42	6	0	1.037526	-2.958678	-0.958297
43	6	0	-2.185852	-1.472747	-0.239788
44	6	0	-1.629307	-3.877558	-1.051148
45	6	0	0.734005	-4.252239	-1.364110
46	1	0	2.064166	-2.620399	-0.947208
47	6	0	-3.567009	-1.360806	-0.087260
48	6	0	-0.584648	-4.716145	-1.407667
49	1	0	-2.657980	-4.222106	-1.097511
50	1	0	1.543534	-4.912596	-1.659053
51	6	0	-4.122905	-0.165710	0.350290
52	1	0	-4.208767	-2.210743	-0.304573
53	1	0	-0.789150	-5.731633	-1.731248
54	6	0	-3.258330	0.902909	0.641381
55	1	0	-3.674702	1.840495	0.998222
56	6	0	-1.881308	0.811013	0.498969
57	1	0	-1.254779	1.656107	0.748210
58	6	0	-5.624932	-0.024506	0.519339
59	1	0	-6.071354	-0.985126	0.235145
60	6	0	-6.011046	0.251849	1.977278
61	1	0	-7.099848	0.293158	2.085607
62	1	0	-5.631288	-0.529614	2.642543
63	1	0	-5.606356	1.210370	2.319524
64	6	0	-6.203186	1.048108	-0.411329
65	1	0	-5.804507	2.039096	-0.168992

```
     66          1           0       -5.962615    0.836311   -1.457631
     67          1           0       -7.292828    1.095108   -0.314236
     68          1           0        5.983074   -2.136597    1.489144
 ---------------------------------------------------------------------

Step2

 Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=acetonitrile)

 Excited State   1:      Singlet-A      4.2979 eV  288.48 nm  f=0.3018
<S**2>=0.000
     118 ->120         0.17486
     119 ->120         0.63866

Step3

 Method: cam-b3lyp/6-31+G(d,p)
SCRF(Solvent=acetonitrile,NonEquilibrium=Save)
 SCF Done: E(RCAM-B3LYP) = -1318.89873996 a.u.

Step4

 Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
 SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Read)

 After PCM corrections, the energy is -1318.74049788 a.u.

 Excited State   1:      Singlet-A      4.2935 eV  288.77 nm  f=0.2377
<S**2>=0.000
     117 ->120         0.10169
     118 ->120         0.19545
     119 ->120         0.63393

Step5

 Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

 Total Energy, E(TD-HF/TD-DFT) = -1318.68184577 a.u.
 Lowest frequency =  19.8571

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          5           0        1.238953   -0.038082    0.084305
      2          6           0        4.175362    0.016102   -0.587660
      3          1           0        3.565469   -0.036540   -1.495993
      4          1           0        4.164265    1.064084   -0.272388
      5          1           0        5.205730   -0.243451   -0.847833
      6          6           0        2.443146    1.945314    2.012627
      7          1           0        2.644241    2.811777    2.649305
      8          1           0        1.691756    1.319347    2.506393
      9          1           0        3.357211    1.345326    1.965353
     10          6           0        0.429666    1.142699   -2.629634
     11          1           0        1.063150    0.261652   -2.781510
     12          1           0       -0.580065    0.773328   -2.417538
     13          1           0        0.379167    1.691899   -3.574062
     14          6           0        1.685758    5.751914   -1.139809
```

15	1	0	0.872612	6.298871	-0.646635
16	1	0	2.624932	6.180576	-0.775602
17	1	0	1.612390	5.957853	-2.211620
18	6	0	1.606692	4.274371	-0.858681
19	6	0	2.056933	3.743442	0.349905
20	1	0	2.477538	4.416247	1.095051
21	6	0	1.971712	2.387346	0.648253
22	6	0	1.405236	1.471705	-0.289024
23	6	0	0.965372	2.019407	-1.526975
24	6	0	1.067834	3.385417	-1.782353
25	1	0	0.730181	3.764847	-2.744969
26	6	0	1.878417	-1.909850	1.815896
27	6	0	2.819452	-2.755888	2.399735
28	1	0	2.493059	-3.461102	3.160391
29	6	0	4.159681	-2.698862	2.044173
30	6	0	4.559472	-1.773645	1.086894
31	1	0	5.604518	-1.726277	0.790247
32	6	0	3.648174	-0.913582	0.478629
33	6	0	2.263868	-0.962699	0.823839
34	6	0	0.458714	-1.995065	2.314364
35	1	0	-0.214849	-2.458620	1.584696
36	1	0	0.403004	-2.592976	3.228446
37	1	0	0.053535	-1.000535	2.533188
38	7	0	-0.084994	-0.687853	-0.320794
39	6	0	-0.246224	-1.795630	-1.149601
40	6	0	-1.341728	-0.286455	0.076029
41	6	0	-1.617129	-2.114417	-1.285015
42	6	0	0.750386	-2.540161	-1.771466
43	6	0	-2.336991	-1.120192	-0.490590
44	6	0	-1.997974	-3.189944	-2.058214
45	6	0	0.346409	-3.622553	-2.556487
46	1	0	1.795667	-2.290122	-1.639954
47	6	0	-3.665470	-0.877493	-0.226596
48	6	0	-0.999387	-3.943589	-2.696791
49	1	0	-3.043220	-3.455955	-2.176325
50	1	0	1.096255	-4.223329	-3.059420
51	6	0	-4.026015	0.199819	0.608785
52	1	0	-4.441929	-1.504789	-0.653773
53	1	0	-1.286248	-4.793207	-3.306935
54	6	0	-3.023829	1.010925	1.156661
55	1	0	-3.303304	1.841348	1.796341
56	6	0	-1.676298	0.790775	0.901523
57	1	0	-0.906941	1.430548	1.314937
58	6	0	-5.488094	0.471397	0.898253
59	1	0	-6.069483	-0.293540	0.371353
60	6	0	-5.800455	0.345119	2.394961
61	1	0	-6.871879	0.484383	2.569149
62	1	0	-5.517039	-0.639326	2.778734
63	1	0	-5.266429	1.102360	2.978127
64	6	0	-5.923069	1.840450	0.359067
65	1	0	-5.391028	2.653025	0.864363
66	1	0	-5.729053	1.925144	-0.714211
67	1	0	-6.994592	1.988212	0.525540
68	1	0	4.883847	-3.362731	2.506991

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Save)

After PCM corrections, the energy is -1318.78596032 a.u.

Excited State 1: Singlet-A 2.7222 eV 455.46 nm f=0.0433
<S**2>=0.000
111 ->120 -0.11015
119 ->120 0.68249

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=acetonitrile,
NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1318.87670962 a.u.

Results

Absorb Energy =	0.158 a.u.	4.306 eV	287.934 nm
Emission Energy =	0.091 a.u.	2.469 eV	502.079 nm
Stokes Shift =	0.067 a.u.	1.837 eV	214.145 nm

Compound E-2b n-hexane

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : n-Hexane
SCF Done: E(RCAM-B3LYP) = -1318.81006710 a.u.
Lowest frequency = 21.5132

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.936285	0.455791	-0.107616
2	6	0	3.316167	0.999130	-1.952342
3	1	0	2.718403	0.408241	-2.655515
4	1	0	2.809447	1.958437	-1.823231
5	1	0	4.281486	1.188428	-2.428842
6	6	0	1.469487	2.559391	2.040621
7	1	0	1.675969	3.444031	2.648570
8	1	0	0.754784	1.943317	2.597971
9	1	0	2.394635	1.984385	1.955146
10	6	0	-0.309520	1.480450	-2.634244
11	1	0	0.424596	0.684922	-2.782681
12	1	0	-1.267584	0.995819	-2.418852
13	1	0	-0.416242	2.013640	-3.582703
14	6	0	0.160892	4.732710	-0.765161
15	6	0	0.681501	4.306827	0.447573
16	1	0	0.910913	5.032693	1.222737
17	6	0	0.924245	2.955036	0.688867
18	6	0	0.619857	1.996064	-0.301276
19	6	0	0.075807	2.437844	-1.528911
20	6	0	-0.133736	3.799005	-1.746913
21	1	0	-0.538497	4.126271	-2.700696
22	6	0	2.666744	-0.748646	1.391947

23	6	0	3.970706	-1.115023	1.717066
24	1	0	4.148771	-1.655124	2.644258
25	6	0	5.047802	-0.817483	0.888956
26	6	0	4.787061	-0.128108	-0.290282
27	1	0	5.611182	0.107250	-0.959669
28	6	0	3.500047	0.276868	-0.638683
29	6	0	2.409011	-0.032218	0.200981
30	6	0	1.566532	-1.157735	2.345573
31	1	0	1.029560	-2.036709	1.973845
32	1	0	1.983154	-1.415905	3.322793
33	1	0	0.823991	-0.371176	2.499515
34	7	0	-0.130002	-0.506199	-0.212574
35	6	0	-0.016544	-1.872829	-0.586030
36	6	0	-1.512781	-0.280633	0.029379
37	6	0	-1.284848	-2.477102	-0.581975
38	6	0	1.105329	-2.595663	-0.989818
39	6	0	-2.236496	-1.462959	-0.177959
40	6	0	-1.439366	-3.812577	-0.946241
41	6	0	0.936218	-3.927081	-1.347008
42	1	0	2.086609	-2.143748	-1.026791
43	6	0	-3.613750	-1.503415	0.028772
44	6	0	-0.320748	-4.538128	-1.323430
45	1	0	-2.423000	-4.272608	-0.939940
46	1	0	1.804517	-4.500791	-1.655896
47	6	0	-4.286640	-0.366050	0.454237
48	1	0	-4.161390	-2.427618	-0.137206
49	1	0	-0.420006	-5.580143	-1.610242
50	6	0	-3.541034	0.802769	0.677303
51	1	0	-4.049190	1.698756	1.022003
52	6	0	-2.169329	0.863662	0.481080
53	1	0	-1.636555	1.783810	0.676638
54	6	0	-5.787352	-0.391099	0.680603
55	1	0	-6.130241	-1.406454	0.445969
56	6	0	-6.148633	-0.108310	2.143566
57	1	0	-7.230025	-0.188030	2.296814
58	1	0	-5.654598	-0.814964	2.817035
59	1	0	-5.845317	0.901959	2.438364
60	6	0	-6.520035	0.572959	-0.259927
61	1	0	-6.229627	1.611172	-0.066686
62	1	0	-6.293560	0.352736	-1.307406
63	1	0	-7.603840	0.499708	-0.121109
64	1	0	-0.012260	5.789581	-0.945360
65	6	0	6.452130	-1.204788	1.270718
66	1	0	7.082832	-1.341267	0.387778
67	1	0	6.919917	-0.429701	1.889149
68	1	0	6.467406	-2.133677	1.848075

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=n-hexane)

Excited State 1: Singlet-A 4.2844 eV 289.39 nm f=0.3106
<S**2>=0.000

117	->120	-0.10459
118	->120	-0.19022
119	->120	0.63488

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1318.89398111 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1318.73709556 a.u.

Excited State 1: Singlet-A 4.2774 eV 289.86 nm f=0.2420
<S**2>=0.000
117 ->120 -0.10743
118 ->120 0.21901
119 ->120 0.62753

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1318.67904694 a.u.
Lowest frequency = 17.6885

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.038003	0.510878	-0.136229
2	6	0	3.852726	1.145946	-0.993782
3	1	0	3.206205	0.979422	-1.861882
4	1	0	3.660532	2.172417	-0.667249
5	1	0	4.894354	1.090208	-1.323415
6	6	0	1.960282	2.708307	1.696672
7	1	0	2.034602	3.608077	2.314568
8	1	0	1.382121	1.958132	2.247077
9	1	0	2.966987	2.293356	1.589158
10	6	0	-0.195958	1.460569	-2.787495
11	1	0	0.585062	0.719431	-2.991458
12	1	0	-1.095615	0.904484	-2.500968
13	1	0	-0.423164	1.975845	-3.725109
14	6	0	0.489725	4.771218	-1.108300
15	6	0	1.118542	4.375160	0.065255
16	1	0	1.452261	5.127974	0.775286
17	6	0	1.318502	3.031331	0.368823
18	6	0	0.874430	2.012353	-0.528606
19	6	0	0.240891	2.442533	-1.730574
20	6	0	0.057639	3.796764	-1.996227
21	1	0	-0.418161	4.090446	-2.928847
22	6	0	2.152588	-1.193117	1.529158
23	6	0	3.282463	-1.828281	2.036895
24	1	0	3.155596	-2.580140	2.813571
25	6	0	4.565995	-1.518551	1.602432
26	6	0	4.687313	-0.528510	0.629711
27	1	0	5.679487	-0.268868	0.265119
28	6	0	3.587183	0.131227	0.092310
29	6	0	2.265120	-0.189525	0.526234
30	6	0	0.820474	-1.565783	2.127970
31	1	0	0.204274	-2.159896	1.443756

32	1	0	0.955883	-2.160740	3.035613
33	1	0	0.237753	-0.675968	2.391869
34	7	0	-0.172963	-0.395382	-0.443607
35	6	0	-0.177222	-1.514971	-1.265561
36	6	0	-1.443932	-0.246975	0.055690
37	6	0	-1.464533	-2.100880	-1.295978
38	6	0	0.898272	-2.060115	-1.959447
39	6	0	-2.298955	-1.266027	-0.434751
40	6	0	-1.682959	-3.237370	-2.043577
41	6	0	0.656026	-3.206577	-2.718668
42	1	0	1.882764	-1.615294	-1.892295
43	6	0	-3.622240	-1.289153	-0.059218
44	6	0	-0.607538	-3.785022	-2.761970
45	1	0	-2.660657	-3.707317	-2.080077
46	1	0	1.470619	-3.656115	-3.275963
47	6	0	-4.119491	-0.298558	0.811859
48	1	0	-4.292102	-2.061105	-0.426894
49	1	0	-0.766664	-4.680065	-3.353908
50	6	0	-3.257177	0.702667	1.277049
51	1	0	-3.644532	1.470209	1.938750
52	6	0	-1.920092	0.755017	0.907551
53	1	0	-1.265469	1.548106	1.244818
54	6	0	-5.577151	-0.319620	1.224460
55	1	0	-6.036429	-1.192381	0.745524
56	6	0	-5.732462	-0.486457	2.741531
57	1	0	-6.791371	-0.560043	3.008063
58	1	0	-5.226920	-1.388934	3.097133
59	1	0	-5.312292	0.368763	3.280503
60	6	0	-6.321221	0.927285	0.728585
61	1	0	-5.922346	1.836801	1.189075
62	1	0	-6.237493	1.036226	-0.356576
63	1	0	-7.383197	0.861827	0.985012
64	1	0	0.342181	5.824437	-1.327676
65	6	0	5.775135	-2.235217	2.142691
66	1	0	6.108744	-3.030445	1.464335
67	1	0	6.620415	-1.552380	2.275592
68	1	0	5.563033	-2.701184	3.109551

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1318.77079766 a.u.

Excited State 1: Singlet-A 2.8711 eV 431.83 nm f=0.0380
<S**2>=0.000
111 ->120 -0.11150
119 ->120 0.68299

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,
NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1318.87484357 a.u.

Results

Absorb Energy = | 0.157 a.u. | 4.269 eV | 290.424 nm

Emission Energy =	0.104 a.u.	2.831 eV	437.916 nm
Stokes Shift =	0.053 a.u.	1.438 eV	147.492 nm

Compound E-2b THF

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : TetraHydroFuran
SCF Done: E(RCAM-B3LYP) = -1318.81313841 a.u.
Lowest frequency = 21.5824

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.937652	0.458963	-0.107694
2	6	0	3.323800	0.983400	-1.954958
3	1	0	2.746994	0.376030	-2.661605
4	1	0	2.796795	1.933448	-1.839439
5	1	0	4.291626	1.187913	-2.419779
6	6	0	1.439184	2.571306	2.044177
7	1	0	1.671670	3.458740	2.638352
8	1	0	0.702256	1.988082	2.608091
9	1	0	2.345318	1.965206	1.972102
10	6	0	-0.290886	1.472015	-2.644629
11	1	0	0.454500	0.686881	-2.792705
12	1	0	-1.242349	0.974186	-2.429858
13	1	0	-0.404620	2.003773	-3.592940
14	6	0	0.152637	4.732512	-0.781492
15	6	0	0.665244	4.311930	0.436843
16	1	0	0.885955	5.040904	1.211601
17	6	0	0.910100	2.961138	0.684391
18	6	0	0.617886	1.998216	-0.305724
19	6	0	0.081230	2.434493	-1.538996
20	6	0	-0.131656	3.794456	-1.762880
21	1	0	-0.529929	4.117620	-2.720769
22	6	0	2.663721	-0.738911	1.401051
23	6	0	3.966245	-1.106721	1.731101
24	1	0	4.141348	-1.641461	2.661909
25	6	0	5.046215	-0.816071	0.903259
26	6	0	4.789221	-0.132790	-0.280677
27	1	0	5.615130	0.096621	-0.949871
28	6	0	3.503214	0.272615	-0.634430
29	6	0	2.409833	-0.028544	0.205146
30	6	0	1.560070	-1.136914	2.355613
31	1	0	1.006123	-2.003477	1.979712
32	1	0	1.975805	-1.409708	3.329103
33	1	0	0.832591	-0.337929	2.518357
34	7	0	-0.127791	-0.505012	-0.213342
35	6	0	-0.012514	-1.870332	-0.589274
36	6	0	-1.510412	-0.281649	0.029378
37	6	0	-1.280240	-2.476779	-0.586468
38	6	0	1.110408	-2.590826	-0.995322
39	6	0	-2.233348	-1.464404	-0.180422
40	6	0	-1.433189	-3.812202	-0.953455

41	6	0	0.943406	-3.922105	-1.355330
42	1	0	2.090603	-2.136652	-1.033692
43	6	0	-3.610984	-1.507181	0.026576
44	6	0	-0.313051	-4.535372	-1.332364
45	1	0	-2.415962	-4.274018	-0.947970
46	1	0	1.812262	-4.493723	-1.666464
47	6	0	-4.284892	-0.371157	0.455327
48	1	0	-4.157680	-2.431497	-0.141462
49	1	0	-0.410815	-5.576899	-1.621293
50	6	0	-3.540043	0.798092	0.681782
51	1	0	-4.048670	1.692412	1.030050
52	6	0	-2.168145	0.860664	0.485080
53	1	0	-1.635816	1.780106	0.685122
54	6	0	-5.785593	-0.398418	0.682459
55	1	0	-6.127705	-1.412827	0.443684
56	6	0	-6.145940	-0.121652	2.146856
57	1	0	-7.227275	-0.202433	2.299275
58	1	0	-5.652505	-0.831891	2.817243
59	1	0	-5.842844	0.887571	2.445647
60	6	0	-6.519482	0.569611	-0.253080
61	1	0	-6.230045	1.607239	-0.054952
62	1	0	-6.294699	0.353747	-1.301992
63	1	0	-7.602875	0.494070	-0.113065
64	1	0	-0.022418	5.788231	-0.966404
65	6	0	6.448866	-1.204536	1.290133
66	1	0	7.081520	-1.344828	0.409280
67	1	0	6.915969	-0.427721	1.906850
68	1	0	6.460576	-2.130746	1.871737

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=THF)

Excited State 1: Singlet-A 4.2930 eV 288.80 nm f=0.3140
<S**2>=0.000
117 ->120 -0.10573
118 ->120 -0.17773
119 ->120 0.63764

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1318.89733010 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1318.73959883 a.u.

Excited State 1: Singlet-A 4.2874 eV 289.19 nm f=0.2414
<S**2>=0.000
117 ->120 -0.10983
118 ->120 -0.20331
119 ->120 0.63178

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1318.68092730 a.u.
Lowest frequency = 16.8308

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.030337	0.510856	-0.135142
2	6	0	3.841079	1.162446	-1.013978
3	1	0	3.186424	0.989374	-1.874725
4	1	0	3.647056	2.188309	-0.685888
5	1	0	4.879702	1.111250	-1.353544
6	6	0	1.935529	2.721601	1.696057
7	1	0	2.004289	3.622020	2.313565
8	1	0	1.359183	1.968791	2.245034
9	1	0	2.944797	2.312645	1.588135
10	6	0	-0.204477	1.446016	-2.785521
11	1	0	0.582976	0.710875	-2.986785
12	1	0	-1.097641	0.882076	-2.493898
13	1	0	-0.439005	1.955542	-3.724469
14	6	0	0.452769	4.769061	-1.115559
15	6	0	1.083714	4.381040	0.060467
16	1	0	1.409675	5.138376	0.769393
17	6	0	1.293411	3.038960	0.367128
18	6	0	0.857386	2.014823	-0.527372
19	6	0	0.223885	2.435740	-1.732425
20	6	0	0.029515	3.788736	-2.001884
21	1	0	-0.448523	4.076201	-2.935324
22	6	0	2.170941	-1.170323	1.533483
23	6	0	3.307291	-1.800877	2.035094
24	1	0	3.188887	-2.549001	2.816716
25	6	0	4.586447	-1.491009	1.586749
26	6	0	4.697058	-0.504269	0.608183
27	1	0	5.685494	-0.244079	0.233855
28	6	0	3.589825	0.149577	0.077060
29	6	0	2.272788	-0.175042	0.521307
30	6	0	0.843798	-1.538995	2.145159
31	1	0	0.222427	-2.136375	1.468413
32	1	0	0.985383	-2.128272	3.055561
33	1	0	0.263145	-0.646569	2.405074
34	7	0	-0.166979	-0.399417	-0.432295
35	6	0	-0.164087	-1.529557	-1.244341
36	6	0	-1.444053	-0.251865	0.061030
37	6	0	-1.448666	-2.120175	-1.272106
38	6	0	0.913790	-2.073253	-1.935224
39	6	0	-2.291341	-1.277751	-0.425644
40	6	0	-1.661057	-3.266366	-2.006836
41	6	0	0.678694	-3.230313	-2.681361
42	1	0	1.894618	-1.618142	-1.881178
43	6	0	-3.617558	-1.302931	-0.060021
44	6	0	-0.581539	-3.817016	-2.717101
45	1	0	-2.636637	-3.740416	-2.039287
46	1	0	1.495156	-3.679736	-3.235932
47	6	0	-4.123527	-0.307908	0.801200
48	1	0	-4.281326	-2.079762	-0.427790
49	1	0	-0.735516	-4.719367	-3.298973

50	6	0	-3.266455	0.696380	1.269548
51	1	0	-3.658494	1.463852	1.928511
52	6	0	-1.926327	0.749481	0.908904
53	1	0	-1.274642	1.540762	1.256596
54	6	0	-5.584099	-0.330420	1.203060
55	1	0	-6.038378	-1.204187	0.722117
56	6	0	-5.749798	-0.494716	2.719344
57	1	0	-6.810793	-0.568960	2.977162
58	1	0	-5.246657	-1.396938	3.079249
59	1	0	-5.334477	0.362007	3.259844
60	6	0	-6.325512	0.915215	0.700092
61	1	0	-5.931135	1.825725	1.162699
62	1	0	-6.234468	1.021569	-0.384832
63	1	0	-7.389081	0.847809	0.949152
64	1	0	0.296753	5.820570	-1.337612
65	6	0	5.802215	-2.202971	2.119006
66	1	0	6.130030	-3.000720	1.440892
67	1	0	6.647958	-1.518444	2.239273
68	1	0	5.600142	-2.665073	3.089773

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1318.78168378 a.u.

Excited State 1: Singlet-A 2.7647 eV 448.45 nm f=0.0426
<S**2>=0.000
111 ->120 -0.11081
119 ->120 0.68271

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1318.87643495 a.u.

Results

Absorb Energy =	0.158 a.u.	4.292 eV	288.867 nm
Emission Energy =	0.095 a.u.	2.578 eV	480.874 nm
Stokes Shift =	0.063 a.u.	1.714 eV	192.007 nm

Compound E-2b ACN

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : Acetonitrile
SCF Done: E(RCAM-B3LYP) = -1318.81443232 a.u.
Lowest frequency = 21.3916

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	0.938238	0.460903	-0.108342
2	6	0	3.330107	0.975689	-1.953470
3	1	0	2.765187	0.360450	-2.662929
4	1	0	2.792650	1.920681	-1.845097
5	1	0	4.299677	1.188339	-2.410861
6	6	0	1.428643	2.577149	2.044183
7	1	0	1.668479	3.465580	2.633849
8	1	0	0.684684	2.004412	2.609559
9	1	0	2.328774	1.961583	1.977508
10	6	0	-0.281163	1.469319	-2.650367
11	1	0	0.470075	0.689848	-2.799179
12	1	0	-1.228882	0.964443	-2.435464
13	1	0	-0.399221	2.000738	-3.598273
14	6	0	0.152058	4.733297	-0.790022
15	6	0	0.660873	4.314843	0.430748
16	1	0	0.878129	5.045128	1.205218
17	6	0	0.905761	2.964364	0.681247
18	6	0	0.618020	1.999805	-0.308670
19	6	0	0.085062	2.433924	-1.544530
20	6	0	-0.128229	3.793456	-1.771189
21	1	0	-0.523236	4.115045	-2.730939
22	6	0	2.659175	-0.736047	1.406003
23	6	0	3.960292	-1.105950	1.739814
24	1	0	4.132285	-1.638996	2.672147
25	6	0	5.042897	-0.818781	0.913863
26	6	0	4.789894	-0.137222	-0.272109
27	1	0	5.617756	0.089054	-0.939924
28	6	0	3.505277	0.269679	-0.629807
29	6	0	2.409372	-0.027411	0.208046
30	6	0	1.552549	-1.129333	2.359209
31	1	0	0.994656	-1.992929	1.982221
32	1	0	1.965991	-1.404772	3.332866
33	1	0	0.828943	-0.326750	2.521640
34	7	0	-0.127133	-0.503518	-0.215407
35	6	0	-0.011230	-1.867941	-0.593620
36	6	0	-1.509566	-0.281223	0.028298
37	6	0	-1.278727	-2.475226	-0.591529
38	6	0	1.111988	-2.587039	-1.001834
39	6	0	-2.232265	-1.463932	-0.183442
40	6	0	-1.431132	-3.810357	-0.960771
41	6	0	0.945717	-3.917897	-1.364067
42	1	0	2.091615	-2.131733	-1.041281
43	6	0	-3.610046	-1.507786	0.024153
44	6	0	-0.310527	-4.532178	-1.341319
45	1	0	-2.413531	-4.272888	-0.955775
46	1	0	1.814587	-4.488357	-1.677214
47	6	0	-4.284056	-0.372804	0.455857
48	1	0	-4.156486	-2.431921	-0.145473
49	1	0	-0.407632	-5.573237	-1.632024
50	6	0	-3.539325	0.796350	0.684869
51	1	0	-4.047949	1.689423	1.036272
52	6	0	-2.167489	0.859790	0.487425
53	1	0	-1.635077	1.778459	0.690813
54	6	0	-5.784511	-0.401311	0.684754
55	1	0	-6.127000	-1.414210	0.440653
56	6	0	-6.142337	-0.132788	2.151360
57	1	0	-7.223487	-0.213820	2.304593
58	1	0	-5.648791	-0.847698	2.816785
59	1	0	-5.838051	0.874507	2.455457

60	6	0	-6.519861	0.572345	-0.243782
61	1	0	-6.230742	1.608897	-0.039559
62	1	0	-6.296995	0.362620	-1.294414
63	1	0	-7.602904	0.495186	-0.102405
64	1	0	-0.023199	5.788580	-0.977067
65	6	0	6.443934	-1.209287	1.304589
66	1	0	7.078513	-1.350845	0.425382
67	1	0	6.910495	-0.432764	1.922052
68	1	0	6.452499	-2.134934	1.887087

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=acetonitrile)

Excited State 1: Singlet-A 4.2985 eV 288.43 nm f=0.3049
<S**2>=0.000
117 ->120 -0.10603
118 ->120 -0.17192
119 ->120 0.63902

Step3

Method: cam-b3lyp/6-31+G(d,p)
SCRF(Solvent=acetonitrile,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1318.89875049 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1318.74045688 a.u.

Excited State 1: Singlet-A 4.2947 eV 288.69 nm f=0.2414
<S**2>=0.000
117 ->120 -0.11030
118 ->120 -0.19240
119 ->120 0.63458

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1318.68180722 a.u.
Lowest frequency = 17.4777

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.028804	0.507769	-0.135377
2	6	0	3.841729	1.146767	-1.022690
3	1	0	3.186559	0.968038	-1.881987
4	1	0	3.648125	2.174319	-0.699381
5	1	0	4.880130	1.093388	-1.362461
6	6	0	1.938711	2.718828	1.695824
7	1	0	2.008921	3.618767	2.313786

8	1	0	1.360337	1.966836	2.243850
9	1	0	2.947438	2.308618	1.586821
10	6	0	-0.201010	1.445224	-2.785784
11	1	0	0.585012	0.708143	-2.985395
12	1	0	-1.095196	0.883104	-2.493650
13	1	0	-0.434434	1.954307	-3.725220
14	6	0	0.460751	4.768674	-1.117181
15	6	0	1.090563	4.380035	0.059613
16	1	0	1.417093	5.137120	0.768549
17	6	0	1.297517	3.037456	0.366830
18	6	0	0.859602	2.013706	-0.526966
19	6	0	0.228539	2.434949	-1.733229
20	6	0	0.036399	3.788551	-2.003456
21	1	0	-0.440911	4.076397	-2.937149
22	6	0	2.169162	-1.167317	1.539454
23	6	0	3.304635	-1.798078	2.043968
24	1	0	3.184946	-2.541722	2.829648
25	6	0	4.584300	-1.494066	1.592546
26	6	0	4.696576	-0.513100	0.607928
27	1	0	5.685289	-0.257926	0.230921
28	6	0	3.590085	0.140337	0.074165
29	6	0	2.272905	-0.178476	0.521300
30	6	0	0.841156	-1.528928	2.153205
31	1	0	0.216847	-2.124871	1.477863
32	1	0	0.980659	-2.116768	3.064825
33	1	0	0.264362	-0.633217	2.410500
34	7	0	-0.166687	-0.398808	-0.431844
35	6	0	-0.165708	-1.528221	-1.246586
36	6	0	-1.444983	-0.250808	0.062052
37	6	0	-1.450942	-2.116903	-1.274793
38	6	0	0.910185	-2.068883	-1.942717
39	6	0	-2.292866	-1.274569	-0.426947
40	6	0	-1.665567	-3.260402	-2.013292
41	6	0	0.673442	-3.223903	-2.691751
42	1	0	1.890367	-1.611510	-1.893602
43	6	0	-3.619203	-1.299622	-0.061312
44	6	0	-0.587251	-3.809917	-2.726428
45	1	0	-2.641870	-3.732556	-2.047533
46	1	0	1.488157	-3.671185	-3.250591
47	6	0	-4.124090	-0.305998	0.802267
48	1	0	-4.283435	-2.075359	-0.430124
49	1	0	-0.743085	-4.710099	-3.311072
50	6	0	-3.265737	0.695333	1.274567
51	1	0	-3.656236	1.460338	1.937315
52	6	0	-1.925138	0.747193	0.914461
53	1	0	-1.271441	1.533939	1.268996
54	6	0	-5.584800	-0.328018	1.203566
55	1	0	-6.040107	-1.199047	0.719027
56	6	0	-5.751108	-0.497914	2.719166
57	1	0	-6.812409	-0.571590	2.975857
58	1	0	-5.249815	-1.402706	3.075275
59	1	0	-5.334681	0.356105	3.263154
60	6	0	-6.323860	0.920921	0.705372
61	1	0	-5.928142	1.828917	1.171903
62	1	0	-6.232556	1.030810	-0.379224
63	1	0	-7.387557	0.853897	0.953924
64	1	0	0.306468	5.820345	-1.339694
65	6	0	5.798858	-2.205948	2.127921
66	1	0	6.123725	-3.008429	1.454054
67	1	0	6.646630	-1.523034	2.242723

68	1	0	5.596507	-2.661969	3.101452

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1) SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1318.78593024 a.u.

Excited State 1: Singlet-A 2.7214 eV 455.60 nm f=0.0435 <S**2>=0.000
111 ->120 -0.10988
119 ->120 0.68258

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=acetonitrile, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1318.87666374 a.u.

Results

Absorb Energy =	0.158 a.u.	4.307 eV	287.841 nm
Emission Energy =	0.091 a.u.	2.469 eV	502.167 nm
Stokes Shift =	0.068 a.u.	1.838 eV	214.326 nm

Compound 3 n-hexane

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : n-Hexane
SCF Done: E(RCAM-B3LYP) = -1472.58034145 a.u.
Lowest frequency = 19.0630

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.736475	1.946576	-0.287227
2	6	0	2.407101	0.710493	0.056853
3	6	0	1.416186	-0.275036	0.175635
4	7	0	0.135808	0.289770	-0.063650
5	6	0	0.366626	1.665942	-0.343754
6	6	0	-0.531171	2.670000	-0.714162
7	6	0	-0.038490	3.934183	-0.979012
8	6	0	1.333840	4.220870	-0.899449
9	6	0	2.234782	3.223059	-0.558535
10	6	0	3.748547	0.406111	0.280755
11	6	0	4.119486	-0.883567	0.635091
12	6	0	3.110726	-1.851704	0.769590
13	6	0	1.770034	-1.569823	0.555077
14	6	0	5.576083	-1.232932	0.880560
15	6	0	5.819484	-1.679758	2.326911

16	6	0	6.083228	-2.287462	-0.110154
17	8	0	1.676634	5.507909	-1.185844
18	6	0	3.043216	5.854538	-1.126857
19	1	0	-1.592412	2.480355	-0.795281
20	1	0	-0.709355	4.737843	-1.262349
21	1	0	3.300314	3.410492	-0.507885
22	1	0	4.505504	1.180507	0.184583
23	1	0	3.381466	-2.863402	1.057813
24	1	0	1.027559	-2.345430	0.681586
25	1	0	6.157745	-0.317446	0.715345
26	1	0	6.883844	-1.872287	2.498286
27	1	0	5.491052	-0.915708	3.037807
28	1	0	5.274631	-2.602515	2.553164
29	1	0	7.149292	-2.483687	0.045783
30	1	0	5.943379	-1.958761	-1.144282
31	1	0	5.549376	-3.235744	0.013727
32	1	0	3.099951	6.913181	-1.381510
33	1	0	3.636235	5.277575	-1.846827
34	1	0	3.453711	5.702091	-0.121289
35	5	0	-1.133288	-0.387095	-0.023187
36	6	0	-1.200560	-1.942842	-0.305932
37	6	0	-0.750659	-2.442997	-1.548724
38	6	0	-1.764509	-2.853398	0.612512
39	6	0	-0.883840	-3.797699	-1.845139
40	6	0	-1.858793	-4.205438	0.288743
41	6	0	-1.427211	-4.700341	-0.937212
42	1	0	-0.549420	-4.158517	-2.815250
43	1	0	-2.289950	-4.890935	1.014717
44	6	0	-2.446567	0.434137	0.301952
45	6	0	-3.560763	0.451023	-0.563679
46	6	0	-2.548276	1.122463	1.532096
47	6	0	-4.716165	1.141435	-0.202945
48	6	0	-3.728904	1.781673	1.867209
49	6	0	-4.823824	1.812818	1.010233
50	1	0	-5.560131	1.148248	-0.888854
51	1	0	-3.792943	2.289165	2.827123
52	6	0	-2.240841	-2.415822	1.977358
53	1	0	-1.415522	-2.028459	2.585338
54	1	0	-2.993094	-1.625949	1.912902
55	1	0	-2.677923	-3.255952	2.523261
56	6	0	-0.109588	-1.556765	-2.593128
57	1	0	-0.620707	-0.597857	-2.707821
58	1	0	0.931520	-1.335227	-2.336021
59	1	0	-0.109887	-2.051405	-3.568127
60	6	0	-1.524824	-6.167589	-1.262629
61	1	0	-1.672461	-6.330029	-2.334140
62	1	0	-0.608025	-6.696736	-0.976951
63	1	0	-2.353562	-6.641016	-0.728601
64	6	0	-1.406461	1.183086	2.521865
65	1	0	-0.897670	0.223453	2.641226
66	1	0	-0.649892	1.909235	2.206826
67	1	0	-1.768665	1.491012	3.506367
68	6	0	-3.533579	-0.230164	-1.911506
69	1	0	-2.778465	0.212519	-2.570700
70	1	0	-3.303091	-1.294778	-1.825663
71	1	0	-4.499046	-0.132251	-2.414635
72	6	0	-6.075715	2.566507	1.374719
73	1	0	-6.013534	3.612772	1.052937
74	1	0	-6.957789	2.130963	0.896838
75	1	0	-6.239773	2.569026	2.456108

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=n-hexane)

Excited State 1: Singlet-A 4.1967 eV 295.43 nm f=0.3858 <S**2>=0.000

128	->132	-0.10792
130	->132	-0.17540
131	->132	0.63008
131	->133	0.10706

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1472.67321682 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1472.52023867 a.u.

Excited State 1: Singlet-A 4.1774 eV 296.80 nm f=0.2923 <S**2>=0.000

128	->132	0.12290
130	->132	0.16653
131	->132	-0.63942

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes) TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1472.45320976 a.u.
Lowest frequency = 19.2514

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.968197	1.595169	-0.589856
2	6	0	2.464654	0.424461	0.124058
3	6	0	1.328000	-0.355330	0.413213
4	7	0	0.174252	0.259191	-0.084266
5	6	0	0.556766	1.418521	-0.680058
6	6	0	-0.256923	2.384316	-1.305160
7	6	0	0.354452	3.490439	-1.845720
8	6	0	1.752213	3.662637	-1.764690
9	6	0	2.571514	2.709488	-1.126350
10	6	0	3.717968	-0.005741	0.514250
11	6	0	3.853543	-1.223391	1.201280
12	6	0	2.708656	-1.979555	1.467641
13	6	0	1.434680	-1.569464	1.075506
14	6	0	5.225975	-1.704889	1.633890
15	6	0	5.327847	-1.832873	3.158684
16	6	0	5.608160	-3.020933	0.945429

17	8	0	2.219282	4.788285	-2.323973
18	6	0	3.612360	5.061565	-2.284607
19	1	0	-1.330864	2.256715	-1.335468
20	1	0	-0.219735	4.267333	-2.336306
21	1	0	3.642893	2.848734	-1.057975
22	1	0	4.602540	0.585815	0.293735
23	1	0	2.807997	-2.925172	1.991213
24	1	0	0.559300	-2.178190	1.263957
25	1	0	5.949020	-0.943454	1.316807
26	1	0	6.341919	-2.123174	3.451461
27	1	0	5.085925	-0.888080	3.654281
28	1	0	4.640929	-2.595966	3.539146
29	1	0	6.623718	-3.318665	1.225395
30	1	0	5.567066	-2.926633	-0.143666
31	1	0	4.931678	-3.831134	1.236669
32	1	0	3.740981	6.014799	-2.794965
33	1	0	4.180643	4.286677	-2.808548
34	1	0	3.967218	5.148283	-1.252829
35	5	0	-1.270631	-0.286635	-0.011176
36	6	0	-1.515790	-1.675897	-0.675570
37	6	0	-0.914909	-2.083818	-1.900422
38	6	0	-2.349764	-2.638396	-0.028305
39	6	0	-1.134714	-3.356961	-2.418507
40	6	0	-2.542342	-3.898579	-0.584369
41	6	0	-1.943317	-4.289951	-1.779630
42	1	0	-0.670009	-3.623415	-3.366109
43	1	0	-3.174767	-4.609859	-0.056083
44	6	0	-2.292595	0.631139	0.725777
45	6	0	-3.597053	0.834145	0.180290
46	6	0	-1.984223	1.352454	1.914043
47	6	0	-4.491978	1.706807	0.789537
48	6	0	-2.911670	2.216881	2.488794
49	6	0	-4.175250	2.418664	1.944997
50	1	0	-5.472255	1.847561	0.337600
51	1	0	-2.643800	2.737083	3.406710
52	6	0	-3.012322	-2.363630	1.300698
53	1	0	-2.303257	-1.940470	2.019875
54	1	0	-3.830264	-1.640976	1.223415
55	1	0	-3.421678	-3.286642	1.722037
56	6	0	-0.069837	-1.142330	-2.720416
57	1	0	-0.549511	-0.162431	-2.824388
58	1	0	0.917106	-0.970916	-2.276389
59	1	0	0.094778	-1.544264	-3.724261
60	6	0	-2.146436	-5.672673	-2.340514
61	1	0	-1.928088	-5.703820	-3.412217
62	1	0	-1.491380	-6.406339	-1.853963
63	1	0	-3.175474	-6.017415	-2.196294
64	6	0	-0.675699	1.157933	2.637845
65	1	0	-0.424056	0.095190	2.727609
66	1	0	0.165437	1.640675	2.128073
67	1	0	-0.724071	1.578487	3.646473
68	6	0	-4.041663	0.165384	-1.098201
69	1	0	-3.290424	0.278203	-1.887560
70	1	0	-4.192990	-0.911752	-0.979660
71	1	0	-4.982246	0.598518	-1.451288
72	6	0	-5.155966	3.378786	2.564696
73	1	0	-5.162708	4.343378	2.041625
74	1	0	-6.178146	2.988273	2.528246
75	1	0	-4.909510	3.579321	3.611664

Step6

 Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Save)
 After PCM corrections, the energy is -1472.55468574 a.u.

 Excited State   1:   Singlet-A   2.6902 eV 460.88 nm f=0.0430
<S**2>=0.000
     123 ->132   -0.10790
     131 ->132   0.68027

Step7

  Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,
NonEquilibrium=Read)

 SCF Done: E(RCAM-B3LYP) = -1472.65176275 a.u.

Results

Absorb Energy =	0.153 a.u.	4.163 eV	297.842 nm
Emission Energy =	0.097 a.u.	2.642 eV	469.353 nm
Stokes Shift =	0.056 a.u.	1.521 eV	171.510 nm

Compound 3 THF

Step1

 Method: cam-b3lyp/6-31G(d)
 Solvent : TetraHydroFuran
 SCF Done: E(RCAM-B3LYP) = -1472.58418081 a.u.
 Lowest frequency = 19.4662

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.723028	1.954955	-0.289264
2	6	0	2.400667	0.722608	0.055733
3	6	0	1.414915	-0.268489	0.174124
4	7	0	0.131597	0.288779	-0.066225
5	6	0	0.354540	1.665698	-0.347041
6	6	0	-0.548427	2.664052	-0.720362
7	6	0	-0.062666	3.931404	-0.985341
8	6	0	1.308199	4.226749	-0.903196
9	6	0	2.214914	3.234218	-0.560458
10	6	0	3.744360	0.426678	0.280677
11	6	0	4.122381	-0.861046	0.636064
12	6	0	3.118691	-1.835190	0.770893
13	6	0	1.776270	-1.561058	0.555168
14	6	0	5.580915	-1.201859	0.882902
15	6	0	5.825627	-1.645271	2.330152
16	6	0	6.094065	-2.255847	-0.105395
17	8	0	1.644350	5.515362	-1.189377
18	6	0	3.011832	5.870790	-1.126516

19	1	0	-1.608096	2.467709	-0.805561
20	1	0	-0.739409	4.729435	-1.271258
21	1	0	3.279180	3.428087	-0.508648
22	1	0	4.496516	1.205621	0.184619
23	1	0	3.394844	-2.844927	1.060747
24	1	0	1.038140	-2.340440	0.683785
25	1	0	6.157362	-0.283634	0.716399
26	1	0	6.891014	-1.831735	2.501171
27	1	0	5.494319	-0.881131	3.039847
28	1	0	5.285642	-2.570660	2.557534
29	1	0	7.160984	-2.445160	0.052479
30	1	0	5.954479	-1.929504	-1.140460
31	1	0	5.565488	-3.206891	0.020370
32	1	0	3.062686	6.929440	-1.381264
33	1	0	3.608631	5.296638	-1.844626
34	1	0	3.418714	5.720453	-0.119859
35	5	0	-1.134413	-0.395128	-0.024536
36	6	0	-1.191929	-1.951121	-0.309048
37	6	0	-0.745815	-2.444189	-1.556476
38	6	0	-1.739584	-2.869566	0.611502
39	6	0	-0.867431	-3.799637	-1.855488
40	6	0	-1.823592	-4.222108	0.284754
41	6	0	-1.395660	-4.710156	-0.945573
42	1	0	-0.536854	-4.154797	-2.828955
43	1	0	-2.242778	-4.913485	1.012116
44	6	0	-2.450492	0.420640	0.304344
45	6	0	-3.564649	0.442968	-0.561304
46	6	0	-2.552851	1.100863	1.539398
47	6	0	-4.721715	1.128761	-0.195080
48	6	0	-3.734295	1.756538	1.879535
49	6	0	-4.830124	1.791890	1.022911
50	1	0	-5.565833	1.139002	-0.880715
51	1	0	-3.799049	2.256835	2.843131
52	6	0	-2.204678	-2.441820	1.983324
53	1	0	-1.368798	-2.084174	2.595232
54	1	0	-2.937314	-1.632846	1.932546
55	1	0	-2.660918	-3.279460	2.517068
56	6	0	-0.122906	-1.547984	-2.603575
57	1	0	-0.656186	-0.601624	-2.722541
58	1	0	0.912638	-1.301864	-2.346272
59	1	0	-0.110668	-2.046335	-3.576472
60	6	0	-1.481510	-6.177521	-1.273999
61	1	0	-1.634677	-6.338570	-2.344864
62	1	0	-0.557250	-6.697697	-0.996202
63	1	0	-2.301075	-6.660183	-0.734275
64	6	0	-1.410866	1.154496	2.529660
65	1	0	-0.910748	0.190523	2.651403
66	1	0	-0.647835	1.873446	2.213515
67	1	0	-1.770881	1.467862	3.513127
68	6	0	-3.534867	-0.222086	-1.917095
69	1	0	-2.808374	0.257989	-2.582484
70	1	0	-3.261708	-1.277706	-1.848363
71	1	0	-4.511528	-0.155507	-2.403276
72	6	0	-6.083262	2.540682	1.393446
73	1	0	-6.021679	3.589672	1.080680
74	1	0	-6.964214	2.108585	0.910590
75	1	0	-6.247171	2.534076	2.474770

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=THF)

Excited State 1: Singlet-A 4.2070 eV 294.71 nm f=0.3935 <S**2>=0.000

128	->132	-0.10707
130	->132	-0.16593
131	->132	0.63014
131	->133	0.11886

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1472.67750689 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1472.52343268 a.u.

Excited State 1: Singlet-A 4.1922 eV 295.75 nm f=0.2965 <S**2>=0.000

128	->132	-0.12306
130	->132	-0.16057
131	->132	0.63890

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes) TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1472.45578923 a.u.
Lowest frequency = 19.7458

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.959332	1.603678	-0.586182
2	6	0	2.462300	0.429632	0.120116
3	6	0	1.330362	-0.357457	0.408025
4	7	0	0.171718	0.253951	-0.086156
5	6	0	0.550578	1.421922	-0.677943
6	6	0	-0.265169	2.381329	-1.306654
7	6	0	0.342155	3.494171	-1.840822
8	6	0	1.738144	3.674857	-1.752862
9	6	0	2.560232	2.721948	-1.116547
10	6	0	3.718297	0.005177	0.506344
11	6	0	3.860991	-1.214846	1.189629
12	6	0	2.720504	-1.976419	1.459821
13	6	0	1.443392	-1.570104	1.072366
14	6	0	5.237281	-1.690363	1.616245
15	6	0	5.345627	-1.818342	3.140651
16	6	0	5.621280	-3.005026	0.926075
17	8	0	2.201780	4.803658	-2.305651
18	6	0	3.597045	5.082390	-2.261701
19	1	0	-1.337823	2.245356	-1.351521

20	1	0	-0.235899	4.266129	-2.334856
21	1	0	3.630938	2.863962	-1.046883
22	1	0	4.598596	0.602771	0.286597
23	1	0	2.824823	-2.921007	1.984210
24	1	0	0.570602	-2.179402	1.271512
25	1	0	5.955294	-0.926100	1.296104
26	1	0	6.362405	-2.104573	3.427799
27	1	0	5.103451	-0.873858	3.636915
28	1	0	4.663373	-2.584359	3.523837
29	1	0	6.639363	-3.297495	1.202142
30	1	0	5.576293	-2.909968	-0.162911
31	1	0	4.949484	-3.818041	1.220643
32	1	0	3.722468	6.038256	-2.767404
33	1	0	4.167328	4.311424	-2.787916
34	1	0	3.947173	5.165121	-1.228669
35	5	0	-1.262213	-0.291672	-0.010156
36	6	0	-1.511998	-1.687287	-0.666005
37	6	0	-0.908239	-2.099434	-1.888265
38	6	0	-2.351080	-2.645633	-0.019910
39	6	0	-1.124186	-3.376718	-2.400672
40	6	0	-2.540652	-3.909501	-0.569763
41	6	0	-1.934275	-4.307716	-1.759997
42	1	0	-0.654747	-3.647674	-3.344684
43	1	0	-3.175580	-4.618278	-0.040997
44	6	0	-2.292691	0.629255	0.719151
45	6	0	-3.591648	0.837223	0.164655
46	6	0	-1.991791	1.343256	1.913390
47	6	0	-4.490850	1.708901	0.770362
48	6	0	-2.922417	2.208114	2.485002
49	6	0	-4.181665	2.415066	1.932149
50	1	0	-5.466791	1.854766	0.310625
51	1	0	-2.659885	2.725013	3.406322
52	6	0	-3.024997	-2.360998	1.301185
53	1	0	-2.324368	-1.921182	2.018278
54	1	0	-3.849580	-1.647551	1.206635
55	1	0	-3.428916	-3.282047	1.731903
56	6	0	-0.063898	-1.159163	-2.710448
57	1	0	-0.546646	-0.181308	-2.819257
58	1	0	0.920362	-0.980464	-2.263310
59	1	0	0.106168	-1.565598	-3.711579
60	6	0	-2.132819	-5.694354	-2.313617
61	1	0	-1.909629	-5.731683	-3.384047
62	1	0	-1.478267	-6.423497	-1.819816
63	1	0	-3.161456	-6.040604	-2.170483
64	6	0	-0.687781	1.144078	2.643976
65	1	0	-0.445306	0.079911	2.744279
66	1	0	0.158521	1.613526	2.130319
67	1	0	-0.734980	1.575910	3.647874
68	6	0	-4.024410	0.174851	-1.121213
69	1	0	-3.262806	0.289954	-1.900445
70	1	0	-4.179932	-0.902311	-1.006608
71	1	0	-4.959743	0.611538	-1.483650
72	6	0	-5.165266	3.374969	2.548424
73	1	0	-5.164230	4.341914	2.029877
74	1	0	-6.188331	2.988224	2.500186
75	1	0	-4.927036	3.569907	3.598266

Step6

```
 Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Save)
 After PCM corrections, the energy is -1472.56810644 a.u.

 Excited State   1:      Singlet-A      2.5539 eV  485.46 nm  f=0.0479
<S**2>=0.000
     123 ->132        -0.10457
     131 ->132         0.68053

Step7

  Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF, NonEquilibrium=Read)

 SCF Done: E(RCAM-B3LYP) = -1472.65375269 a.u.

                              Results
 ------------------------------------------------------------------------
     Absorb Energy     =  | 0.154 a.u. | 4.193 eV | 295.723 nm
 --------------------------|------------|----------|----------------
     Emission Energy   =  | 0.086 a.u. | 2.331 eV | 531.995 nm
 --------------------------|------------|----------|----------------
     Stokes Shift      =  | 0.068 a.u. | 1.862 eV | 236.271 nm
 ------------------------------------------------------------------------

Compound 3 ACN

Step1

 Method: cam-b3lyp/6-31G(d)
 Solvent : Acetonitrile
 SCF Done: E(RCAM-B3LYP) = -1472.58576987 a.u.
 Lowest frequency =  19.6517

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.713445    1.960947   -0.289273
      2          6           0        2.395975    0.731630    0.057389
      3          6           0        1.413870   -0.263106    0.177198
      4          7           0        0.128586    0.288628   -0.064482
      5          6           0        0.345967    1.665872   -0.347091
      6          6           0       -0.560726    2.659848   -0.723141
      7          6           0       -0.079826    3.928905   -0.989792
      8          6           0        1.289935    4.230184   -0.906788
      9          6           0        2.200639    3.241805   -0.561947
     10          6           0        3.741077    0.441437    0.282643
     11          6           0        4.123948   -0.844420    0.640245
     12          6           0        3.123763   -1.822204    0.777498
     13          6           0        1.780168   -1.553513    0.561312
     14          6           0        5.583943   -1.179377    0.886768
     15          6           0        5.830837   -1.622133    2.333843
     16          6           0        6.100619   -2.231478   -0.101743
     17          8           0        1.621098    5.519650   -1.194438
     18          6           0        2.988485    5.880552   -1.133258
     19          1           0       -1.619333    2.458735   -0.810388
     20          1           0       -0.760135    4.723069   -1.278255
     21          1           0        3.264074    3.439987   -0.509634
     22          1           0        4.490097    1.223126    0.184990
```

23	1	0	3.403654	-2.830169	1.069918
24	1	0	1.044888	-2.335117	0.692783
25	1	0	6.156606	-0.258968	0.720096
26	1	0	6.897113	-1.803930	2.503987
27	1	0	5.497170	-0.859207	3.043847
28	1	0	5.295041	-2.549972	2.561239
29	1	0	7.168139	-2.416828	0.056392
30	1	0	5.960558	-1.905102	-1.136809
31	1	0	5.575355	-3.184401	0.023945
32	1	0	3.035009	6.938884	-1.389787
33	1	0	3.586230	5.307218	-1.850863
34	1	0	3.396258	5.733171	-0.126791
35	5	0	-1.134936	-0.400622	-0.023692
36	6	0	-1.184920	-1.956272	-0.311550
37	6	0	-0.736522	-2.443227	-1.560842
38	6	0	-1.725862	-2.880788	0.606963
39	6	0	-0.849143	-3.798748	-1.863365
40	6	0	-1.801451	-4.233190	0.276529
41	6	0	-1.370698	-4.715321	-0.955255
42	1	0	-0.517253	-4.149169	-2.838082
43	1	0	-2.215639	-4.929223	1.002276
44	6	0	-2.453395	0.410559	0.307203
45	6	0	-3.567200	0.434709	-0.558876
46	6	0	-2.557160	1.086146	1.544855
47	6	0	-4.725797	1.117066	-0.190251
48	6	0	-3.739739	1.738851	1.887218
49	6	0	-4.835644	1.775541	1.030305
50	1	0	-5.569688	1.128572	-0.876120
51	1	0	-3.805716	2.235162	2.852771
52	6	0	-2.190884	-2.460823	1.981236
53	1	0	-1.352894	-2.117464	2.598443
54	1	0	-2.914928	-1.643886	1.936135
55	1	0	-2.656874	-3.298641	2.506140
56	6	0	-0.121911	-1.539749	-2.606737
57	1	0	-0.666067	-0.599622	-2.726299
58	1	0	0.910401	-1.281785	-2.347993
59	1	0	-0.102489	-2.037748	-3.579636
60	6	0	-1.446837	-6.182380	-1.287395
61	1	0	-1.602428	-6.341635	-2.358153
62	1	0	-0.517533	-6.696023	-1.014409
63	1	0	-2.260434	-6.672580	-0.745527
64	6	0	-1.415465	1.136795	2.535733
65	1	0	-0.919227	0.170902	2.658686
66	1	0	-0.649434	1.852478	2.219330
67	1	0	-1.774810	1.452513	3.518637
68	6	0	-3.535080	-0.222505	-1.918429
69	1	0	-2.820036	0.273224	-2.584776
70	1	0	-3.244560	-1.273951	-1.857631
71	1	0	-4.515370	-0.168526	-2.398758
72	6	0	-6.090278	2.520555	1.403457
73	1	0	-6.031317	3.570235	1.092562
74	1	0	-6.970480	2.087483	0.920180
75	1	0	-6.252954	2.511667	2.484911

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=acetonitrile)

```
 Excited State   1:      Singlet-A      4.2119 eV  294.37 nm  f=0.3827
<S**2>=0.000
     128 ->132        -0.10727
     130 ->132        -0.16112
     131 ->132         0.63112
     131 ->133         0.11895

Step3

 Method: cam-b3lyp/6-31+G(d,p)
SCRF(Solvent=acetonitrile,NonEquilibrium=Save)
 SCF Done: E(RCAM-B3LYP) = -1472.67930140 a.u.

Step4

 Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
 SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Read)

 After PCM corrections, the energy is -1472.52455129 a.u.

 Excited State   1:      Singlet-A      4.2020 eV  295.06 nm  f=0.2990
<S**2>=0.000
     128 ->132        -0.12160
     130 ->132        -0.15788
     131 ->132         0.63812

Step5

 Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

 Total Energy, E(TD-HF/TD-DFT) = -1472.45693756 a.u.
 Lowest frequency =  18.2327

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        1.960925    1.605148   -0.586342
      2          6           0        2.459223    0.426050    0.116046
      3          6           0        1.324335   -0.358289    0.399942
      4          7           0        0.168192    0.258464   -0.093836
      5          6           0        0.552495    1.428396   -0.682300
      6          6           0       -0.258658    2.390990   -1.310295
      7          6           0        0.353049    3.506084   -1.836228
      8          6           0        1.748804    3.683721   -1.741263
      9          6           0        2.566640    2.724613   -1.108186
     10          6           0        3.712757   -0.002437    0.505132
     11          6           0        3.849552   -1.223721    1.188297
     12          6           0        2.706080   -1.981632    1.456545
     13          6           0        1.431149   -1.570682    1.066320
     14          6           0        5.223191   -1.703390    1.618625
     15          6           0        5.326325   -1.832987    3.143281
     16          6           0        5.604921   -3.018866    0.928685
     17          8           0        2.217457    4.814613   -2.284870
     18          6           0        3.614659    5.088739   -2.234268
     19          1           0       -1.331082    2.254919   -1.364499
     20          1           0       -0.221927    4.280522   -2.330083
     21          1           0        3.637388    2.863287   -1.034242
```

22	1	0	4.595223	0.592955	0.288887
23	1	0	2.805907	-2.925773	1.982623
24	1	0	0.555405	-2.175630	1.267304
25	1	0	5.944249	-0.941163	1.301205
26	1	0	6.341570	-2.122185	3.432751
27	1	0	5.085878	-0.887916	3.639349
28	1	0	4.640873	-2.597519	3.523841
29	1	0	6.621038	-3.314649	1.208328
30	1	0	5.564757	-2.922290	-0.160404
31	1	0	4.929252	-3.829787	1.220379
32	1	0	3.744506	6.047786	-2.732649
33	1	0	4.183558	4.319524	-2.764076
34	1	0	3.961041	5.162600	-1.199543
35	5	0	-1.262877	-0.283735	-0.016858
36	6	0	-1.507249	-1.684944	-0.669166
37	6	0	-0.925887	-2.083014	-1.905709
38	6	0	-2.314798	-2.656863	-0.005846
39	6	0	-1.136498	-3.361412	-2.419090
40	6	0	-2.500904	-3.921593	-0.555916
41	6	0	-1.918673	-4.305863	-1.763064
42	1	0	-0.685359	-3.622382	-3.374759
43	1	0	-3.111996	-4.641683	-0.014531
44	6	0	-2.297623	0.631466	0.712756
45	6	0	-3.606305	0.817906	0.172269
46	6	0	-1.992061	1.361003	1.897019
47	6	0	-4.507813	1.686963	0.778132
48	6	0	-2.925453	2.223118	2.469129
49	6	0	-4.192899	2.410974	1.927986
50	1	0	-5.490487	1.816996	0.328078
51	1	0	-2.658026	2.753168	3.381545
52	6	0	-2.954005	-2.384115	1.334863
53	1	0	-2.230869	-1.955785	2.037357
54	1	0	-3.777201	-1.665951	1.268304
55	1	0	-3.350325	-3.307799	1.766890
56	6	0	-0.110638	-1.126673	-2.738453
57	1	0	-0.605567	-0.152620	-2.825073
58	1	0	0.881219	-0.941463	-2.310875
59	1	0	0.041577	-1.521432	-3.747084
60	6	0	-2.112394	-5.692650	-2.318505
61	1	0	-1.913355	-5.722503	-3.393863
62	1	0	-1.437255	-6.415137	-1.843148
63	1	0	-3.132741	-6.052912	-2.152743
64	6	0	-0.678662	1.182436	2.615857
65	1	0	-0.415586	0.122538	2.705624
66	1	0	0.154284	1.671249	2.098217
67	1	0	-0.725684	1.607150	3.622791
68	6	0	-4.047344	0.135310	-1.100003
69	1	0	-3.296436	0.250559	-1.889515
70	1	0	-4.189133	-0.942062	-0.969666
71	1	0	-4.992037	0.556869	-1.455890
72	6	0	-5.179592	3.368301	2.543387
73	1	0	-5.195033	4.328162	2.012084
74	1	0	-6.199034	2.970436	2.511823
75	1	0	-4.931089	3.579911	3.587565

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Save)

After PCM corrections, the energy is -1472.57319406 a.u.

Excited State 1: Singlet-A 2.5096 eV 494.05 nm f=0.0504
<S**2>=0.000
123 ->132 0.10339
131 ->132 -0.68065

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=acetonitrile,
NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1472.65438144 a.u.

Results

Absorb Energy =	0.155 a.u.	4.211 eV	294.432 nm
Emission Energy =	0.081 a.u.	2.209 eV	561.212 nm
Stokes Shift =	0.074 a.u.	2.002 eV	266.780 nm

Compound 4 n-hexane

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : n-Hexane
SCF Done: E(RCAM-B3LYP) = -1695.06807929 a.u.
Lowest frequency = 15.5059

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.231344	0.568713	-0.120318
2	6	0	-1.526621	1.796244	0.181088
3	6	0	-0.163739	1.476720	0.245470
4	7	0	0.023641	0.087654	0.010571
5	6	0	-1.265502	-0.449756	-0.209064
6	6	0	-1.642399	-1.749906	-0.549191
7	6	0	-2.986439	-2.013142	-0.755608
8	6	0	-3.949544	-1.004084	-0.643864
9	6	0	-3.577633	0.294025	-0.332663
10	6	0	-1.968852	3.097568	0.411711
11	6	0	-1.055002	4.095816	0.718613
12	6	0	0.304774	3.751238	0.799101
13	6	0	0.765397	2.462652	0.576610
14	6	0	-1.516285	5.519731	0.970634
15	6	0	-1.202027	5.975638	2.400342
16	6	0	-0.931988	6.496565	-0.056514
17	1	0	-0.914034	-2.541406	-0.654233
18	1	0	-3.296902	-3.017622	-1.021533
19	1	0	-4.322992	1.078842	-0.268294
20	1	0	-3.029247	3.329948	0.357559
21	1	0	1.031629	4.518295	1.050090
22	1	0	1.820670	2.242302	0.659228

23	1	0	-2.606884	5.529081	0.852825
24	1	0	-1.593795	6.982391	2.579162
25	1	0	-1.645337	5.300116	3.137970
26	1	0	-0.121798	6.003409	2.579032
27	1	0	-1.320891	7.506999	0.107173
28	1	0	-1.182972	6.194756	-1.077733
29	1	0	0.159618	6.544565	0.019102
30	5	0	1.278814	-0.630882	-0.000603
31	6	0	2.604940	0.131413	-0.391706
32	6	0	2.700862	0.766757	-1.649658
33	6	0	3.739423	0.139974	0.448916
34	6	0	3.895945	1.370758	-2.035531
35	6	0	4.907474	0.777031	0.037745
36	6	0	5.009561	1.397489	-1.203712
37	1	0	3.956088	1.837381	-3.016067
38	1	0	5.766632	0.781777	0.704515
39	6	0	1.298487	-2.163320	0.379889
40	6	0	1.853339	-3.140122	-0.475539
41	6	0	0.815616	-2.576757	1.641390
42	6	0	1.898128	-4.473324	-0.075563
43	6	0	0.902225	-3.916289	2.015450
44	6	0	1.429751	-4.884606	1.168638
45	1	0	2.319338	-5.212009	-0.753530
46	1	0	0.542927	-4.211417	2.998637
47	6	0	3.724450	-0.501559	1.816732
48	1	0	2.937589	-0.083529	2.453619
49	1	0	3.551571	-1.579235	1.757593
50	1	0	4.676380	-0.340123	2.329102
51	6	0	1.542142	0.826691	-2.619878
52	1	0	0.989474	-0.114095	-2.681546
53	1	0	0.824435	1.601400	-2.330245
54	1	0	1.897128	1.067718	-3.625311
55	6	0	6.278571	2.092053	-1.621906
56	1	0	6.368777	2.137348	-2.710706
57	1	0	6.304652	3.122546	-1.248579
58	1	0	7.162000	1.581980	-1.227055
59	6	0	0.192839	-1.614903	2.628831
60	1	0	0.711841	-0.654442	2.673708
61	1	0	-0.850221	-1.403129	2.370625
62	1	0	0.199823	-2.042257	3.634990
63	6	0	2.382891	-2.791830	-1.846988
64	1	0	1.616756	-2.319650	-2.471191
65	1	0	3.225340	-2.097558	-1.792042
66	1	0	2.719291	-3.690366	-2.370582
67	6	0	1.474705	-6.333967	1.574656
68	1	0	0.579641	-6.866328	1.232040
69	1	0	2.340596	-6.843372	1.142125
70	1	0	1.522213	-6.442863	2.661689
71	6	0	-5.393467	-1.351506	-0.823158
72	9	0	-5.925731	-1.890883	0.292006
73	9	0	-5.573535	-2.255067	-1.804806
74	9	0	-6.141063	-0.275455	-1.126407

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=n-hexane)

Excited State 1: Singlet-A 4.2399 eV 292.43 nm f=0.2926
<S**2>=0.000

```
     135 ->140         0.10564
     138 ->140         0.15373
     139 ->140         0.64708

Step3

 Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,NonEquilibrium=Save)
 SCF Done: E(RCAM-B3LYP) = -1695.17723825 a.u.

Step4

 Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
 SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Read)

 After PCM corrections, the energy is -1695.02133983 a.u.

 Excited State   1:      Singlet-A      4.2437 eV  292.16 nm  f=0.2332
<S**2>=0.000
     135 ->140         0.10767
     138 ->140         0.16668
     139 ->140         0.64270

Step5

 Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

 Total Energy, E(TD-HF/TD-DFT) = -1694.93295102 a.u.
 Lowest frequency =  14.9584

                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -2.277011    0.299862   -0.200768
      2          6           0       -1.739563    1.540600    0.350413
      3          6           0       -0.338302    1.335405    0.457035
      4          7           0        0.009032    0.090109    0.010551
      5          6           0       -1.162203   -0.547400   -0.395541
      6          6           0       -1.293109   -1.832973   -0.901929
      7          6           0       -2.578168   -2.263333   -1.236145
      8          6           0       -3.677963   -1.433760   -1.053155
      9          6           0       -3.539009   -0.137573   -0.530583
     10          6           0       -2.288765    2.738655    0.740843
     11          6           0       -1.454419    3.757652    1.246304
     12          6           0       -0.072727    3.535229    1.338276
     13          6           0        0.509245    2.339957    0.946258
     14          6           0       -2.055607    5.079012    1.676522
     15          6           0       -1.830155    5.338563    3.171970
     16          6           0       -1.524243    6.242527    0.828836
     17          1           0       -0.430577   -2.476197   -1.017656
     18          1           0       -2.722248   -3.257007   -1.642885
     19          1           0       -4.411978    0.492667   -0.400337
     20          1           0       -3.357830    2.913920    0.664931
     21          1           0        0.565609    4.324998    1.719688
     22          1           0        1.578395    2.181008    0.993734
     23          1           0       -3.137000    5.012720    1.509710
     24          1           0       -2.324042    6.267728    3.472273
     25          1           0       -2.231677    4.525114    3.783069
```

26	1	0	-0.764543	5.438130	3.401829
27	1	0	-2.017849	7.175528	1.117482
28	1	0	-1.705567	6.075285	-0.236751
29	1	0	-0.447164	6.377709	0.969896
30	5	0	1.431808	-0.501064	-0.013462
31	6	0	2.481394	0.306448	-0.837679
32	6	0	2.188053	0.914096	-2.090959
33	6	0	3.795279	0.514393	-0.318238
34	6	0	3.136968	1.693614	-2.747197
35	6	0	4.711159	1.298282	-1.010257
36	6	0	4.408079	1.907422	-2.227328
37	1	0	2.880101	2.131708	-3.709773
38	1	0	5.698137	1.451205	-0.577594
39	6	0	1.635032	-1.830605	0.779164
40	6	0	2.417588	-2.884494	0.217734
41	6	0	1.039256	-2.085997	2.045852
42	6	0	2.559306	-4.093491	0.889809
43	6	0	1.206613	-3.313718	2.681034
44	6	0	1.960362	-4.339805	2.123941
45	1	0	3.150124	-4.881218	0.426041
46	1	0	0.745871	-3.466374	3.655114
47	6	0	4.227126	-0.048613	1.014019
48	1	0	3.484949	0.158696	1.792544
49	1	0	4.345272	-1.136155	0.992158
50	1	0	5.182603	0.385301	1.322867
51	6	0	0.872300	0.683147	-2.789299
52	1	0	0.595708	-0.377313	-2.777116
53	1	0	0.045296	1.232971	-2.325734
54	1	0	0.924334	1.005172	-3.833149
55	6	0	5.415869	2.771340	-2.938076
56	1	0	5.139495	2.926186	-3.985072
57	1	0	5.497938	3.761076	-2.471872
58	1	0	6.415019	2.324080	-2.915912
59	6	0	0.258245	-1.025642	2.778869
60	1	0	0.784273	-0.064113	2.769233
61	1	0	-0.731147	-0.853579	2.339493
62	1	0	0.098567	-1.312266	3.822086
63	6	0	3.073536	-2.763622	-1.136764
64	1	0	2.371350	-2.385917	-1.887581
65	1	0	3.917454	-2.067265	-1.135106
66	1	0	3.444573	-3.736867	-1.471020
67	6	0	2.111427	-5.670601	2.812066
68	1	0	1.456924	-6.430300	2.367072
69	1	0	3.136492	-6.047698	2.736461
70	1	0	1.855310	-5.601440	3.873310
71	6	0	-5.056573	-1.937970	-1.360218
72	9	0	-5.680951	-2.379519	-0.252768
73	9	0	-5.040191	-2.954469	-2.235542
74	9	0	-5.830919	-0.967409	-1.878005

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1) SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1695.04858119 a.u.

Excited State 1: Singlet-A 3.0663 eV 404.35 nm f=0.0452 <S**2>=0.000
131 ->140 0.10821

139 ->140 0.67911

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1695.16012992 a.u.

Results

Absorb Energy =	0.156 a.u.	4.242 eV	292.263 nm
Emission Energy =	0.112 a.u.	3.035 eV	408.461 nm
Stokes Shift =	0.044 a.u.	1.207 eV	116.198 nm

Compound 4 THF

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : TetraHydroFuran
SCF Done: E(RCAM-B3LYP) = -1695.07115732 a.u.
Lowest frequency = 15.9229

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.223930	0.589656	-0.121577
2	6	0	-1.507635	1.810468	0.180599
3	6	0	-0.147859	1.477163	0.245834
4	7	0	0.026002	0.086661	0.010617
5	6	0	-1.267245	-0.438038	-0.210245
6	6	0	-1.656067	-1.734443	-0.552035
7	6	0	-3.002389	-1.985507	-0.759308
8	6	0	-3.955991	-0.966983	-0.646999
9	6	0	-3.572850	0.328032	-0.334689
10	6	0	-1.937813	3.116290	0.411336
11	6	0	-1.014009	4.105374	0.719515
12	6	0	0.342664	3.747210	0.801475
13	6	0	0.790630	2.453936	0.578721
14	6	0	-1.461545	5.533712	0.972027
15	6	0	-1.146978	5.984166	2.403463
16	6	0	-0.862895	6.506038	-0.051192
17	1	0	-0.935063	-2.532192	-0.659796
18	1	0	-3.320645	-2.987300	-1.026145
19	1	0	-4.310100	1.120410	-0.269504
20	1	0	-2.995748	3.359009	0.356400
21	1	0	1.076974	4.506543	1.054138
22	1	0	1.843371	2.222976	0.664125
23	1	0	-2.551353	5.554453	0.850424
24	1	0	-1.528674	6.994893	2.581303
25	1	0	-1.601263	5.313223	3.138801
26	1	0	-0.067080	6.000040	2.585662
27	1	0	-1.242343	7.519801	0.113673
28	1	0	-1.114139	6.209386	-1.074006

29	1	0	0.228850	6.542579	0.028962
30	5	0	1.275050	-0.644260	0.000424
31	6	0	2.607130	0.106051	-0.394254
32	6	0	2.707572	0.729782	-1.657922
33	6	0	3.740796	0.116717	0.447611
34	6	0	3.906904	1.322501	-2.049148
35	6	0	4.913892	0.741442	0.030636
36	6	0	5.020896	1.349256	-1.217029
37	1	0	3.970612	1.779356	-3.034016
38	1	0	5.772564	0.747281	0.697967
39	6	0	1.278612	-2.176198	0.384645
40	6	0	1.815933	-3.163396	-0.470236
41	6	0	0.795651	-2.579224	1.649811
42	6	0	1.844379	-4.496198	-0.066051
43	6	0	0.864920	-3.918919	2.027909
44	6	0	1.375317	-4.897406	1.181528
45	1	0	2.252550	-5.242661	-0.743419
46	1	0	0.506489	-4.205902	3.013789
47	6	0	3.717694	-0.503081	1.825229
48	1	0	2.959047	-0.038924	2.464782
49	1	0	3.495630	-1.572493	1.786467
50	1	0	4.682785	-0.376099	2.322232
51	6	0	1.549223	0.787913	-2.628917
52	1	0	0.998354	-0.153945	-2.690614
53	1	0	0.829994	1.561497	-2.339823
54	1	0	1.904370	1.029604	-3.634034
55	6	0	6.295099	2.030496	-1.641544
56	1	0	6.383852	2.067943	-2.730693
57	1	0	6.329546	3.063129	-1.274969
58	1	0	7.174512	1.516295	-1.243256
59	6	0	0.193479	-1.604475	2.637540
60	1	0	0.739012	-0.659038	2.688041
61	1	0	-0.842221	-1.363463	2.375326
62	1	0	0.184106	-2.035309	3.642088
63	6	0	2.341126	-2.827638	-1.846412
64	1	0	1.569407	-2.369900	-2.474489
65	1	0	3.177305	-2.125211	-1.801085
66	1	0	2.684545	-3.729516	-2.359405
67	6	0	1.402284	-6.346051	1.591898
68	1	0	0.500828	-6.867888	1.249910
69	1	0	2.261613	-6.867252	1.160474
70	1	0	1.447252	-6.452043	2.679256
71	6	0	-5.402307	-1.300290	-0.827175
72	9	0	-5.943780	-1.831072	0.289162
73	9	0	-5.592242	-2.206027	-1.805717
74	9	0	-6.140682	-0.218983	-1.135141

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=THF)

Excited State 1: Singlet-A 4.2488 eV 291.81 nm f=0.2935 <S**2>=0.000

135	->140	0.10153
138	->140	0.14832
139	->140	0.64799

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1695.18089053 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1695.02419206 a.u.

Excited State 1: Singlet-A 4.2543 eV 291.43 nm f=0.2311
<S**2>=0.000
135 ->140 0.10561
138 ->140 0.16006
139 ->140 0.64372

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1694.93493514 a.u.
Lowest frequency = 15.5407

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.272357	0.319813	-0.199539
2	6	0	-1.723725	1.559488	0.344026
3	6	0	-0.325505	1.344245	0.452945
4	7	0	0.013006	0.090866	0.010351
5	6	0	-1.166076	-0.538153	-0.393206
6	6	0	-1.307537	-1.820905	-0.903739
7	6	0	-2.596542	-2.241571	-1.234594
8	6	0	-3.689012	-1.402730	-1.047145
9	6	0	-3.538935	-0.106849	-0.526647
10	6	0	-2.264932	2.763563	0.728186
11	6	0	-1.423205	3.777470	1.231593
12	6	0	-0.044208	3.542893	1.331315
13	6	0	0.528212	2.339826	0.946565
14	6	0	-2.014989	5.104953	1.655890
15	6	0	-1.795533	5.364250	3.152304
16	6	0	-1.467320	6.261986	0.809810
17	1	0	-0.450214	-2.469127	-1.030848
18	1	0	-2.747877	-3.233219	-1.643535
19	1	0	-4.404639	0.532955	-0.395781
20	1	0	-3.332344	2.945875	0.649761
21	1	0	0.599766	4.326214	1.716449
22	1	0	1.594938	2.169452	1.009939
23	1	0	-3.095519	5.048077	1.482666
24	1	0	-2.282716	6.298580	3.447481
25	1	0	-2.209599	4.555500	3.761407
26	1	0	-0.730269	5.453933	3.388078
27	1	0	-1.954706	7.199385	1.094748
28	1	0	-1.645031	6.094576	-0.256453
29	1	0	-0.389889	6.387468	0.957539
30	5	0	1.420456	-0.508907	-0.011770
31	6	0	2.489638	0.289402	-0.825153

32	6	0	2.209301	0.900490	-2.080684
33	6	0	3.803313	0.479430	-0.300429
34	6	0	3.169171	1.673286	-2.729562
35	6	0	4.731492	1.256384	-0.985325
36	6	0	4.440148	1.873723	-2.201565
37	1	0	2.921565	2.116923	-3.692068
38	1	0	5.717828	1.398038	-0.547483
39	6	0	1.612993	-1.850561	0.771100
40	6	0	2.377876	-2.911606	0.202449
41	6	0	1.022453	-2.099967	2.041664
42	6	0	2.507262	-4.125950	0.869520
43	6	0	1.175881	-3.332473	2.672108
44	6	0	1.911559	-4.368125	2.106231
45	1	0	3.084249	-4.920341	0.399790
46	1	0	0.718792	-3.481759	3.648516
47	6	0	4.221614	-0.094019	1.031443
48	1	0	3.475961	0.119455	1.805074
49	1	0	4.328090	-1.182811	1.003384
50	1	0	5.179747	0.327911	1.348408
51	6	0	0.894868	0.682142	-2.784991
52	1	0	0.613590	-0.377204	-2.782667
53	1	0	0.069745	1.230020	-2.315902
54	1	0	0.950318	1.015446	-3.825111
55	6	0	5.456882	2.735074	-2.902927
56	1	0	5.244590	2.811203	-3.973425
57	1	0	5.464974	3.755688	-2.500211
58	1	0	6.469589	2.336831	-2.785399
59	6	0	0.259642	-1.029702	2.779228
60	1	0	0.798630	-0.075462	2.767317
61	1	0	-0.727704	-0.842751	2.341270
62	1	0	0.098181	-1.315474	3.822405
63	6	0	3.027608	-2.792344	-1.155028
64	1	0	2.323837	-2.402197	-1.898218
65	1	0	3.880078	-2.106196	-1.152676
66	1	0	3.384793	-3.768026	-1.497118
67	6	0	2.042583	-5.704296	2.788658
68	1	0	1.292547	-6.417007	2.423618
69	1	0	3.024725	-6.152184	2.608162
70	1	0	1.904197	-5.615059	3.870247
71	6	0	-5.071134	-1.897059	-1.350987
72	9	0	-5.695245	-2.342985	-0.243674
73	9	0	-5.065933	-2.909930	-2.231807
74	9	0	-5.844648	-0.921407	-1.860522

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1695.05948001 a.u.

Excited State 1: Singlet-A 2.9664 eV 417.97 nm f=0.0496
<S**2>=0.000
131 ->140 0.10408
139 ->140 0.67851

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1695.16216726 a.u.

Results

Absorb Energy =	0.157 a.u.	4.264 eV	290.771 nm
Emission Energy =	0.103 a.u.	2.794 eV	443.710 nm
Stokes Shift =	0.054 a.u.	1.470 eV	152.939 nm

Compound 4 ACN

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : Acetonitrile
SCF Done: E(RCAM-B3LYP) = -1695.07240266 a.u.
Lowest frequency = 16.4569

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.208588	0.634089	-0.119727
2	6	0	-1.466177	1.840096	0.179040
3	6	0	-0.113744	1.477850	0.244497
4	7	0	0.030323	0.083392	0.011641
5	6	0	-1.274074	-0.414045	-0.206865
6	6	0	-1.691208	-1.702624	-0.545068
7	6	0	-3.042839	-1.925364	-0.750422
8	6	0	-3.974214	-0.886174	-0.639440
9	6	0	-3.563203	0.401229	-0.330711
10	6	0	-1.868830	3.155325	0.407077
11	6	0	-0.924047	4.125228	0.713186
12	6	0	0.424831	3.738336	0.796147
13	6	0	0.845191	2.435263	0.575853
14	6	0	-1.341202	5.563227	0.963160
15	6	0	-1.019053	6.008637	2.394534
16	6	0	-0.720005	6.521207	-0.060192
17	1	0	-0.987898	-2.515924	-0.652733
18	1	0	-3.382314	-2.920847	-1.014704
19	1	0	-4.282802	1.209705	-0.266372
20	1	0	-2.921412	3.420129	0.351914
21	1	0	1.175166	4.482077	1.048032
22	1	0	1.892627	2.182298	0.663431
23	1	0	-2.430016	5.607160	0.839821
24	1	0	-1.379151	7.027641	2.569985
25	1	0	-1.489526	5.349043	3.130067
26	1	0	0.060659	6.001361	2.578408
27	1	0	-1.078253	7.542866	0.103114
28	1	0	-0.976296	6.229072	-1.083127
29	1	0	0.372125	6.534638	0.021968
30	5	0	1.263654	-0.673733	-0.001028
31	6	0	2.610908	0.051790	-0.393291
32	6	0	2.724918	0.664595	-1.661534
33	6	0	3.740601	0.055226	0.453570
34	6	0	3.933189	1.239047	-2.052277
35	6	0	4.924053	0.660818	0.036245

36	6	0	5.044250	1.257844	-1.215312
37	1	0	4.006984	1.687037	-3.040496
38	1	0	5.779961	0.660208	0.707095
39	6	0	1.234014	-2.206892	0.379585
40	6	0	1.731361	-3.209086	-0.481784
41	6	0	0.757036	-2.596276	1.651796
42	6	0	1.732878	-4.541813	-0.074735
43	6	0	0.797100	-3.936627	2.031404
44	6	0	1.271594	-4.929246	1.179898
45	1	0	2.112496	-5.299241	-0.756481
46	1	0	0.445176	-4.212879	3.022660
47	6	0	3.701149	-0.545025	1.839208
48	1	0	2.987612	-0.019958	2.483956
49	1	0	3.405290	-1.596735	1.820123
50	1	0	4.681100	-0.477470	2.318316
51	6	0	1.570647	0.727297	-2.637129
52	1	0	1.018862	-0.213915	-2.701977
53	1	0	0.851729	1.501846	-2.349868
54	1	0	1.930264	0.969485	-3.640486
55	6	0	6.328820	1.919412	-1.639807
56	1	0	6.430737	1.931463	-2.728390
57	1	0	6.366524	2.959951	-1.296674
58	1	0	7.199165	1.408127	-1.218711
59	6	0	0.192251	-1.604170	2.644383
60	1	0	0.770919	-0.678619	2.695313
61	1	0	-0.835263	-1.326531	2.386177
62	1	0	0.171304	-2.037097	3.647798
63	6	0	2.229201	-2.892151	-1.872286
64	1	0	1.422499	-2.515233	-2.511011
65	1	0	3.014243	-2.132375	-1.861504
66	1	0	2.630514	-3.787747	-2.353174
67	6	0	1.268414	-6.377308	1.593354
68	1	0	0.342605	-6.873107	1.278811
69	1	0	2.099308	-6.923993	1.138584
70	1	0	1.341066	-6.482411	2.679307
71	6	0	-5.427226	-1.188915	-0.817784
72	9	0	-5.978644	-1.709129	0.299166
73	9	0	-5.637951	-2.090321	-1.796336
74	9	0	-6.143904	-0.092762	-1.124272

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=acetonitrile)

Excited State 1: Singlet-A 4.2723 eV 290.21 nm f=0.2860
<S**2>=0.000
138 ->140 0.14801
139 ->140 0.64711

Step3

Method: cam-b3lyp/6-31+G(d,p)
SCRF(Solvent=acetonitrile,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1695.18232082 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1695.02453267 a.u.

Excited State 1: Singlet-A 4.2788 eV 289.76 nm f=0.2310
<S**2>=0.000
135 ->140 0.10501
138 ->140 0.15771
139 ->140 0.64337

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1694.93583202 a.u.
Lowest frequency = 16.6593

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.271525	0.325596	-0.198184
2	6	0	-1.719603	1.565192	0.342609
3	6	0	-0.322352	1.347223	0.452241
4	7	0	0.013776	0.091159	0.010658
5	6	0	-1.167727	-0.535347	-0.391813
6	6	0	-1.311949	-1.817094	-0.904243
7	6	0	-2.602012	-2.235249	-1.233634
8	6	0	-3.692557	-1.394008	-1.043915
9	6	0	-3.539501	-0.098207	-0.524130
10	6	0	-2.258585	2.771031	0.724899
11	6	0	-1.414778	3.783447	1.227740
12	6	0	-0.036684	3.545208	1.330467
13	6	0	0.532923	2.339724	0.948021
14	6	0	-2.003811	5.113113	1.649044
15	6	0	-1.780604	5.377697	3.143937
16	6	0	-1.456016	6.266054	0.797423
17	1	0	-0.455711	-2.465866	-1.036393
18	1	0	-2.755315	-3.226053	-1.643940
19	1	0	-4.403128	0.544215	-0.393096
20	1	0	-3.325495	2.955225	0.645834
21	1	0	0.608785	4.326293	1.717648
22	1	0	1.598660	2.165354	1.018268
23	1	0	-3.084601	5.057098	1.478266
24	1	0	-2.266429	6.313622	3.436305
25	1	0	-2.194655	4.571656	3.756688
26	1	0	-0.714719	5.467370	3.377060
27	1	0	-1.941301	7.205197	1.080241
28	1	0	-1.637154	6.094876	-0.267703
29	1	0	-0.377968	6.390003	0.942266
30	5	0	1.416066	-0.510641	-0.011615
31	6	0	2.491237	0.284609	-0.822100
32	6	0	2.214807	0.895403	-2.078486
33	6	0	3.804813	0.470931	-0.295132
34	6	0	3.177716	1.667400	-2.725158
35	6	0	4.735884	1.246450	-0.977380
36	6	0	4.447902	1.865204	-2.194528
37	1	0	2.932521	2.112792	-3.687418
38	1	0	5.721341	1.386780	-0.537092

39	6	0	1.606623	-1.855872	0.768648
40	6	0	2.364842	-2.919908	0.196469
41	6	0	1.019841	-2.102755	2.040875
42	6	0	2.491214	-4.135356	0.861735
43	6	0	1.169610	-3.337244	2.670146
44	6	0	1.898706	-4.375566	2.101218
45	1	0	3.062115	-4.932380	0.388942
46	1	0	0.714311	-3.485463	3.647507
47	6	0	4.218625	-0.104812	1.037086
48	1	0	3.471102	0.110091	1.808547
49	1	0	4.322775	-1.193871	1.006916
50	1	0	5.176847	0.314483	1.357096
51	6	0	0.901379	0.679144	-2.784984
52	1	0	0.620358	-0.380308	-2.785831
53	1	0	0.075834	1.224949	-2.314221
54	1	0	0.957515	1.016265	-3.823825
55	6	0	5.469548	2.722599	-2.893657
56	1	0	5.219952	2.858370	-3.949927
57	1	0	5.532168	3.720634	-2.442446
58	1	0	6.470530	2.283196	-2.835091
59	6	0	0.263797	-1.029320	2.780631
60	1	0	0.807014	-0.077501	2.767230
61	1	0	-0.723286	-0.837396	2.344177
62	1	0	0.102748	-1.314671	3.823984
63	6	0	3.009437	-2.801246	-1.163482
64	1	0	2.302999	-2.408033	-1.902628
65	1	0	3.864157	-2.117771	-1.162606
66	1	0	3.362162	-3.777477	-1.508502
67	6	0	2.030025	-5.712366	2.782564
68	1	0	1.339436	-6.450074	2.355585
69	1	0	3.039852	-6.120893	2.674259
70	1	0	1.806944	-5.638491	3.850863
71	6	0	-5.075242	-1.887190	-1.346022
72	9	0	-5.692139	-2.350465	-0.241303
73	9	0	-5.073156	-2.888845	-2.240189
74	9	0	-5.855041	-0.907806	-1.838167

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1) SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1695.06377344 a.u.

Excited State 1: Singlet-A 2.9268 eV 423.62 nm f=0.0511 <S**2>=0.000
139 ->140 0.67838

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=acetonitrile, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1695.16254690 a.u.

Results

Absorb Energy =	0.158 a.u.	4.294 eV	288.763 nm
Emission Energy =	0.099 a.u.	2.688 eV	461.291 nm

Stokes Shift =	0.059 a.u.	1.606 eV	172.529 nm

Compound 5 n-hexane

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : n-Hexane
SCF Done: E(RCAM-B3LYP) = -1393.77783157 a.u.
Lowest frequency = 18.8655

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.584364	-0.220907	-0.046159
2	6	0	-2.640716	-1.354851	-1.981755
3	1	0	-2.030094	-0.619249	-2.514029
4	1	0	-2.054387	-2.276409	-1.925991
5	1	0	-3.523170	-1.555170	-2.595307
6	6	0	-0.782909	-2.918608	1.383865
7	1	0	-0.548522	-3.867251	1.874306
8	1	0	-0.622756	-2.122416	2.116778
9	1	0	-1.852007	-2.917538	1.151976
10	6	0	1.132504	-0.223078	-2.550506
11	1	0	0.232084	0.394636	-2.588676
12	1	0	1.938331	0.409579	-2.165415
13	1	0	1.391780	-0.491291	-3.578207
14	6	0	2.178495	-5.076300	-2.011072
15	1	0	3.113154	-5.241276	-1.462489
16	1	0	1.563317	-5.971367	-1.877987
17	1	0	2.431513	-4.990575	-3.071271
18	6	0	1.471859	-3.843770	-1.512840
19	6	0	0.702483	-3.879361	-0.352549
20	1	0	0.598512	-4.819583	0.184400
21	6	0	0.054074	-2.750447	0.134959
22	6	0	0.191825	-1.507151	-0.528328
23	6	0	0.958593	-1.471443	-1.713855
24	6	0	1.571787	-2.633271	-2.184003
25	1	0	2.145101	-2.585859	-3.106941
26	6	0	-2.598672	0.157114	1.540436
27	6	0	-3.944581	0.010216	1.868429
28	1	0	-4.289771	0.354048	2.840749
29	6	0	-4.860468	-0.552178	0.985626
30	6	0	-4.392405	-0.973675	-0.255135
31	1	0	-5.093997	-1.398375	-0.969438
32	6	0	-3.049417	-0.869522	-0.609442
33	6	0	-2.123526	-0.296604	0.289615
34	6	0	-1.696972	0.816074	2.560922
35	1	0	-1.420825	1.829124	2.252470
36	1	0	-2.204027	0.890039	3.526507
37	1	0	-0.763502	0.268707	2.720281
38	6	0	-6.307568	-0.718004	1.367510
39	1	0	-6.960832	-0.660113	0.492276
40	1	0	-6.480459	-1.692747	1.838727
41	1	0	-6.623023	0.048625	2.080805

42	7	0	0.089092	1.069255	0.048832
43	6	0	-0.476809	2.265138	-0.477835
44	6	0	1.462758	1.342074	0.248296
45	6	0	0.545024	3.204590	-0.699438
46	6	0	-1.793674	2.567503	-0.829629
47	6	0	1.772781	2.606421	-0.237498
48	6	0	2.444966	0.579129	0.952965
49	6	0	0.263762	4.451719	-1.256303
50	6	0	-2.058492	3.816044	-1.375271
51	1	0	-2.598073	1.862437	-0.679540
52	6	0	3.091489	3.109829	-0.205033
53	6	0	3.777613	1.091818	0.953255
54	6	0	2.183208	-0.586852	1.710857
55	6	0	-1.044517	4.755142	-1.590797
56	1	0	1.060461	5.170764	-1.422035
57	1	0	-3.081977	4.063905	-1.639054
58	6	0	4.076612	2.344839	0.344222
59	1	0	3.309499	4.089433	-0.618934
60	6	0	4.794136	0.363475	1.617360
61	6	0	3.185180	-1.253667	2.367264
62	1	0	1.170849	-0.952868	1.790209
63	1	0	-1.286170	5.721856	-2.020897
64	1	0	5.103242	2.697832	0.368543
65	6	0	4.513647	-0.789268	2.302078
66	1	0	5.807701	0.753787	1.589620
67	1	0	2.950023	-2.141301	2.946001
68	1	0	5.303788	-1.330103	2.813311

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=n-hexane)

Excited State 1: Singlet-A 3.9277 eV 315.67 nm f=0.2326
<S**2>=0.000
123 ->125 0.23242
124 ->125 0.62910

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1393.86204896 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1393.71917752 a.u.

Excited State 1: Singlet-A 3.9014 eV 317.79 nm f=0.1647
<S**2>=0.000
123 ->125 -0.19224
124 ->125 -0.64483

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1393.65321527 a.u.
Lowest frequency = 19.9275

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.565192	-0.393994	-0.117039
2	6	0	-3.020877	-1.780300	-1.218089
3	1	0	-2.428213	-1.330650	-2.021773
4	1	0	-2.534957	-2.732549	-0.985571
5	1	0	-4.018358	-2.002103	-1.609027
6	6	0	-0.900504	-2.966149	1.421732
7	1	0	-0.709432	-3.901944	1.955310
8	1	0	-0.629534	-2.133207	2.079013
9	1	0	-1.981184	-2.883729	1.271046
10	6	0	1.014324	-0.690259	-2.770485
11	1	0	0.062563	-0.200964	-3.001050
12	1	0	1.681828	0.080425	-2.371096
13	1	0	1.448832	-1.032975	-3.713827
14	6	0	1.877032	-5.520611	-1.848646
15	1	0	2.875223	-5.628182	-1.405577
16	1	0	1.286178	-6.382792	-1.524314
17	1	0	1.998519	-5.584238	-2.934446
18	6	0	1.227860	-4.223920	-1.443367
19	6	0	0.454880	-4.127527	-0.290246
20	1	0	0.309932	-5.016507	0.320899
21	6	0	-0.128959	-2.933588	0.122668
22	6	0	0.043749	-1.734238	-0.635313
23	6	0	0.824262	-1.848978	-1.822458
24	6	0	1.390662	-3.064064	-2.193965
25	1	0	1.966586	-3.111271	-3.116392
26	6	0	-2.232769	0.708917	1.594103
27	6	0	-3.517383	0.881691	2.099440
28	1	0	-3.663695	1.565129	2.933888
29	6	0	-4.616323	0.201904	1.584313
30	6	0	-4.385029	-0.661594	0.517975
31	1	0	-5.229159	-1.186888	0.074924
32	6	0	-3.116665	-0.865305	-0.019432
33	6	0	-1.981702	-0.184222	0.514795
34	6	0	-1.121161	1.479545	2.261553
35	1	0	-0.777265	2.322858	1.651762
36	1	0	-1.455300	1.891316	3.218225
37	1	0	-0.250803	0.844215	2.455516
38	6	0	-5.993124	0.375653	2.169011
39	1	0	-6.770367	0.223633	1.413654
40	1	0	-6.181673	-0.344551	2.975003
41	1	0	-6.125217	1.375808	2.593163
42	7	0	0.245183	0.905028	-0.355452
43	6	0	-0.256448	1.932413	-1.191247
44	6	0	1.444324	1.319825	0.123104
45	6	0	0.652359	3.000230	-1.245147
46	6	0	-1.456088	1.966111	-1.879375
47	6	0	1.760746	2.612932	-0.407914
48	6	0	2.358648	0.670607	1.034927
49	6	0	0.370335	4.127499	-2.001420
50	6	0	-1.727203	3.106078	-2.645886
51	1	0	-2.165072	1.152123	-1.813866
52	6	0	2.943672	3.266323	-0.088602

53	6	0	3.556874	1.382212	1.349681
54	6	0	2.154841	-0.582027	1.633582
55	6	0	-0.833846	4.170349	-2.707813
56	1	0	1.063853	4.961629	-2.043896
57	1	0	-2.659445	3.157248	-3.198356
58	6	0	3.823978	2.654473	0.778601
59	1	0	3.166345	4.242031	-0.506877
60	6	0	4.486462	0.814482	2.248671
61	6	0	3.084497	-1.111258	2.510800
62	1	0	1.266559	-1.144246	1.392672
63	1	0	-1.075061	5.042759	-3.305449
64	1	0	4.750730	3.151619	1.047421
65	6	0	4.254883	-0.411330	2.827786
66	1	0	5.392469	1.368519	2.475377
67	1	0	2.900702	-2.086288	2.949532
68	1	0	4.976254	-0.836697	3.517443

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1393.74431918 a.u.

Excited State 1: Singlet-A 2.8366 eV 437.09 nm f=0.0435
<S**2>=0.000
123 ->125 0.10034
124 ->125 0.67910

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,
NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1393.84716648 a.u.

Results

Absorb Energy =	0.143 a.u.	3.888 eV	318.911 nm
Emission Energy =	0.103 a.u.	2.799 eV	443.019 nm
Stokes Shift =	0.040 a.u.	1.089 eV	124.108 nm

Compound 5 THF

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : TetraHydroFuran
SCF Done: E(RCAM-B3LYP) = -1393.78151870 a.u.
Lowest frequency = 18.1416

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.585914	-0.225452	-0.049532

2	6	0	-2.648664	-1.379552	-1.968953
3	1	0	-2.035297	-0.651831	-2.508665
4	1	0	-2.067524	-2.304071	-1.906440
5	1	0	-3.533540	-1.580762	-2.578503
6	6	0	-0.769869	-2.926428	1.378432
7	1	0	-0.526931	-3.872083	1.870100
8	1	0	-0.618168	-2.127766	2.110273
9	1	0	-1.838616	-2.936518	1.144690
10	6	0	1.118306	-0.219374	-2.561382
11	1	0	0.205450	0.379112	-2.612221
12	1	0	1.906332	0.431177	-2.169304
13	1	0	1.395083	-0.485845	-3.584814
14	6	0	2.201188	-5.065848	-2.020551
15	1	0	3.135915	-5.227115	-1.471049
16	1	0	1.590351	-5.963884	-1.888259
17	1	0	2.454800	-4.976880	-3.080259
18	6	0	1.488105	-3.837515	-1.520962
19	6	0	0.720781	-3.877547	-0.359031
20	1	0	0.623805	-4.818162	0.178373
21	6	0	0.065419	-2.752280	0.129207
22	6	0	0.194188	-1.508239	-0.534658
23	6	0	0.958006	-1.468217	-1.722419
24	6	0	1.578630	-2.626132	-2.193331
25	1	0	2.148757	-2.575864	-3.118050
26	6	0	-2.594785	0.160217	1.542160
27	6	0	-3.939940	0.015571	1.875341
28	1	0	-4.282195	0.365421	2.846501
29	6	0	-4.858874	-0.552912	0.998936
30	6	0	-4.394284	-0.983405	-0.240434
31	1	0	-5.098004	-1.413177	-0.949511
32	6	0	-3.052005	-0.881912	-0.599346
33	6	0	-2.123135	-0.301894	0.292590
34	6	0	-1.690410	0.823428	2.557787
35	1	0	-1.410388	1.833339	2.242523
36	1	0	-2.197343	0.906023	3.522598
37	1	0	-0.759454	0.273005	2.721264
38	6	0	-6.304889	-0.715653	1.386152
39	1	0	-6.960357	-0.663934	0.512285
40	1	0	-6.475929	-1.687439	1.863996
41	1	0	-6.617455	0.055206	2.096031
42	7	0	0.086676	1.067071	0.042378
43	6	0	-0.479179	2.259753	-0.489488
44	6	0	1.458190	1.343208	0.248192
45	6	0	0.540907	3.202927	-0.705477
46	6	0	-1.794860	2.556882	-0.851479
47	6	0	1.767925	2.608571	-0.236356
48	6	0	2.439148	0.583144	0.958347
49	6	0	0.259012	4.449361	-1.264967
50	6	0	-2.060870	3.804320	-1.399636
51	1	0	-2.597176	1.847924	-0.708345
52	6	0	3.085450	3.115864	-0.197579
53	6	0	3.770842	1.099251	0.964647
54	6	0	2.176293	-0.582574	1.716971
55	6	0	-1.048547	4.747703	-1.608222
56	1	0	1.054080	5.171143	-1.426224
57	1	0	-3.083199	4.048002	-1.671586
58	6	0	4.070098	2.353273	0.356685
59	1	0	3.303098	4.095847	-0.610635
60	6	0	4.786418	0.373598	1.634175
61	6	0	3.176887	-1.246543	2.379292

62	1	0	1.164285	-0.950162	1.793852
63	1	0	-1.290945	5.713216	-2.040488
64	1	0	5.095667	2.708773	0.385583
65	6	0	4.505132	-0.779402	2.319067
66	1	0	5.799207	0.765975	1.610766
67	1	0	2.940905	-2.132878	2.959629
68	1	0	5.293953	-1.317881	2.834632

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=THF)

Excited State 1: Singlet-A 3.9286 eV 315.59 nm f=0.2383 <S**2>=0.000

123 ->125	0.24047
124 ->125	0.62557

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1393.86601871 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1393.72245248 a.u.

Excited State 1: Singlet-A 3.9036 eV 317.61 nm f=0.1669 <S**2>=0.000

123 ->125	-0.20144
124 ->125	-0.64130

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes) TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1393.65549567 a.u.
Lowest frequency = 23.0622

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.556789	-0.397247	-0.116628
2	6	0	-2.972928	-1.836518	-1.253273
3	1	0	-2.387185	-1.359810	-2.046405
4	1	0	-2.462876	-2.777273	-1.025152
5	1	0	-3.960718	-2.081440	-1.654666
6	6	0	-0.828594	-2.996460	1.402757
7	1	0	-0.615300	-3.930635	1.930458
8	1	0	-0.584029	-2.161852	2.068208
9	1	0	-1.909901	-2.943494	1.242771
10	6	0	1.033204	-0.632634	-2.762577
11	1	0	0.068933	-0.162765	-2.981124
12	1	0	1.684972	0.149001	-2.358243

13	1	0	1.470242	-0.955948	-3.711595
14	6	0	2.040482	-5.443571	-1.872715
15	1	0	3.027423	-5.537330	-1.402438
16	1	0	1.461063	-6.325082	-1.581390
17	1	0	2.194834	-5.482288	-2.955346
18	6	0	1.350944	-4.169512	-1.461219
19	6	0	0.570632	-4.105060	-0.309767
20	1	0	0.450581	-5.002438	0.294465
21	6	0	-0.049964	-2.931495	0.109170
22	6	0	0.091368	-1.722107	-0.637920
23	6	0	0.875678	-1.804352	-1.824450
24	6	0	1.480424	-3.000030	-2.203391
25	1	0	2.060617	-3.022865	-3.124068
26	6	0	-2.265408	0.635931	1.593630
27	6	0	-3.558549	0.773018	2.092212
28	1	0	-3.726754	1.442963	2.933411
29	6	0	-4.637669	0.074479	1.560611
30	6	0	-4.378881	-0.771327	0.484893
31	1	0	-5.207664	-1.310134	0.029180
32	6	0	-3.102029	-0.938177	-0.045257
33	6	0	-1.988053	-0.235720	0.503975
34	6	0	-1.175061	1.422635	2.277182
35	1	0	-0.843318	2.277998	1.677424
36	1	0	-1.524332	1.818327	3.235248
37	1	0	-0.292547	0.803435	2.468993
38	6	0	-6.023353	0.209281	2.135350
39	1	0	-6.789429	0.113639	1.359490
40	1	0	-6.225603	-0.567165	2.883646
41	1	0	-6.159425	1.176375	2.628596
42	7	0	0.214212	0.915906	-0.337544
43	6	0	-0.314079	1.945624	-1.157185
44	6	0	1.416701	1.346361	0.130284
45	6	0	0.579315	3.026208	-1.211611
46	6	0	-1.517935	1.964597	-1.838809
47	6	0	1.707228	2.645617	-0.395387
48	6	0	2.343844	0.707967	1.034613
49	6	0	0.272811	4.156242	-1.953605
50	6	0	-1.815646	3.108746	-2.590042
51	1	0	-2.209468	1.134667	-1.785268
52	6	0	2.886820	3.311890	-0.091682
53	6	0	3.539564	1.431830	1.334921
54	6	0	2.153363	-0.540113	1.647884
55	6	0	-0.940172	4.187954	-2.646938
56	1	0	0.953957	5.000115	-1.996157
57	1	0	-2.752107	3.149479	-3.136116
58	6	0	3.787410	2.705645	0.759919
59	1	0	3.091957	4.292026	-0.507975
60	6	0	4.482158	0.876279	2.228888
61	6	0	3.092630	-1.054505	2.524896
62	1	0	1.264988	-1.108785	1.422358
63	1	0	-1.200187	5.062696	-3.232979
64	1	0	4.712580	3.211925	1.015924
65	6	0	4.263039	-0.345652	2.822178
66	1	0	5.386457	1.437927	2.442341
67	1	0	2.917509	-2.024452	2.978483
68	1	0	4.993434	-0.760351	3.508663

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1393.75634247 a.u.

Excited State 1: Singlet-A 2.7214 eV 455.59 nm f=0.0470
<S**2>=0.000
124 ->125 0.68084

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1393.84902497 a.u.

Results

Absorb Energy =	0.144 a.u.	3.907 eV	317.368 nm
Emission Energy =	0.093 a.u.	2.522 eV	491.607 nm
Stokes Shift =	0.051 a.u.	1.385 eV	174.239 nm

Compound 5 ACN

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : Acetonitrile
SCF Done: E(RCAM-B3LYP) = -1393.78312542 a.u.
Lowest frequency = 18.7150

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.586902	-0.228896	-0.051399
2	6	0	-2.649856	-1.401760	-1.960498
3	1	0	-2.033645	-0.679770	-2.504451
4	1	0	-2.072510	-2.328319	-1.891994
5	1	0	-3.535335	-1.603638	-2.568851
6	6	0	-0.758264	-2.931880	1.375147
7	1	0	-0.507874	-3.874479	1.868759
8	1	0	-0.614969	-2.130632	2.105727
9	1	0	-1.826453	-2.952167	1.139177
10	6	0	1.110572	-0.215230	-2.567398
11	1	0	0.190800	0.372175	-2.623269
12	1	0	1.889137	0.445385	-2.173138
13	1	0	1.394893	-0.480377	-3.589040
14	6	0	2.225960	-5.054693	-2.023165
15	1	0	3.160753	-5.211473	-1.472493
16	1	0	1.619694	-5.955846	-1.891473
17	1	0	2.480332	-4.963801	-3.082487
18	6	0	1.505848	-3.830335	-1.523807
19	6	0	0.739342	-3.874371	-0.361254
20	1	0	0.648447	-4.815231	0.176684
21	6	0	0.076746	-2.752799	0.126451
22	6	0	0.197873	-1.508290	-0.538087
23	6	0	0.960287	-1.464401	-1.726868

24	6	0	1.588061	-2.618715	-2.197510
25	1	0	2.156464	-2.565861	-3.123130
26	6	0	-2.594201	0.159494	1.541800
27	6	0	-3.938897	0.014591	1.877076
28	1	0	-4.280743	0.368677	2.846817
29	6	0	-4.857981	-0.559877	1.004452
30	6	0	-4.393821	-0.996714	-0.232996
31	1	0	-5.097542	-1.431606	-0.938892
32	6	0	-3.051919	-0.895193	-0.593736
33	6	0	-2.122954	-0.308250	0.293860
34	6	0	-1.690147	0.827920	2.554442
35	1	0	-1.410409	1.836511	2.234707
36	1	0	-2.197414	0.914729	3.518649
37	1	0	-0.759292	0.278225	2.720825
38	6	0	-6.303469	-0.722221	1.393734
39	1	0	-6.959614	-0.675651	0.520130
40	1	0	-6.472769	-1.691952	1.876294
41	1	0	-6.615973	0.051492	2.100475
42	7	0	0.083175	1.065857	0.038977
43	6	0	-0.484295	2.256139	-0.495562
44	6	0	1.453054	1.345800	0.248633
45	6	0	0.533407	3.203011	-0.707680
46	6	0	-1.799527	2.548220	-0.863936
47	6	0	1.760802	2.612325	-0.234803
48	6	0	2.434365	0.588496	0.961594
49	6	0	0.249315	4.448838	-1.268066
50	6	0	-2.067892	3.794826	-1.412999
51	1	0	-2.599493	1.835608	-0.725677
52	6	0	3.077018	3.123301	-0.192650
53	6	0	3.764934	1.107960	0.970724
54	6	0	2.172594	-0.577627	1.720334
55	6	0	-1.058064	4.742389	-1.616581
56	1	0	1.042328	5.173518	-1.426195
57	1	0	-3.089751	4.034593	-1.690081
58	6	0	4.062496	2.363045	0.363663
59	1	0	3.293166	4.103869	-0.605021
60	6	0	4.781084	0.384594	1.642316
61	6	0	3.173570	-1.239347	2.384821
62	1	0	1.161239	-0.947144	1.796458
63	1	0	-1.302282	5.707034	-2.049681
64	1	0	5.087062	2.721114	0.394763
65	6	0	4.501072	-0.769193	2.326821
66	1	0	5.792962	0.779312	1.621016
67	1	0	2.938332	-2.125432	2.965818
68	1	0	5.290053	-1.305706	2.844092

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=acetonitrile)

Excited State 1: Singlet-A 3.9297 eV 315.51 nm f=0.2312
<S**2>=0.000
123 ->125 0.24281
124 ->125 0.62456

Step3

Method: cam-b3lyp/6-31+G(d,p)
SCRF(Solvent=acetonitrile,NonEquilibrium=Save)

SCF Done: E(RCAM-B3LYP) = -1393.86774954 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1393.72358682 a.u.

Excited State 1: Singlet-A 3.9098 eV 317.11 nm f=0.1693
<S**2>=0.000
123 ->125 -0.21015
124 ->125 -0.63795

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1393.65661875 a.u.
Lowest frequency = 22.3397

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-0.555037	-0.398303	-0.118314
2	6	0	-2.951798	-1.857667	-1.275613
3	1	0	-2.369079	-1.366746	-2.062337
4	1	0	-2.431533	-2.793960	-1.051888
5	1	0	-3.934896	-2.111295	-1.682911
6	6	0	-0.800267	-3.013017	1.386180
7	1	0	-0.576538	-3.946787	1.910093
8	1	0	-0.571695	-2.178798	2.057718
9	1	0	-1.881150	-2.975593	1.218539
10	6	0	1.043122	-0.600679	-2.759370
11	1	0	0.072762	-0.141588	-2.973675
12	1	0	1.685835	0.186850	-2.351864
13	1	0	1.482890	-0.913969	-3.710467
14	6	0	2.124093	-5.399450	-1.885771
15	1	0	3.109713	-5.480007	-1.410411
16	1	0	1.557099	-6.291193	-1.601366
17	1	0	2.285164	-5.430306	-2.967625
18	6	0	1.412754	-4.138129	-1.471830
19	6	0	0.625720	-4.091349	-0.323710
20	1	0	0.516784	-4.993377	0.275629
21	6	0	-0.014963	-2.929292	0.097697
22	6	0	0.112300	-1.714167	-0.642161
23	6	0	0.901255	-1.778824	-1.826670
24	6	0	1.526705	-2.963429	-2.208519
25	1	0	2.110800	-2.973024	-3.126947
26	6	0	-2.281674	0.598765	1.593900
27	6	0	-3.578307	0.718066	2.089217
28	1	0	-3.756658	1.379270	2.935208
29	6	0	-4.648121	0.012473	1.547755
30	6	0	-4.376673	-0.821960	0.465815
31	1	0	-5.198194	-1.365582	0.002767
32	6	0	-3.096046	-0.970573	-0.061048
33	6	0	-1.992125	-0.260021	0.497248

34	6	0	-1.201336	1.390573	2.287435
35	1	0	-0.873924	2.252327	1.694474
36	1	0	-1.558121	1.777185	3.246417
37	1	0	-0.314044	0.777902	2.478345
38	6	0	-6.037346	0.128219	2.118329
39	1	0	-6.799388	0.031700	1.338687
40	1	0	-6.234555	-0.657032	2.858708
41	1	0	-6.184742	1.089216	2.620040
42	7	0	0.198943	0.921636	-0.328230
43	6	0	-0.339514	1.953215	-1.140292
44	6	0	1.401984	1.357936	0.136951
45	6	0	0.547917	3.038750	-1.193279
46	6	0	-1.544487	1.967157	-1.820300
47	6	0	1.682777	2.660187	-0.385060
48	6	0	2.333712	0.722770	1.038122
49	6	0	0.232652	4.170325	-1.929214
50	6	0	-1.851891	3.113461	-2.564652
51	1	0	-2.229302	1.131222	-1.772736
52	6	0	2.860833	3.330988	-0.086220
53	6	0	3.528764	1.450661	1.333310
54	6	0	2.147799	-0.523649	1.656550
55	6	0	-0.983163	4.198332	-2.618172
56	1	0	0.909346	5.017681	-1.970927
57	1	0	-2.789475	3.150684	-3.109023
58	6	0	3.769320	2.725757	0.758349
59	1	0	3.059019	4.313405	-0.500211
60	6	0	4.476409	0.898597	2.224364
61	6	0	3.090940	-1.033530	2.532695
62	1	0	1.258671	-1.093895	1.437645
63	1	0	-1.249916	5.074249	-3.199328
64	1	0	4.693907	3.235102	1.009968
65	6	0	4.261852	-0.322323	2.822167
66	1	0	5.380270	1.462617	2.432983
67	1	0	2.918542	-2.001474	2.991713
68	1	0	4.995807	-0.733781	3.506736

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1) SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1393.76111474 a.u.

Excited State 1: Singlet-A 2.6784 eV 462.91 nm f=0.0483 <S**2>=0.000
124 ->125 0.68164

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=acetonitrile, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1393.84947540 a.u.

Results

Absorb Energy =	0.144 a.u.	3.923 eV	316.055 nm
Emission Energy =	0.088 a.u.	2.404 eV	515.652 nm

Stokes Shift = | 0.056 a.u. | 1.518 eV | 199.597 nm

Compound 6 n-hexane

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : n-Hexane
SCF Done: E(RCAM-B3LYP) = -1511.64745787 a.u.
Lowest frequency = 17.5817

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.529025	0.738154	-0.034502
2	6	0	0.218641	2.976742	2.003795
3	1	0	-0.229693	2.067027	2.414543
4	1	0	1.300749	2.886711	2.134833
5	1	0	-0.124521	3.816735	2.613694
6	6	0	3.031145	2.237246	-0.957730
7	1	0	4.049412	2.500761	-1.256182
8	1	0	2.549363	1.764345	-1.818642
9	1	0	2.486886	3.167087	-0.768401
10	6	0	0.886473	-0.918943	2.484316
11	1	0	-0.075071	-0.411932	2.374467
12	1	0	0.782306	-1.905354	2.021585
13	1	0	1.056099	-1.076561	3.552856
14	6	0	5.681088	0.423547	2.868975
15	1	0	6.353338	-0.299248	2.392107
16	1	0	6.197616	1.388122	2.878061
17	1	0	5.537278	0.103585	3.904518
18	6	0	4.370766	0.508038	2.132335
19	6	0	4.249255	1.269806	0.972770
20	1	0	5.112196	1.825159	0.612122
21	6	0	3.053988	1.350352	0.267529
22	6	0	1.921291	0.618291	0.698579
23	6	0	2.037123	-0.142550	1.882702
24	6	0	3.247593	-0.175561	2.575988
25	1	0	3.309555	-0.755946	3.493647
26	6	0	-0.455037	2.433175	-1.730123
27	6	0	-0.895930	3.709871	-2.071405
28	1	0	-1.183773	3.909418	-3.101031
29	6	0	-0.989130	4.732026	-1.132854
30	6	0	-0.623646	4.445077	0.178802
31	1	0	-0.706622	5.223327	0.933991
32	6	0	-0.152018	3.189223	0.553533
33	6	0	-0.060762	2.154160	-0.402446
34	6	0	-0.427361	1.386548	-2.822133
35	1	0	-1.230270	0.654450	-2.691842
36	1	0	-0.559736	1.853666	-3.801537
37	1	0	0.510918	0.825024	-2.849189
38	6	0	-1.451326	6.109918	-1.526948
39	1	0	-1.965819	6.610008	-0.701474
40	1	0	-0.602616	6.742630	-1.812304
41	1	0	-2.132062	6.073662	-2.382099
42	7	0	-0.262823	-0.446825	-0.338806

43	6	0	-1.657943	-0.523874	-0.060967
44	6	0	0.167998	-1.779462	-0.535731
45	6	0	-2.044153	-1.870078	0.020581
46	6	0	-2.597049	0.479498	0.185769
47	6	0	-0.876131	-2.660428	-0.279512
48	6	0	1.409483	-2.263046	-1.053458
49	6	0	-3.358045	-2.222816	0.329184
50	6	0	-3.898607	0.105965	0.483019
51	1	0	-2.335879	1.526872	0.142003
52	6	0	-0.700384	-4.059220	-0.356730
53	6	0	1.577424	-3.680262	-1.100457
54	6	0	2.438406	-1.455386	-1.593451
55	6	0	-4.305000	-1.236844	0.561543
56	1	0	-3.640365	-3.271040	0.386359
57	1	0	-4.627232	0.891851	0.660243
58	6	0	0.516673	-4.552766	-0.721108
59	1	0	-1.525667	-4.724196	-0.121833
60	6	0	2.797530	-4.212235	-1.583353
61	6	0	3.597030	-2.003168	-2.080409
62	1	0	2.304702	-0.385279	-1.639925
63	1	0	0.686869	-5.623990	-0.773190
64	6	0	3.793204	-3.398052	-2.054624
65	1	0	2.919862	-5.291785	-1.591623
66	1	0	4.364183	-1.356400	-2.494316
67	1	0	4.718740	-3.823427	-2.429638
68	6	0	-5.741315	-1.600886	0.890709
69	1	0	-5.800909	-2.696343	0.897783
70	6	0	-6.150112	-1.107201	2.283486
71	1	0	-7.168914	-1.428843	2.524135
72	1	0	-5.477696	-1.495666	3.054192
73	1	0	-6.125467	-0.013641	2.339015
74	6	0	-6.716252	-1.092137	-0.177696
75	1	0	-6.714022	0.002039	-0.226326
76	1	0	-6.449612	-1.470623	-1.168978
77	1	0	-7.738934	-1.412615	0.047640

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=n-hexane)

Excited State 1: Singlet-A 3.9160 eV 316.61 nm f=0.2458
<S**2>=0.000
135 ->137 0.26010
136 ->137 0.61597

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1511.74110004 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1511.59845354 a.u.

Excited State 1: Singlet-A 3.8946 eV 318.35 nm f=0.1786
<S**2>=0.000

135 ->137 0.22272
136 ->137 0.63335

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes) TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1511.52315977 a.u.
Lowest frequency = 17.5170

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.707149	0.717110	0.060782
2	6	0	0.668335	3.424891	1.411965
3	1	0	0.212465	2.657623	2.046649
4	1	0	1.748771	3.325764	1.553061
5	1	0	0.371623	4.407063	1.791901
6	6	0	3.355744	2.038895	-0.518411
7	1	0	4.420716	2.228401	-0.682319
8	1	0	2.955861	1.533024	-1.403499
9	1	0	2.847870	3.007233	-0.476890
10	6	0	0.611625	-0.825523	2.750002
11	1	0	-0.228267	-0.123340	2.740077
12	1	0	0.311663	-1.691311	2.150553
13	1	0	0.740170	-1.176028	3.778009
14	6	0	5.436326	0.135062	3.602410
15	1	0	6.024116	-0.741309	3.301196
16	1	0	6.098857	1.003911	3.541426
17	1	0	5.162460	-0.007143	4.652497
18	6	0	4.217889	0.309691	2.735226
19	6	0	4.256760	1.072452	1.572135
20	1	0	5.188944	1.561799	1.295800
21	6	0	3.153377	1.222530	0.737163
22	6	0	1.910625	0.588115	1.046326
23	6	0	1.878611	-0.177329	2.248371
24	6	0	3.008319	-0.301059	3.050476
25	1	0	2.936089	-0.882236	3.968004
26	6	0	-0.253101	1.996704	-2.028687
27	6	0	-0.684239	3.168056	-2.643161
28	1	0	-1.044207	3.118645	-3.669229
29	6	0	-0.657433	4.399652	-1.996946
30	6	0	-0.190085	4.418157	-0.686393
31	1	0	-0.183265	5.362169	-0.144520
32	6	0	0.250652	3.270833	-0.031950
33	6	0	0.242156	2.006415	-0.694429
34	6	0	-0.300904	0.731229	-2.847929
35	1	0	-1.120867	0.070931	-2.543210
36	1	0	-0.450667	0.960577	-3.906914
37	1	0	0.627138	0.157377	-2.757051
38	6	0	-1.094119	5.662056	-2.692171
39	1	0	-1.504399	6.387782	-1.983036
40	1	0	-0.255270	6.150375	-3.203816
41	1	0	-1.858788	5.459145	-3.448317
42	7	0	-0.218866	-0.512562	-0.111140
43	6	0	-1.574072	-0.462949	0.289466
44	6	0	0.007811	-1.749401	-0.625333

45	6	0	-2.201531	-1.689515	0.036270
46	6	0	-2.271587	0.595861	0.845019
47	6	0	-1.186004	-2.534991	-0.546327
48	6	0	1.207312	-2.312392	-1.199759
49	6	0	-3.540369	-1.872250	0.342287
50	6	0	-3.619270	0.391346	1.154329
51	1	0	-1.798171	1.553005	1.017424
52	6	0	-1.227458	-3.849588	-0.991000
53	6	0	1.119623	-3.662396	-1.660301
54	6	0	2.430443	-1.639348	-1.348298
55	6	0	-4.270160	-0.820830	0.913752
56	1	0	-4.031491	-2.820273	0.139991
57	1	0	-4.175105	1.214075	1.592951
58	6	0	-0.087363	-4.398846	-1.539857
59	1	0	-2.140726	-4.430039	-0.915521
60	6	0	2.250341	-4.270000	-2.251346
61	6	0	3.518478	-2.261766	-1.931518
62	1	0	2.523111	-0.627074	-0.987553
63	1	0	-0.100620	-5.422529	-1.900753
64	6	0	3.431851	-3.582001	-2.392455
65	1	0	2.165915	-5.296857	-2.594423
66	1	0	4.451907	-1.716476	-2.023270
67	1	0	4.293013	-4.058921	-2.848466
68	6	0	-5.738080	-1.003169	1.253154
69	1	0	-6.005566	-2.031688	0.981603
70	6	0	-5.998378	-0.838650	2.755261
71	1	0	-7.050787	-1.033413	2.985024
72	1	0	-5.386484	-1.529207	3.343060
73	1	0	-5.768764	0.178891	3.088398
74	6	0	-6.629286	-0.061358	0.434428
75	1	0	-6.421215	0.986964	0.672726
76	1	0	-6.470918	-0.197514	-0.639399
77	1	0	-7.685837	-0.248522	0.651290

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1511.62365680 a.u.

Excited State 1: Singlet-A 2.8300 eV 438.11 nm f=0.0446
<S**2>=0.000
135 ->137 0.10664
136 ->137 0.67779

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,
NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1511.72625198 a.u.

Results

Absorb Energy =	0.143 a.u.	3.882 eV	319.414 nm
Emission Energy =	0.103 a.u.	2.792 eV	444.108 nm
Stokes Shift =	0.040 a.u.	1.090 eV	124.694 nm

Compound 6 THF

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : TetraHydroFuran
SCF Done: E(RCAM-B3LYP) = -1511.65114647 a.u.
Lowest frequency = 16.9991

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.528936	0.744052	-0.030738
2	6	0	0.216938	2.993382	1.997574
3	1	0	-0.225317	2.083605	2.414596
4	1	0	1.299971	2.910488	2.126077
5	1	0	-0.128871	3.835177	2.603257
6	6	0	3.039053	2.241946	-0.938200
7	1	0	4.059134	2.501845	-1.232995
8	1	0	2.556769	1.775438	-1.802170
9	1	0	2.499312	3.173719	-0.744936
10	6	0	0.867241	-0.907553	2.492938
11	1	0	-0.086365	-0.382875	2.396357
12	1	0	0.743770	-1.885836	2.017861
13	1	0	1.041279	-1.082199	3.557973
14	6	0	5.670167	0.406299	2.891949
15	1	0	6.341562	-0.316478	2.413933
16	1	0	6.189794	1.369038	2.905518
17	1	0	5.521802	0.082326	3.925522
18	6	0	4.362502	0.498009	2.151322
19	6	0	4.247825	1.262740	0.992589
20	1	0	5.114340	1.814740	0.635623
21	6	0	3.054404	1.350640	0.283958
22	6	0	1.917168	0.622470	0.709912
23	6	0	2.025492	-0.139901	1.894249
24	6	0	3.233914	-0.180517	2.591225
25	1	0	3.289994	-0.761225	3.509027
26	6	0	-0.459913	2.429150	-1.733636
27	6	0	-0.907414	3.702563	-2.079692
28	1	0	-1.196748	3.896852	-3.109862
29	6	0	-1.004971	4.728315	-1.144904
30	6	0	-0.636067	4.448419	0.167708
31	1	0	-0.721874	5.229335	0.919738
32	6	0	-0.157573	3.196181	0.546843
33	6	0	-0.063034	2.156986	-0.404861
34	6	0	-0.426453	1.379966	-2.823289
35	1	0	-1.224248	0.642631	-2.690791
36	1	0	-0.563214	1.844179	-3.803339
37	1	0	0.515954	0.825476	-2.850307
38	6	0	-1.475048	6.102096	-1.543938
39	1	0	-1.991180	6.602439	-0.719750
40	1	0	-0.629530	6.737834	-1.831856
41	1	0	-2.155237	6.058639	-2.399093
42	7	0	-0.260061	-0.444150	-0.337416
43	6	0	-1.653842	-0.526292	-0.057834
44	6	0	0.174156	-1.773945	-0.541503

45	6	0	-2.037515	-1.874038	0.015398
46	6	0	-2.594634	0.473597	0.198348
47	6	0	-0.867666	-2.659826	-0.290303
48	6	0	1.416937	-2.251475	-1.062587
49	6	0	-3.350766	-2.231935	0.323445
50	6	0	-3.895307	0.095665	0.494947
51	1	0	-2.334802	1.521703	0.163538
52	6	0	-0.688218	-4.058158	-0.375459
53	6	0	1.589050	-3.668273	-1.116907
54	6	0	2.443052	-1.437767	-1.599843
55	6	0	-4.299306	-1.249034	0.564127
56	1	0	-3.630769	-3.281055	0.374163
57	1	0	-4.624813	0.878927	0.679876
58	6	0	0.530621	-4.546400	-0.742343
59	1	0	-1.511445	-4.726953	-0.144400
60	6	0	2.811030	-4.194422	-1.602887
61	6	0	3.603422	-1.979669	-2.090505
62	1	0	2.305721	-0.367934	-1.642949
63	1	0	0.703870	-5.616782	-0.799958
64	6	0	3.804172	-3.374500	-2.070882
65	1	0	2.936860	-5.273439	-1.616474
66	1	0	4.367600	-1.328891	-2.503556
67	1	0	4.730746	-3.795040	-2.448553
68	6	0	-5.734421	-1.618066	0.893621
69	1	0	-5.792423	-2.713406	0.891243
70	6	0	-6.140287	-1.136583	2.291594
71	1	0	-7.158160	-1.461830	2.530858
72	1	0	-5.466439	-1.531987	3.057710
73	1	0	-6.116915	-0.043454	2.356386
74	6	0	-6.712808	-1.100745	-0.167545
75	1	0	-6.712396	-0.006111	-0.206126
76	1	0	-6.449415	-1.471026	-1.162957
77	1	0	-7.733984	-1.425026	0.058642

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=THF)

Excited State 1: Singlet-A 3.9147 eV 316.71 nm f=0.2503
<S**2>=0.000
135 ->137 0.26730
136 ->137 0.61220

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1511.74509184 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1511.60190208 a.u.

Excited State 1: Singlet-A 3.8946 eV 318.34 nm f=0.1804
<S**2>=0.000
135 ->137 0.23393
136 ->137 0.62842

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1511.52551106 a.u.
Lowest frequency = 18.3753

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.694186	0.722286	0.058303
2	6	0	0.622654	3.422404	1.436193
3	1	0	0.179085	2.642275	2.063997
4	1	0	1.705494	3.336663	1.568414
5	1	0	0.314985	4.396439	1.827933
6	6	0	3.329303	2.078058	-0.533173
7	1	0	4.390359	2.282116	-0.703990
8	1	0	2.929746	1.570772	-1.417650
9	1	0	2.809132	3.039408	-0.479939
10	6	0	0.633744	-0.824017	2.739032
11	1	0	-0.212966	-0.130108	2.727987
12	1	0	0.341630	-1.693374	2.140651
13	1	0	0.768215	-1.171698	3.767242
14	6	0	5.459405	0.171825	3.562856
15	1	0	6.082013	-0.662518	3.216120
16	1	0	6.086191	1.068797	3.545320
17	1	0	5.193865	-0.035499	4.603954
18	6	0	4.232436	0.339347	2.705812
19	6	0	4.256830	1.108275	1.545138
20	1	0	5.183054	1.606286	1.264237
21	6	0	3.145750	1.252046	0.718915
22	6	0	1.911957	0.604104	1.033052
23	6	0	1.892758	-0.163999	2.232695
24	6	0	3.030098	-0.282162	3.027356
25	1	0	2.969066	-0.868124	3.942623
26	6	0	-0.286199	2.010352	-2.013367
27	6	0	-0.741334	3.179929	-2.616890
28	1	0	-1.103631	3.132969	-3.642227
29	6	0	-0.735767	4.405881	-1.959346
30	6	0	-0.263671	4.421828	-0.649256
31	1	0	-0.272596	5.361095	-0.099149
32	6	0	0.199906	3.276430	-0.007012
33	6	0	0.208872	2.018098	-0.679657
34	6	0	-0.309535	0.750472	-2.842120
35	1	0	-1.112321	0.069109	-2.537883
36	1	0	-0.468988	0.983718	-3.898843
37	1	0	0.631121	0.196389	-2.756536
38	6	0	-1.199599	5.666777	-2.640272
39	1	0	-1.664832	6.357249	-1.929797
40	1	0	-0.363870	6.202083	-3.107979
41	1	0	-1.926680	5.451246	-3.428967
42	7	0	-0.212433	-0.508296	-0.115096
43	6	0	-1.571104	-0.475206	0.280539
44	6	0	0.034175	-1.751404	-0.617154
45	6	0	-2.177695	-1.714357	0.037861
46	6	0	-2.284794	0.574654	0.833239

47	6	0	-1.146122	-2.552428	-0.530555
48	6	0	1.239339	-2.296242	-1.193714
49	6	0	-3.513601	-1.916154	0.342535
50	6	0	-3.630759	0.352531	1.139841
51	1	0	-1.825373	1.537770	1.010869
52	6	0	-1.167930	-3.872802	-0.958917
53	6	0	1.173615	-3.653960	-1.638129
54	6	0	2.446727	-1.600083	-1.367818
55	6	0	-4.261767	-0.870920	0.903894
56	1	0	-3.988038	-2.873968	0.148420
57	1	0	-4.199064	1.168663	1.574716
58	6	0	-0.018732	-4.410312	-1.502294
59	1	0	-2.071784	-4.466573	-0.877233
60	6	0	2.310913	-4.246304	-2.233653
61	6	0	3.539763	-2.206157	-1.960279
62	1	0	2.522279	-0.580612	-1.023356
63	1	0	-0.016031	-5.438237	-1.850444
64	6	0	3.475835	-3.535205	-2.400076
65	1	0	2.243821	-5.279097	-2.561810
66	1	0	4.459479	-1.642129	-2.075690
67	1	0	4.341082	-4.000170	-2.860451
68	6	0	-5.727908	-1.074321	1.238702
69	1	0	-5.976342	-2.110080	0.978536
70	6	0	-5.999073	-0.895120	2.737205
71	1	0	-7.049308	-1.105969	2.962405
72	1	0	-5.379217	-1.568589	3.336557
73	1	0	-5.789639	0.130501	3.058837
74	6	0	-6.629600	-0.157210	0.403413
75	1	0	-6.438570	0.897307	0.628696
76	1	0	-6.464839	-0.306756	-0.667789
77	1	0	-7.683780	-0.358596	0.618813

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1511.63540054 a.u.

Excited State 1: Singlet-A 2.7206 eV 455.73 nm f=0.0484
<S**2>=0.000
136 ->137 0.67922

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1511.72825557 a.u.

Results

Absorb Energy =	0.143 a.u.	3.896 eV	318.203 nm
Emission Energy =	0.093 a.u.	2.527 eV	490.693 nm
Stokes Shift =	0.050 a.u.	1.370 eV	172.491 nm

Compound 6 ACN

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : Acetonitrile
SCF Done: E(RCAM-B3LYP) = -1511.65278025 a.u.
Lowest frequency = 17.1009

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.527158	0.747373	-0.029435
2	6	0	0.213510	2.997446	1.998894
3	1	0	-0.224474	2.086156	2.416978
4	1	0	1.297137	2.919574	2.125869
5	1	0	-0.134770	3.838254	2.604430
6	6	0	3.038709	2.244588	-0.935169
7	1	0	4.058927	2.502332	-1.231075
8	1	0	2.553789	1.780956	-1.799124
9	1	0	2.502011	3.177491	-0.738680
10	6	0	0.861952	-0.900785	2.496367
11	1	0	-0.088947	-0.370435	2.403988
12	1	0	0.731797	-1.876933	2.018571
13	1	0	1.038025	-1.079641	3.560301
14	6	0	5.669287	0.400886	2.891942
15	1	0	6.339459	-0.322070	2.412466
16	1	0	6.190345	1.362777	2.905893
17	1	0	5.520920	0.075675	3.925074
18	6	0	4.361314	0.495526	2.152168
19	6	0	4.247387	1.260945	0.993598
20	1	0	5.114739	1.811273	0.636247
21	6	0	3.053397	1.351738	0.285833
22	6	0	1.915038	0.625666	0.712246
23	6	0	2.022265	-0.136763	1.896797
24	6	0	3.231246	-0.180621	2.592921
25	1	0	3.286533	-0.761004	3.510960
26	6	0	-0.466006	2.430361	-1.731845
27	6	0	-0.917310	3.702638	-2.077527
28	1	0	-1.207892	3.896313	-3.107427
29	6	0	-1.016899	4.728202	-1.142481
30	6	0	-0.645726	4.449270	0.169823
31	1	0	-0.732887	5.229938	0.921895
32	6	0	-0.163393	3.198242	0.548464
33	6	0	-0.067220	2.159054	-0.403279
34	6	0	-0.430035	1.381858	-2.822182
35	1	0	-1.224690	0.641191	-2.689108
36	1	0	-0.570124	1.846181	-3.801647
37	1	0	0.514791	0.831606	-2.850988
38	6	0	-1.491399	6.100642	-1.540851
39	1	0	-2.008098	6.599200	-0.715998
40	1	0	-0.647758	6.738732	-1.829029
41	1	0	-2.171641	6.055298	-2.395811
42	7	0	-0.259194	-0.442801	-0.337440
43	6	0	-1.652568	-0.528813	-0.057971
44	6	0	0.178362	-1.771101	-0.543163
45	6	0	-2.033199	-1.877641	0.013062
46	6	0	-2.595741	0.468466	0.200246
47	6	0	-0.861201	-2.660210	-0.293258
48	6	0	1.422357	-2.244895	-1.064986

49	6	0	-3.345901	-2.239371	0.319992
50	6	0	-3.895767	0.087066	0.495648
51	1	0	-2.337989	1.517210	0.168764
52	6	0	-0.677945	-4.058177	-0.379372
53	6	0	1.598767	-3.661282	-1.119545
54	6	0	2.445608	-1.427854	-1.603096
55	6	0	-4.296849	-1.258907	0.561920
56	1	0	-3.623306	-3.289205	0.368965
57	1	0	-4.626917	0.868339	0.682346
58	6	0	0.542666	-4.542819	-0.745743
59	1	0	-1.499336	-4.729505	-0.149271
60	6	0	2.822700	-4.183674	-1.605301
61	6	0	3.607924	-1.966088	-2.093696
62	1	0	2.304243	-0.358611	-1.648233
63	1	0	0.718992	-5.612640	-0.803588
64	6	0	3.813393	-3.360439	-2.073208
65	1	0	2.952063	-5.262223	-1.618939
66	1	0	4.369367	-1.313076	-2.508216
67	1	0	4.741334	-3.777989	-2.450712
68	6	0	-5.731233	-1.631781	0.890586
69	1	0	-5.787387	-2.727081	0.883748
70	6	0	-6.137059	-1.156469	2.290739
71	1	0	-7.154296	-1.484475	2.528757
72	1	0	-5.462617	-1.554504	3.055063
73	1	0	-6.115430	-0.063570	2.359864
74	6	0	-6.711207	-1.111511	-0.167722
75	1	0	-6.713070	-0.016715	-0.201333
76	1	0	-6.448220	-1.477461	-1.164920
77	1	0	-7.731405	-1.438967	0.058062

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=acetonitrile)

Excited State 1: Singlet-A 3.9200 eV 316.28 nm f=0.2434
<S**2>=0.000
135 ->137 0.26815
136 ->137 0.61158

Step3

Method: cam-b3lyp/6-31+G(d,p)
SCRF(Solvent=acetonitrile,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1511.74686954 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1511.60297477 a.u.

Excited State 1: Singlet-A 3.9049 eV 317.51 nm f=0.1829
<S**2>=0.000
135 ->137 0.24134
136 ->137 0.62483

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1511.52666871 a.u.
Lowest frequency = 19.8071

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.689016	0.724190	0.058673
2	6	0	0.606483	3.419525	1.450323
3	1	0	0.165611	2.634547	2.073993
4	1	0	1.689977	3.337640	1.580129
5	1	0	0.295440	4.390306	1.847261
6	6	0	3.321233	2.092946	-0.530232
7	1	0	4.381349	2.299765	-0.703083
8	1	0	2.919958	1.590078	-1.416437
9	1	0	2.799808	3.053177	-0.468238
10	6	0	0.638038	-0.830900	2.732257
11	1	0	-0.210515	-0.139255	2.721871
12	1	0	0.348483	-1.699881	2.132048
13	1	0	0.773653	-1.180138	3.759753
14	6	0	5.463595	0.171746	3.553062
15	1	0	6.087585	-0.659250	3.200924
16	1	0	6.088282	1.070176	3.538552
17	1	0	5.200255	-0.041844	4.593396
18	6	0	4.234771	0.340265	2.698721
19	6	0	4.255461	1.114823	1.541321
20	1	0	5.180068	1.616181	1.261166
21	6	0	3.142479	1.259327	0.717490
22	6	0	1.911190	0.606303	1.030067
23	6	0	1.895039	-0.166271	2.226834
24	6	0	3.034254	-0.285420	3.019500
25	1	0	2.975974	-0.875556	3.932240
26	6	0	-0.293738	2.019849	-2.006279
27	6	0	-0.754474	3.190280	-2.604892
28	1	0	-1.115685	3.146371	-3.630722
29	6	0	-0.756030	4.413136	-1.941247
30	6	0	-0.285053	4.425389	-0.630340
31	1	0	-0.299513	5.361948	-0.075811
32	6	0	0.183865	3.279019	0.006589
33	6	0	0.198755	2.024061	-0.671619
34	6	0	-0.309062	0.763524	-2.840629
35	1	0	-1.106036	0.074676	-2.537977
36	1	0	-0.471805	1.000081	-3.896078
37	1	0	0.635572	0.215722	-2.757911
38	6	0	-1.226244	5.674903	-2.616353
39	1	0	-1.696035	6.359048	-1.902852
40	1	0	-0.392897	6.217311	-3.080058
41	1	0	-1.950711	5.459183	-3.407313
42	7	0	-0.211456	-0.505450	-0.118668
43	6	0	-1.571799	-0.478277	0.273924
44	6	0	0.042136	-1.750042	-0.617869
45	6	0	-2.171348	-1.721091	0.032346
46	6	0	-2.290797	0.567399	0.827897
47	6	0	-1.133857	-2.556184	-0.530820
48	6	0	1.249523	-2.288138	-1.194926
49	6	0	-3.506444	-1.929649	0.335620

50	6	0	-3.636332	0.339102	1.132484
51	1	0	-1.835655	1.531705	1.010467
52	6	0	-1.148423	-3.878150	-0.954033
53	6	0	1.192118	-3.648556	-1.633610
54	6	0	2.450811	-1.583474	-1.378486
55	6	0	-4.260804	-0.887501	0.895216
56	1	0	-3.975236	-2.890322	0.142577
57	1	0	-4.208636	1.152067	1.568035
58	6	0	0.004741	-4.411709	-1.493830
59	1	0	-2.049170	-4.476347	-0.871734
60	6	0	2.332252	-4.235415	-2.229652
61	6	0	3.546082	-2.183729	-1.973592
62	1	0	2.519378	-0.561052	-1.041146
63	1	0	0.013312	-5.440947	-1.837686
64	6	0	3.491132	-3.516040	-2.404763
65	1	0	2.271867	-5.270327	-2.552160
66	1	0	4.460386	-1.612753	-2.098060
67	1	0	4.358120	-3.976787	-2.866016
68	6	0	-5.726024	-1.098915	1.229006
69	1	0	-5.969738	-2.134470	0.964402
70	6	0	-5.997543	-0.927188	2.728364
71	1	0	-7.046972	-1.143244	2.952287
72	1	0	-5.375326	-1.601443	3.324443
73	1	0	-5.791986	0.097863	3.054402
74	6	0	-6.631965	-0.182088	0.398026
75	1	0	-6.446613	0.872302	0.628797
76	1	0	-6.466597	-0.326172	-0.673881
77	1	0	-7.684978	-0.390316	0.612466

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1) SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1511.64014217 a.u.

Excited State 1: Singlet-A 2.6778 eV 463.01 nm f=0.0498 <S**2>=0.000
136 ->137 0.67998

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=acetonitrile, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1511.72876162 a.u.

Results

Absorb Energy =	0.144 a.u.	3.916 eV	316.644 nm
Emission Energy =	0.089 a.u.	2.411 eV	514.146 nm
Stokes Shift =	0.055 a.u.	1.504 eV	197.503 nm

Compound 7 n-hexane

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : n-Hexane
SCF Done: E(RCAM-B3LYP) = -1508.25482631 a.u.
Lowest frequency = 19.6136

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.437739	-1.600627	0.146264
2	6	0	-1.371440	-2.506466	-0.199164
3	6	0	-0.250804	-1.738318	-0.495906
4	7	0	-0.531290	-0.370496	-0.282179
5	6	0	-1.917238	-0.304319	0.050539
6	6	0	-2.737865	0.791020	0.338441
7	6	0	-4.054527	0.558250	0.687282
8	6	0	-4.577237	-0.742891	0.774138
9	6	0	-3.768664	-1.835381	0.506357
10	6	0	-1.346670	-3.915922	-0.281724
11	6	0	-0.203203	-4.533687	-0.691138
12	6	0	0.928187	-3.776078	-1.112054
13	6	0	0.911904	-2.349221	-1.061403
14	8	0	-5.890237	-0.819103	1.130225
15	6	0	-6.469582	-2.101059	1.237669
16	6	0	2.066145	-4.432347	-1.640073
17	6	0	3.123198	-3.726369	-2.150837
18	6	0	3.073246	-2.318742	-2.173012
19	6	0	1.997747	-1.653262	-1.643553
20	1	0	-2.372143	1.806180	0.287167
21	1	0	-4.719168	1.387518	0.903592
22	1	0	-4.141769	-2.850210	0.568796
23	1	0	-2.227517	-4.491682	-0.014670
24	1	0	-0.148350	-5.616685	-0.748166
25	1	0	-7.508465	-1.942343	1.528139
26	1	0	-5.968805	-2.706107	2.003288
27	1	0	-6.439638	-2.637541	0.281492
28	1	0	2.073910	-5.518766	-1.650768
29	1	0	3.983889	-4.245976	-2.560004
30	1	0	3.887102	-1.755251	-2.618251
31	1	0	1.974352	-0.575088	-1.689240
32	5	0	0.389779	0.724626	-0.011708
33	6	0	-0.070219	2.196435	-0.344700
34	6	0	-0.008861	3.227198	0.618098
35	6	0	-0.490994	2.526780	-1.652470
36	6	0	-0.362570	4.528772	0.269829
37	6	0	-0.810567	3.845248	-1.968536
38	6	0	-0.760835	4.862280	-1.020892
39	1	0	-0.321897	5.306530	1.028984
40	1	0	-1.113709	4.084049	-2.985322
41	6	0	1.795680	0.460305	0.654366
42	6	0	1.888409	-0.313062	1.832388
43	6	0	2.974621	1.077095	0.171241
44	6	0	3.119507	-0.468270	2.470320
45	6	0	4.186547	0.876996	0.822481
46	6	0	4.283711	0.103455	1.976421
47	1	0	3.165113	-1.055508	3.384604
48	1	0	5.083199	1.345338	0.422748
49	6	0	2.984187	1.963506	-1.054488

50	1	0	2.417051	1.542388	-1.890004
51	1	0	2.546376	2.943589	-0.843572
52	1	0	4.008681	2.122929	-1.401483
53	6	0	0.694204	-0.974958	2.483917
54	1	0	-0.215905	-0.373881	2.418828
55	1	0	0.471233	-1.942673	2.023613
56	1	0	0.894929	-1.156315	3.543269
57	6	0	5.610783	-0.113659	2.653588
58	1	0	5.482972	-0.391965	3.703233
59	1	0	6.172438	-0.919466	2.166674
60	1	0	6.232897	0.785405	2.611752
61	6	0	0.410934	2.967560	2.047183
62	1	0	-0.098341	2.098891	2.475157
63	1	0	1.485359	2.777781	2.124240
64	1	0	0.176441	3.829581	2.677478
65	6	0	-0.613283	1.493147	-2.750333
66	1	0	0.264652	0.844656	-2.823302
67	1	0	-1.476015	0.839945	-2.587243
68	1	0	-0.744308	1.980312	-3.720104
69	6	0	-1.153632	6.272740	-1.372933
70	1	0	-2.225783	6.434542	-1.210668
71	1	0	-0.618131	7.001843	-0.758303
72	1	0	-0.947096	6.494259	-2.423813

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=n-hexane)

Excited State 1: Singlet-A 3.9006 eV 317.86 nm f=0.2557 <S**2>=0.000

131 ->133 -0.40351

132 ->133 0.51499

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,NonEquilibrium=Save)

SCF Done: E(RCAM-B3LYP) = -1508.34530902 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1) SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1508.20275922 a.u.

Excited State 1: Singlet-A 3.8883 eV 318.87 nm f=0.1873 <S**2>=0.000

128 ->133 0.10169

131 ->133 -0.42882

132 ->133 0.49434

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes) TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1508.13157621 a.u.

Lowest frequency = 23.6117

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.626360	-1.189530	0.331856
2	6	0	-1.842723	-2.206573	-0.349577
3	6	0	-0.569164	-1.661955	-0.558137
4	7	0	-0.517562	-0.364160	-0.017799
5	6	0	-1.753092	-0.087764	0.502338
6	6	0	-2.197127	1.090430	1.130835
7	6	0	-3.497453	1.135802	1.583181
8	6	0	-4.363704	0.040307	1.413661
9	6	0	-3.927071	-1.140824	0.775967
10	6	0	-2.176289	-3.490835	-0.779832
11	6	0	-1.223542	-4.230416	-1.441683
12	6	0	0.072140	-3.716885	-1.684579
13	6	0	0.443238	-2.406509	-1.235086
14	8	0	-5.605883	0.210838	1.888882
15	6	0	-6.555094	-0.837444	1.756310
16	6	0	1.023026	-4.500756	-2.389256
17	6	0	2.278713	-4.025167	-2.646536
18	6	0	2.645312	-2.740129	-2.194069
19	6	0	1.756528	-1.954311	-1.505225
20	1	0	-1.539166	1.941469	1.235921
21	1	0	-3.890293	2.019662	2.071201
22	1	0	-4.594749	-1.981784	0.638401
23	1	0	-3.168184	-3.894395	-0.602952
24	1	0	-1.457611	-5.229337	-1.796243
25	1	0	-7.471904	-0.464724	2.210415
26	1	0	-6.225065	-1.737035	2.285247
27	1	0	-6.738179	-1.071925	0.702987
28	1	0	0.727528	-5.491597	-2.721735
29	1	0	2.996248	-4.634377	-3.186671
30	1	0	3.648033	-2.369825	-2.381098
31	1	0	2.062331	-0.984672	-1.144204
32	5	0	0.637337	0.664608	0.088463
33	6	0	0.357749	2.027707	-0.623421
34	6	0	0.645872	3.260790	0.036630
35	6	0	-0.241187	2.125282	-1.911525
36	6	0	0.348727	4.476991	-0.571854
37	6	0	-0.521557	3.363595	-2.480424
38	6	0	-0.237674	4.560911	-1.831626
39	1	0	0.572199	5.396616	-0.034106
40	1	0	-0.962803	3.394770	-3.475027
41	6	0	1.880658	0.287222	0.954737
42	6	0	1.820317	-0.493938	2.144966
43	6	0	3.183783	0.700542	0.538536
44	6	0	2.976074	-0.827321	2.844025
45	6	0	4.311699	0.345095	1.272671
46	6	0	4.240847	-0.423189	2.430402
47	1	0	2.883309	-1.412845	3.756858
48	1	0	5.287659	0.670311	0.917090
49	6	0	3.419423	1.488980	-0.729255
50	1	0	2.863061	1.074858	-1.576535
51	1	0	3.098364	2.531521	-0.644500
52	1	0	4.483201	1.488685	-0.984781
53	6	0	0.509874	-0.943388	2.741517
54	1	0	-0.193426	-0.109526	2.840267
55	1	0	0.015314	-1.712216	2.138451

56	1	0	0.665848	-1.367054	3.737594
57	6	0	5.480507	-0.822678	3.186009
58	1	0	5.271344	-0.962569	4.251114
59	1	0	5.894324	-1.767446	2.811479
60	1	0	6.266917	-0.067314	3.093086
61	6	0	1.222008	3.313410	1.432025
62	1	0	0.698446	2.628974	2.108385
63	1	0	2.274986	3.018331	1.466827
64	1	0	1.145729	4.326065	1.839035
65	6	0	-0.548727	0.899821	-2.735009
66	1	0	0.286005	0.191273	-2.729825
67	1	0	-1.428759	0.359602	-2.368001
68	1	0	-0.750647	1.171931	-3.775065
69	6	0	-0.574614	5.890842	-2.452538
70	1	0	-1.564414	6.244494	-2.137220
71	1	0	0.148036	6.661354	-2.166354
72	1	0	-0.587068	5.829379	-3.545032

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1508.22900206 a.u.

Excited State 1: Singlet-A 2.7954 eV 443.53 nm f=0.0337
<S**2>=0.000
132 ->133 0.68131

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,
NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1508.33015391 a.u.

Results

Absorb Energy =	0.143 a.u.	3.879 eV	319.631 nm
Emission Energy =	0.101 a.u.	2.752 eV	450.445 nm
Stokes Shift =	0.041 a.u.	1.126 eV	130.814 nm

Compound 7 THF

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : TetraHydroFuran
SCF Done: E(RCAM-B3LYP) = -1508.25929561 a.u.
Lowest frequency = 19.5822

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.433214	-1.605468	0.145619

2	6	0	-1.365487	-2.508094	-0.204445
3	6	0	-0.246494	-1.736065	-0.498698
4	7	0	-0.529283	-0.369834	-0.280025
5	6	0	-1.914322	-0.307619	0.055186
6	6	0	-2.736421	0.784821	0.350216
7	6	0	-4.052675	0.548004	0.699504
8	6	0	-4.573733	-0.754817	0.780127
9	6	0	-3.763497	-1.844930	0.505985
10	6	0	-1.338487	-3.917676	-0.291680
11	6	0	-0.193492	-4.531883	-0.703263
12	6	0	0.936503	-3.770035	-1.121891
13	6	0	0.917322	-2.343043	-1.066911
14	8	0	-5.885985	-0.835617	1.137217
15	6	0	-6.463481	-2.122373	1.240519
16	6	0	2.076038	-4.422633	-1.652409
17	6	0	3.131467	-3.712487	-2.161990
18	6	0	3.078238	-2.304440	-2.180655
19	6	0	2.001346	-1.642773	-1.648078
20	1	0	-2.372166	1.800830	0.305490
21	1	0	-4.716721	1.376508	0.921349
22	1	0	-4.134730	-2.860625	0.564260
23	1	0	-2.218069	-4.496020	-0.026361
24	1	0	-0.136416	-5.614499	-0.763503
25	1	0	-7.502029	-1.967023	1.533022
26	1	0	-5.959345	-2.727784	2.002713
27	1	0	-6.432783	-2.653402	0.282060
28	1	0	2.086376	-5.508922	-1.666231
29	1	0	3.992994	-4.228838	-2.573302
30	1	0	3.889776	-1.738171	-2.626538
31	1	0	1.975088	-0.564594	-1.692270
32	5	0	0.389930	0.728489	-0.009259
33	6	0	-0.073525	2.198008	-0.346358
34	6	0	-0.014460	3.232291	0.613216
35	6	0	-0.497285	2.523322	-1.654886
36	6	0	-0.374310	4.531685	0.261919
37	6	0	-0.822869	3.839794	-1.974314
38	6	0	-0.776325	4.860042	-1.029332
39	1	0	-0.335491	5.311783	1.018697
40	1	0	-1.127591	4.074713	-2.991487
41	6	0	1.794269	0.464967	0.660999
42	6	0	1.884303	-0.308257	1.839829
43	6	0	2.975123	1.079928	0.179586
44	6	0	3.114716	-0.467062	2.478923
45	6	0	4.186582	0.876364	0.831774
46	6	0	4.281376	0.101708	1.985623
47	1	0	3.157972	-1.053369	3.393897
48	1	0	5.084503	1.342992	0.433111
49	6	0	2.988381	1.969330	-1.043979
50	1	0	2.419256	1.553736	-1.880695
51	1	0	2.555233	2.950612	-0.828597
52	1	0	4.013397	2.125629	-1.390329
53	6	0	0.687588	-0.965195	2.492254
54	1	0	-0.218232	-0.357122	2.431911
55	1	0	0.456591	-1.929814	2.029319
56	1	0	0.890175	-1.151827	3.550207
57	6	0	5.607391	-0.118343	2.664029
58	1	0	5.477827	-0.397112	3.713254
59	1	0	6.167702	-0.924970	2.176989
60	1	0	6.231357	0.779289	2.621923
61	6	0	0.410260	2.980342	2.042320

62	1	0	-0.091195	2.109479	2.474853
63	1	0	1.486471	2.799303	2.116685
64	1	0	0.171741	3.843103	2.669888
65	6	0	-0.614371	1.487602	-2.751609
66	1	0	0.269979	0.848267	-2.828016
67	1	0	-1.470142	0.826141	-2.585092
68	1	0	-0.753937	1.973160	-3.720856
69	6	0	-1.175213	6.267895	-1.384931
70	1	0	-2.247905	6.424996	-1.221865
71	1	0	-0.642695	7.000617	-0.772169
72	1	0	-0.971215	6.486799	-2.436777

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=THF)

Excited State 1: Singlet-A 3.8994 eV 317.95 nm f=0.2608
<S**2>=0.000
131 ->133 -0.36025
132 ->133 0.54664

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1508.35024421 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1508.20728418 a.u.

Excited State 1: Singlet-A 3.8879 eV 318.90 nm f=0.1898
<S**2>=0.000
131 ->133 -0.37292
132 ->133 0.53846

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1508.13479607 a.u.
Lowest frequency = 23.9302

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.610610	-1.224847	0.325712
2	6	0	-1.804509	-2.232914	-0.344909
3	6	0	-0.538150	-1.666838	-0.552362
4	7	0	-0.510263	-0.368497	-0.017692
5	6	0	-1.759689	-0.109863	0.498157
6	6	0	-2.223244	1.056393	1.128208
7	6	0	-3.529750	1.081458	1.570517
8	6	0	-4.378018	-0.025536	1.392676

9	6	0	-3.915959	-1.199524	0.759728
10	6	0	-2.113332	-3.525058	-0.765942
11	6	0	-1.144030	-4.252749	-1.420105
12	6	0	0.140865	-3.715940	-1.669247
13	6	0	0.486773	-2.394465	-1.230861
14	8	0	-5.626468	0.124259	1.857749
15	6	0	-6.557231	-0.943482	1.718450
16	6	0	1.104305	-4.485789	-2.372712
17	6	0	2.348203	-3.985175	-2.644394
18	6	0	2.688098	-2.687518	-2.208631
19	6	0	1.786354	-1.915756	-1.517717
20	1	0	-1.578163	1.915439	1.249893
21	1	0	-3.936258	1.958084	2.060681
22	1	0	-4.566681	-2.052908	0.618540
23	1	0	-3.097972	-3.945010	-0.588872
24	1	0	-1.359253	-5.258796	-1.765919
25	1	0	-7.483549	-0.586982	2.165805
26	1	0	-6.213544	-1.835593	2.250211
27	1	0	-6.727294	-1.180451	0.664063
28	1	0	0.827956	-5.485514	-2.694360
29	1	0	3.074960	-4.583364	-3.184258
30	1	0	3.679450	-2.295058	-2.411135
31	1	0	2.071534	-0.933869	-1.173008
32	5	0	0.621092	0.670592	0.088605
33	6	0	0.323017	2.040261	-0.609715
34	6	0	0.598985	3.272459	0.056172
35	6	0	-0.278403	2.137389	-1.896719
36	6	0	0.286655	4.489206	-0.544471
37	6	0	-0.575243	3.376300	-2.458307
38	6	0	-0.304185	4.573461	-1.803006
39	1	0	0.499531	5.408366	-0.001619
40	1	0	-1.020441	3.407857	-3.451124
41	6	0	1.878875	0.308225	0.947561
42	6	0	1.828930	-0.471992	2.138323
43	6	0	3.175495	0.734641	0.527184
44	6	0	2.991474	-0.798067	2.832021
45	6	0	4.310697	0.387057	1.254959
46	6	0	4.251415	-0.384452	2.412115
47	1	0	2.907338	-1.384991	3.744811
48	1	0	5.282334	0.720777	0.895407
49	6	0	3.396600	1.531909	-0.737632
50	1	0	2.840694	1.115171	-1.583990
51	1	0	3.063671	2.570015	-0.643164
52	1	0	4.458849	1.545464	-0.998622
53	6	0	0.523689	-0.929695	2.740211
54	1	0	-0.187544	-0.102068	2.832837
55	1	0	0.035030	-1.706028	2.141870
56	1	0	0.684882	-1.345969	3.738570
57	6	0	5.498236	-0.775531	3.160975
58	1	0	5.294375	-0.924435	4.225774
59	1	0	5.919739	-1.713775	2.778968
60	1	0	6.276912	-0.012206	3.068713
61	6	0	1.176963	3.322405	1.450870
62	1	0	0.659701	2.628522	2.122441
63	1	0	2.233263	3.038359	1.480222
64	1	0	1.090954	4.331372	1.864803
65	6	0	-0.574573	0.912361	-2.724838
66	1	0	0.270174	0.215565	-2.728122
67	1	0	-1.443314	0.357888	-2.352194
68	1	0	-0.789261	1.186917	-3.761684

69	6	0	-0.658563	5.903121	-2.415310
70	1	0	-1.650847	6.243242	-2.093325
71	1	0	0.055974	6.680373	-2.127197
72	1	0	-0.675923	5.847316	-3.507954

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1508.24232448 a.u.

Excited State 1: Singlet-A 2.6746 eV 463.56 nm f=0.0378
<S**2>=0.000
132 ->133 -0.68168

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1508.33295072 a.u.

Results

Absorb Energy =	0.143 a.u.	3.890 eV	318.714 nm
Emission Energy =	0.091 a.u.	2.466 eV	502.761 nm
Stokes Shift =	0.052 a.u.	1.424 eV	184.047 nm

Compound 7 ACN

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : Acetonitrile
SCF Done: E(RCAM-B3LYP) = -1508.26117905 a.u.
Lowest frequency = 18.7382

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.427704	-1.611848	0.145369
2	6	0	-1.357477	-2.510522	-0.207563
3	6	0	-0.241060	-1.734009	-0.500676
4	7	0	-0.527820	-0.369389	-0.278881
5	6	0	-1.912231	-0.312160	0.058223
6	6	0	-2.736606	0.777177	0.358448
7	6	0	-4.052095	0.535783	0.708020
8	6	0	-4.570019	-0.768840	0.784172
9	6	0	-3.757184	-1.856144	0.505942
10	6	0	-1.325914	-3.920041	-0.297597
11	6	0	-0.178853	-4.529618	-0.710825
12	6	0	0.948335	-3.762949	-1.128936
13	6	0	0.924180	-2.335981	-1.071527
14	8	0	-5.881799	-0.854376	1.141511
15	6	0	-6.456357	-2.144172	1.240270

16	6	0	2.089873	-4.410625	-1.661785
17	6	0	3.142074	-3.695614	-2.171803
18	6	0	3.083418	-2.287548	-2.188851
19	6	0	2.004629	-1.630658	-1.653682
20	1	0	-2.374523	1.794183	0.318088
21	1	0	-4.717393	1.362305	0.933786
22	1	0	-4.125787	-2.872929	0.561432
23	1	0	-2.203321	-4.501910	-0.032958
24	1	0	-0.118167	-5.611890	-0.772846
25	1	0	-7.495210	-1.992477	1.533266
26	1	0	-5.950289	-2.750441	2.000143
27	1	0	-6.423825	-2.671176	0.279924
28	1	0	2.104355	-5.496802	-1.677360
29	1	0	4.004913	-4.208066	-2.585116
30	1	0	3.891631	-1.717726	-2.636222
31	1	0	1.973986	-0.552536	-1.697312
32	5	0	0.388716	0.731920	-0.007555
33	6	0	-0.077957	2.199485	-0.347342
34	6	0	-0.019048	3.236458	0.609781
35	6	0	-0.506300	2.520822	-1.655510
36	6	0	-0.384516	4.533850	0.256896
37	6	0	-0.837382	3.835698	-1.976775
38	6	0	-0.791837	4.858100	-1.033984
39	1	0	-0.345911	5.315744	1.011804
40	1	0	-1.145293	4.067595	-2.993642
41	6	0	1.791727	0.469072	0.665864
42	6	0	1.879115	-0.303810	1.844970
43	6	0	2.974315	1.082378	0.185635
44	6	0	3.109106	-0.465484	2.485187
45	6	0	4.184949	0.875917	0.838328
46	6	0	4.277347	0.100784	1.992632
47	1	0	3.150503	-1.051537	3.400358
48	1	0	5.084115	1.340622	0.440243
49	6	0	2.989691	1.973475	-1.036652
50	1	0	2.415876	1.563269	-1.872692
51	1	0	2.563132	2.956857	-0.817298
52	1	0	4.014645	2.124741	-1.385181
53	6	0	0.680038	-0.956661	2.497388
54	1	0	-0.221603	-0.341793	2.442547
55	1	0	0.440877	-1.917405	2.030516
56	1	0	0.884250	-1.149778	3.553797
57	6	0	5.602591	-0.118316	2.672935
58	1	0	5.470925	-0.468860	3.699971
59	1	0	6.196876	-0.870411	2.141220
60	1	0	6.195205	0.801160	2.697394
61	6	0	0.412278	2.990258	2.037948
62	1	0	-0.080069	2.116032	2.473886
63	1	0	1.490378	2.818754	2.108462
64	1	0	0.169130	3.852309	2.664625
65	6	0	-0.621405	1.483442	-2.751011
66	1	0	0.266014	0.848614	-2.829153
67	1	0	-1.473693	0.818064	-2.582104
68	1	0	-0.765549	1.967683	-3.720185
69	6	0	-1.196445	6.263990	-1.390796
70	1	0	-2.264177	6.424890	-1.201169
71	1	0	-0.647111	7.000198	-0.797326
72	1	0	-1.019001	6.473724	-2.449210

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=acetonitrile)

Excited State 1: Singlet-A 3.8993 eV 317.97 nm f=0.2522
<S**2>=0.000
131 ->133 -0.34286
132 ->133 0.55779

Step3

Method: cam-b3lyp/6-31+G(d,p)
SCRF(Solvent=acetonitrile,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1508.35232888 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1508.20905877 a.u.

Excited State 1: Singlet-A 3.8898 eV 318.74 nm f=0.1908
<S**2>=0.000
131 ->133 -0.35026
132 ->133 0.55353

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1508.13627257 a.u.
Lowest frequency = 23.2124

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.606496	-1.234019	0.320922
2	6	0	-1.793196	-2.239359	-0.345604
3	6	0	-0.528752	-1.666669	-0.552259
4	7	0	-0.508271	-0.368465	-0.019616
5	6	0	-1.762867	-0.115076	0.494157
6	6	0	-2.232260	1.046896	1.125202
7	6	0	-3.540794	1.065323	1.564417
8	6	0	-4.383253	-0.045244	1.383907
9	6	0	-3.913135	-1.216594	0.752194
10	6	0	-2.094181	-3.533826	-0.763396
11	6	0	-1.119341	-4.258174	-1.414345
12	6	0	0.162122	-3.714202	-1.665661
13	6	0	0.500005	-2.389054	-1.231451
14	8	0	-5.633550	0.097513	1.846499
15	6	0	-6.557208	-0.977819	1.707247
16	6	0	1.129313	-4.479717	-2.368831
17	6	0	2.369150	-3.971104	-2.646309
18	6	0	2.700245	-2.669183	-2.217210
19	6	0	1.794572	-1.901762	-1.525234
20	1	0	-1.591131	1.908140	1.253226
21	1	0	-3.951278	1.939339	2.056089

22	1	0	-4.557778	-2.074417	0.610417
23	1	0	-3.076806	-3.958408	-0.586980
24	1	0	-1.328656	-5.266484	-1.756975
25	1	0	-7.486464	-0.627253	2.153103
26	1	0	-6.207369	-1.866484	2.240354
27	1	0	-6.723915	-1.217004	0.653033
28	1	0	0.859070	-5.482282	-2.686553
29	1	0	3.098445	-4.565877	-3.186425
30	1	0	3.687257	-2.269247	-2.426472
31	1	0	2.072611	-0.915329	-1.187497
32	5	0	0.615850	0.672232	0.088661
33	6	0	0.314402	2.045003	-0.604568
34	6	0	0.585906	3.276332	0.064468
35	6	0	-0.285552	2.142982	-1.892291
36	6	0	0.269840	4.493756	-0.533178
37	6	0	-0.586523	3.382609	-2.451116
38	6	0	-0.320623	4.579154	-1.792208
39	1	0	0.478418	5.412281	0.012383
40	1	0	-1.031581	3.415175	-3.443937
41	6	0	1.877234	0.312846	0.946412
42	6	0	1.828194	-0.468192	2.136588
43	6	0	3.172771	0.742936	0.527171
44	6	0	2.991806	-0.794065	2.829714
45	6	0	4.309044	0.395868	1.253991
46	6	0	4.251223	-0.378287	2.409846
47	1	0	2.908673	-1.382351	3.741704
48	1	0	5.280060	0.731839	0.894897
49	6	0	3.391733	1.545289	-0.734772
50	1	0	2.835158	1.131203	-1.581962
51	1	0	3.057963	2.582629	-0.634236
52	1	0	4.453552	1.561119	-0.997102
53	6	0	0.523454	-0.927832	2.738303
54	1	0	-0.189688	-0.101726	2.828832
55	1	0	0.036564	-1.705690	2.140431
56	1	0	0.684801	-1.342634	3.737210
57	6	0	5.499054	-0.768904	3.157505
58	1	0	5.295281	-0.923241	4.221482
59	1	0	5.923166	-1.704279	2.771464
60	1	0	6.275747	-0.003251	3.068265
61	6	0	1.162426	3.324092	1.459812
62	1	0	0.645053	2.627800	2.128808
63	1	0	2.219332	3.042104	1.488413
64	1	0	1.074232	4.331783	1.876211
65	6	0	-0.576891	0.918739	-2.723256
66	1	0	0.271749	0.226604	-2.729874
67	1	0	-1.441289	0.358229	-2.349572
68	1	0	-0.795925	1.194940	-3.758723
69	6	0	-0.679679	5.909201	-2.401105
70	1	0	-1.672561	6.245280	-2.076864
71	1	0	0.032516	6.688086	-2.111705
72	1	0	-0.698634	5.855729	-3.493791

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1508.24768443 a.u.

Excited State 1: Singlet-A 2.6278 eV 471.82 nm f=0.0392
<S**2>=0.000
132 ->133 -0.68182

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=acetonitrile, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1508.33373209 a.u.

Results

Absorb Energy =	0.143 a.u.	3.899 eV	318.024 nm
Emission Energy =	0.086 a.u.	2.341 eV	529.513 nm
Stokes Shift =	0.057 a.u.	1.557 eV	211.489 nm

Compound 8 n-hexane

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : n-Hexane
SCF Done: E(RCAM-B3LYP) = -1730.74265509 a.u.
Lowest frequency = 14.3761

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.802081	0.715867	-0.027069
2	6	0	0.805466	2.983019	2.001788
3	1	0	0.237898	2.142384	2.412084
4	1	0	1.865120	2.751016	2.141545
5	1	0	0.572390	3.863189	2.606828
6	6	0	3.511039	1.843110	-0.884335
7	1	0	4.562485	1.949386	-1.164350
8	1	0	2.976512	1.458435	-1.757844
9	1	0	3.113821	2.844221	-0.692653
10	6	0	0.857731	-0.993259	2.483193
11	1	0	-0.007914	-0.331944	2.394935
12	1	0	0.597415	-1.931799	1.984121
13	1	0	0.992873	-1.216057	3.544802
14	6	0	5.787072	-0.363258	2.975944
15	1	0	6.339090	-1.196232	2.525169
16	1	0	6.453297	0.504538	2.975520
17	1	0	5.578037	-0.633263	4.014594
18	6	0	4.519033	-0.083748	2.214247
19	6	0	4.533632	0.695299	1.060171
20	1	0	5.475167	1.122327	0.722450
21	6	0	3.377829	0.953046	0.331757
22	6	0	2.142586	0.389483	0.733491
23	6	0	2.121905	-0.389613	1.912036
24	6	0	3.299585	-0.601448	2.628759
25	1	0	3.258050	-1.190627	3.541819

26	6	0	0.088771	2.526275	-1.737906
27	6	0	-0.165034	3.851290	-2.084608
28	1	0	-0.412448	4.086858	-3.117036
29	6	0	-0.121886	4.878750	-1.148168
30	6	0	0.189652	4.547261	0.167040
31	1	0	0.210895	5.331765	0.919852
32	6	0	0.477759	3.239098	0.548088
33	6	0	0.428584	2.198476	-0.405940
34	6	0	-0.017979	1.484905	-2.830346
35	1	0	-0.926749	0.884560	-2.722532
36	1	0	-0.054247	1.964960	-3.811646
37	1	0	0.823857	0.786761	-2.836785
38	6	0	-0.383517	6.306508	-1.548055
39	1	0	-0.823965	6.877235	-0.725699
40	1	0	0.547237	6.811059	-1.832781
41	1	0	-1.060205	6.363799	-2.405174
42	7	0	-0.152600	-0.345370	-0.351238
43	6	0	-1.538543	-0.223189	-0.083452
44	6	0	0.084886	-1.722084	-0.576106
45	6	0	-2.119685	-1.503594	-0.041038
46	6	0	-2.314597	0.907425	0.186956
47	6	0	-1.077898	-2.448599	-0.351455
48	6	0	1.251933	-2.368819	-1.089919
49	6	0	-3.470865	-1.668467	0.250109
50	6	0	-3.658643	0.731999	0.467642
51	1	0	-1.894018	1.901981	0.176217
52	6	0	-1.109011	-3.855946	-0.463739
53	6	0	1.210639	-3.793498	-1.172462
54	6	0	2.397799	-1.707903	-1.591495
55	6	0	-4.236604	-0.543122	0.499801
56	1	0	-3.916347	-2.656293	0.286141
57	1	0	-4.274601	1.600376	0.674368
58	6	0	0.028021	-4.511271	-0.829058
59	1	0	-2.025600	-4.398568	-0.254933
60	6	0	2.346939	-4.487130	-1.653870
61	6	0	3.471677	-2.408172	-2.077642
62	1	0	2.425487	-0.629150	-1.608389
63	1	0	0.041418	-5.594032	-0.908463
64	6	0	3.459503	-3.816626	-2.088908
65	1	0	2.309321	-5.572229	-1.690449
66	1	0	4.333161	-1.871312	-2.461822
67	1	0	4.318608	-4.364106	-2.463367
68	6	0	-5.704218	-0.669529	0.759041
69	9	0	-6.118997	0.184736	1.713718
70	9	0	-6.437031	-0.396037	-0.339016
71	9	0	-6.046150	-1.908808	1.153978

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=n-hexane)

Excited State 1: Singlet-A 3.9561 eV 313.40 nm f=0.2261
<S**2>=0.000
139 ->141 -0.23510
140 ->141 0.62295

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,NonEquilibrium=Save)

SCF Done: E(RCAM-B3LYP) = -1730.84930507 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1730.70547374 a.u.

Excited State 1: Singlet-A 3.9271 eV 315.71 nm f=0.1594
<S**2>=0.000
139 ->141 0.18508
140 ->141 0.64198

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1730.61504263 a.u.
Lowest frequency = 10.7260

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.946781	0.692590	0.062507
2	6	0	1.159793	3.374063	1.454238
3	1	0	0.634378	2.645189	2.080205
4	1	0	2.226284	3.171885	1.591081
5	1	0	0.957486	4.374384	1.848212
6	6	0	3.711644	1.759105	-0.495521
7	1	0	4.789994	1.848806	-0.656352
8	1	0	3.266570	1.308022	-1.388755
9	1	0	3.298425	2.770642	-0.438187
10	6	0	0.691437	-0.863435	2.731761
11	1	0	-0.077015	-0.083831	2.716530
12	1	0	0.313202	-1.699373	2.133822
13	1	0	0.779303	-1.221473	3.761348
14	6	0	5.588714	-0.405686	3.594092
15	1	0	6.153200	-1.265165	3.211032
16	1	0	6.281613	0.440640	3.635357
17	1	0	5.289039	-0.646365	4.618498
18	6	0	4.394014	-0.099224	2.730578
19	6	0	4.511058	0.674299	1.578947
20	1	0	5.487780	1.072751	1.310573
21	6	0	3.429807	0.946595	0.747130
22	6	0	2.129721	0.433319	1.046355
23	6	0	2.018293	-0.340842	2.237116
24	6	0	3.129412	-0.589787	3.037119
25	1	0	2.998142	-1.173623	3.946226
26	6	0	0.115689	2.087223	-2.007018
27	6	0	-0.203697	3.302156	-2.605178
28	1	0	-0.563283	3.301229	-3.632459
29	6	0	-0.065929	4.516121	-1.940401
30	6	0	0.397805	4.472655	-0.629047
31	1	0	0.490899	5.404124	-0.073787
32	6	0	0.729080	3.280222	0.008929
33	6	0	0.604010	2.032139	-0.671700

34	6	0	-0.044785	0.843798	-2.845851
35	1	0	-0.930021	0.262573	-2.562566
36	1	0	-0.157387	1.101396	-3.902833
37	1	0	0.821810	0.181061	-2.752515
38	6	0	-0.383072	5.823443	-2.616964
39	1	0	-0.739098	6.569115	-1.899358
40	1	0	0.501917	6.246196	-3.108666
41	1	0	-1.151749	5.700321	-3.385955
42	7	0	-0.093368	-0.440800	-0.124647
43	6	0	-1.444613	-0.259445	0.255292
44	6	0	0.017455	-1.687089	-0.644493
45	6	0	-2.186943	-1.418008	-0.022184
46	6	0	-2.032306	0.859301	0.819243
47	6	0	-1.251616	-2.355265	-0.591963
48	6	0	1.163170	-2.362566	-1.211424
49	6	0	-3.539987	-1.475303	0.263850
50	6	0	-3.396240	0.793766	1.109645
51	1	0	-1.462659	1.757097	1.015308
52	6	0	-1.416353	-3.654959	-1.046381
53	6	0	0.948514	-3.694631	-1.682291
54	6	0	2.445618	-1.811788	-1.343159
55	6	0	-4.139492	-0.351788	0.834627
56	1	0	-4.127079	-2.363456	0.057752
57	1	0	-3.885758	1.649069	1.560798
58	6	0	-0.326047	-4.310393	-1.582582
59	1	0	-2.383023	-4.143345	-0.989431
60	6	0	2.019390	-4.407189	-2.264412
61	6	0	3.475816	-2.536188	-1.919716
62	1	0	2.633412	-0.815254	-0.976499
63	1	0	-0.434586	-5.325727	-1.950454
64	6	0	3.265935	-3.837270	-2.388711
65	1	0	1.838666	-5.418672	-2.615376
66	1	0	4.458509	-2.083580	-1.998421
67	1	0	4.080696	-4.394549	-2.838450
68	6	0	-5.614444	-0.360143	1.101210
69	9	0	-5.938626	0.419330	2.145641
70	9	0	-6.316514	0.090712	0.045114
71	9	0	-6.064315	-1.600119	1.364410

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=n-hexane,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1730.72830911 a.u.

Excited State 1: Singlet-A 2.9340 eV 422.58 nm f=0.0460
<S**2>=0.000
140 ->141 0.68081

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=n-hexane,
NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1730.83474599 a.u.

Results

Absorb Energy = | 0.144 a.u. | 3.914 eV | 316.783 nm

Emission Energy =	0.106 a.u.	2.896 eV	428.079 nm
Stokes Shift =	0.037 a.u.	1.018 eV	111.295 nm

Compound 8 THF

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : TetraHydroFuran
SCF Done: E(RCAM-B3LYP) = -1730.74638108 a.u.
Lowest frequency = 14.4483

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.802040	0.720299	-0.024127
2	6	0	0.812282	2.994492	1.998199
3	1	0	0.251702	2.151534	2.413066
4	1	0	1.874206	2.770251	2.134142
5	1	0	0.576475	3.875275	2.601118
6	6	0	3.515964	1.843673	-0.872098
7	1	0	4.567624	1.942189	-1.153561
8	1	0	2.976231	1.467499	-1.745911
9	1	0	3.128175	2.847401	-0.674162
10	6	0	0.845730	-0.985599	2.488583
11	1	0	-0.013059	-0.314380	2.408186
12	1	0	0.574388	-1.917451	1.982734
13	1	0	0.981998	-1.218388	3.547801
14	6	0	5.778683	-0.379269	2.987189
15	1	0	6.328293	-1.213291	2.535455
16	1	0	6.448030	0.486000	2.988108
17	1	0	5.566827	-0.650635	4.024841
18	6	0	4.512755	-0.093955	2.223992
19	6	0	4.531828	0.687000	1.070829
20	1	0	5.475412	1.110677	0.734870
21	6	0	3.377500	0.950762	0.341320
22	6	0	2.139522	0.391249	0.740554
23	6	0	2.114012	-0.389012	1.918611
24	6	0	3.290079	-0.607230	2.636655
25	1	0	3.244891	-1.196464	3.549491
26	6	0	0.084379	2.525497	-1.738785
27	6	0	-0.172587	3.849444	-2.088185
28	1	0	-0.422228	4.082313	-3.120651
29	6	0	-0.128923	4.879531	-1.154061
30	6	0	0.186870	4.551714	0.161388
31	1	0	0.208825	5.338137	0.912101
32	6	0	0.478473	3.244751	0.544783
33	6	0	0.427954	2.201266	-0.406476
34	6	0	-0.020394	1.482471	-2.830032
35	1	0	-0.923939	0.875112	-2.717641
36	1	0	-0.065176	1.961997	-3.811115
37	1	0	0.827390	0.791578	-2.840449
38	6	0	-0.394394	6.305813	-1.556680
39	1	0	-0.833441	6.877421	-0.734282
40	1	0	0.535074	6.810962	-1.844402

41	1	0	-1.072335	6.359353	-2.412969
42	7	0	-0.151948	-0.343307	-0.349436
43	6	0	-1.536745	-0.224326	-0.080174
44	6	0	0.087700	-1.718234	-0.580177
45	6	0	-2.117032	-1.505759	-0.044575
46	6	0	-2.313441	0.904296	0.197855
47	6	0	-1.074080	-2.448076	-0.359225
48	6	0	1.256301	-2.361359	-1.095857
49	6	0	-3.468199	-1.673780	0.245854
50	6	0	-3.657300	0.726714	0.477859
51	1	0	-1.893201	1.899024	0.194976
52	6	0	-1.103096	-3.855474	-0.476519
53	6	0	1.217679	-3.786155	-1.182569
54	6	0	2.401000	-1.696547	-1.595892
55	6	0	-4.234131	-0.549668	0.502227
56	1	0	-3.911820	-2.662641	0.275827
57	1	0	-4.272671	1.594178	0.690094
58	6	0	0.035771	-4.507708	-0.842683
59	1	0	-2.018802	-4.400433	-0.270350
60	6	0	2.355968	-4.476631	-1.665108
61	6	0	3.476829	-2.393501	-2.083723
62	1	0	2.426229	-0.617717	-1.612141
63	1	0	0.051366	-5.590131	-0.925181
64	6	0	3.467689	-3.802389	-2.097933
65	1	0	2.320683	-5.561630	-1.704574
66	1	0	4.336649	-1.854062	-2.467910
67	1	0	4.328111	-4.346976	-2.473376
68	6	0	-5.700838	-0.678319	0.761034
69	9	0	-6.118155	0.170309	1.720420
70	9	0	-6.436193	-0.398646	-0.335339
71	9	0	-6.044690	-1.919343	1.148862

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=THF)

Excited State 1: Singlet-A 3.9601 eV 313.09 nm f=0.2309
<S**2>=0.000
139 ->141 -0.24140
140 ->141 0.61985

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF,NonEquilibrium=Save)
SCF Done: E(RCAM-B3LYP) = -1730.85361738 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1730.70901064 a.u.

Excited State 1: Singlet-A 3.9322 eV 315.30 nm f=0.1607
<S**2>=0.000
137 ->141 -0.10755
139 ->141 -0.19098
140 ->141 0.63920

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes)
TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1730.61738604 a.u.
Lowest frequency = 14.6872

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.936286	0.694073	0.061108
2	6	0	1.136333	3.366820	1.484732
3	1	0	0.614782	2.625895	2.099579
4	1	0	2.204749	3.170896	1.616942
5	1	0	0.926906	4.360391	1.891697
6	6	0	3.702703	1.776489	-0.493922
7	1	0	4.780180	1.871112	-0.656973
8	1	0	3.257140	1.330845	-1.389607
9	1	0	3.286153	2.786009	-0.423850
10	6	0	0.693987	-0.879379	2.715141
11	1	0	-0.079805	-0.105264	2.695847
12	1	0	0.324295	-1.717582	2.114917
13	1	0	0.781141	-1.237317	3.744848
14	6	0	5.593153	-0.416666	3.576063
15	1	0	6.160096	-1.269801	3.182879
16	1	0	6.283339	0.431448	3.624414
17	1	0	5.295447	-0.669730	4.597975
18	6	0	4.396152	-0.106169	2.716650
19	6	0	4.510118	0.676367	1.569992
20	1	0	5.485798	1.078060	1.302718
21	6	0	3.426212	0.951924	0.741930
22	6	0	2.128820	0.432463	1.038374
23	6	0	2.019107	-0.348423	2.224356
24	6	0	3.132676	-0.601043	3.021866
25	1	0	3.003896	-1.192402	3.926470
26	6	0	0.107120	2.111011	-1.991390
27	6	0	-0.218674	3.330856	-2.578659
28	1	0	-0.575935	3.338066	-3.606740
29	6	0	-0.090455	4.539027	-1.900842
30	6	0	0.370591	4.485372	-0.588086
31	1	0	0.456225	5.411786	-0.023184
32	6	0	0.707200	3.287722	0.038180
33	6	0	0.589280	2.046624	-0.654535
34	6	0	-0.041515	0.873836	-2.841574
35	1	0	-0.919483	0.280199	-2.561455
36	1	0	-0.158279	1.139565	-3.896104
37	1	0	0.831415	0.218686	-2.753099
38	6	0	-0.414790	5.851518	-2.564655
39	1	0	-0.777249	6.587161	-1.840057
40	1	0	0.468632	6.285346	-3.049400
41	1	0	-1.179960	5.730934	-3.337411
42	7	0	-0.092664	-0.433006	-0.133365
43	6	0	-1.448652	-0.259860	0.240388
44	6	0	0.029693	-1.687119	-0.642161
45	6	0	-2.178439	-1.428165	-0.028906
46	6	0	-2.045811	0.854690	0.802543
47	6	0	-1.232116	-2.364723	-0.584407

48	6	0	1.179539	-2.350940	-1.211081
49	6	0	-3.531140	-1.496241	0.255192
50	6	0	-3.410111	0.779974	1.089925
51	1	0	-1.483683	1.755712	1.005709
52	6	0	-1.384788	-3.670980	-1.023206
53	6	0	0.978535	-3.691178	-1.667184
54	6	0	2.451559	-1.781980	-1.367860
55	6	0	-4.141617	-0.373659	0.817585
56	1	0	-4.107824	-2.392193	0.054386
57	1	0	-3.906175	1.632873	1.538365
58	6	0	-0.287190	-4.321364	-1.552850
59	1	0	-2.346098	-4.168666	-0.961570
60	6	0	2.053480	-4.394166	-2.254680
61	6	0	3.484605	-2.495183	-1.955210
62	1	0	2.628637	-0.777968	-1.016346
63	1	0	-0.385704	-5.341961	-1.908057
64	6	0	3.289233	-3.805580	-2.404214
65	1	0	1.883830	-5.411979	-2.591891
66	1	0	4.458043	-2.027292	-2.057498
67	1	0	4.106251	-4.355011	-2.859222
68	6	0	-5.616076	-0.393810	1.083015
69	9	0	-5.949718	0.387632	2.124009
70	9	0	-6.323118	0.047975	0.024843
71	9	0	-6.058484	-1.635109	1.351224

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1)
SCRF(Solvent=THF,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1730.74132518 a.u.

Excited State 1: Singlet-A 2.8051 eV 441.99 nm f=0.0486
<S**2>=0.000
140 ->141 0.68289

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=THF, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1730.83664204 a.u.

Results

Absorb Energy =	0.145 a.u.	3.935 eV	315.085 nm
Emission Energy =	0.095 a.u.	2.594 eV	478.020 nm
Stokes Shift =	0.049 a.u.	1.341 eV	162.935 nm

Compound 8 ACN

Step1

Method: cam-b3lyp/6-31G(d)
Solvent : Acetonitrile
SCF Done: E(RCAM-B3LYP) = -1730.74792317 a.u.
Lowest frequency = 14.6367

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.800736	0.724718	-0.021457
2	6	0	0.814128	3.001658	1.998657
3	1	0	0.257488	2.157417	2.416000
4	1	0	1.877304	2.781545	2.131906
5	1	0	0.577162	3.882526	2.600901
6	6	0	3.517744	1.848894	-0.860538
7	1	0	4.569571	1.944866	-1.141932
8	1	0	2.976076	1.479475	-1.735936
9	1	0	3.134147	2.853083	-0.656551
10	6	0	0.836730	-0.979866	2.492026
11	1	0	-0.017199	-0.301881	2.416605
12	1	0	0.557434	-1.907286	1.982329
13	1	0	0.973482	-1.218693	3.549793
14	6	0	5.773429	-0.397658	2.989564
15	1	0	6.321402	-1.230103	2.532964
16	1	0	6.444768	0.465997	2.995243
17	1	0	5.560550	-0.674715	4.025466
18	6	0	4.508357	-0.104969	2.227666
19	6	0	4.530060	0.680052	1.077143
20	1	0	5.475092	1.101407	0.742473
21	6	0	3.376306	0.950980	0.348813
22	6	0	2.136441	0.394035	0.746002
23	6	0	2.107928	-0.388782	1.922528
24	6	0	3.283413	-0.614311	2.639560
25	1	0	3.236070	-1.205384	3.551089
26	6	0	0.079770	2.528039	-1.737011
27	6	0	-0.179617	3.851485	-2.086829
28	1	0	-0.430690	4.083529	-3.119104
29	6	0	-0.136236	4.882335	-1.153251
30	6	0	0.182148	4.555747	0.161960
31	1	0	0.204191	5.342634	0.912135
32	6	0	0.476336	3.249326	0.545693
33	6	0	0.425531	2.204891	-0.404710
34	6	0	-0.023416	1.484991	-2.828516
35	1	0	-0.922410	0.871584	-2.712778
36	1	0	-0.075536	1.965128	-3.808879
37	1	0	0.829198	0.800115	-2.843366
38	6	0	-0.404656	6.307911	-1.556361
39	1	0	-0.843605	6.879142	-0.733687
40	1	0	0.523780	6.814323	-1.845146
41	1	0	-1.083158	6.359627	-2.412287
42	7	0	-0.151392	-0.340693	-0.349547
43	6	0	-1.536008	-0.225452	-0.079354
44	6	0	0.091219	-1.714396	-0.583376
45	6	0	-2.113896	-1.508223	-0.047339
46	6	0	-2.314774	0.900949	0.202337
47	6	0	-1.068921	-2.447635	-0.364169
48	6	0	1.261276	-2.353751	-1.100693
49	6	0	-3.464887	-1.679819	0.242360
50	6	0	-3.658300	0.720140	0.481810
51	1	0	-1.896158	1.896358	0.203608
52	6	0	-1.094508	-3.855057	-0.484009
53	6	0	1.226462	-3.778664	-1.189458
54	6	0	2.403778	-1.684941	-1.600875
55	6	0	-4.232712	-0.557622	0.502009

56	1	0	-3.906369	-2.669709	0.268992
57	1	0	-4.274884	1.586015	0.696974
58	6	0	0.046248	-4.503928	-0.850844
59	1	0	-2.008765	-4.402747	-0.278851
60	6	0	2.366859	-4.465441	-1.672977
61	6	0	3.481669	-2.378220	-2.089893
62	1	0	2.425545	-0.605991	-1.616927
63	1	0	0.064537	-5.586162	-0.934828
64	6	0	3.476679	-3.787330	-2.105238
65	1	0	2.334806	-5.550455	-1.713842
66	1	0	4.339332	-1.835909	-2.474815
67	1	0	4.338564	-4.328931	-2.481540
68	6	0	-5.699038	-0.689625	0.760334
69	9	0	-6.118386	0.154864	1.722689
70	9	0	-6.435344	-0.406978	-0.335136
71	9	0	-6.041704	-1.932330	1.143555

Step2

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=3) SCRF(solvent=acetonitrile)

Excited State 1: Singlet-A 3.9630 eV 312.86 nm f=0.2239 <S**2>=0.000

139 ->141	-0.24342
140 ->141	0.61894

Step3

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=acetonitrile,NonEquilibrium=Save)

SCF Done: E(RCAM-B3LYP) = -1730.85537834 a.u.

Step4

Method: CAM-B3LYP/6-31+G(d,p) TD(NStates=1,Root=1) SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Read)

After PCM corrections, the energy is -1730.71008936 a.u.

Excited State 1: Singlet-A 3.9411 eV 314.59 nm f=0.1632 <S**2>=0.000

137 ->141	-0.11139
139 ->141	-0.20076
140 ->141	0.63549

Step5

Method: cam-b3lyp/6-31G(d) opt freq(savenormalmodes) TD(NStates=1,Root=1)

Total Energy, E(TD-HF/TD-DFT) = -1730.61849005 a.u.

Lowest frequency = 13.9033

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.929564	0.697962	0.062357

2	6	0	1.126335	3.361530	1.507715
3	1	0	0.606080	2.613890	2.115519
4	1	0	2.195528	3.167471	1.637141
5	1	0	0.914436	4.350927	1.923343
6	6	0	3.697884	1.787209	-0.489217
7	1	0	4.774933	1.882845	-0.653918
8	1	0	3.250492	1.349201	-1.387732
9	1	0	3.281889	2.796202	-0.408093
10	6	0	0.692136	-0.887415	2.706472
11	1	0	-0.081981	-0.113742	2.685371
12	1	0	0.323738	-1.726107	2.106056
13	1	0	0.778610	-1.245018	3.736353
14	6	0	5.595235	-0.441078	3.559018
15	1	0	6.157532	-1.294442	3.159839
16	1	0	6.288967	0.404013	3.608557
17	1	0	5.299850	-0.698110	4.580577
18	6	0	4.396619	-0.122218	2.704773
19	6	0	4.509304	0.668812	1.563462
20	1	0	5.485039	1.070768	1.296914
21	6	0	3.423558	0.952101	0.740009
22	6	0	2.126676	0.431380	1.034975
23	6	0	2.017482	-0.356060	2.216513
24	6	0	3.132745	-0.616525	3.009957
25	1	0	3.004912	-1.213794	3.910795
26	6	0	0.100478	2.130447	-1.978130
27	6	0	-0.226587	3.354436	-2.557012
28	1	0	-0.583413	3.368661	-3.585154
29	6	0	-0.100341	4.557945	-1.870183
30	6	0	0.359957	4.495560	-0.557149
31	1	0	0.443653	5.417991	0.014504
32	6	0	0.697497	3.293559	0.060540
33	6	0	0.580815	2.057567	-0.641007
34	6	0	-0.045675	0.898686	-2.836551
35	1	0	-0.920060	0.299386	-2.557388
36	1	0	-0.166787	1.171075	-3.888871
37	1	0	0.829801	0.246064	-2.754452
38	6	0	-0.426295	5.874886	-2.524519
39	1	0	-0.792553	6.603768	-1.795067
40	1	0	0.457388	6.314906	-3.003142
41	1	0	-1.188575	5.758273	-3.300655
42	7	0	-0.093631	-0.427397	-0.139251
43	6	0	-1.452057	-0.260538	0.231202
44	6	0	0.036058	-1.683615	-0.644841
45	6	0	-2.174317	-1.434031	-0.035969
46	6	0	-2.055567	0.850634	0.793268
47	6	0	-1.221508	-2.367977	-0.585453
48	6	0	1.189050	-2.340119	-1.214605
49	6	0	-3.526954	-1.509306	0.246616
50	6	0	-3.420004	0.769219	1.078592
51	1	0	-1.498234	1.753693	1.000798
52	6	0	-1.365662	-3.677435	-1.017078
53	6	0	0.997660	-3.685010	-1.662241
54	6	0	2.454489	-1.759959	-1.384106
55	6	0	-4.144412	-0.388836	0.805973
56	1	0	-4.097608	-2.409325	0.047141
57	1	0	-3.920646	1.619611	1.526675
58	6	0	-0.263062	-4.323900	-1.542062
59	1	0	-2.323642	-4.181107	-0.954004
60	6	0	2.076484	-4.382181	-2.249882
61	6	0	3.490916	-2.466773	-1.974255

62	1	0	2.623562	-0.751071	-1.042677
63	1	0	-0.354827	-5.347183	-1.891033
64	6	0	3.305955	-3.782688	-2.411097
65	1	0	1.914802	-5.403859	-2.578930
66	1	0	4.458577	-1.989552	-2.088172
67	1	0	4.125539	-4.327663	-2.866757
68	6	0	-5.618803	-0.416854	1.070193
69	9	0	-5.957957	0.363086	2.110949
70	9	0	-6.327894	0.021826	0.011563
71	9	0	-6.055919	-1.659857	1.338145

Step6

Method: cam-b3lyp/6-31+G(d,p) TD(NStates=1, Root=1) SCRF(Solvent=acetonitrile,ExternalIteration,NonEquilibrium=Save)
After PCM corrections, the energy is -1730.74656548 a.u.

Excited State 1: Singlet-A 2.7546 eV 450.10 nm f=0.0498 <S**2>=0.000
140 ->141 0.68381

Step7

Method: cam-b3lyp/6-31+G(d,p) SCRF(Solvent=acetonitrile, NonEquilibrium=Read)

SCF Done: E(RCAM-B3LYP) = -1730.83696192 a.u.

Results

Absorb Energy =	0.145 a.u.	3.954 eV	313.605 nm
Emission Energy =	0.090 a.u.	2.460 eV	504.039 nm
Stokes Shift =	0.055 a.u.	1.494 eV	190.434 nm