Supporting information

The effects of bromine atom on the photophysical and photochemical properties of 3-cinnamoylcoumarin derivatives

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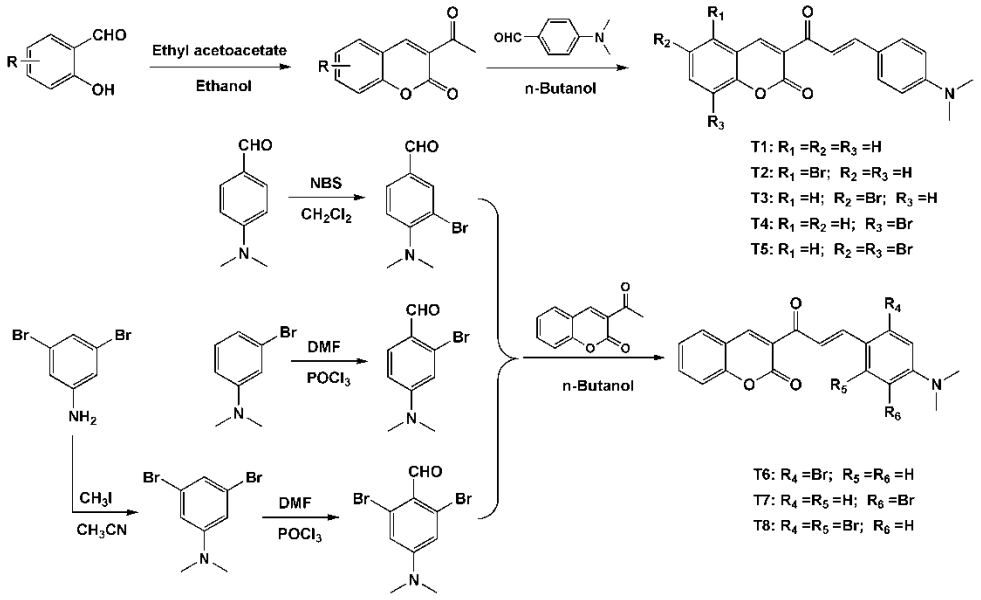
1. The synthesizes of T1–T8.



3-bromo-4-(dimethylamino)benzaldehyde

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 2.95 (s, 6H, $-CH_3$), 7.07 (d, 1H, J = 8.0 Hz, phenyl-H), 7.73 (d, 1H, J = 8.0 Hz, phenyl-H), 8.03 (s, 1H, phenyl-H), 9.81 (s, 1H, -CHO).

2-bromo-4-(dimethylamino)benzaldehyde

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 3.08 (s, 6H, $-CH_3$), 6.65 (d, 1H, J = 8.0 Hz, phenyl-H), 6.81 (s, 1H, phenyl-H), 7.80 (d, 1H, J = 8.0 Hz, phenyl-H), 10.09 (s, 1H, -CHO).

2,6-dibromo-4-(dimethylamino)benzaldehyde

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 3.07 (s, 6H, -CH_3), 6.86 (s, 2H phenyl-H), 10.15 (s, 1H, -CHO).

3-(3-(4-(dimethylamino)phenyl)acryloyl)-2*H*-chromen-2-one (**T1**)

4-(dimethylamino)benzaldehyde (0.22 g, 1.5 mmol) and 3-acetyl-2*H*-chromen-2-one (0.40 g, 1.5 mmol) were dissolved in *n*-butanol under stirring. Then 0.2 mL of glacial acetic acid and 0.2 mL of piperidine were added to the solution. The reaction mixture was refluxed for 4 h under nitrogen atmosphere, and then the solvent was removed in vacuum. The crude product was purified by silica gel column chromatography using petroleum ether: ethyl acetate (5:1) as eluent to give the target PS **T1** (0.17 g, yield 36%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 3.06 (s, 6H, -CH_3), 6.69 (d, 2H, J = 8.0 Hz, phenyl-H), 7.32-7.36 (m, 1H, coumarin-H), 7.39 (d, 1H, J = 8.0 Hz, coumarin-H), 7.59 (d, 1H, J = 8.0 Hz, phenyl-H), 7.63-7.67 (m, 1H, coumarin-H), 7.74 (d, 1H, J = 16.0 Hz, -C=C-H), 7.88 (d, 1H, J = 16.0 Hz, -C=C-H), 8.56 (s, 1H, coumarin-H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 185.95, 159.42, 155.09, 152.25, 146.41, 133.72, 131.11, 129.82, 126.11, 124.81, 122.86, 118.78, 116.61, 111.87, 40.17. MS (EI): m/z Calcd for $C_{29}H_{17}NO_3$ 319.12; found 319.10.

3-(3-(4-(dimethylamino)phenyl)acryloyl)-5-bromo-2*H*-chromen-2-one (**T2**)

T2 was prepared by an analogous method to that used for **T1**. The crude product was purified by column chromatography on SiO_2 using petroleum ether: ethyl acetate (5:1) as eluent to give **T2** (0.12 g, yield 20%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 3.12 (s, 6H, -CH_3), 7.15 (d, 2H, J = 8.0 Hz, phenyl-H), 7.35 (d, 1H, J = 8.0 Hz, coumarin-H), 7.46-7.50 (m, 1H, coumarin-H), 7.58 (d, 1H, J = 8.0 Hz, coumarin-H), 7.68 (d, 2H, J = 8.0 Hz, phenyl-H), 7.77 (d, 1H, J = 12.0 Hz, -C=C-H), 7.87 (d, 1H, J = 16.0 Hz, -C=C-H), 8.86 (s, 1H, coumarin-H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 185.53, 158.73, 155.60, 152.30, 146.77, 145.60, 133.81, 131.18, 128.89, 127.11, 124.32, 122.76, 118.97, 118.57, 116.10, 111.89, 40.18. MS (EI): m/z Calcd for $C_{20}H_{16}NO_3Br$ 397.03; found 397.00.

3-(3-(4-(dimethylamino)phenyl)acryloyl)-6,8-dibromo-2*H*-chromen-2-one (**T3**)

T3 was prepared by an analogous method to that used for **T1**. The crude product was purified by column chromatography on SiO_2 using petroleum ether: ethyl acetate (5:1) as eluent to give **T3** (0.21 g, yield 35%).

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 3.11 (s, 6H, -CH_3), 7.11 (d, 2H, J = 8.0 Hz, phenyl-H), 7.29 (d, 1H, J = 8.0 Hz, coumarin-H), 7.66 (d, 2H, J = 8.0 Hz, phenyl-H), 7.73 (d, 1H, J = 8.0 Hz, coumarin-H), 7.78 (d, 1H, J = 16.0 Hz, -C=C-H), 7.80 (s, 1H, coumarin-H), 7.82 (d, 1H, J = 16.0 Hz, -C=C-H), 8.48 (s, 1H, coumarin-H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 185.62, 158.32, 153.63, 151.67, 146.34, 145.68, 136.33, 132.04, 131.65, 126.85, 120.09, 118.97, 117.88, 117.24, 112.64, 40.58. MS (EI): m/z Calcd for $C_{20}H_{16}NO_3Br$ 397.03; found 397.00.

3-(3-(4-(dimethylamino)phenyl)acryloyl)-8-bromo-2*H*-chromen-2-one (**T4**)

T4 was prepared by an analogous method to that used for **T1**. The crude product was purified by column chromatography on SiO_2 using petroleum ether: ethyl acetate (5:1) as eluent to give **T4** (0.20 g, yield 33%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 3.10 (s, 6H, -CH_3), 7.00 (d, 2H, J = 8.0 Hz, phenyl-H), 7.21-7.26 (m, 1H, coumarin-H), 7.62 (d, 1H, J = 8.0 Hz, coumarin-H), 7.64 (d, 2H, J = 8.0 Hz, phenyl-H), 7.76 (d, 1H, J = 16.0 Hz, -C=C-H), 7.87 (d, 1H, J = 8.0 Hz, coumarin-H), 7.88 (d, 1H, J = 16.0 Hz, -C=C-H), 8.52 (s, 1H, coumarin-H). δ (ppm) 185.43, 158.38, 153.63, 146.67, 136.99, 134.64, 131.20, 130.45, 128.99, 127.91, 125.47, 123.50, 118.75, 113.65, 112.22, 110.68, 40.41. MS (EI): m/z Calcd for $C_{20}H_{16}NO_3Br$ 397.03; found 397.00.

3-(3-(4-(dimethylamino)phenyl)acryloyl)-6,8-dibromo-2*H*-chromen-2-one (**T5**)

T5 was prepared by an analogous method to that used for **T1**. The crude product was purified by column chromatography on SiO_2 using petroleum ether: ethyl acetate (5:1) as eluent to give **T5** (0.08 g, yield 12%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 3.11 (s, 6H, -CH_3), 7.10 (d, 2H, J = 8.0 Hz, phenyl-H), 7.66 (d, 2H, J = 8.0 Hz, phenyl-H), 7.74 (d, 1H, J = 16.0 Hz, -C=C-H), 7.74 (s, 1H, coumarin-H), 7.87 (d, 1H, J = 16.0 Hz, -C=C-H), 7.98 (s, 1H, J = 8.0 Hz, coumarin-H), 8.43 (s, 1H, coumarin-H). δ (ppm) 184.96, 157.83, 153.63, 150.87, 147.21, 145.26, 138.94, 131.36, 131.04, 127.78, 121.06, 118.42, 117.29, 112.24, 111.21, 40.42. MS (EI): m/z Calcd for

$C_{20}H_{15}NO_3Br_2$ 474.94; found 474.90.

3-(3-(2-bromo-4-(dimethylamino)phenyl)acryloyl)-2*H*-chromen-2-one (**T6**)

T6 was prepared by an analogous method to that used for **T1**. The crude product was purified by column chromatography on SiO_2 using petroleum ether: ethyl acetate (5:1) as eluent to give **T6** (0.31 g, yield 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 3.04 (s, 6H, -CH_3), 6.66 (d, 1H, J = 8.0 Hz, phenyl-H), 6.90 (s, 1H, phenyl-H), 7.33-7.36 (m, 1H, coumarin-H), 7.39 (d, 1H, J = 8.0 Hz, coumarin-H), 7.62-7.68 (m, 2H, coumarin-H), 7.74 (d, 1H, J = 16.0 Hz, -C=C-H), 7.76 (d, 1H, J = 8.0 Hz, phenyl-H), 8.26 (d, 1H, J = 16.0 Hz, -C=C-H), 8.57 (s, 1H, coumarin-H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 186.07, 159.71, 155.40, 152.72, 147.77, 144.48, 134.13, 130.18, 129.38, 126.11, 125.13, 121.95, 119.00, 116.90, 115.81, 111.57, 40.35. MS (EI): m/z Calcd for $C_{20}H_{16}NO_3Br$ 397.03; found 397.00.

3-(3-(3-bromo-4-(dimethylamino)phenyl)acryloyl)-2*H*-chromen-2-one (**T7**)

T7 was prepared by an analogous method to that used for **T1**. The crude product was purified by column chromatography on SiO_2 using petroleum ether: ethyl acetate (5:1) as eluent to give **T7** (0.10 g, yield 26%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 2.94 (s, 6H, -CH_3), 7.19 (d, 1H, J = 8.0 Hz, phenyl-H), 7.34-7.38 (m, 1H, coumarin-H), 7.41 (d, 1H, J = 8.0 Hz, coumarin-H), 7.58 (d, 1H, J = 8.0 Hz, phenyl-H), 7.65-7.69 (m, 1H, coumarin-H), 7.68 (d, 1H, J = 8.0 Hz, coumarin-H), 7.76 (d, 1H, J = 16.0 Hz, -C=C-H), 7.84 (d, 1H, J = 12.0 Hz, -C=C-H), 7.88 (s, 1H, phenyl-H), 8.59 (s, 1H, coumarin-H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 186.39, 159.62, 155.52, 148.27, 143.68, 134.87, 134.47, 130.29, 129.26, 125.64, 125.24, 123.13, 120.40, 118.88, 118.15, 116.99, 40.35. MS (EI): m/z Calcd for $C_{20}H_{16}NO_3Br$ 397.03; found 397.00.

3-(3-(2,6-dibromo-4-(dimethylamino)phenyl)acryloyl)-2*H*-chromen-2-one (**T8**)

T8 was prepared by an analogous method to that used for **T1**. The crude product was purified by column chromatography on SiO_2 using petroleum ether: ethyl acetate (5:1) as eluent to give **T8** (0.05 g, yield 11%). ^{1}H

NMR (400 MHz, $CDCl_3$) δ (ppm) 3.04 (s, 6H, $-CH_3$), 7.13 (s, 2H, phenyl-H), 7.34-7.40 (m, 1H, coumarin-H), 7.39 (d, 1H, J = 8.0 Hz, coumarin-H), 7.66-7.69 (m, 1H, coumarin-H), 7.68 (d, 1H, J = 8.0 Hz, coumarin-H), 7.79 (d, 1H, J = 16.0 Hz, -C=C-H), 8.04 (d, 1H, J = 16.0 Hz, -C=C-H), 8.58 (s, 1H, coumarin-H). δ (ppm) 186.70, 159.36, 155.50, 151.21, 147.85, 143.43, 134.24, 130.20, 128.26, 126.64, 125.12, 121.70, 118.91, 116.96, 116.42, 40.25. MS (EI): m/z Calcd for $C_{20}H_{15}NO_3Br_2$ 474.94; found 474.90.

Figure S1. The photostability of the PSs T1–T8 with the irradiation time in toluene solution

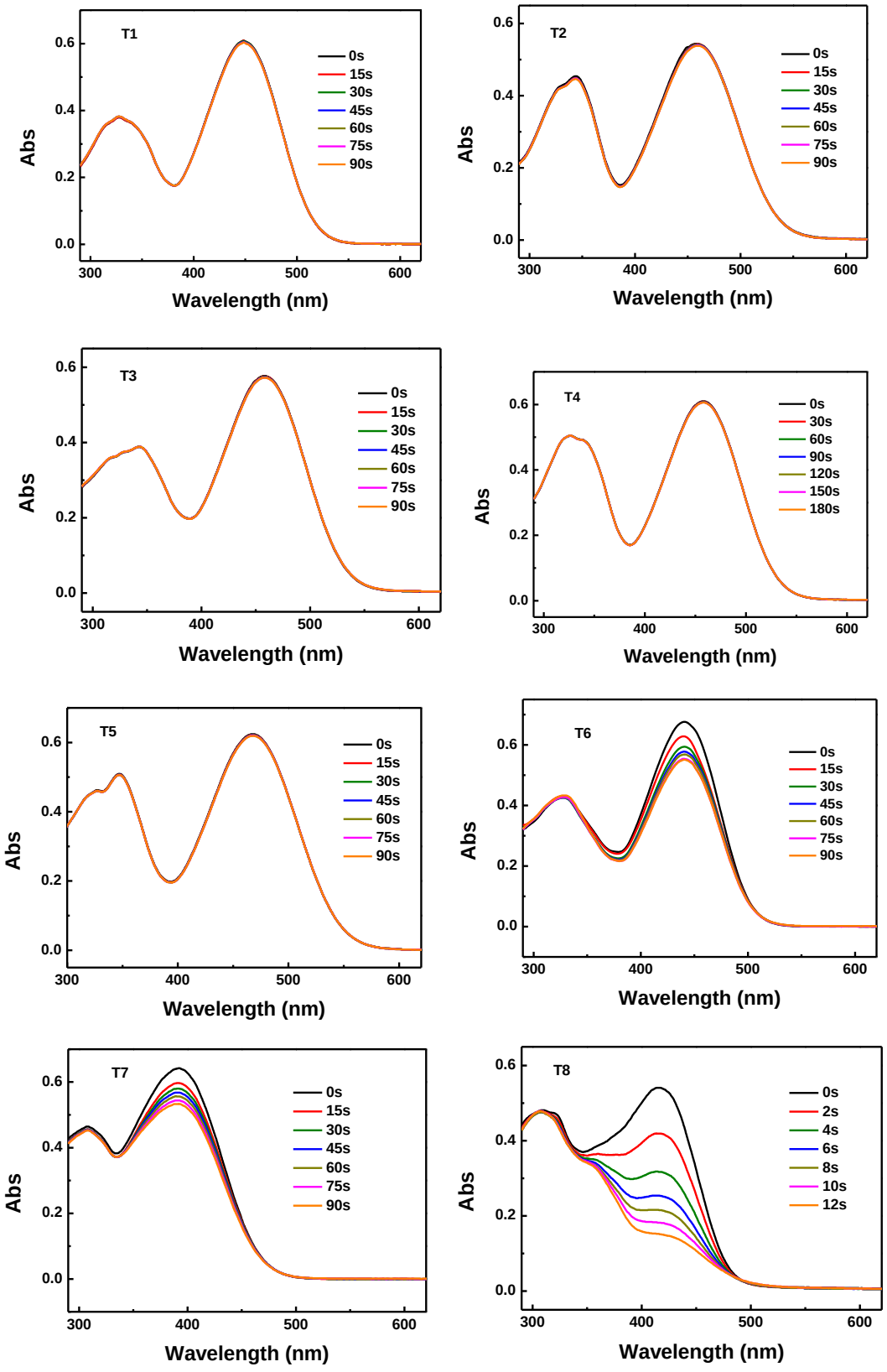


Figure S2. The cyclic voltammetry of the PSs T1–T8 in acetonitrile (0.1 M TBAPF6)

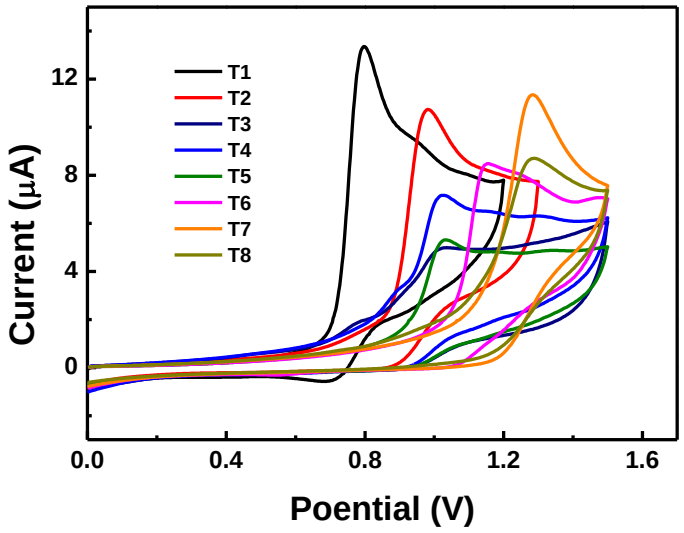


Table S1 The obtained absorption and emission spectra (λ_{max}^{abs} and λ_{max}^{fl}, in nm) from three different functionals (PBE1PBE, CAM-B3LYP and WB97XD) and experiments

	Method	Compound							
		T1	**T2**	**T3**	**T4**	**T5**	**T6**	**T7**	**T8**
λ_{max}^{abs}	PBE1PBE	476	499	496	493	514	458	434	442
	CAM-B3LYP	375	383	383	382	390	367	343	356
	WB97XD	363	369	369	369	375	357	334	354
	Exp.	448	459	459	458	468	440	391	416
f_a	PBE1PBE	0.62	0.55	0.58	0.57	0.53	0.65	0.63	0.57
	CAM-B3LYP	1.14	1.06	1.09	1.07	1.02	1.16	1.21	0.47
	WB97XD	1.29	1.24	1.26	1.23	1.20	1.29	1.36	0.17
λ_{max}^{fl}	PBE1PBE	600	642	639	633	670	567	573	576
	CAM-B3LYP	427	448	445	442	461	416	372	437
	WB97XD	420	422	421	419	431	405	361	437
	Exp.	584	612	608	604	620	562	560	536
f_e	PBE1PBE	0.38	0.36	0.37	0.37	0.35	0.40	0.38	0.28
	CAM-B3LYP	1.02	0.87	0.90	0.89	0.80	1.12	1.12	0.18
	WB97XD	1.26	1.15	1.19	1.17	1.09	1.29	1.28	0.06

λ_{max}^{abs} is the absorption maximum, f_a is the absorption oscillator strengths, λ_{max}^{fl} is the fluorescence emission maximum, f_e is the emission oscillator strengths.

Table S2. The Cartesian Coordinates (in Å) of species studied, optimized with PBE1PBE+IDSCRF/6-31G(d) .

Compounds	Cartesian coordinates				Species	Cartesian coordinates			
T1(ground state)	H	7.01483	4.63155	-5.50954	**T1** (excited state)	H	-5.89879	2.73048	-0.00016
	C	7.39154	4.91463	-4.53176		C	-5.96346	1.64635	-0.00014
	C	7.63736	6.23750	-4.19396		C	-7.19662	0.98714	-0.00026
	C	8.12407	6.58157	-2.92497		C	-7.23769	-0.41230	-0.00024
	C	8.36563	5.59282	-1.98926		C	-6.06765	-1.14960	-0.00011
	C	8.12503	4.24402	-2.30564		C	-4.80009	-0.51079	0.00003
	C	7.63821	3.92665	-3.58199		C	-4.79402	0.90789	0.00000
	O	7.39287	2.64175	-3.92846		O	-3.61413	1.59775	0.00013
	C	7.59197	1.56032	-3.08701		C	-2.36504	0.98880	0.00037
	C	8.10019	1.86318	-1.74718		C	-2.34331	-0.44735	0.00026
	C	8.34410	3.15879	-1.40743		C	-3.56393	-1.16755	0.00012
	H	7.44837	7.01658	-4.92748		H	-8.11641	1.56426	-0.00037
	H	8.31013	7.62287	-2.67981		H	-8.19648	-0.92457	-0.00034
	H	8.74302	5.84040	-1.00023		H	-6.09834	-2.23646	-0.00011
	H	8.72100	3.34783	-0.40433		H	-3.51648	-2.25108	0.00007
	C	8.38157	0.82570	-0.68760		C	-1.11620	-1.21796	0.00024
	O	8.80739	1.22451	0.39732		O	-1.11033	-2.45317	-0.00007
	O	7.32185	0.47919	-3.55629		O	-1.42751	1.77659	0.00010
	C	8.14814	-0.58681	-0.96809		C	0.23241	-0.53108	0.00020
	H	7.77240	-0.85339	-1.94768		H	0.22904	0.55363	0.00035
	C	8.40491	-1.50824	-0.00840		C	1.35652	-1.27346	0.00001
	H	8.78086	-1.12374	0.94060		H	1.24034	-2.35637	-0.00011
	C	8.24088	-2.93946	-0.09018		C	2.70806	-0.75088	-0.00002
	C	8.56429	-3.73654	1.02180		C	3.79710	-1.65171	-0.00005
	C	7.76757	-3.60839	-1.23538		C	3.00957	0.63317	-0.00002
	C	8.42992	-5.11148	1.00790		C	5.10121	-1.21802	-0.00007
	C	7.62625	-4.97958	-1.26961		C	4.30431	1.08732	-0.00004
	C	7.95417	-5.77724	-0.14492		C	5.39701	0.17373	-0.00006
	H	8.93322	-3.25354	1.92454		H	3.59265	-2.71899	-0.00005
	H	7.50368	-3.03741	-2.12174		H	2.20215	1.35847	-0.00001
	H	8.69524	-5.67379	1.89594		H	5.90038	-1.94961	-0.00008
	N	7.81509	-7.13688	-0.17597		N	6.67831	0.61646	-0.00009
	C	7.32626	-7.79015	-1.36866		C	6.96723	2.03944	-0.00007
	H	7.98314	-7.60974	-2.23042		H	6.55213	2.52390	0.89099
	H	7.28633	-8.86658	-1.19682		H	8.04634	2.18544	-0.00021
	H	6.31490	-7.45245	-1.63279		H	6.55192	2.52395	-0.89100
	C	8.15726	-7.92475	0.98563		C	7.78419	-0.32433	-0.00005
	H	7.54679	-7.65114	1.85707		H	7.75708	-0.96168	-0.89120
	H	7.98047	-8.97913	0.76927		H	8.72314	0.22718	-0.00007
	H	9.21484	-7.80815	1.25925		H	7.75708	-0.96162	0.89114
	H	7.25728	-5.44322	-2.17755		H	4.48420	2.15574	-0.00003

T2(ground state)					**T2** (excited state)				
	H	-4.58570	3.77402	-0.13944		H	-4.42435	3.79623	0.00122
	C	-4.73427	2.70157	-0.06974		C	-4.62552	2.72961	0.00087
	C	-5.99667	2.13492	-0.00636		C	-5.93117	2.22964	0.00071
	C	-6.16608	0.74847	0.08319		C	-6.15182	0.85075	0.00027
	C	-5.05312	-0.07024	0.10880		C	-5.07521	-0.01617	-0.00002
	C	-3.74935	0.46240	0.04650		C	-3.72815	0.43776	0.00010
	C	-3.62606	1.85918	-0.04259		C	-3.55938	1.85059	0.00056
	O	-2.40722	2.43769	-0.10585		O	-2.30812	2.39248	0.00074
	C	-1.20829	1.74289	-0.08983		C	-1.13479	1.64336	0.00053
	C	-1.31068	0.28617	0.00323		C	-1.28437	0.21772	-0.00005
	C	-2.53989	-0.29298	0.06598		C	-2.57764	-0.35568	-0.00016
	H	-6.87427	2.77481	-0.02623		H	-6.77547	2.91163	0.00093
	H	-7.15935	0.31581	0.13228		H	-7.16118	0.45242	0.00016
	H	-2.57636	-1.37732	0.13302		H	-2.65877	-1.43592	-0.00047
	C	-0.12631	-0.65214	0.03541		C	-0.15295	-0.69488	-0.00056
	O	-0.36326	-1.85844	0.10114		O	-0.29564	-1.91913	-0.00070
	O	-0.21195	2.42263	-0.15564		O	-0.11369	2.31715	0.00094
	C	1.22850	-0.11597	-0.00770		C	1.26699	-0.17194	-0.00123
	H	1.34804	0.95826	-0.06646		H	1.39269	0.90523	-0.00337
	C	2.28307	-0.96691	0.02723		C	2.29419	-1.04245	0.00089
	H	2.04316	-2.02932	0.08603		H	2.05088	-2.10409	0.00286
	C	3.68657	-0.63637	-0.00335		C	3.69877	-0.68401	0.00056
	C	4.64051	-1.66827	0.04372		C	4.67312	-1.70724	0.00193
	C	4.17846	0.68117	-0.07831		C	4.16093	0.65452	-0.00100
	C	5.99882	-1.41837	0.01885		C	6.01953	-1.43060	0.00163
	C	5.53005	0.95178	-0.10430		C	5.50009	0.95287	-0.00132
	C	6.48644	-0.09334	-0.05618		C	6.47728	-0.08342	-0.00012
	H	4.29652	-2.69907	0.10197		H	4.34413	-2.74294	0.00326
	H	3.48186	1.51455	-0.11718		H	3.44499	1.47022	-0.00186
	H	6.68722	-2.25484	0.05798		H	6.72669	-2.25142	0.00276
	N	7.82692	0.17179	-0.08138		N	7.80154	0.20545	-0.00058
	C	8.29657	1.53648	-0.15649		C	8.25611	1.58455	-0.00214
	H	7.96462	2.12977	0.70635		H	7.90188	2.11518	0.88888
	H	9.38727	1.53997	-0.16658		H	9.34488	1.60237	-0.00341
	H	7.94871	2.03699	-1.07027		H	7.89991	2.11371	-0.89322
	C	8.77933	-0.91342	-0.02768		C	8.78913	-0.85883	0.00132
	H	8.66474	-1.59736	-0.87966		H	8.68689	-1.49025	-0.88857
	H	9.79052	-0.50561	-0.05783		H	9.78644	-0.42165	0.00012
	H	8.67763	-1.49854	0.89653		H	8.68740	-1.48667	0.89381
	H	5.85411	1.98474	-0.16241		H	5.80474	1.99256	-0.00242
	Br	-5.29994	-1.93572	0.22981		Br	-5.41182	-1.88074	-0.00060

T3(ground state)					**T3**(excited state)				
	H	7.01458	4.64017	-5.50819		H	-4.23762	3.19326	0.00008
	C	7.39186	4.91710	-4.52898		C	-4.35506	2.11394	0.00005
	C	7.63581	6.24025	-4.19774		C	-5.62600	1.53002	0.00006
	C	8.12263	6.56733	-2.92625		C	-5.72050	0.13715	0.00003
	C	8.36814	5.58865	-1.98324		C	-4.60707	-0.67761	-0.00001
	C	8.12504	4.24325	-2.30625		C	-3.30981	-0.10138	-0.00001
	C	7.63782	3.92607	-3.58146		C	-3.22647	1.31554	0.00002
	O	7.39177	2.64409	-3.92943		O	-2.01396	1.93901	0.00002
	C	7.59129	1.56113	-3.08731		C	-0.79765	1.26132	-0.00001
	C	8.10055	1.86464	-1.74698		C	-0.85714	-0.17261	-0.00005
	C	8.34542	3.15819	-1.40528		C	-2.11260	-0.82537	-0.00005
	H	7.45040	7.02653	-4.92236		H	-6.51907	2.14402	0.00008
	H	8.74563	5.84641	-0.99838		H	-4.71063	-1.75784	-0.00003
	H	8.72282	3.34693	-0.40242		H	-2.12518	-1.90985	-0.00008
	C	8.38260	0.82524	-0.68609		C	0.32975	-1.01175	-0.00010
	O	8.80874	1.22756	0.39696		O	0.26237	-2.24276	-0.00013
	O	7.32080	0.48131	-3.55622		O	0.18100	1.99534	-0.00001
	C	8.14887	-0.58550	-0.96687		C	1.71495	-0.40272	-0.00008
	H	7.77265	-0.85288	-1.94593		H	1.77442	0.68013	-0.00006
	C	8.40616	-1.50754	-0.00681		C	2.79296	-1.20904	-0.00007
	H	8.78263	-1.12315	0.94198		H	2.61447	-2.28348	-0.00008
	C	8.24188	-2.93777	-0.08885		C	4.17396	-0.76700	-0.00005
	C	8.56567	-3.73562	1.02292		C	5.20739	-1.73033	0.00009
	C	7.76774	-3.60593	-1.23447		C	4.55529	0.59654	-0.00016
	C	8.43087	-5.11023	1.00827		C	6.53508	-1.37399	0.00013
	C	7.62601	-4.97674	-1.26939		C	5.87444	0.97409	-0.00013
	C	7.95430	-5.77523	-0.14501		C	6.91166	-0.00198	0.00002
	H	8.93513	-3.25312	1.92568		H	4.94075	-2.78381	0.00018
	H	7.50357	-3.03457	-2.12048		H	3.79204	1.36818	-0.00029
	H	8.69636	-5.67317	1.89581		H	7.28983	-2.15127	0.00025
	N	7.81477	-7.13418	-0.17693		N	8.21647	0.36553	0.00005
	C	7.32520	-7.78666	-1.37011		C	8.58779	1.76938	0.00002
	H	7.98185	-7.60555	-2.23179		H	8.20134	2.27712	0.89098
	H	7.28526	-8.86316	-1.19903		H	9.67356	1.85228	0.00015
	H	6.31380	-7.44854	-1.63325		H	8.20157	2.27702	-0.89110
	C	8.15703	-7.92340	0.98414		C	9.26583	-0.63791	0.00014
	H	7.54688	-7.65011	1.85580		H	9.20157	-1.27266	-0.89095
	H	7.97960	-8.97745	0.76690		H	10.23526	-0.14201	0.00003
	H	9.21475	-7.80749	1.25719		H	9.20166	-1.27243	0.89141
	H	7.25648	-5.43987	-2.17732		H	6.11659	2.03010	-0.00023
	Br	8.44586	8.37954	-2.50290		Br	-7.44634	-0.65879	0.00003

T4(ground state)					**T4**(excited state)				
	C	7.39219	4.92372	-4.52963		C	5.06950	-0.34434	0.00002
	C	7.63854	6.24621	-4.19152		C	6.20281	0.47341	0.00004
	C	8.12490	6.57773	-2.92250		C	6.03940	1.86173	0.00005
	C	8.36483	5.58445	-1.99120		C	4.77766	2.42531	0.00003
	C	8.12081	4.24058	-2.31718		C	3.61633	1.61104	0.00001
	C	7.63297	3.91591	-3.59212		C	3.79537	0.20114	0.00000
	O	7.38851	2.63777	-3.93663		O	2.72706	-0.63661	-0.00002
	C	7.58827	1.55249	-3.09300		C	1.40093	-0.20102	-0.00004
	C	8.09713	1.85811	-1.75464		C	1.18957	1.21713	-0.00004
	C	8.34009	3.15310	-1.41870		C	2.30154	2.09168	-0.00001
	H	7.44844	7.02216	-4.92648		H	7.18870	0.02253	0.00006
	H	8.74257	5.82497	-1.00113		H	4.65228	3.50473	0.00004
	H	8.71764	3.34550	-0.41656		H	2.11172	3.15953	-0.00001
	C	8.38022	0.82183	-0.69191		C	-0.13379	1.81736	-0.00006
	O	8.80685	1.22613	0.39038		O	-0.30083	3.03907	-0.00002
	O	7.31769	0.47446	-3.56350		O	0.58243	-1.10877	-0.00007
	C	8.14712	-0.58924	-0.97079		C	-1.37690	0.95530	-0.00003
	H	7.77072	-0.85797	-1.94946		H	-1.22708	-0.11875	-0.00002
	C	8.40487	-1.51035	-0.01010		C	-2.59109	1.53681	-0.00002
	H	8.78143	-1.12498	0.93832		H	-2.62643	2.62540	-0.00003
	C	8.24113	-2.94067	-0.09056		C	-3.85822	0.83167	-0.00001
	C	8.56530	-3.73677	1.02224		C	-5.06174	1.57173	0.00003
	C	7.76727	-3.61055	-1.23531		C	-3.96275	-0.58051	-0.00005
	C	8.43110	-5.11142	1.00949		C	-6.29275	0.95988	0.00004
	C	7.62616	-4.98144	-1.26830		C	-5.18107	-1.21143	-0.00004
	C	7.95482	-5.77814	-0.14283		C	-6.39074	-0.45958	0.00001
	H	8.93456	-3.25290	1.92434		H	-5.00875	2.65714	0.00006
	H	7.50285	-3.04054	-2.12211		H	-3.06229	-1.18639	-0.00009
	H	8.69683	-5.67307	1.89777		H	-7.18636	1.57250	0.00008
	N	7.81594	-7.13726	-0.17271		N	-7.59708	-1.07780	0.00002
	C	7.32668	-7.79195	-1.36466		C	-7.68358	-2.52732	0.00004
	H	7.98318	-7.61196	-2.22672		H	-7.20442	-2.94864	0.89101
	H	7.28732	-8.86819	-1.19172		H	-8.73152	-2.82321	0.00011
	H	6.31508	-7.45480	-1.62834		H	-7.20454	-2.94866	-0.89099
	C	8.15860	-7.92442	0.98939		C	-8.82422	-0.30193	0.00003
	H	7.54834	-7.65014	1.86070		H	-8.88685	0.33293	-0.89110
	H	7.98170	-8.97891	0.77374		H	-9.67635	-0.97986	-0.00005
	H	9.21628	-7.80756	1.26228		H	-8.88692	0.33281	0.89125
	H	7.25684	-5.44597	-2.17560		H	-5.20954	-2.29449	-0.00007
	Br	6.73905	4.48312	-6.23506		Br	5.28378	-2.22230	0.00001
	H	8.31117	7.61882	-2.67771		H	6.91895	2.49985	0.00007

T5(ground state)					**T5**(excited state)				
	C	7.39246	4.92681	-4.52890		C	-3.87285	1.21103	-0.00002
	C	7.63758	6.24936	-4.19357		C	-5.09082	0.52342	-0.00012
	C	8.12354	6.56536	-2.92164		C	-5.05788	-0.87081	-0.00007
	C	8.36662	5.58037	-1.98447		C	-3.87604	-1.58099	0.00008
	C	8.12019	4.24020	-2.31883		C	-2.63819	-0.88839	0.00019
	C	7.63276	3.91642	-3.59281		C	-2.66462	0.53270	0.00014
	O	7.38808	2.64065	-3.93922		O	-1.51470	1.24958	0.00025
	C	7.58807	1.55365	-3.09531		C	-0.24110	0.67196	0.00052
	C	8.09717	1.85942	-1.75624		C	-0.18666	-0.76003	0.00039
	C	8.34047	3.15265	-1.41827		C	-1.38384	-1.50896	0.00028
	H	7.45135	7.03340	-4.91927		H	-6.02807	1.06511	-0.00024
	H	8.74400	5.82958	-0.99776		H	-3.87991	-2.66576	0.00010
	H	8.71799	3.34491	-0.41619		H	-1.31120	-2.59113	0.00022
	C	8.38067	0.82132	-0.69247		C	1.06771	-1.50261	0.00033
	O	8.80677	1.22868	0.38853		O	1.09454	-2.73345	0.00015
	O	7.31768	0.47683	-3.56592		O	0.67053	1.48424	0.00018
	C	8.14753	-0.58821	-0.97155		C	2.39825	-0.78408	0.00027
	H	7.77123	-0.85794	-1.94988		H	2.37025	0.29984	0.00035
	C	8.40537	-1.50955	-0.01002		C	3.53833	-1.49879	0.00011
	H	8.78184	-1.12383	0.93824		H	3.45044	-2.58443	0.00004
	C	8.24157	-2.93900	-0.09048		C	4.87875	-0.94354	0.00004
	C	8.56562	-3.73515	1.02272		C	5.98802	-1.81774	-0.00012
	C	7.76767	-3.60896	-1.23556		C	5.14501	0.44669	0.00012
	C	8.43130	-5.10946	1.00995		C	7.28163	-1.35220	-0.00020
	C	7.62644	-4.97958	-1.26857		C	6.42822	0.93286	0.00005
	C	7.95498	-5.77628	-0.14270		C	7.54283	0.04628	-0.00012
	H	8.93481	-3.25120	1.92478		H	5.81012	-2.88980	-0.00018
	H	7.50343	-3.03898	-2.12242		H	4.32053	1.15256	0.00025
	H	8.69681	-5.67123	1.89819		H	8.09838	-2.06406	-0.00032
	N	7.81603	-7.13481	-0.17252		N	8.81248	0.52101	-0.00020
	C	7.32673	-7.78974	-1.36463		C	9.06565	1.95095	-0.00008
	H	7.98348	-7.60995	-2.22644		H	8.63850	2.42461	0.89105
	H	7.28726	-8.86589	-1.19149		H	10.14073	2.12390	-0.00014
	H	6.31522	-7.45250	-1.62822		H	8.63838	2.42477	-0.89108
	C	8.15848	-7.92237	0.98977		C	9.94179	-0.39163	-0.00038
	H	7.54800	-7.64797	1.86077		H	9.93039	-1.02928	-0.89164
	H	7.98146	-8.97673	0.77387		H	10.86655	0.18329	-0.00047
	H	9.21611	-7.80553	1.26253		H	9.93060	-1.02938	0.89081
	H	7.25721	-5.44418	-2.17582		H	6.58150	2.00536	0.00011
	Br	6.74036	4.49280	-6.23305		Br	-3.88965	3.09707	-0.00009
	Br	8.44787	8.37309	-2.49315		Br	-6.70557	-1.81057	-0.00022

T6(ground state)					**T6**(excited state)				
	H	6.33252	4.63909	-5.20053		H	-6.75142	-2.69453	-0.00008
	C	6.94784	4.91340	-4.34953		C	-6.72457	-1.60883	-0.00005
	C	7.32448	6.22654	-4.10806		C	-7.89722	-0.84800	-0.00008
	C	8.11999	6.55972	-3.00261		C	-7.82017	0.55002	-0.00003
	C	8.54031	5.56975	-2.13404		C	-6.59218	1.18599	0.00004
	C	8.17285	4.23054	-2.35545		C	-5.38338	0.44263	0.00010
	C	7.37656	3.92402	-3.46857		C	-5.49727	-0.97086	0.00005
	O	6.99996	2.64855	-3.71917		O	-4.37924	-1.75764	0.00013
	C	7.35193	1.56746	-2.93031		C	-3.08520	-1.25779	0.00044
	C	8.18363	1.85898	-1.76072		C	-2.94032	0.17327	0.00013
	C	8.55812	3.14508	-1.51587		C	-4.09592	0.99319	0.00007
	H	6.99556	7.00674	-4.78911		H	-8.86248	-1.34535	-0.00015
	H	8.40402	7.59360	-2.83117		H	-8.73234	1.14125	-0.00008
	H	9.15752	5.80870	-1.27159		H	-6.53105	2.27153	0.00005
	H	9.17584	3.32602	-0.63851		H	-3.95682	2.06878	-0.00009
	C	8.66985	0.81951	-0.78176		C	-1.65480	0.83669	-0.00019
	O	9.36345	1.20323	0.15909		O	-1.53876	2.06768	0.00002
	O	6.93036	0.49503	-3.29769		O	-2.21775	-2.12223	-0.00030
	C	8.31341	-0.58593	-0.97048		C	-0.37497	0.03321	-0.00013
	H	7.69910	-0.83691	-1.82556		H	-0.48145	-1.04615	-0.00013
	C	8.75832	-1.50510	-0.08253		C	0.81291	0.67656	-0.00012
	H	9.36868	-1.12903	0.73614		H	0.78760	1.76303	-0.00013
	C	8.51008	-2.92812	-0.10554		C	2.10122	0.02332	-0.00008
	C	9.01995	-3.80749	0.86965		C	3.32306	0.75148	-0.00002
	C	7.73493	-3.54024	-1.11245		C	2.22810	-1.39006	-0.00009
	C	8.78804	-5.17015	0.85627		C	4.55270	0.13393	0.00001
	C	7.48432	-4.89296	-1.15617		C	3.43840	-2.03021	-0.00005
	C	8.00817	-5.75626	-0.16406		C	4.64932	-1.28164	-0.00000
	H	9.21702	-5.77576	1.64401		H	5.44224	0.75035	0.00006
	N	7.77231	-7.09983	-0.18803		N	5.85532	-1.89662	0.00003
	C	6.96981	-7.67487	-1.24459		C	5.94272	-3.34674	0.00008
	H	7.41634	-7.50339	-2.23313		H	5.46480	-3.76836	-0.89130
	H	6.89617	-8.75216	-1.09150		H	6.99112	-3.64085	0.00012
	H	5.95153	-7.26369	-1.25101		H	5.46474	-3.76830	0.89145
	C	8.32380	-7.95064	0.84229		C	7.08100	-1.11804	0.00006
	H	7.95641	-7.67121	1.83897		H	7.14184	-0.48340	0.89155
	H	8.02739	-8.98271	0.65178		H	7.93446	-1.79419	-0.00002
	H	9.42134	-7.91070	0.85705		H	7.14179	-0.48325	-0.89133
	H	6.87850	-5.28708	-1.96371		H	3.45926	-3.11318	-0.00007
	H	7.31311	-2.91513	-1.89427		H	1.32613	-1.99273	-0.00013
	Br	10.08532	-3.15567	2.29985		Br	3.31085	2.63488	0.00001

T6a(ground state)					**T6a**(excited state)				
	H	6.45441	5.05162	-5.11932		H	-6.45715	-2.39338	0.00018
	C	7.07031	5.22186	-4.24195		C	-6.47838	-1.30754	0.00012
	C	7.51331	6.48841	-3.88981		C	-7.68359	-0.59939	0.00012
	C	8.30833	6.68676	-2.75207		C	-7.66820	0.80065	0.00005
	C	8.66106	5.60792	-1.96284		C	-6.46929	1.49001	-0.00001
	C	8.22548	4.31332	-2.29708		C	-5.22874	0.80090	-0.00001
	C	7.43120	4.14191	-3.44029		C	-5.28020	-0.61629	0.00006
	O	6.99055	2.91405	-3.79836		O	-4.12900	-1.35279	0.00006
	C	7.27159	1.75328	-3.09616		C	-2.85669	-0.79702	-0.00004
	C	8.09985	1.90408	-1.89715		C	-2.77523	0.64021	-0.00007
	C	8.53871	3.14390	-1.54466		C	-3.96678	1.40773	-0.00006
	H	7.23749	7.33810	-4.50844		H	-8.62592	-1.13893	0.00017
	H	8.64496	7.68618	-2.49350		H	-8.60551	1.35118	0.00005
	H	9.27678	5.74188	-1.07691		H	-6.45618	2.57724	-0.00006
	H	9.15160	3.22015	-0.64885		H	-3.87588	2.48842	-0.00010
	C	8.51417	0.76414	-1.00105		C	-1.52182	1.35907	-0.00010
	O	9.21296	1.03508	-0.02469		O	-1.46412	2.59554	-0.00009
	O	6.79923	0.73979	-3.55395		O	-1.95296	-1.62115	0.00009
	C	8.08364	-0.60228	-1.30985		C	-0.20437	0.61011	-0.00006
	H	7.47215	-0.75151	-2.18573		H	-0.25703	-0.46926	-0.00006
	C	8.47889	-1.59489	-0.47784		C	0.93661	1.33695	-0.00004
	H	9.09404	-1.25625	0.35724		H	0.78293	2.41621	-0.00004
	C	8.25135	-3.02399	-0.46840		C	2.32411	0.93376	-0.00001
	C	8.84899	-3.73476	0.59688		C	3.26565	2.00000	0.00004
	C	7.51715	-3.82656	-1.36787		C	2.88954	-0.37478	-0.00003
	C	8.74482	-5.09639	0.77399		C	4.62311	1.82293	0.00006
	C	7.39350	-5.19591	-1.21794		C	4.25237	-0.57813	0.00000
	C	8.00371	-5.87629	-0.14134		C	5.16386	0.50795	0.00004
	H	9.42683	-3.16276	1.31937		H	2.87125	3.01214	0.00005
	H	9.23805	-5.55628	1.62226		H	5.27081	2.69110	0.00011
	N	7.87801	-7.22744	0.00106		N	6.50090	0.29490	0.00006
	C	7.11075	-7.99129	-0.95696		C	7.03395	-1.05603	0.00013
	H	7.52660	-7.90723	-1.97003		H	6.70935	-1.60483	-0.89124
	H	7.12907	-9.04401	-0.67258		H	8.12186	-1.01129	0.00018
	H	6.06172	-7.66744	-0.98803		H	6.70926	-1.60478	0.89149
	C	8.51419	-7.89640	1.11353		C	7.42419	1.41637	0.00008
	H	8.13965	-7.52695	2.07765		H	7.28538	2.03818	0.89164
	H	8.30213	-8.96474	1.05763		H	8.44522	1.03808	-0.00005
	H	9.60464	-7.76638	1.09584		H	7.28522	2.03832	-0.89135
	H	6.81228	-5.73817	-1.95271		H	4.61403	-1.59822	-0.00002
	Br	6.62662	-3.10248	-2.87344		Br	1.83897	-1.93292	-0.00010

T7(ground state)					**T7**(excited state)				
	H	6.79826	4.70669	-5.39075		H	6.41190	-2.82603	0.48595
	C	7.27133	4.96624	-4.44903		C	6.58246	-1.76760	0.31258
	C	7.58958	6.27649	-4.12305		C	7.87342	-1.24058	0.21760
	C	8.20078	6.59091	-2.90085		C	8.05101	0.13010	-0.00624
	C	8.49437	5.58482	-1.99967		C	6.95854	0.96824	-0.13483
	C	8.18233	4.24784	-2.30488		C	5.63510	0.46457	-0.04412
	C	7.57151	3.96025	-3.53454		C	5.49107	-0.92749	0.18339
	O	7.25469	2.68791	-3.86912		O	4.24912	-1.48973	0.28417
	C	7.49381	1.59194	-3.06006		C	3.06739	-0.77115	0.18197
	C	8.12771	1.86406	-1.76805		C	3.18395	0.64368	-0.05749
	C	8.44559	3.14708	-1.43932		C	4.46860	1.23092	-0.16103
	H	7.35979	7.06961	-4.82934		H	8.73249	-1.89708	0.31795
	H	8.44171	7.62304	-2.66513		H	9.05519	0.53973	-0.07988
	H	8.96779	5.80895	-1.04705		H	7.09523	2.03276	-0.30882
	H	8.91747	3.31397	-0.47314		H	4.52608	2.29971	-0.33625
	C	8.46300	0.80571	-0.75079		C	2.03976	1.51492	-0.19568
	O	9.01368	1.16225	0.28872		O	2.14835	2.73264	-0.38948
	O	7.15285	0.52348	-3.51153		O	2.05739	-1.44936	0.31162
	C	8.12910	-0.59880	-1.01135		C	0.63540	0.96138	-0.13389
	H	7.64937	-0.83814	-1.95218		H	0.53258	-0.11840	-0.09728
	C	8.42816	-1.53196	-0.08315		C	-0.41192	1.80734	-0.12114
	H	8.91606	-1.17947	0.82591		H	-0.19792	2.87474	-0.14359
	C	8.17695	-2.95899	-0.15542		C	-1.80616	1.41129	-0.05436
	C	8.58023	-3.78435	0.90222		C	-2.80483	2.39818	0.10023
	C	7.52352	-3.56863	-1.23975		C	-2.23086	0.07135	-0.15624
	C	8.37352	-5.15379	0.86730		C	-4.13269	2.06448	0.19702
	C	7.30103	-4.93136	-1.26026		C	-3.56091	-0.27631	-0.06679
	C	7.74218	-5.78143	-0.21917		C	-4.56940	0.71165	0.16118
	H	9.08326	-3.34241	1.75922		H	-2.50959	3.44096	0.17426
	H	7.15370	-2.96937	-2.06555		H	-1.50640	-0.71265	-0.34883
	N	7.50979	-7.15765	-0.24598		N	-5.89245	0.43535	0.33074
	C	8.18271	-7.92445	-1.28554		C	-6.39986	-0.74025	1.01918
	H	8.15934	-7.39450	-2.23746		H	-5.60707	-1.24712	1.56541
	H	9.23341	-8.12702	-1.01931		H	-7.15990	-0.40490	1.73401
	H	7.66705	-8.88133	-1.41745		H	-6.86182	-1.44434	0.31889
	C	7.52193	-7.85126	1.02363		C	-6.89543	1.44952	0.06978
	H	6.92767	-7.30197	1.75868		H	-6.59888	2.07742	-0.77150
	H	7.06571	-8.83635	0.88148		H	-7.83034	0.94486	-0.18810
	H	8.53607	-8.00860	1.43078		H	-7.07781	2.07744	0.95298
	Br	6.28268	-5.62129	-2.70035		Br	-3.98808	-2.07161	-0.44238
	H	8.72770	-5.76056	1.69418		H	-4.86040	2.84795	0.37572

T7a(ground state)					**T7a**(excited state)				
	H	6.78155	4.53847	-5.45780		H	6.08609	0.67889	-2.91837
	C	7.20442	4.84127	-4.50517		C	6.35612	0.26663	-1.95062
	C	7.44429	6.17256	-4.19763		C	7.64944	-0.19000	-1.68607
	C	7.99146	6.54319	-2.96091		C	7.95179	-0.71158	-0.42396
	C	8.30009	5.57242	-2.02663		C	6.98245	-0.77921	0.56121
	C	8.06705	4.21521	-2.31265		C	5.66015	-0.32525	0.32778
	C	7.51879	3.87126	-3.55720		C	5.39168	0.20026	-0.96295
	O	7.27824	2.57759	-3.87362		O	4.13923	0.67824	-1.29037
	C	7.54082	1.51256	-3.03132		C	3.10413	0.64519	-0.40260
	C	8.11466	1.84315	-1.72513		C	3.33274	0.10027	0.89706
	C	8.35330	3.14755	-1.41366		C	4.61318	-0.37232	1.26485
	H	7.20278	6.93798	-4.93008		H	8.41039	-0.13610	-2.45836
	H	8.17140	7.59092	-2.74006		H	8.95673	-1.06801	-0.21290
	H	8.72498	5.84016	-1.06246		H	7.21983	-1.18775	1.54036
	H	8.77958	3.35824	-0.43491		H	4.76703	-0.77710	2.25924
	C	8.46962	0.82485	-0.67376		C	2.21495	0.11642	1.76989
	O	8.94097	1.23322	0.38531		O	2.18471	-0.21026	2.96832
	O	7.26551	0.41932	-3.46892		O	2.03203	1.11160	-0.79546
	C	8.25242	-0.60300	-0.92933		C	0.90249	0.62297	1.23135
	H	7.83523	-0.88649	-1.88738		H	0.71881	1.68783	1.35986
	C	8.57604	-1.50348	0.02270		C	-0.12846	-0.21745	0.90215
	H	8.99160	-1.10874	0.95013		H	0.07185	-1.28669	0.88500
	C	8.43074	-2.94539	-0.05095		C	-1.45413	0.18809	0.58177
	C	8.84591	-3.72254	1.04084		C	-2.42772	-0.80145	0.29907
	C	7.90766	-3.62148	-1.16389		C	-1.87247	1.54212	0.49178
	C	8.74148	-5.10246	1.02412		C	-3.72728	-0.48529	-0.00990
	C	7.78635	-4.99859	-1.16674		C	-3.16448	1.86540	0.18520
	C	8.18338	-5.79167	-0.07230		C	-4.16821	0.87587	-0.03603
	H	9.28639	-3.23865	1.90805		H	-2.12716	-1.84446	0.28848
	H	7.57279	-3.06228	-2.03291		H	-1.16540	2.34208	0.68247
	N	8.07895	-7.18357	-0.09429		N	-5.44658	1.26620	-0.26395
	C	7.98804	-7.81731	-1.39191		C	-5.73663	2.61255	-0.72472
	H	8.74070	-7.40267	-2.06768		H	-4.96168	2.96156	-1.40861
	H	8.19190	-8.88584	-1.26742		H	-6.68459	2.58674	-1.26814
	H	6.99400	-7.71970	-1.86217		H	-5.83727	3.31803	0.11082
	C	7.17804	-7.79823	0.87101		C	-6.62119	0.52630	0.17465
	H	7.26457	-7.31797	1.84540		H	-6.35247	-0.24535	0.89296
	H	6.12865	-7.73638	0.53816		H	-7.29499	1.23633	0.66644
	H	7.44320	-8.85406	0.98887		H	-7.14529	0.06668	-0.66934
	H	7.35143	-5.48336	-2.03474		H	-3.45161	2.91036	0.17384
	Br	9.46796	-6.04738	2.49555		Br	-4.83095	-1.90915	-0.57358

T8(ground state)					**T8**(excited state)				
	H	-6.17914	-2.61008	-0.19592		H	-6.72786	-1.87421	1.98096
	C	-6.15428	-1.52734	-0.12445		C	-6.75459	-1.05822	1.26480
	C	-7.31380	-0.76707	-0.08038		C	-7.96029	-0.49137	0.84590
	C	-7.26006	0.63098	0.01224		C	-7.95137	0.55967	-0.07917
	C	-6.03550	1.27043	0.06087		C	-6.75678	1.04241	-0.58216
	C	-4.84455	0.52371	0.01788		C	-5.51624	0.48818	-0.17762
	C	-4.92582	-0.87372	-0.07472		C	-5.56134	-0.57288	0.75891
	O	-3.80541	-1.63097	-0.11842		O	-4.40719	-1.15888	1.19820
	C	-2.52065	-1.11675	-0.07674		C	-3.14162	-0.77823	0.78484
	C	-2.40741	0.34047	0.01492		C	-3.06472	0.29756	-0.17699
	C	-3.53991	1.09542	0.06169		C	-4.25673	0.90524	-0.63344
	H	-8.27777	-1.26711	-0.11846		H	-8.89915	-0.86869	1.23994
	H	-8.17939	1.20777	0.04553		H	-8.88997	1.00054	-0.40502
	H	-5.97347	2.35342	0.13271		H	-6.74851	1.85842	-1.30065
	H	-3.41982	2.17437	0.13551		H	-4.17177	1.71184	-1.35344
	C	-1.09935	1.08396	0.06979		C	-1.81827	0.80380	-0.69156
	O	-1.13970	2.30460	0.20450		O	-1.76504	1.73250	-1.51618
	O	-1.62874	-1.93089	-0.11787		O	-2.23406	-1.41412	1.29786
	C	0.17025	0.35209	-0.04442		C	-0.50833	0.18623	-0.28578
	H	0.12872	-0.71172	-0.22609		H	-0.53529	-0.69614	0.34330
	C	1.31787	1.04150	0.12753		C	0.63068	0.75427	-0.72227
	H	1.19473	2.09291	0.38124		H	0.54478	1.67931	-1.29180
	C	2.69377	0.57927	0.08062		C	1.96088	0.29308	-0.36916
	C	3.68715	1.25182	0.83017		C	2.95494	1.22151	0.04733
	C	3.20029	-0.49341	-0.68665		C	2.38801	-1.06335	-0.42481
	C	5.02047	0.89787	0.85810		C	4.23016	0.85696	0.40580
	C	4.52926	-0.87293	-0.69323		C	3.65448	-1.45969	-0.06094
	C	5.48159	-0.19286	0.09303		C	4.61168	-0.50854	0.37257
	H	5.69629	1.46974	1.48009		H	4.92116	1.62380	0.73045
	N	6.79208	-0.56900	0.10707		N	5.85932	-0.89203	0.73579
	C	7.23322	-1.68335	-0.70199		C	6.21996	-2.29894	0.76712
	H	7.08409	-1.49560	-1.77422		H	6.22410	-2.72596	-0.24285
	H	8.29799	-1.84782	-0.53325		H	7.21764	-2.40181	1.19084
	H	6.70319	-2.60729	-0.43673		H	5.51926	-2.86437	1.38969
	C	7.74916	0.17862	0.89179		C	6.85949	0.09628	1.10061
	H	7.49522	0.16347	1.95995		H	6.57715	0.61804	2.02264
	H	8.73577	-0.27112	0.77548		H	7.81236	-0.40445	1.26412
	H	7.81325	1.22613	0.56730		H	6.98822	0.83209	0.30016
	H	4.82274	-1.69842	-1.32816		H	3.91014	-2.50809	-0.13965
	Br	3.21063	2.72539	1.92795		Br	2.51095	3.04486	0.15382
	Br	2.09163	-1.47788	-1.86500		Br	1.23684	-2.40646	-1.05617

Table S3. The Cartesian Coordinates (in Å) of species studied, optimized with CAM-B3LYP+IDSCRF/6-31G(d).

Compounds	Cartesian coordinates				Species	Cartesian coordinates			
T1(ground state)	H	7.01688	4.63849	-5.50505	**T1** (excited state)	H	-5.89301	2.73422	-0.00007
	C	7.39375	4.92233	-4.52886		C	-5.95149	1.65106	-0.00006
	C	7.63986	6.24225	-4.19113		C	-7.17018	0.98267	-0.00018
	C	8.12682	6.58331	-2.92300		C	-7.20381	-0.41646	-0.00018
	C	8.36747	5.59426	-1.99045		C	-6.02886	-1.14229	-0.00005
	C	8.12595	4.24858	-2.30858		C	-4.77692	-0.49156	0.00011
	C	7.64044	3.93572	-3.58012		C	-4.77873	0.91399	0.00010
	O	7.39325	2.64611	-3.92881		O	-3.59874	1.60495	0.00026
	C	7.59180	1.56733	-3.09013		C	-2.35529	1.00931	0.00071
	C	8.10196	1.87012	-1.74727		C	-2.32248	-0.44987	0.00030
	C	8.34561	3.15864	-1.40801		C	-3.52364	-1.14838	0.00013
	H	7.45152	7.02199	-4.92247		H	-8.09486	1.55056	-0.00030
	H	8.31376	7.62294	-2.67624		H	-8.15828	-0.93367	-0.00030
	H	8.74505	5.84046	-1.00237		H	-6.04910	-2.22824	-0.00008
	H	8.72252	3.35060	-0.40749		H	-3.47317	-2.23067	-0.00008
	C	8.38156	0.82543	-0.69158		C	-1.09421	-1.22978	-0.00003
	O	8.80719	1.21833	0.39174		O	-1.12680	-2.47907	-0.00021
	O	7.32327	0.48501	-3.55338		O	-1.41961	1.78596	-0.00019
	C	8.14752	-0.59274	-0.96996		C	0.21337	-0.55865	-0.00007
	H	7.77194	-0.86052	-1.94683		H	0.22526	0.52250	-0.00009
	C	8.40460	-1.50511	-0.01234		C	1.36655	-1.30804	-0.00010
	H	8.78069	-1.12158	0.93488		H	1.24549	-2.38777	-0.00005
	C	8.23990	-2.94432	-0.09163		C	2.68613	-0.78190	-0.00012
	C	8.56401	-3.73672	1.01717		C	3.80022	-1.66918	0.00009
	C	7.76615	-3.61028	-1.23280		C	2.98087	0.61425	-0.00032
	C	8.42938	-5.11172	1.00412		C	5.08988	-1.21965	0.00012
	C	7.62435	-4.98129	-1.26664		C	4.26579	1.07851	-0.00027
	C	7.95307	-5.77643	-0.14470		C	5.37270	0.17937	-0.00004
	H	8.93397	-3.25421	1.91839		H	3.60788	-2.73779	0.00023
	H	7.50139	-3.03987	-2.11781		H	2.16689	1.33027	-0.00052
	H	8.69562	-5.67227	1.89096		H	5.89869	-1.93829	0.00029
	N	7.81326	-7.14080	-0.17477		N	6.64616	0.63552	0.00002
	C	7.32175	-7.79553	-1.36915		C	6.91918	2.06557	-0.00002
	H	7.97576	-7.61541	-2.23164		H	6.50013	2.54769	0.88950
	H	7.28233	-8.87092	-1.19706		H	7.99603	2.22272	0.00016
	H	6.31132	-7.45853	-1.63279		H	6.50044	2.54760	-0.88973
	C	8.15779	-7.92946	0.98930		C	7.76633	-0.29453	0.00017
	H	7.55023	-7.65585	1.86126		H	7.75036	-0.93292	-0.88949
	H	7.98055	-8.98291	0.77385		H	8.69713	0.26929	0.00004
	H	9.21439	-7.81327	1.26210		H	7.75040	-0.93260	0.89006
	H	7.25439	-5.44410	-2.17258		H	4.43535	2.14711	-0.00043

T2(ground state)					**T2** (excited state)				
	H	-4.58951	3.77085	-0.11043		H	4.40623	3.80064	-0.00069
	C	-4.74052	2.69850	-0.06696		C	4.60879	2.73546	-0.00052
	C	-6.00084	2.13142	-0.05119		C	5.90604	2.23449	-0.00049
	C	-6.16779	0.74401	0.00527		C	6.12400	0.85613	-0.00027
	C	-5.05653	-0.07130	0.04591		C	5.04779	-0.00815	-0.00009
	C	-3.75538	0.46408	0.03184		C	3.71025	0.45055	-0.00012
	C	-3.63413	1.85670	-0.02520		C	3.54514	1.85218	-0.00033
	O	-2.41086	2.44131	-0.04169		O	2.29026	2.39326	-0.00041
	C	-1.21492	1.74988	-0.00554		C	1.12373	1.65515	-0.00006
	C	-1.31753	0.28797	0.05294		C	1.26827	0.20885	0.00009
	C	-2.53991	-0.29237	0.07069		C	2.54740	-0.34807	0.00006
	H	-6.87807	2.76941	-0.08299		H	6.75170	2.91348	-0.00064
	H	-7.15987	0.30906	0.01718		H	7.13194	0.45783	-0.00025
	H	-2.57839	-1.37530	0.11677		H	2.62566	-1.42637	0.00016
	C	-0.12609	-0.64432	0.09736		C	0.14330	-0.70832	0.00028
	O	-0.35712	-1.84767	0.17309		O	0.31051	-1.94287	0.00043
	O	-0.21600	2.42579	-0.02468		O	0.10424	2.31931	0.00012
	C	1.23457	-0.10965	0.04436		C	-1.24120	-0.19206	0.00035
	H	1.35568	0.96189	-0.01975		H	-1.37881	0.88037	0.00062
	C	2.27967	-0.96028	0.07609		C	-2.29258	-1.07181	0.00007
	H	2.04034	-2.02046	0.14294		H	-2.04338	-2.12950	-0.00031
	C	3.69141	-0.63190	0.03072		C	-3.66710	-0.70779	0.00014
	C	4.63974	-1.66236	0.07292		C	-4.66383	-1.72361	-0.00055
	C	4.18137	0.68071	-0.05616		C	-4.12607	0.64202	0.00088
	C	5.99813	-1.41460	0.03157		C	-5.99832	-1.43372	-0.00064
	C	5.53279	0.94964	-0.09857		C	-5.45655	0.94860	0.00080
	C	6.48576	-0.09411	-0.05539		C	-6.44724	-0.07862	-0.00005
	H	4.29568	-2.69142	0.13981		H	-4.34330	-2.76090	-0.00100
	H	3.48596	1.51369	-0.09189		H	-3.40401	1.45057	0.00155
	H	6.68419	-2.25104	0.06656		H	-6.71442	-2.24456	-0.00109
	N	7.83107	0.16956	-0.09656		N	-7.76392	0.22079	-0.00027
	C	8.30206	1.53496	-0.20186		C	-8.20839	1.60833	0.00083
	H	7.97690	2.14410	0.65064		H	-7.85065	2.13718	-0.88846
	H	9.39170	1.53708	-0.21853		H	-9.29620	1.63347	0.00048
	H	7.94871	2.01997	-1.12071		H	-7.85126	2.13560	0.89131
	C	8.78359	-0.92046	-0.06785		C	-8.76528	-0.83748	-0.00119
	H	8.65636	-1.59683	-0.92279		H	-8.67304	-1.46820	0.88890
	H	9.79412	-0.51447	-0.10755		H	-9.75668	-0.38906	-0.00212
	H	8.69411	-1.51384	0.85067		H	-8.67138	-1.46811	-0.89113
	H	5.85658	1.98033	-0.16636		H	-5.75377	1.98875	0.00140
	Br	-5.30614	-1.94670	0.12185		Br	5.38800	-1.87734	0.00020

T3(ground state)					**T3**(excited state)			
	H	7.01578	4.64667	-5.50468		H	-4.22272	3.20050	-0.00010
	C	7.39278	4.92481	-4.52706		C	-4.33986	2.12236	-0.00006
	C	7.63663	6.24488	-4.19493		C	-5.60043	1.53478	-0.00010
	C	8.12292	6.56929	-2.92486		C	-5.69466	0.14289	-0.00005
	C	8.36738	5.59061	-1.98575		C	-4.57775	-0.66426	0.00004
	C	8.12426	4.24799	-2.30994		C	-3.29108	-0.08409	0.00007
	C	7.63889	3.93520	-3.58050		C	-3.21181	1.32112	0.00003
	O	7.39169	2.64865	-3.93084		O	-1.99555	1.94308	0.00007
	C	7.59083	1.56825	-3.09166		C	-0.78674	1.27476	0.00018
	C	8.10140	1.87165	-1.74792		C	-0.84017	-0.18030	0.00017
	C	8.34537	3.15812	-1.40655		C	-2.08203	-0.81376	0.00014
	H	7.45175	7.03161	-4.91740		H	-6.49522	2.14495	-0.00016
	H	8.74461	5.84685	-1.00169		H	-4.67554	-1.74399	0.00007
	H	8.72231	3.35009	-0.40617		H	-2.09552	-1.89664	0.00015
	C	8.38145	0.82464	-0.69124		C	0.34041	-1.02543	0.00018
	O	8.80628	1.22063	0.39074		O	0.24651	-2.26857	-0.00002
	O	7.32213	0.48733	-3.55466		O	0.19115	1.99809	0.00014
	C	8.14763	-0.59175	-0.97037		C	1.69001	-0.42660	0.00012
	H	7.77223	-0.86030	-1.94698		H	1.76240	0.65217	0.00012
	C	8.40492	-1.50445	-0.01220		C	2.79342	-1.24075	0.00008
	H	8.78070	-1.12066	0.93501		H	2.60921	-2.31164	0.00009
	C	8.24078	-2.94281	-0.09133		C	4.14344	-0.79389	0.00003
	C	8.56396	-3.73495	1.01827		C	5.20019	-1.74727	0.00002
	C	7.76842	-3.60907	-1.23309		C	4.51970	0.58126	-0.00000
	C	8.42958	-5.10969	1.00531		C	6.51467	-1.37683	-0.00002
	C	7.62696	-4.97984	-1.26684		C	5.82929	0.96799	-0.00005
	C	7.95459	-5.77474	-0.14415		C	6.88058	0.00305	-0.00006
	H	8.93281	-3.25212	1.91973		H	4.94333	-2.80214	0.00004
	H	7.50461	-3.03906	-2.11863		H	3.75008	1.34468	-0.00000
	H	8.69488	-5.67007	1.89248		H	7.27864	-2.14276	-0.00003
	N	7.81514	-7.13862	-0.17414		N	8.17687	0.38210	-0.00010
	C	7.32490	-7.79390	-1.36900		C	8.53597	1.79411	-0.00009
	H	7.97992	-7.61397	-2.23068		H	8.14693	2.29945	0.88977
	H	7.28538	-8.86919	-1.19650		H	9.62024	1.88552	-0.00007
	H	6.31475	-7.45698	-1.63358		H	8.14696	2.29946	-0.88995
	C	8.15837	-7.92735	0.99054		C	9.24082	-0.61317	-0.00014
	H	7.54958	-7.65375	1.86155		H	9.18637	-1.24847	-0.89010
	H	7.98151	-8.98078	0.77477		H	10.20307	-0.10519	-0.00024
	H	9.21460	-7.81098	1.26440		H	9.18651	-1.24840	0.88989
	H	7.25823	-5.44294	-2.17308		H	6.06275	2.02431	-0.00008
	Br	8.44833	8.38721	-2.49641		Br	-7.42190	-0.65895	-0.00009

T4(ground state)					**T4**(excited state)			
	C	7.39365	4.93183	-4.52756		C	5.05767	-0.34245	-0.00002
	C	7.63980	6.25068	-4.18868		C	6.17602	0.48211	-0.00009
	C	8.12562	6.57985	-2.92043		C	6.00641	1.86850	-0.00010
	C	8.36430	5.58584	-1.99268		C	4.74145	2.42130	-0.00005
	C	8.11997	4.24524	-2.32070		C	3.59507	1.59978	0.00005
	C	7.63412	3.92573	-3.59158		C	3.78219	0.20331	0.00006
	O	7.38866	2.64252	-3.93786		O	2.71214	-0.63683	0.00016
	C	7.58779	1.55991	-3.09693		C	1.39409	-0.21448	0.00040
	C	8.09783	1.86543	-1.75515		C	1.16706	1.22287	0.00014
	C	8.33994	3.15332	-1.41938		C	2.26552	2.07902	0.00004
	H	7.45066	7.02757	-4.92106		H	7.16561	0.04119	-0.00014
	H	8.74164	5.82472	-1.00322		H	4.60745	3.49860	-0.00008
	H	8.71688	3.34885	-0.41965		H	2.07273	3.14478	-0.00011
	C	8.37882	0.82159	-0.69644		C	-0.15404	1.82645	-0.00008
	O	8.80421	1.21976	0.38468		O	-0.29910	3.06508	-0.00004
	O	7.31933	0.48063	-3.56145		O	0.57719	-1.11397	-0.00014
	C	8.14580	-0.59530	-0.97358		C	-1.36125	0.97857	-0.00009
	H	7.77024	-0.86528	-1.94980		H	-1.22267	-0.09367	-0.00012
	C	8.40366	-1.50704	-0.01475		C	-2.60355	1.56040	-0.00006
	H	8.77951	-1.12224	0.93207		H	-2.63436	2.64658	-0.00001
	C	8.24011	-2.94556	-0.09237		C	-3.83842	0.85528	-0.00005
	C	8.56391	-3.73622	1.01807		C	-5.06354	1.57998	0.00007
	C	7.76779	-3.61331	-1.23331		C	-3.93473	-0.56748	-0.00016
	C	8.43015	-5.11104	1.00674		C	-6.27836	0.95599	0.00009
	C	7.62696	-4.98420	-1.26539		C	-5.14163	-1.20629	-0.00014
	C	7.95520	-5.77762	-0.14185		C	-6.36333	-0.46907	-0.00001
	H	8.93274	-3.25219	1.91890		H	-5.02125	2.66485	0.00016
	H	7.50351	-3.04449	-2.11948		H	-3.02918	-1.16334	-0.00027
	H	8.69590	-5.67030	1.89449		H	-7.17918	1.55506	0.00019
	N	7.81637	-7.14163	-0.17012		N	-7.55897	-1.09767	0.00001
	C	7.32618	-7.79878	-1.36396		C	-7.63088	-2.55264	-0.00005
	H	7.98089	-7.61969	-2.22605		H	-7.14921	-2.97101	0.88969
	H	7.28725	-8.87386	-1.18997		H	-8.67545	-2.85738	0.00004
	H	6.31579	-7.46274	-1.62875		H	-7.14937	-2.97094	-0.88990
	C	8.16023	-7.92870	0.99541		C	-8.79902	-0.33332	0.00010
	H	7.55152	-7.65430	1.86625		H	-8.87186	0.30033	-0.88978
	H	7.98380	-8.98249	0.78101		H	-9.64146	-1.02201	0.00003
	H	9.21648	-7.81152	1.26891		H	-8.87185	0.30013	0.89013
	H	7.25823	-5.44848	-2.17104		H	-5.16082	-2.28796	-0.00023
	Br	6.73807	4.49226	-6.24020		Br	5.27916	-2.22326	0.00001
	H	8.31250	7.61910	-2.67321		H	6.88090	2.51125	-0.00017

T5(ground state)					**T5**(excited state)				
	C	7.39373	4.93432	-4.52722		C	3.85782	1.21544	-0.00001
	C	7.63884	6.25307	-4.19080		C	5.06645	0.52696	-0.00008
	C	8.12406	6.56728	-2.92052		C	5.03540	-0.86555	-0.00008
	C	8.36574	5.58208	-1.98733		C	3.85213	-1.57058	-0.00003
	C	8.11931	4.24479	-2.32251		C	2.62249	-0.87862	0.00004
	C	7.63381	3.92596	-3.59239		C	2.65225	0.53174	0.00005
	O	7.38818	2.64510	-3.94019		O	1.49617	1.24674	0.00012
	C	7.58758	1.56093	-3.09881		C	0.23179	0.67689	0.00025
	C	8.09793	1.86677	-1.75628		C	0.17011	-0.77360	0.00014
	C	8.34034	3.15290	-1.41883		C	1.35895	-1.50562	0.00007
	H	7.45345	7.03762	-4.91424		H	6.00453	1.06551	-0.00012
	H	8.74272	5.82979	-1.00135		H	3.85320	-2.65434	-0.00005
	H	8.71730	3.34876	-0.41929		H	1.28818	-2.58599	0.00001
	C	8.37930	0.82095	-0.69654		C	-1.07439	-1.51961	0.00010
	O	8.80425	1.22199	0.38328		O	-1.08509	-2.76378	-0.00002
	O	7.31929	0.48283	-3.56319		O	-0.68011	1.48012	0.00006
	C	8.14615	-0.59433	-0.97405		C	-2.37400	-0.81029	0.00009
	H	7.77063	-0.86509	-1.95000		H	-2.35636	0.27072	0.00011
	C	8.40407	-1.50637	-0.01460		C	-3.53866	-1.52884	0.00005
	H	8.77991	-1.12137	0.93211		H	-3.44562	-2.61159	0.00004
	C	8.24048	-2.94408	-0.09225		C	-4.84740	-0.96974	0.00004
	C	8.56414	-3.73474	1.01852		C	-5.97914	-1.83173	0.00004
	C	7.76818	-3.61184	-1.23348		C	-5.10587	0.43170	0.00003
	C	8.43028	-5.10927	1.00716		C	-7.25791	-1.35282	0.00004
	C	7.62725	-4.98248	-1.26558		C	-6.37772	0.92724	0.00002
	C	7.95536	-5.77591	-0.14170		C	-7.50651	0.05319	0.00003
	H	8.93288	-3.25067	1.91934		H	-5.81133	-2.90432	0.00005
	H	7.50408	-3.04308	-2.11972		H	-4.27497	1.12790	0.00002
	H	8.69581	-5.66863	1.89488		H	-8.08340	-2.05189	0.00004
	N	7.81647	-7.13939	-0.16998		N	-8.76485	0.53944	0.00002
	C	7.32631	-7.79664	-1.36397		C	-9.00466	1.97730	-0.00001
	H	7.98126	-7.61768	-2.22584		H	-8.57479	2.44751	-0.89006
	H	7.28727	-8.87165	-1.18986		H	-10.07742	2.15875	-0.00003
	H	6.31601	-7.46050	-1.62873		H	-8.57481	2.44755	0.89002
	C	8.16011	-7.92683	0.99564		C	-9.90961	-0.36280	0.00004
	H	7.55118	-7.65241	1.86624		H	-9.90839	-0.99978	0.89021
	H	7.98359	-8.98050	0.78094		H	-10.82530	0.22477	0.00008
	H	9.21631	-7.80970	1.26909		H	-9.90844	-0.99976	-0.89015
	H	7.25865	-5.44683	-2.17120		H	-6.52163	1.99934	0.00001
	Br	6.73915	4.50081	-6.23835		Br	3.87135	3.10624	-0.00000
	Br	8.45087	8.38052	-2.48646		Br	6.68562	-1.81021	-0.00018

T6a(ground state)					**T6a**(excited state)				
	H	6.33402	4.64147	-5.19814		H	-6.78103	-2.67721	-0.00087
	C	6.94871	4.91779	-4.34884		C	-6.73604	-1.59350	-0.00059
	C	7.32423	6.22851	-4.10845		C	-7.88358	-0.81162	-0.00058
	C	8.11912	6.56018	-3.00393		C	-7.78663	0.58511	-0.00022
	C	8.53849	5.57095	-2.13731		C	-6.54855	1.19623	0.00013
	C	8.17116	4.23432	-2.35923		C	-5.36641	0.42822	0.00014
	C	7.37800	3.93082	-3.46804		C	-5.49813	-0.96931	-0.00024
	O	7.00004	2.65020	-3.71951		O	-4.38893	-1.76567	-0.00025
	C	7.35186	1.57256	-2.93251		C	-3.09602	-1.28917	0.00006
	C	8.18535	1.86553	-1.76027		C	-2.92740	0.16435	0.00046
	C	8.55806	3.14511	-1.51649		C	-4.05428	0.96529	0.00048
	H	6.99594	7.00856	-4.78820		H	-8.85814	-1.28911	-0.00086
	H	8.40336	7.59276	-2.83181		H	-8.68848	1.18912	-0.00022
	H	9.15518	5.80977	-1.27585		H	-6.46480	2.27909	0.00041
	H	9.17480	3.33003	-0.64156		H	-3.90235	2.03861	0.00077
	C	8.66880	0.82010	-0.78362		C	-1.62813	0.83417	0.00080
	O	9.36073	1.19902	0.15612		O	-1.55886	2.08295	0.00032
	O	6.93344	0.49844	-3.29320		O	-2.23558	-2.14625	-0.00019
	C	8.31328	-0.59152	-0.96949		C	-0.39618	0.04911	0.00063
	H	7.70044	-0.84441	-1.82213		H	-0.48743	-1.02764	0.00074
	C	8.75869	-1.50081	-0.08300		C	0.82541	0.69640	0.00041
	H	9.36740	-1.12411	0.73325		H	0.79440	1.77950	0.00032
	C	8.51033	-2.93277	-0.10401		C	2.08237	0.04497	0.00028
	C	9.01861	-3.80779	0.86795		C	3.32747	0.75554	-0.00004
	C	7.73730	-3.54058	-1.10905		C	2.20326	-1.38132	0.00047
	C	8.78675	-5.16974	0.85446		C	4.54138	0.12498	-0.00017
	C	7.48656	-4.89308	-1.15302		C	3.40384	-2.02743	0.00033
	C	8.00883	-5.75470	-0.16344		C	4.62613	-1.29460	0.00001
	H	9.21487	-5.77437	1.64085		H	5.43826	0.72771	-0.00040
	N	7.77191	-7.10244	-0.18797		N	5.82540	-1.92165	-0.00012
	C	6.96772	-7.67796	-1.24718		C	5.89647	-3.37544	0.00011
	H	7.41297	-7.50633	-2.23495		H	5.41495	-3.79555	-0.88948
	H	6.89395	-8.75429	-1.09450		H	6.94118	-3.68040	-0.00004
	H	5.95063	-7.26705	-1.25472		H	5.41529	-3.79526	0.89001
	C	8.32431	-7.95539	0.84452		C	7.06173	-1.15417	-0.00043
	H	7.95819	-7.67683	1.84055		H	7.13367	-0.51923	0.88934
	H	8.02776	-8.98628	0.65356		H	7.90678	-1.83992	-0.00053
	H	9.42064	-7.91601	0.86049		H	7.13332	-0.51940	-0.89035
	H	6.88166	-5.28608	-1.95961		H	3.41631	-3.10919	0.00049
	H	7.31599	-2.91642	-1.89001		H	1.29750	-1.97553	0.00072
	Br	10.08878	-3.15626	2.30567		Br	3.33426	2.64602	-0.00030

T7(ground state)					**T7**(excited state)				
	H	6.77807	4.71550	-5.37525		H	6.56499	-2.77503	0.40800
	C	7.25846	4.97462	-4.43850		C	6.68582	-1.70786	0.25814
	C	7.57998	6.28152	-4.11377		C	7.93593	-1.11494	0.16833
	C	8.20067	6.59119	-2.89688		C	8.05549	0.26557	-0.02513
	C	8.49945	5.58366	-2.00210		C	6.92415	1.05140	-0.12850
	C	8.18355	4.25027	-2.30782		C	5.64486	0.47552	-0.04101
	C	7.56513	3.96893	-3.52841		C	5.55823	-0.90652	0.15261
	O	7.24293	2.69234	-3.86407		O	4.33944	-1.52001	0.24530
	C	7.48723	1.59817	-3.06074		C	3.14028	-0.86984	0.15944
	C	8.13313	1.86812	-1.77052		C	3.19967	0.58982	-0.03795
	C	8.45364	3.14369	-1.44332		C	4.42658	1.21142	-0.13689
	H	7.34606	7.07611	-4.81532		H	8.82630	-1.72998	0.24929
	H	8.44493	7.62119	-2.66029		H	9.03866	0.71928	-0.09410
	H	8.98030	5.80527	-1.05389		H	7.00654	2.12386	-0.27886
	H	8.93293	3.31192	-0.48311		H	4.48136	2.28391	-0.28780
	C	8.47336	0.80170	-0.76093		C	1.99614	1.36294	-0.13518
	O	9.03432	1.15057	0.27204		O	2.16687	2.64155	-0.34307
	O	7.14403	0.52894	-3.50477		O	2.14644	-1.54962	0.25263
	C	8.13247	-0.60735	-1.01691		C	0.64879	0.89758	-0.05950
	H	7.64264	-0.84557	-1.95026		H	0.53778	-0.17538	0.00728
	C	8.43896	-1.53360	-0.09474		C	-0.40906	1.75330	-0.07553
	H	8.93683	-1.18481	0.80804		H	-0.21892	2.82348	-0.09825
	C	8.18122	-2.96781	-0.16480		C	-1.80935	1.37281	-0.03455
	C	8.59426	-3.79102	0.88447		C	-2.79102	2.35927	0.11145
	C	7.51682	-3.57081	-1.24070		C	-2.24364	0.04337	-0.15066
	C	8.38061	-5.15951	0.85205		C	-4.13500	2.03425	0.17653
	C	7.28814	-4.93166	-1.25850		C	-3.58636	-0.27113	-0.10298
	C	7.73172	-5.77867	-0.22303		C	-4.58048	0.70926	0.08562
	H	9.10711	-3.35146	1.73534		H	-2.49063	3.40007	0.19395
	H	7.14766	-2.97039	-2.06399		H	-1.52992	-0.75593	-0.31279
	N	7.49115	-7.16207	-0.25365		N	-5.94380	0.37306	0.13006
	C	8.22259	-7.92056	-1.26381		C	-6.38389	-0.37235	1.30515
	H	8.19788	-7.40910	-2.22433		H	-5.68613	-1.17534	1.53623
	H	9.27343	-8.07679	-0.97186		H	-6.47915	0.28000	2.18803
	H	7.74932	-8.89867	-1.38909		H	-7.36008	-0.82108	1.09974
	C	7.47399	-7.84972	1.02328		C	-6.88529	1.41660	-0.22680
	H	6.86506	-7.29540	1.74055		H	-6.56613	1.91229	-1.14607
	H	7.02162	-8.83492	0.87875		H	-7.86068	0.95563	-0.40681
	H	8.47743	-8.00317	1.45426		H	-7.01680	2.17905	0.55922
	Br	6.27072	-5.62624	-2.70585		Br	-4.06724	-2.08748	-0.39020
	H	8.73761	-5.76688	1.67530		H	-4.86042	2.82731	0.31514

T8(ground state)					**T8**(excited state)				
	H	-6.14034	-2.63201	-0.04377		H	-6.95518	-1.74147	1.90038
	C	-6.12907	-1.54793	-0.03257		C	-6.91166	-0.94168	1.16925
	C	-7.29445	-0.80049	-0.03394		C	-8.05603	-0.32078	0.69078
	C	-7.25400	0.59951	-0.01888		C	-7.96183	0.70854	-0.25197
	C	-6.03741	1.25133	-0.00288		C	-6.72507	1.11482	-0.71441
	C	-4.84144	0.51611	-0.00133		C	-5.54871	0.50216	-0.24654
	C	-4.90980	-0.87917	-0.01579		C	-5.67622	-0.52410	0.69696
	O	-3.77703	-1.62902	-0.01348		O	-4.56813	-1.15685	1.19028
	C	-2.50181	-1.10059	0.00444		C	-3.28417	-0.85806	0.82082
	C	-2.40398	0.36390	0.01202		C	-3.11874	0.22319	-0.16330
	C	-3.53821	1.10524	0.01314		C	-4.23555	0.85705	-0.67087
	H	-8.25259	-1.31050	-0.04678		H	-9.02854	-0.63817	1.05284
	H	-8.17771	1.16813	-0.01992		H	-8.86236	1.18869	-0.62081
	H	-5.98683	2.33612	0.00874		H	-6.64273	1.91280	-1.44656
	H	-3.43358	2.18642	0.02573		H	-4.11617	1.64628	-1.40452
	C	-1.09864	1.11679	0.02691		C	-1.81477	0.61379	-0.60481
	O	-1.14552	2.33939	0.09436		O	-1.73598	1.53534	-1.51148
	O	-1.59755	-1.89965	0.01500		O	-2.40743	-1.51012	1.33715
	C	0.18540	0.39346	-0.04608		C	-0.55597	0.04577	-0.20499
	H	0.15858	-0.67666	-0.17541		H	-0.58559	-0.89747	0.31804
	C	1.31969	1.09754	0.08287		C	0.59398	0.70407	-0.52547
	H	1.20318	2.16037	0.27432		H	0.48828	1.69946	-0.94678
	C	2.70027	0.61383	0.05487		C	1.94826	0.27176	-0.26375
	C	3.67720	1.23292	0.85703		C	2.94995	1.22022	0.05570
	C	3.20147	-0.42724	-0.74694		C	2.42560	-1.05870	-0.32093
	C	5.00356	0.85852	0.89813		C	4.26030	0.90418	0.32727
	C	4.52393	-0.82670	-0.74161		C	3.72989	-1.41219	-0.05110
	C	5.46588	-0.19863	0.09316		C	4.68946	-0.43870	0.29331
	H	5.67216	1.38941	1.55991		H	4.94624	1.70119	0.57456
	N	6.77519	-0.59431	0.11653		N	5.98017	-0.77972	0.57188
	C	7.22273	-1.66822	-0.74749		C	6.39194	-2.17008	0.52473
	H	7.09222	-1.42188	-1.80901		H	6.28094	-2.59304	-0.48125
	H	8.28246	-1.84956	-0.57112		H	7.44143	-2.24060	0.80740
	H	6.68287	-2.60052	-0.54339		H	5.81089	-2.78380	1.22277
	C	7.72715	0.10506	0.95588		C	6.95163	0.24972	0.89000
	H	7.44986	0.04717	2.01536		H	6.66541	0.80980	1.78811
	H	8.70849	-0.35409	0.84123		H	7.91740	-0.21750	1.07781
	H	7.81366	1.16413	0.68165		H	7.07291	0.96086	0.06399
	H	4.81926	-1.62782	-1.40313		H	4.00498	-2.45390	-0.12764
	Br	3.18467	2.66619	2.01223		Br	2.49857	3.06486	0.16321
	Br	2.09469	-1.34797	-1.99068		Br	1.30369	-2.49308	-0.86645

Table S4. The Cartesian Coordinates (in Å) of species studied, optimized with WB97XD+IDSCRF/6-31G(d) .

Compounds	Cartesian coordinates				Species	Cartesian coordinates			
T1(ground state)	H	7.01107	4.62632	-5.51155	**T1** (excited state)	H	5.90393	2.74133	0.00101
	C	7.38757	4.91315	-4.53567		C	5.95554	1.65751	0.00074
	C	7.63033	6.23634	-4.20237		C	7.16922	0.98189	0.00085
	C	8.11724	6.58484	-2.93449		C	7.20175	-0.41942	0.00049
	C	8.36152	5.59935	-1.99674		C	6.02285	-1.14156	0.00002
	C	8.12340	4.25047	-2.31042		C	4.77654	-0.48262	-0.00013
	C	7.63788	3.92949	-3.58156		C	4.77712	0.92093	0.00023
	O	7.39424	2.64013	-3.92612		O	3.60301	1.61190	0.00009
	C	7.59586	1.56573	-3.08419		C	2.35965	1.01908	-0.00062
	C	8.10625	1.87308	-1.73969		C	2.32278	-0.44889	-0.00057
	C	8.34716	3.16491	-1.40375		C	3.51610	-1.14137	-0.00048
	H	7.43927	7.01253	-4.93721		H	8.09639	1.54677	0.00124
	H	8.30114	7.62634	-2.69215		H	8.15549	-0.93813	0.00061
	H	8.73885	5.85099	-1.00941		H	6.03778	-2.22810	-0.00022
	H	8.72423	3.36538	-0.40395		H	3.46632	-2.22547	-0.00056
	C	8.38959	0.83081	-0.67760		C	1.08589	-1.24206	-0.00055
	O	8.81576	1.22765	0.40366		O	1.14452	-2.49300	-0.00085
	O	7.32957	0.48148	-3.54575		O	1.42544	1.79362	0.00014
	C	8.15560	-0.58961	-0.95417		C	-0.20844	-0.57616	-0.00048
	H	7.77897	-0.85954	-1.93126		H	-0.22637	0.50576	-0.00083
	C	8.41313	-1.50365	0.00394		C	-1.37609	-1.32952	-0.00013
	H	8.79033	-1.12411	0.95359		H	-1.25900	-2.41066	0.00028
	C	8.24568	-2.94430	-0.08154		C	-2.68690	-0.79832	-0.00011
	C	8.56738	-3.74169	1.02611		C	-3.81257	-1.67975	0.00077
	C	7.77191	-3.60508	-1.22713		C	-2.97638	0.60445	-0.00094
	C	8.42995	-5.11797	1.00772		C	-5.09933	-1.22073	0.00092
	C	7.62738	-4.97747	-1.26640		C	-4.26090	1.07505	-0.00076
	C	7.95321	-5.77831	-0.14571		C	-5.37420	0.18251	0.00023
	H	8.93747	-3.26485	1.93105		H	-3.62931	-2.75073	0.00133
	H	7.50877	-3.03308	-2.11245		H	-2.16069	1.31972	-0.00177
	H	8.69488	-5.68055	1.89490		H	-5.91142	-1.93726	0.00157
	N	7.81069	-7.14239	-0.18093		N	-6.64742	0.64714	0.00048
	C	7.32012	-7.79082	-1.37928		C	-6.90853	2.07810	-0.00049
	H	7.97880	-7.60859	-2.23877		H	-6.48670	2.55617	-0.89236
	H	7.27640	-8.86774	-1.21312		H	-7.98463	2.24633	0.00040
	H	6.31021	-7.44891	-1.64179		H	-6.48507	2.55760	0.88982
	C	8.15348	-7.93542	0.98082		C	-7.77166	-0.27617	0.00092
	H	7.54393	-7.66272	1.85265		H	-7.75947	-0.91432	0.89221
	H	7.97486	-8.98898	0.76320		H	-8.70116	0.29158	0.00124
	H	9.21142	-7.82141	1.25254		H	-7.76011	-0.91447	-0.89030
	H	7.25753	-5.43370	-2.17684		H	-4.42255	2.14605	-0.00147

T2(ground state)	H	-4.57786	3.77944	-0.09013	**T2** (excited state)	H	4.41560	3.80795	0.04612
	C	-4.73133	2.70640	-0.06934		C	4.61224	2.74139	0.03690
	C	-5.99436	2.14279	-0.09918		C	5.90459	2.23337	0.04338
	C	-6.16844	0.75390	-0.07123		C	6.12288	0.85269	0.03118
	C	-5.05987	-0.06730	-0.01286		C	5.04303	-0.00964	0.01251
	C	-3.75566	0.46452	0.01943		C	3.70978	0.45841	0.00508
	C	-3.62745	1.85887	-0.01022		C	3.54333	1.85679	0.01798
	O	-2.40515	2.44059	0.01857		O	2.29453	2.39881	0.01227
	C	-1.21320	1.74599	0.07704		C	1.12786	1.66539	-0.00780
	C	-1.31874	0.28105	0.10402		C	1.26905	0.20819	-0.01805
	C	-2.54339	-0.29792	0.07923		C	2.53841	-0.34301	-0.01367
	H	-6.86831	2.78478	-0.14497		H	6.75302	2.90964	0.05802
	H	-7.16330	0.32434	-0.09516		H	7.13176	0.45551	0.03627
	H	-2.58647	-1.38272	0.10700		H	2.61401	-1.42375	-0.02424
	C	-0.12861	-0.65772	0.16262		C	0.13884	-0.72213	-0.03541
	O	-0.36364	-1.85875	0.25470		O	0.33395	-1.95656	-0.05828
	O	-0.21339	2.42133	0.10349		O	0.11087	2.32767	-0.01241
	C	1.23395	-0.12491	0.09383		C	-1.22974	-0.21079	-0.03501
	H	1.35679	0.94687	0.01878		H	-1.37541	0.86117	-0.05759
	C	2.28097	-0.97574	0.12454		C	-2.29623	-1.09642	-0.01386
	H	2.04628	-2.03720	0.20419		H	-2.05023	-2.15552	0.01097
	C	3.69276	-0.64142	0.06137		C	-3.66161	-0.72553	-0.01210
	C	4.64591	-1.66948	0.09692		C	-4.67113	-1.73490	0.04330
	C	4.17638	0.67397	-0.03711		C	-4.11581	0.63059	-0.06113
	C	6.00433	-1.41658	0.03704		C	-6.00361	-1.43388	0.05220
	C	5.52787	0.94811	-0.09779		C	-5.44636	0.94478	-0.05174
	C	6.48642	-0.09301	-0.06295		C	-6.44452	-0.07450	0.00533
	H	4.30847	-2.70076	0.17314		H	-4.35989	-2.77522	0.08055
	H	3.47940	1.50675	-0.06680		H	-3.39158	1.43708	-0.10722
	H	6.69210	-2.25303	0.06776		H	-6.72352	-2.24162	0.09610
	N	7.83010	0.17559	-0.12396		N	-7.76191	0.23451	0.01397
	C	8.29317	1.54278	-0.24191		C	-8.19391	1.62384	-0.02951
	H	7.97964	2.15224	0.61575		H	-7.84290	2.11716	-0.94298
	H	9.38306	1.55129	-0.27731		H	-9.28228	1.66089	-0.01855
	H	7.92158	2.02120	-1.15793		H	-7.82183	2.18020	0.83848
	C	8.78656	-0.91136	-0.10490		C	-8.76797	-0.81562	0.07772
	H	8.64544	-1.59232	-0.95496		H	-8.66602	-1.40531	0.99596
	H	9.79620	-0.50369	-0.16512		H	-9.75842	-0.36285	0.07109
	H	8.71466	-1.49783	0.82055		H	-8.69246	-1.48723	-0.78493
	H	5.84415	1.98159	-0.17342		H	-5.73530	1.98783	-0.08931
	Br	-5.31616	-1.94078	0.02385		Br	5.37512	-1.87603	-0.00351

T3(ground state)					**T3**(excited state)				
	H	7.01295	4.63822	-5.51125		H	-4.23010	3.21037	0.00016
	C	7.39019	4.91811	-4.53386		C	-4.34148	2.13132	0.00010
	C	7.63357	6.24082	-4.20617		C	-5.59710	1.53783	0.00014
	C	8.12072	6.57103	-2.93574		C	-5.69280	0.14296	0.00006
	C	8.36667	5.59507	-1.99136		C	-4.57108	-0.66123	-0.00007
	C	8.12370	4.25019	-2.31199		C	-3.29009	-0.07344	-0.00014
	C	7.63768	3.93087	-3.58215		C	-3.20848	1.32852	-0.00005
	O	7.39114	2.64505	-3.92835		O	-1.99769	1.94994	-0.00012
	C	7.59089	1.56855	-3.08579		C	-0.78970	1.28423	-0.00045
	C	8.10286	1.87510	-1.74057		C	-0.84012	-0.18160	-0.00026
	C	8.34671	3.16436	-1.40259		C	-2.07365	-0.80737	-0.00020
	H	7.44712	7.02355	-4.93349		H	-6.49314	2.14799	0.00025
	H	8.74431	5.85370	-1.00725		H	-4.66206	-1.74251	-0.00011
	H	8.72433	3.36447	-0.40310		H	-2.08954	-1.89197	-0.00013
	C	8.38511	0.82997	-0.67739		C	0.34645	-1.04103	-0.00011
	O	8.81032	1.22965	0.40267		O	0.22497	-2.28565	-0.00041
	O	7.32258	0.48624	-3.54732		O	0.18672	2.00455	0.00028
	C	8.15188	-0.58865	-0.95530		C	1.68066	-0.44756	-0.00013
	H	7.77599	-0.85948	-1.93233		H	1.75997	0.63154	-0.00018
	C	8.40962	-1.50312	0.00338		C	2.79969	-1.26685	-0.00006
	H	8.78599	-1.12324	0.95316		H	2.61870	-2.33924	0.00003
	C	8.24361	-2.94301	-0.08168		C	4.13996	-0.81330	-0.00004
	C	8.56626	-3.73977	1.02650		C	5.21048	-1.75985	0.00017
	C	7.77033	-3.60462	-1.22724		C	4.50990	0.56941	-0.00024
	C	8.43035	-5.11596	1.00852		C	6.52192	-1.37735	0.00023
	C	7.62732	-4.97691	-1.26602		C	5.81873	0.96466	-0.00019
	C	7.95429	-5.77722	-0.14496		C	6.87820	0.00764	0.00006
	H	8.93581	-3.26217	1.93124		H	4.96438	-2.81808	0.00031
	H	7.50628	-3.03351	-2.11283		H	3.73739	1.33102	-0.00045
	H	8.69602	-5.67735	1.89611		H	7.29146	-2.13933	0.00041
	N	7.81344	-7.14096	-0.17999		N	8.17457	0.39620	0.00012
	C	7.32265	-7.79032	-1.37801		C	8.52135	1.80988	0.00002
	H	7.98033	-7.60702	-2.23794		H	8.12809	2.31231	0.89117
	H	7.28114	-8.86726	-1.21173		H	9.60552	1.91277	0.00020
	H	6.31186	-7.45029	-1.63938		H	8.12840	2.31211	-0.89139
	C	8.15584	-7.93390	0.98229		C	9.24310	-0.59229	0.00032
	H	7.54505	-7.66194	1.85339		H	9.19312	-1.22806	-0.89103
	H	7.97844	-8.98754	0.76433		H	10.20421	-0.08015	0.00026
	H	9.21337	-7.81899	1.25480		H	9.19307	-1.22778	0.89186
	H	7.25775	-5.43392	-2.17615		H	6.04118	2.02446	-0.00035
	Br	8.44475	8.38870	-2.51449		Br	-7.41486	-0.65906	0.00015

T4(ground state)					**T4**(excited state)				
	C	7.39040	4.92392	-4.53422		C	5.05869	-0.34934	0.00004
	C	7.63492	6.24628	-4.20070		C	6.17155	0.48118	0.00009
	C	8.12133	6.58190	-2.93260		C	6.00154	1.86948	0.00010
	C	8.36236	5.59145	-1.99945		C	4.73350	2.41922	0.00006
	C	8.11964	4.24777	-2.32229		C	3.59372	1.59168	0.00001
	C	7.63330	3.92053	-3.59240		C	3.77811	0.19804	0.00000
	O	7.38945	2.63822	-3.93459		O	2.71340	-0.64074	-0.00004
	C	7.59006	1.55967	-3.09087		C	1.39689	-0.22145	-0.00009
	C	8.10099	1.86891	-1.74759		C	1.16455	1.22568	-0.00007
	C	8.34218	3.15980	-1.41506		C	2.25599	2.07310	-0.00002
	H	7.44466	7.02138	-4.93556		H	7.16434	0.04499	0.00012
	H	8.73991	5.83588	-1.01092		H	4.59535	3.49651	0.00007
	H	8.71963	3.36331	-0.41611		H	2.06449	3.14090	-0.00001
	C	8.38451	0.82701	-0.68262		C	-0.16541	1.84207	-0.00010
	O	8.80951	1.22891	0.39687		O	-0.28336	3.08727	-0.00007
	O	7.32203	0.47896	-3.55386		O	0.58102	-1.11801	-0.00017
	C	8.15150	-0.59196	-0.95890		C	-1.35872	1.00237	-0.00010
	H	7.77557	-0.86347	-1.93575		H	-1.22708	-0.07152	-0.00014
	C	8.40923	-1.50583	0.00025		C	-2.61735	1.58568	-0.00004
	H	8.78565	-1.12509	0.94972		H	-2.65261	2.67267	0.00001
	C	8.24336	-2.94582	-0.08337		C	-3.84082	0.87490	-0.00003
	C	8.56617	-3.74089	1.02595		C	-5.07864	1.58893	0.00008
	C	7.77023	-3.60911	-1.22812		C	-3.92792	-0.55408	-0.00011
	C	8.43060	-5.11711	1.00999		C	-6.28753	0.95270	0.00010
	C	7.62756	-4.98147	-1.26486		C	-5.13182	-1.20221	-0.00008
	C	7.95469	-5.78003	-0.14259		C	-6.36070	-0.47556	0.00002
	H	8.93560	-3.26191	1.93001		H	-5.04853	2.67501	0.00014
	H	7.50612	-3.03920	-2.11447		H	-3.01901	-1.14639	-0.00020
	H	8.69625	-5.67758	1.89819		H	-7.19290	1.54685	0.00019
	N	7.81404	-7.14381	-0.17594		N	-7.55384	-1.11484	0.00005
	C	7.32335	-7.79459	-1.37317		C	-7.61159	-2.56904	0.00000
	H	7.98103	-7.61236	-2.23334		H	-7.12626	-2.98320	0.89121
	H	7.28185	-8.87136	-1.20567		H	-8.65347	-2.88617	0.00006
	H	6.31255	-7.45498	-1.63506		H	-7.12638	-2.98313	-0.89130
	C	8.15649	-7.93519	0.98723		C	-8.79804	-0.35964	0.00015
	H	7.54563	-7.66227	1.85800		H	-8.87601	0.27333	-0.89122
	H	7.97930	-8.98916	0.77061		H	-9.63767	-1.05325	0.00013
	H	9.21402	-7.81978	1.25966		H	-8.87595	0.27321	0.89161
	H	7.25816	-5.44047	-2.17410		H	-5.13921	-2.28516	-0.00015
	Br	6.73554	4.47460	-6.24216		Br	5.28021	-2.22554	0.00003
	H	8.30661	7.62280	-2.69015		H	6.87570	2.51272	0.00014

T5(ground state)					**T5**(excited state)				
	C	7.39051	4.92552	-4.53397		C	3.85772	1.22300	-0.00001
	C	7.63367	6.24793	-4.20343		C	5.06181	0.52967	0.00016
	C	8.11949	6.56861	-2.93281		C	5.03249	-0.86560	0.00010
	C	8.36370	5.58699	-1.99369		C	3.84497	-1.56824	-0.00012
	C	8.11891	4.24685	-2.32408		C	2.62137	-0.87064	-0.00032
	C	7.63308	3.92016	-3.59314		C	2.64769	0.53593	-0.00027
	O	7.38919	2.64017	-3.93677		O	1.49640	1.24966	-0.00046
	C	7.59010	1.56019	-3.09243		C	0.23406	0.68291	-0.00093
	C	8.10126	1.87003	-1.74838		C	0.16845	-0.77882	-0.00059
	C	8.34258	3.15914	-1.41428		C	1.35013	-1.50249	-0.00041
	H	7.44643	7.02945	-4.93106		H	6.00235	1.06689	0.00035
	H	8.74086	5.83843	-1.00789		H	3.84031	-2.65295	-0.00012
	H	8.71992	3.36281	-0.41541		H	1.28203	-2.58464	-0.00023
	C	8.38524	0.82648	-0.68185		C	-1.08111	-1.53755	-0.00030
	O	8.80999	1.23182	0.39602		O	-1.06660	-2.78620	-0.00046
	O	7.32237	0.48061	-3.55523		O	-0.67655	1.48317	-0.00016
	C	8.15250	-0.59097	-0.95779		C	-2.36546	-0.83447	-0.00021
	H	7.77658	-0.86388	-1.93420		H	-2.35448	0.24736	-0.00022
	C	8.41050	-1.50472	0.00230		C	-3.54689	-1.55599	-0.00012
	H	8.78689	-1.12362	0.95162		H	-3.45779	-2.64000	-0.00011
	C	8.24448	-2.94388	-0.08158		C	-4.84430	-0.98982	-0.00002
	C	8.56704	-3.73967	1.02756		C	-5.98998	-1.84271	0.00008
	C	7.77116	-3.60635	-1.22697		C	-5.09430	0.41877	-0.00002
	C	8.43100	-5.11559	1.01071		C	-7.26424	-1.35076	0.00018
	C	7.62802	-4.97839	-1.26462		C	-6.36400	0.92412	0.00007
	C	7.95488	-5.77776	-0.14251		C	-7.50119	0.05967	0.00018
	H	8.93653	-3.26132	1.93190		H	-5.83420	-2.91790	0.00008
	H	7.50733	-3.03576	-2.11298		H	-4.26000	1.11210	-0.00009
	H	8.69644	-5.67644	1.89869		H	-8.09535	-2.04483	0.00026
	N	7.81380	-7.14094	-0.17671		N	-8.75793	0.55684	0.00028
	C	7.32288	-7.79084	-1.37459		C	-8.98345	1.99567	0.00026
	H	7.98085	-7.60810	-2.23435		H	-8.54949	2.46203	-0.89128
	H	7.28097	-8.86764	-1.20777		H	-10.05492	2.18989	0.00034
	H	6.31230	-7.45047	-1.63606		H	-8.54934	2.46208	0.89170
	C	8.15586	-7.93361	0.98604		C	-9.90794	-0.33677	0.00040
	H	7.54495	-7.66089	1.85676		H	-9.91200	-0.97362	0.89205
	H	7.97821	-8.98725	0.76840		H	-10.82133	0.25611	0.00050
	H	9.21338	-7.81861	1.25843		H	-9.91219	-0.97363	-0.89125
	H	7.25856	-5.43678	-2.17409		H	-6.49635	1.99881	0.00007
	Br	6.73689	4.48254	-6.24039		Br	3.87033	3.10927	0.00007
	Br	8.44294	8.38223	-2.50742		Br	6.67817	-1.80910	0.00038

T6a(ground state)					**T6a**(excited state)				
	H	6.33071	4.63974	-5.20283		H	-6.80201	-2.67605	0.00056
	C	6.94559	4.91624	-4.35322		C	-6.74856	-1.59241	0.00042
	C	7.32038	6.22902	-4.11440		C	-7.88999	-0.80223	0.00050
	C	8.11605	6.56453	-3.00957		C	-7.78919	0.59623	0.00031
	C	8.53745	5.57649	-2.14015		C	-6.54675	1.20176	0.00005
	C	8.17084	4.23786	-2.36051		C	-5.37127	0.42464	-0.00004
	C	7.37697	3.92979	-3.46937		C	-5.50439	-0.97169	0.00014
	O	7.00036	2.65042	-3.71913		O	-4.40221	-1.77007	0.00005
	C	7.35337	1.57534	-2.93089		C	-3.10834	-1.29807	-0.00026
	C	8.18826	1.86920	-1.75677		C	-2.93290	0.16134	-0.00028
	C	8.56056	3.15109	-1.51412		C	-4.05211	0.96005	-0.00023
	H	6.99077	7.00747	-4.79579		H	-8.86737	-1.27505	0.00072
	H	8.39898	7.59811	-2.83963		H	-8.68920	1.20317	0.00038
	H	9.15435	5.81786	-1.27894		H	-6.45642	2.28459	-0.00010
	H	9.17784	3.34304	-0.64008		H	-3.89842	2.03488	-0.00032
	C	8.67428	0.82368	-0.77626		C	-1.62236	0.84013	-0.00039
	O	9.36593	1.20370	0.16280		O	-1.57329	2.09093	-0.00030
	O	6.93488	0.50060	-3.29169		O	-2.25061	-2.15537	-0.00047
	C	8.31776	-0.58971	-0.96319		C	-0.40148	0.05731	-0.00031
	H	7.70425	-0.84288	-1.81672		H	-0.48992	-1.02066	-0.00033
	C	8.76296	-1.50108	-0.07655		C	0.83242	0.70637	-0.00022
	H	9.37271	-1.12634	0.74168		H	0.80316	1.79096	-0.00020
	C	8.51230	-2.93452	-0.10065		C	2.08252	0.05296	-0.00014
	C	9.02053	-3.81185	0.87175		C	3.33653	0.75885	0.00002
	C	7.73831	-3.54090	-1.10741		C	2.20088	-1.37848	-0.00021
	C	8.78748	-5.17555	0.85690		C	4.54865	0.12287	0.00011
	C	7.48634	-4.89483	-1.15286		C	3.40137	-2.02766	-0.00013
	C	8.00827	-5.75901	-0.16324		C	4.62772	-1.29912	0.00004
	H	9.21595	-5.78120	1.64402		H	5.44828	0.72382	0.00024
	N	7.77028	-7.10652	-0.18941		N	5.82699	-1.93104	0.00012
	C	6.96559	-7.67871	-1.25012		C	5.89122	-3.38408	0.00009
	H	7.41372	-7.50546	-2.23714		H	5.40834	-3.80169	-0.89125
	H	6.88927	-8.75609	-1.10097		H	6.93478	-3.69600	0.00018
	H	5.94852	-7.26569	-1.25493		H	5.40817	-3.80174	0.89132
	C	8.32216	-7.96063	0.84252		C	7.06415	-1.16670	0.00030
	H	7.95393	-7.68180	1.83853		H	7.13741	-0.53245	0.89175
	H	8.02565	-8.99235	0.65185		H	7.90957	-1.85335	0.00031
	H	9.41927	-7.92146	0.85646		H	7.13757	-0.53229	-0.89102
	H	6.88050	-5.28448	-1.96164		H	3.40743	-3.11053	-0.00019
	H	7.31583	-2.91807	-1.88975		H	1.29471	-1.97354	-0.00035
	Br	10.08968	-3.16413	2.30880		Br	3.34929	2.64734	0.00013

T7(ground state)					**T7**(excited state)				
	H	6.77908	4.69864	-5.38482		H	6.53727	-2.79360	0.38276
	C	7.25267	4.96232	-4.44541		C	6.66494	-1.72545	0.24319
	C	7.55655	6.27444	-4.11907		C	7.92075	-1.14069	0.16057
	C	8.16926	6.59343	-2.89862		C	8.05268	0.24180	-0.02007
	C	8.47811	5.58934	-2.00099		C	6.92647	1.03898	-0.11760
	C	8.18005	4.25064	-2.30842		C	5.64206	0.47138	-0.03678
	C	7.56937	3.95934	-3.53228		C	5.54230	-0.91237	0.14333
	O	7.26482	2.68110	-3.86999		O	4.32098	-1.51795	0.22761
	C	7.51959	1.59060	-3.06649		C	3.12760	-0.85948	0.14667
	C	8.15651	1.86714	-1.77033		C	3.19628	0.60485	-0.03534
	C	8.46130	3.14788	-1.44071		C	4.42866	1.22088	-0.12603
	H	7.31488	7.06571	-4.82219		H	8.80603	-1.76420	0.23698
	H	8.39911	7.62698	-2.66178		H	9.03997	0.68793	-0.08357
	H	8.95256	5.81783	-1.05065		H	7.01816	2.11259	-0.25763
	H	8.93529	3.32552	-0.47848		H	4.49613	2.29487	-0.26596
	C	8.50514	0.80306	-0.75635		C	1.99718	1.38944	-0.12130
	O	9.07300	1.15503	0.27136		O	2.18080	2.67109	-0.29284
	O	7.19325	0.51754	-3.51535		O	2.13004	-1.53570	0.23128
	C	8.15717	-0.60744	-1.00671		C	0.64745	0.92763	-0.05658
	H	7.66297	-0.84687	-1.93874		H	0.53799	-0.14575	0.02056
	C	8.46208	-1.53527	-0.08339		C	-0.41459	1.77965	-0.08637
	H	8.96644	-1.19232	0.81927		H	-0.23490	2.85196	-0.12426
	C	8.19250	-2.96964	-0.15660		C	-1.81505	1.38603	-0.04553
	C	8.61105	-3.80007	0.88674		C	-2.80475	2.36700	0.09092
	C	7.51243	-3.56206	-1.23015		C	-2.23621	0.05086	-0.15203
	C	8.38790	-5.16870	0.85035		C	-4.14809	2.03088	0.15800
	C	7.27355	-4.92339	-1.25057		C	-3.57912	-0.27390	-0.10644
	C	7.72232	-5.77766	-0.22177		C	-4.58148	0.70079	0.07408
	H	9.13590	-3.36874	1.73525		H	-2.51436	3.41180	0.16597
	H	7.13876	-2.95578	-2.04838		H	-1.51573	-0.74530	-0.30603
	N	7.47063	-7.15990	-0.26288		N	-5.94190	0.34645	0.12167
	C	8.22548	-7.90786	-1.26431		C	-6.36337	-0.35730	1.32949
	H	8.21677	-7.38855	-2.22275		H	-5.65587	-1.14760	1.58166
	H	9.27247	-8.05899	-0.95314		H	-6.45097	0.32758	2.18938
	H	7.75854	-8.88748	-1.40586		H	-7.33889	-0.82043	1.15144
	C	7.44155	-7.85233	1.01180		C	-6.89235	1.37475	-0.25756
	H	6.83203	-7.29453	1.72719		H	-6.57438	1.85377	-1.18708
	H	6.98092	-8.83342	0.86041		H	-7.86327	0.90033	-0.43080
	H	8.44262	-8.01620	1.44745		H	-7.03280	2.15199	0.51396
	Br	6.24269	-5.61016	-2.68813		Br	-4.04868	-2.09302	-0.37617
	H	8.75011	-5.78165	1.66840		H	-4.87988	2.82036	0.29068

T8(ground state)					**T8**(excited state)				
	H	-6.06621	-2.67336	0.07929		H	-6.91037	-1.79145	1.90713
	C	-6.07494	-1.58977	0.03385		C	-6.87991	-0.98344	1.18390
	C	-7.25587	-0.86695	-0.02683		C	-8.03554	-0.37385	0.71552
	C	-7.24458	0.53408	-0.08472		C	-7.96265	0.66739	-0.21800
	C	-6.04078	1.21257	-0.08224		C	-6.73268	1.09773	-0.68235
	C	-4.82945	0.50253	-0.02144		C	-5.54622	0.49676	-0.22419
	C	-4.86805	-0.89428	0.03638		C	-5.65105	-0.54093	0.70917
	O	-3.72316	-1.61948	0.09745		O	-4.53364	-1.16155	1.19090
	C	-2.46017	-1.06511	0.10907		C	-3.25705	-0.84225	0.82127
	C	-2.38931	0.40190	0.03937		C	-3.11076	0.25285	-0.15789
	C	-3.53862	1.12094	-0.01665		C	-4.23793	0.87849	-0.65300
	H	-8.20319	-1.39751	-0.02921		H	-9.00163	-0.71009	1.07874
	H	-8.17987	1.08200	-0.13151		H	-8.87254	1.13715	-0.57767
	H	-6.01270	2.29780	-0.12688		H	-6.66575	1.90464	-1.40699
	H	-3.45923	2.20442	-0.05964		H	-4.14174	1.67924	-1.37909
	C	-1.09702	1.18198	0.03217		C	-1.81184	0.66444	-0.60344
	O	-1.16443	2.40478	0.05357		O	-1.78255	1.61192	-1.49527
	O	-1.54147	-1.84532	0.17984		O	-2.36969	-1.48491	1.32988
	C	0.19987	0.47621	-0.01362		C	-0.54331	0.12493	-0.21218
	H	0.19359	-0.60104	-0.09352		H	-0.56867	-0.78300	0.37308
	C	1.32953	1.19495	0.06964		C	0.60849	0.74545	-0.58681
	H	1.22279	2.26825	0.21126		H	0.53435	1.70763	-1.08780
	C	2.70412	0.68536	0.04203		C	1.95872	0.28808	-0.29298
	C	3.68369	1.24923	0.87978		C	2.96684	1.21333	0.05351
	C	3.18577	-0.33721	-0.79501		C	2.40717	-1.04860	-0.34751
	C	5.00146	0.83862	0.92342		C	4.27025	0.87165	0.34817
	C	4.49919	-0.77232	-0.78910		C	3.70294	-1.43150	-0.05663
	C	5.44598	-0.20068	0.08289		C	4.67418	-0.47860	0.31098
	H	5.67490	1.32620	1.61510		H	4.96560	1.65588	0.61499
	N	6.74417	-0.63265	0.10825		N	5.95591	-0.84710	0.61091
	C	7.17184	-1.69024	-0.78530		C	6.34185	-2.24291	0.54679
	H	7.06206	-1.40340	-1.83976		H	6.23899	-2.64797	-0.46867
	H	8.22431	-1.90907	-0.60354		H	7.38604	-2.33985	0.84447
	H	6.60246	-2.61298	-0.61641		H	5.73908	-2.85659	1.22789
	C	7.70150	0.00896	0.98655		C	6.94043	0.16390	0.94207
	H	7.40948	-0.08785	2.04015		H	6.65130	0.72899	1.83733
	H	8.67486	-0.46671	0.86444		H	7.89609	-0.31954	1.14539
	H	7.81470	1.07644	0.75510		H	7.08790	0.87270	0.11665
	H	4.78249	-1.55548	-1.47882		H	3.95773	-2.47958	-0.13435
	Br	3.19887	2.64505	2.07759		Br	2.53740	3.06181	0.16746
	Br	2.06601	-1.17220	-2.08372		Br	1.25940	-2.45294	-0.91460