Theoretical Study on Photophysical Properties of Thiophene-Fused-Type BODIPY Series Molecules in Fluorescence Imaging and Photodynamic Therapy

Jianfang Cao, [*a] Xinyu Chen, [a] Xue Ma, [a] Tianci Zhang, [a] and Wen Sun [*b]

[a] School of Chemical Engineering, Ocean and Life Sciences, Dalian University of Technology, Panjin Campus, Panjin, 124221, China

[b] State Key Laboratory of Fine Chemicals, Dalian University of Technology, No. 2 Linggong Road, High-tech District, Dalian, 116024, China

*Corresponding author E-mail: sunwen@dlut.edu.cn, caojf@dlut.edu.cn

List of Figure and Table

Table S1. The main bond lengths, bond angles and dihedral angles of **thieno-fused BODIPYs** in S_0 state, S_1 state, T_1 state and T_2 state. The four carbon atoms we selected are labeled as C1, C2, C3, and C4, representing the Cartesian coordinates of all atoms as C1, C6, C23, and C27 of thieno-fused BODIPYs.

Compound		S_0 State	S_1 State	T_1 State	T_2 State
PY-BODIPY	Bond Length (Å) C2-C3	1.48796	1.48365	1.48733	1.48614
	Bond Angle (°) C2-C3-C4	120.67268	121.09377	121.22662	121.14302
	Dihedral Angle (°) C1-C2-C3-C4	98.36639	107.52498	104.05061	106.54507
PH-BODIPY	Bond Length (Å) C2-C3	1.48749	1.48227	1.48988	1.48803
	Bond Angle (°) C2-C3-C4	119.97279	120.34751	120.48396	120.24374
	Dihedral Angle (°) C1-C2-C3-C4	78.40109	75.77424	80.79959	75.20968
MeO-BODIPY	Bond Length (Å) C2-C3	1.48390	1.48413	1.48881	1.48673
	Bond Angle (°) C2-C3-C4	120.40799	120.80012	120.87838	120.80525
	Dihedral Angle (°) C1-C2-C3-C4	73.66560	74.65567	81.77093	75.10703
DMA-BODIPY	Bond Length (Å)C2-C3	1.47783	1.48261	1.48796	1.43154
	Bond Angle (°) C2-C3-C4	120.88755	121.21358	121.24578	121.53722
	Dihedral Angle (°) C1-C2-C3-C4	67.89207	73.82960	82.09652	46.96493

Table S2. The main bond lengths, bond angles and dihedral angles of **thieno-pyrrole-fused BODIPYs** in S_0 state, S_1 state, S_2 State, T_1 state and T_2 state.

Compound		S_0 State	S_1 State	S_2 State	T_1 State	T_2 State
SBDPiR690	Bond Length (Å) C2-C3	1.46763	1.45099	1.46578	1.45703	1.46713
	Bond Angle (°) S1-C2-C3	119.19373	119.85947	120.00602	119.97025	119.74379
	Dihedral Angle (°) S1-C2-C3-C4	26.24437	13.81367	-27.58247	16.63516	-29.34571
SBDPiR688	Bond Length (Å) C2-C3	1.46863	1.45234	1.46524	1.45821	1.46642
	Bond Angle (°) S1-C2-C3	119.19072	119.80616	120.17813	120.01495	119.80341
	Dihedral Angle (°) S1-C2-C3-C4	27.44457	14.19720	-22.08699	16.93403	-28.44904
SBDPiR698	Bond Length (Å) C2-C3	1.46695	1.45053	1.46615	1.45621	1.46697
	Bond Angle (°) S1-C2-C3	119.15894	119.88483	120.01912	119.98403	119.80674
	Dihedral Angle (°) S1-C2-C3-C4	27.62688	15.24278	-28.20102	17.04600	-30.74159
SBDPiR710	Bond Length (Å) C2-C3	1.46552	1.44747	1.46524	1.45433	1.46598
	Bond Angle (°) S1-C2-C3	119.22686	120.06730	119.98196	119.93473	119.71584
	Dihedral Angle (°) S1-C2-C3-C4	24.79347	5.37134	-26.43537	15.65810	-29.22379
SBDPiR731	Bond Length (Å) C2-C3	1.46338	1.44315	1.46480	1.44840	1.46791
	Bond Angle (°) S1-C2-C3	119.40899	120.20107	119.80743	120.10372	119.76413
	Dihedral Angle (°) S1-C2-C3-C4	19.88882	4.89380	26.06526	12.63735	27.80297

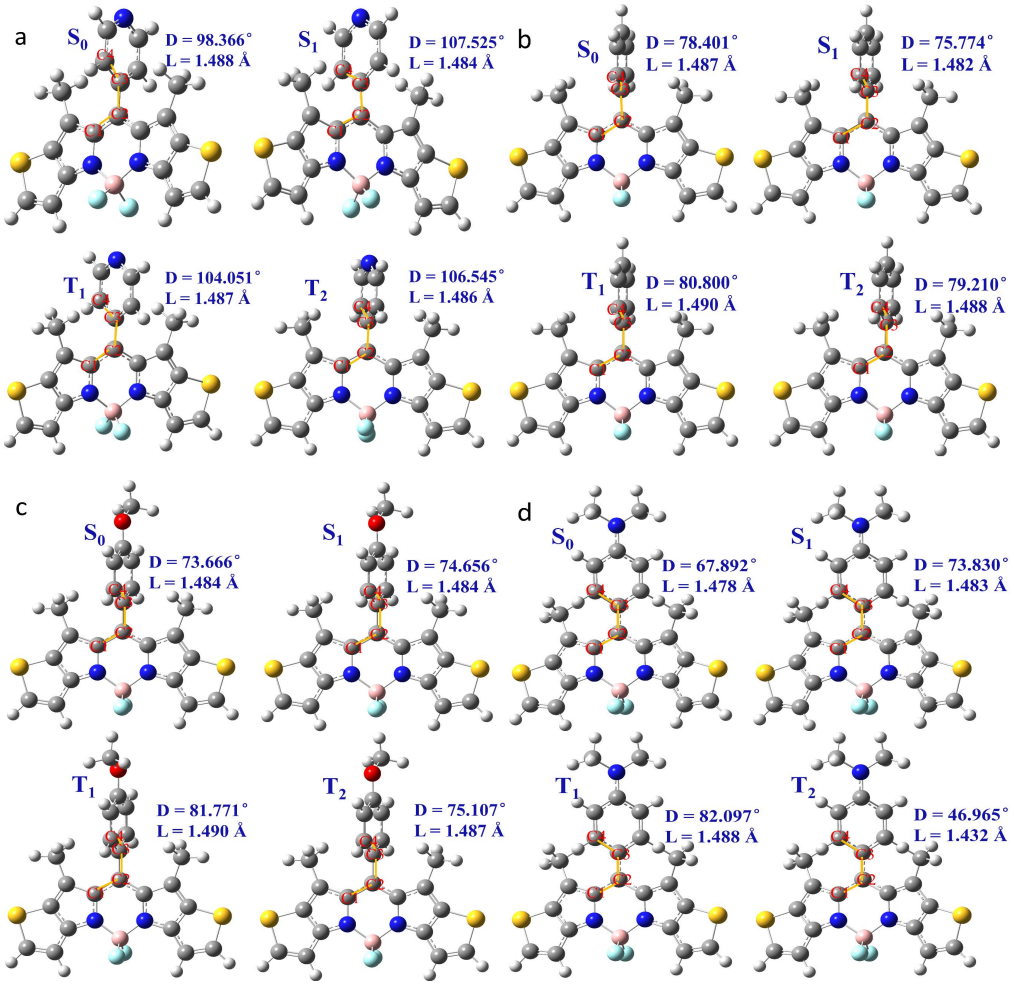


Figure S1. Optimized configuration of **PY-BODIPY** (a), **PH-BODIPY** (b), **MeO-BODIPY** (c), **and DMA-BODIPY** (d).

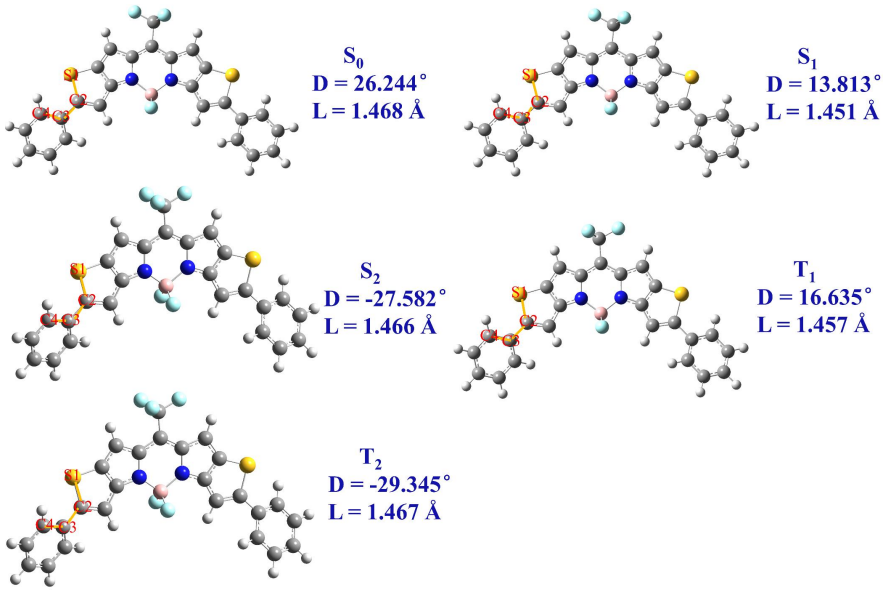


Figure S2. Optimized configuration of **SBDPiR690.**

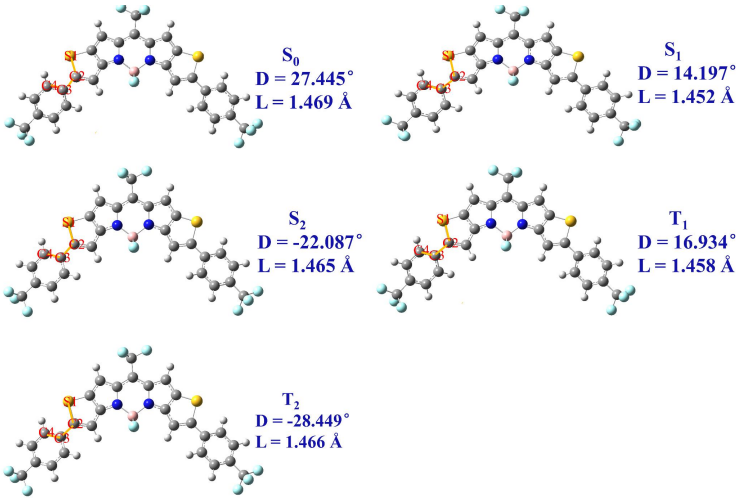


Figure S3. Optimized configuration of **SBDPiR688.**

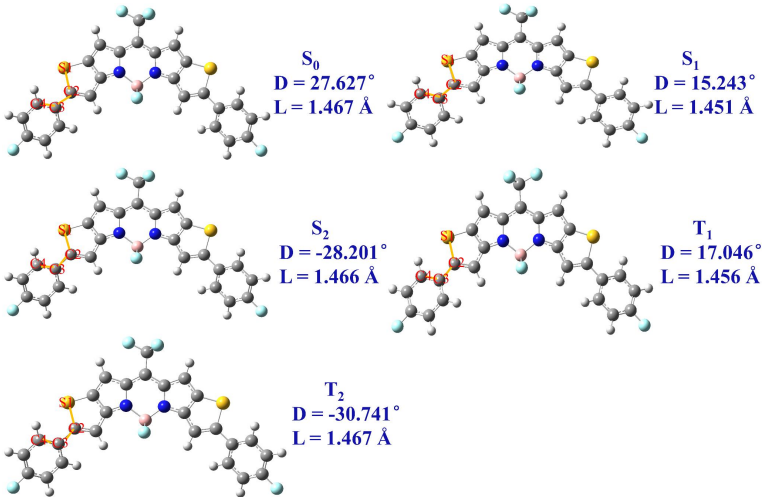


Figure S4. Optimized configuration of **SBDPiR698.**

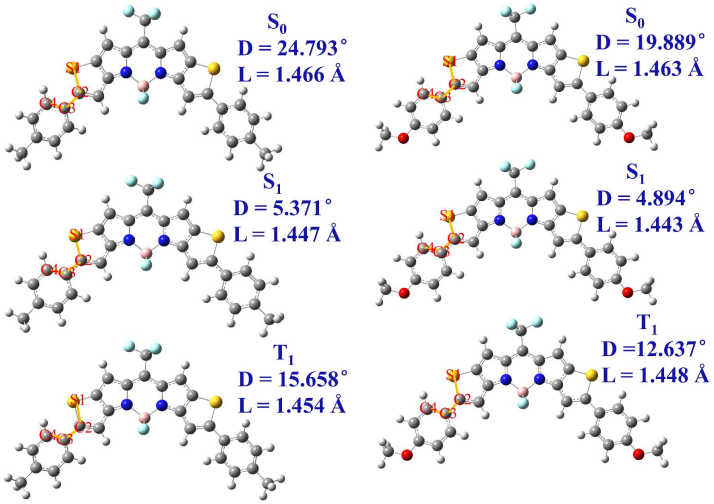


Figure S5. Optimized configuration of **SBDPiR710** (left) and **SBDPiR731** (right)**.**

Table S3. the energy separations for the absorption ΔE_{abs}(nm) and corresponding oscillator strengths of the low-lying electronically excited states for **thiophene-fused-type BODIPY**.

Compound	Transition	Energy (eV)	Maximum absorption wavelength (nm)	Oscillator strengths f	Composition	CI
PY-BODIPY	$S_0 \rightarrow S_1$	2.5302	490.01	1.1021	HOMO→LUMO	0.70142
	$S_0 \rightarrow S_2$	2.9696	417.51	0.0054	HOMO-1→LUMO	0.69699
	$S_0 \rightarrow S_3$	3.2014	387.28	0.0215	HOMO-2→LUMO	0.70050
	$S_0 \rightarrow S_4$	4.4999	275.53	0.4159	HOMO-3→LUMO	0.67401
	$S_0 \rightarrow S_5$	4.5141	274.66	0.0037	HOMO-4→LUMO	0.69597
	$S_0 \rightarrow S_6$	4.6636	265.86	0.0069	HOMO→LUMO+1	0.68067
PH-BODIPY	$S_0 \rightarrow S_1$	2.5473	486.73	1.0915	HOMO→LUMO	0.70069
	$S_0 \rightarrow S_2$	3.0005	413.21	0.0075	HOMO-1→LUMO	0.69645
	$S_0 \rightarrow S_3$	3.2350	383.25	0.0200	HOMO-2→LUMO	0.70038
	$S_0 \rightarrow S_4$	3.9059	317.43	0.0914	HOMO-3→LUMO	0.68348
	$S_0 \rightarrow S_5$	4.3155	287.30	0.0021	HOMO-4→LUMO	0.70040
	$S_0 \rightarrow S_6$	4.5691	271.35	0.3666	HOMO-5→LUMO	0.67798
MeO-BODIPY	$S_0 \rightarrow S_1$	2.5524	485.76	1.0770	HOMO→LUMO	0.70047
	$S_0 \rightarrow S_2$	3.0083	412.14	0.0080	HOMO-1→LUMO	0.69620
	$S_0 \rightarrow S_3$	3.2275	384.15	0.0003	HOMO-2→LUMO	0.67374
	$S_0 \rightarrow S_4$	3.3125	374.29	0.1449	HOMO-3→LUMO	0.67034
	$S_0 \rightarrow S_5$	4.3938	282.18	0.0052	HOMO-4→LUMO	0.69461
	$S_0 \rightarrow S_6$	4.5669	271.48	0.3856	HOMO-5→LUMO	0.68703
DMA-BODIPY	$S_0 \rightarrow S_1$	2.5695	482.53	1.0465	HOMO-1→LUMO	0.69625
	$S_0 \rightarrow S_2$	2.5850	479.64	0.2136	HOMO→LUMO	0.68792
	$S_0 \rightarrow S_3$	3.0356	408.43	0.0080	HOMO-2→LUMO	0.69604
	$S_0 \rightarrow S_4$	3.2712	379.02	0.0313	HOMO-3→LUMO	0.69975
	$S_0 \rightarrow S_5$	4.2677	290.52	0.0004	HOMO-4→LUMO	0.67501
	$S_0 \rightarrow S_6$	4.5458	272.74	0.4620	HOMO-5→LUMO	0.67888
SBDPiR690	$S_0 \rightarrow S_1$	2.0646	600.51	1.5864	HOMO→LUMO	0.70106
	$S_0 \rightarrow S_2$	2.7635	448.64	0.0153	HOMO-1→LUMO	0.68300
	$S_0 \rightarrow S_3$	2.9563	419.39	0.0004	HOMO-2→LUMO	0.63940
	$S_0 \rightarrow S_4$	3.6807	336.85	0.5620	HOMO-3→LUMO	0.64436
	$S_0 \rightarrow S_5$	4.2258	293.40	0.0345	HOMO-6→LUMO	0.64455
	$S_0 \rightarrow S_6$	4.2819	289.55	0.3069	HOMO→LUMO+1	0.68006
SBDPiR688	$S_0 \rightarrow S_1$	2.0966	591.37	1.5994	HOMO→LUMO	0.70087
	$S_0 \rightarrow S_2$	2.7364	453.10	0.0190	HOMO-1→LUMO	0.68713

	$S_0 \rightarrow S_3$	2.9360	422.28	0.0010	HOMO-2→LUMO	0.68098
	$S_0 \rightarrow S_4$	3.8198	324.58	0.6031	HOMO-3→LUMO	0.67999
	$S_0 \rightarrow S_5$	4.1972	295.40	0.3109	HOMO→LUMO+1	0.68136
	$S_0 \rightarrow S_6$	4.3682	283.84	0.0608	HOMO-6→LUMO	0.60512
SBDPiR698	$S_0 \rightarrow S_1$	2.0718	598.43	1.5774	HOMO→LUMO	0.70098
	$S_0 \rightarrow S_2$	2.7757	446.67	0.0161	HOMO-1→LUMO	0.68107
	$S_0 \rightarrow S_3$	2.9690	417.59	0.0005	HOMO-2→LUMO	0.61433
	$S_0 \rightarrow S_4$	3.6643	338.36	0.5479	HOMO-3→LUMO	0.62137
	$S_0 \rightarrow S_5$	4.1944	295.60	0.0362	HOMO-4→LUMO	0.673
	$S_0 \rightarrow S_6$	4.3185	287.10	0.2958	HOMO→LUMO+1	0.68148
	$S_0 \rightarrow S_1$	2.0265	611.81	1.6528	HOMO→LUMO	0.70041
	$S_0 \rightarrow S_2$	2.7772	446.44	0.0139	HOMO-2→LUMO	0.64682
SBDPiR710	$S_0 \rightarrow S_3$	2.9633	418.41	0.0031	HOMO-1→LUMO	0.50438
	$S_0 \rightarrow S_4$	3.5432	349.92	0.5927	HOMO-3→LUMO	0.51194
	$S_0 \rightarrow S_5$	4.0664	304.90	0.0384	HOMO-4→LUMO	0.67604
	$S_0 \rightarrow S_6$	4.2470	291.93	0.3390	HOMO→LUMO+1	0.67828
	$S_0 \rightarrow S_1$	1.9557	633.96	1.7424	HOMO→LUMO	0.69895
	$S_0 \rightarrow S_2$	2.8053	441.97	0.0137	HOMO-2→LUMO	0.68663
SBDPiR731	$S_0 \rightarrow S_3$	2.9710	417.31	0.0293	HOMO-3→LUMO	0.56519
	$S_0 \rightarrow S_4$	3.3254	372.84	0.5498	HOMO-1→LUMO	0.56659
	$S_0 \rightarrow S_5$	3.8295	323.76	0.0342	HOMO-4→LUMO	0.68065
	$S_0 \rightarrow S_6$	4.1562	298.31	0.3267	HOMO→LUMO+1	0.67749

Table S4. the energy separations for the emission ΔE_{em}(nm) and corresponding oscillator strengths of the low-lying electronically excited states for **thiophene-fused-type BODIPY**.

Compound	Transition	Energy (eV)	Maximum emission wavelength (nm)	Oscillator strengths f	Composition	CI
PY-BODIPY	$S_1 \rightarrow S_0$	2.1208	584.61	1.2599	LUMO→HOMO	0.70230
PH-BODIPY	$S_1 \rightarrow S_0$	2.1568	574.84	1.2755	LUMO→HOMO	0.70196
MeO-BODIPY	$S_1 \rightarrow S_0$	2.1655	572.53	1.2723	LUMO→HOMO	0.70189
DMA-BODIPY	$S_1 \rightarrow S_0$	2.1788	569.04	1.2640	LUMO→HOMO	0.70170
SBDPiR690	$S_1 \rightarrow S_0$	1.8773	660.43	1.6416	LUMO→HOMO	0.70337
SBDPiR688	$S_1 \rightarrow S_0$	1.9034	651.38	1.6658	LUMO→HOMO	0.70344
SBDPiR698	$S_1 \rightarrow S_0$	1.8836	658.22	1.6341	LUMO→HOMO	0.70337
SBDPiR710	$S_1 \rightarrow S_0$	1.8251	679.33	1.7179	LUMO→HOMO	0.70269
SBDPiR731	$S_1 \rightarrow S_0$	1.7684	701.12	1.8058	LUMO→HOMO	0.70158

Table S5. the energy of HOMO and HOMO-1 orbitals, and the energy difference between HOMO orbital and HOMO-1 orbital for **thiophene-fused-type BODIPY**. The unit of orbital energy is eV.

	PH-BODIPY	PY-BODIPY	MeO-BODIPY	DMA-BODIPY	SBDPi R690	SBDPi R688	SBDPi R698	SBDPi R710	SBDPi R731
E_{HOMO}	-6.783	-6.737	-6.729	-6.673	-6.640	-6.830	-6.667	-6.330	-6.363
E_{HOMO-1}	-7.568	-7.521	-7.508	-6.702	-7.810	-7.919	-7.844	-7.765	-7.456
ΔE	0.785	0.784	0.779	0.029	1.170	1.089	1.197	1.234	1.222

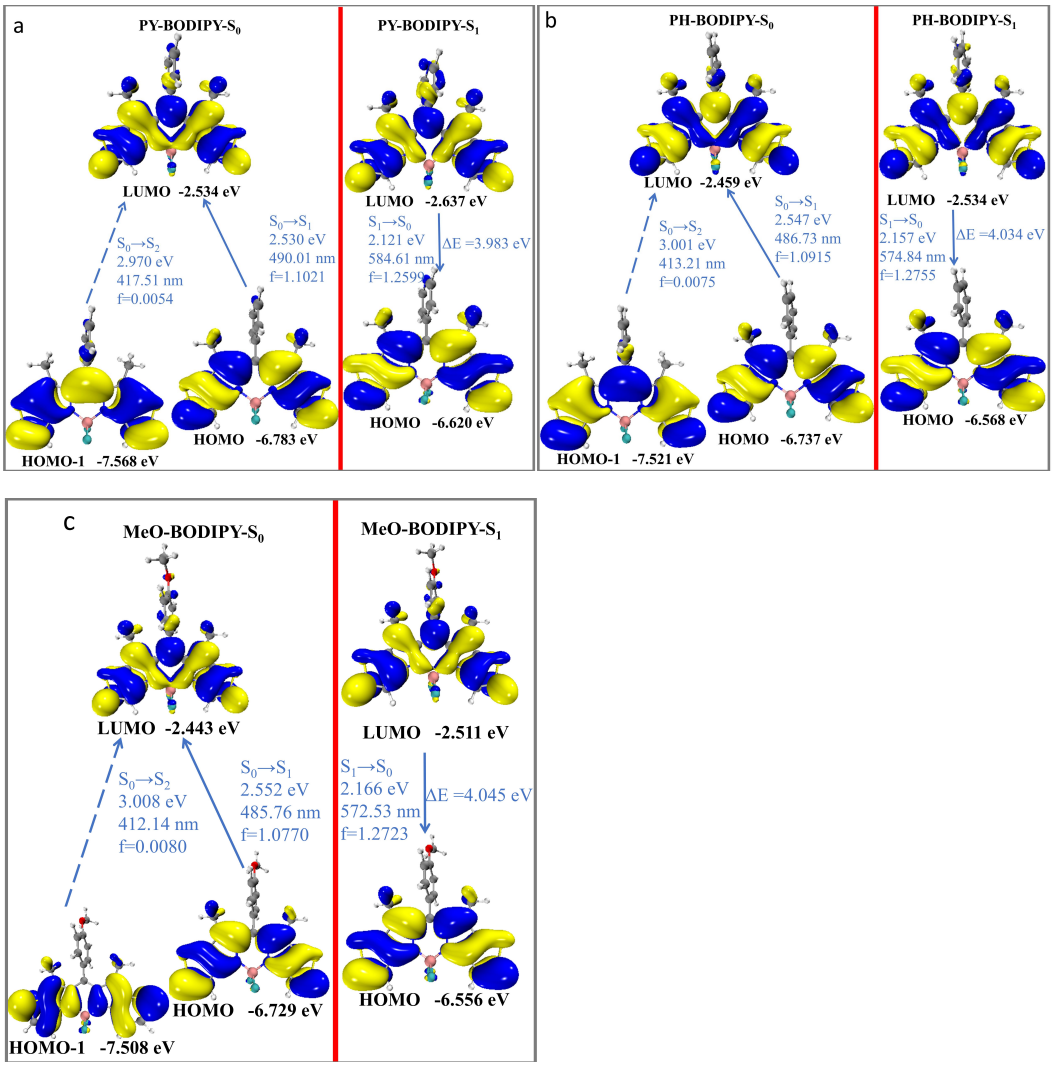


Figure S6. Frontier molecular orbitals of S_0 and S_1 states geometries for the **PY-BODIPY** (a), **PH-BODIPY** (b) and **MeO-BODIPY** (c).

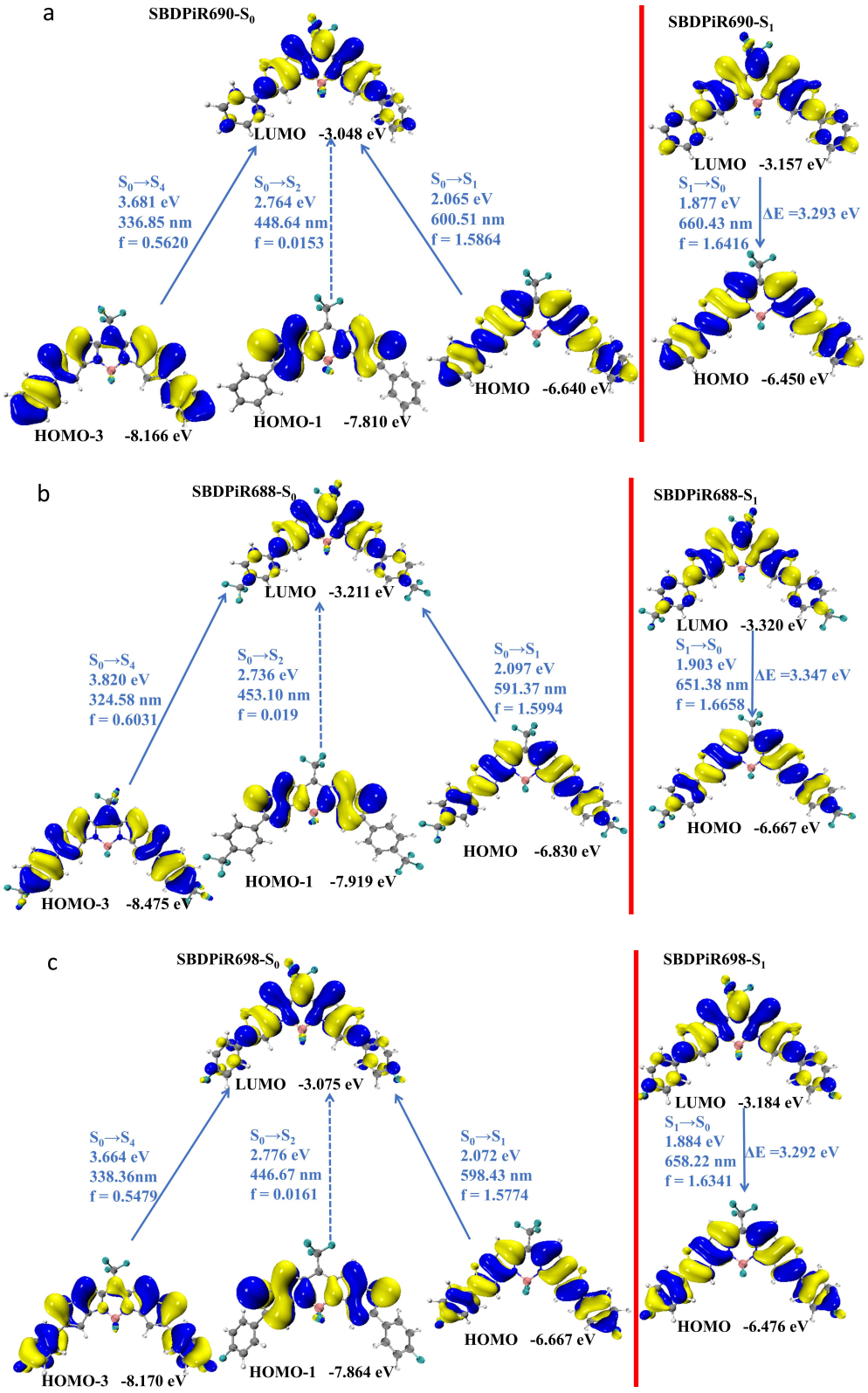


Figure S7. Frontier molecular orbitals of S_0 and S_1 states geometries for the **SBDPiR690** (a), **SBDPiR688** (b), and **SBDPiR698** (c).

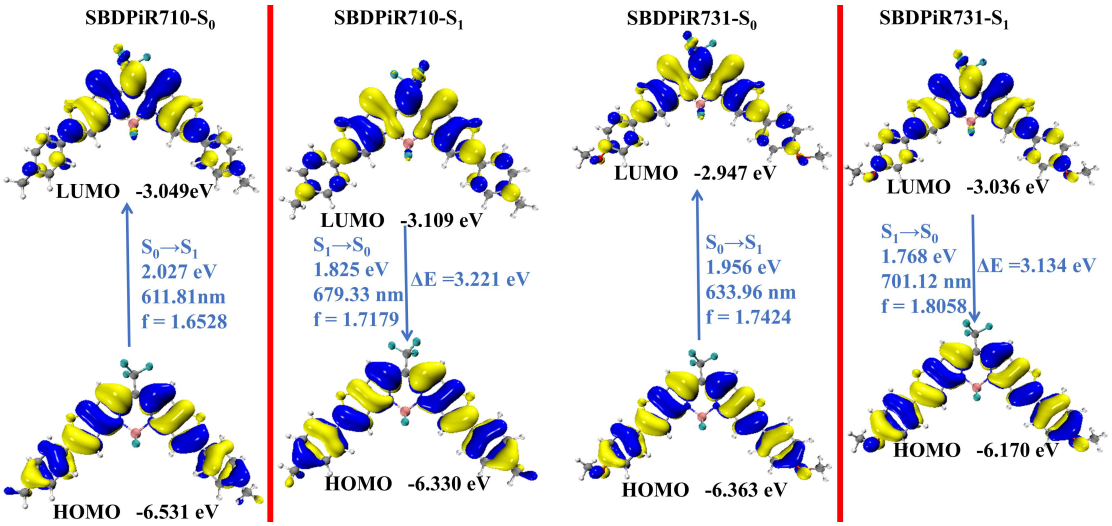


Figure S8. Frontier molecular orbitals of S_0 and S_1 states geometries for the **SBDPiR710** (left)**, SBDPiR731** (right).

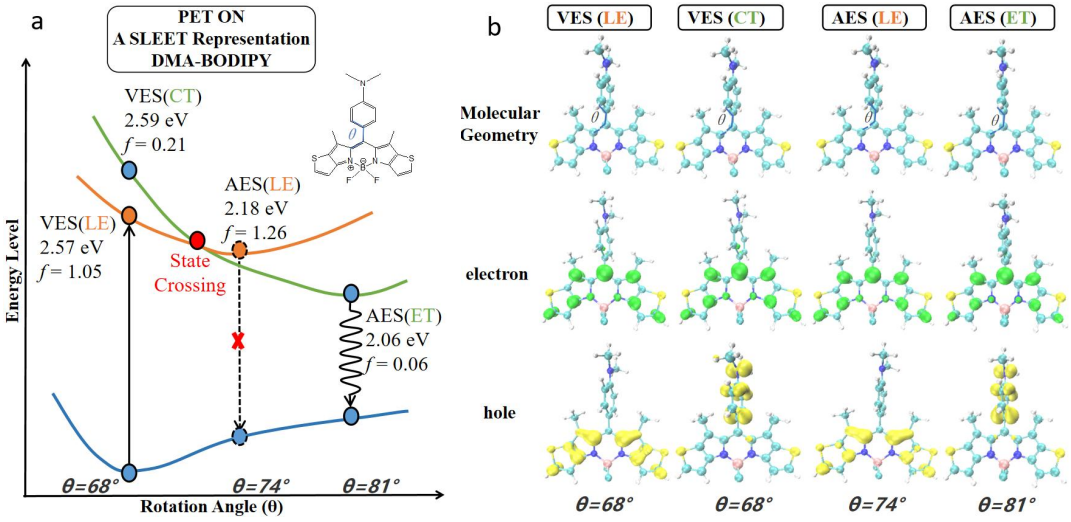


Figure S9.a. Schematic illustration of the state-crossing from a locally excited to an electron-transfer state (SLEET) model and calculated excitation/de-excitation energy (as well as oscillator strength f) of **DMA-BODIPY** in dichloromethane; the inset shows the molecular structure of **DMA-BODIPY**; note that θ values are not drawn to scale for clarification.

Figure S9.b. Optimized molecular structures of **DMA-BODIPY** in the ground and excited states, as well as the corresponding electron and hole distributions in dichloromethane. VES and AES denoted vertically excited state and adiabatic excited state, respectively.

Table S6. Contribution of different fragments of **PY-BODIPY** to important frontier molecular orbitals in S_0, S_1, and T_2 states.

Compound	MO	E (au)	Main Contribution %		
			thiophene-fused BODIPY	Meso substitution	Atom S
	HOMO-3	-0.3248	94.928	5.090	4.422
	HOMO-2	-0.2832	99.619	0.379	35.764
	HOMO-1	-0.2781	99.665	0.337	33.686
S_0 State	HOMO	-0.2493	99.295	0.709	4.000
PY-BODIPY	LUMO	-0.0931	95.008	4.993	3.229
	LUMO+1	-0.0135	15.847	84.146	0.321
	LUMO+2	-0.0010	39.263	60.389	4.159
	LUMO+3	0.0034	71.313	23.749	9.858
	HOMO-3	-0.3224	90.641	9.374	5.296
	HOMO-2	-0.2841	99.056	0.941	33.078
	HOMO-1	-0.2827	99.607	0.394	31.830
S_1 State	HOMO	-0.2433	99.292	0.712	5.283
PY-BODIPY	LUMO	-0.0969	93.527	6.476	3.719
	LUMO+1	-0.0130	17.599	82.434	0.620
	LUMO+2	-0.0021	47.563	51.792	5.297
	LUMO+3	0.0038	74.888	20.770	10.638
	HOMO-3	-0.3229	92.173	7.838	4.412
	HOMO-2	-0.2811	99.742	0.256	34.238
	HOMO-1	-0.2715	99.838	0.160	31.462
T_2 State	HOMO	-0.2558	99.245	0.757	3.854
PY-BODIPY	LUMO	-0.0991	93.384	6.614	2.738
	LUMO+1	-0.0136	16.627	83.411	0.456
	LUMO+2	-0.0015	37.776	61.369	3.826
	LUMO+3	0.0041	69.743	25.946	10.008

Table S7. Contribution of different fragments of **PH-BODIPY** to important frontier molecular orbitals in S_0, S_1, and T_2 states.

Compound	MO	E (au)	Main Contribution %		
			thiophene-fused BODIPY	Meso substitution	Atom S
S_0 State PH-BODIPY	HOMO-3	-0.3102	23.901	74.305	0.942
	HOMO-2	-0.2815	99.536	0.460	35.357
	HOMO-1	-0.2764	99.567	0.434	33.338
	HOMO	-0.2476	99.232	0.771	3.957
	LUMO	-0.0904	94.688	5.271	3.222
	LUMO+1	0.0027	58.564	38.157	7.228
	LUMO+2	0.0052	69.569	26.777	9.622
	LUMO+3	0.00532	24.297	48.469	2.337
S_1 State PH-BODIPY	HOMO-3	-0.3093	29.205	70.802	2.117
	HOMO-2	-0.2823	98.687	1.310	32.583
	HOMO-1	-0.2807	99.356	0.646	31.557
	HOMO	-0.2414	99.312	0.693	5.208
	LUMO	-0.0931	94.440	5.564	3.789
	LUMO+1	0.0015	62.850	35.935	7.788
	LUMO+2	0.0048	24.268	75.542	2.291
	LUMO+3	0.0048	75.851	20.214	10.547
T_2 State PH-BODIPY	HOMO-3	-0.3104	30.114	68.894	1.113
	HOMO-2	-0.2794	99.714	0.283	33.958
	HOMO-1	-0.2698	99.779	0.220	31.187
	HOMO	-0.2538	99.229	0.774	3.820
	LUMO	-0.0953	94.001	5.998	2.785
	LUMO+1	0.0023	56.700	40.797	6.928
	LUMO+2	0.0047	22.986	76.843	1.968
	LUMO+3	0.0057	68.870	28.421	9.700

Table S8. Contribution of different fragments of **MeO-BODIPY** to important frontier molecular orbitals in S_0, S_1, and T_2 states.

Compound	MO	E (au)	Main Contribution %		
			thiophene-fused BODIPY	Meso substitution	Atom S
S_0 State MeO-BODIPY	HOMO-3	-0.2824	48.553	49.057	16.245
	HOMO-2	-0.2801	62.367	35.949	19.395
	HOMO-1	-0.2759	99. 590	0.393	33.246
	HOMO	-0.2473	99.170	0.811	3.929
	LUMO	-0.0898	93.977	5.959	3.180
	LUMO+1	0.0020	52.706	43.630	6.143
	LUMO+2	0.0057	68.650	26.973	9.715
	LUMO+3	0.0124	64.929	32.469	9.715
S_1 State MeO-BODIPY	HOMO-3	-0.2841	57.743	42.249	19.240
	HOMO-2	-0.2803	95.869	4.117	30.236
	HOMO-1	-0.2798	56.051	43.942	15.453
	HOMO	-0.2409	99.291	0. 693	5.166
	LUMO	-0.0923	94.281	5.703	3.780
	LUMO+1	0.0011	57.260	41.574	6.857
	LUMO+2	0.0050	75.377	20.495	10.816
	LUMO+3	0.0116	59.347	39.486	11.890
T_2 State MeO-BODIPY	HOMO-3	-0.2831	11.107	88.889	0.476
	HOMO-2	-0.2789	99.231	0.758	33.627
	HOMO-1	-0.2694	99.790	0.208	31.132
	HOMO	-0.2533	99.246	0.746	3.804
	LUMO	-0.0945	93.946	6.045	2.788
	LUMO+1	0.0018	50.812	47.226	5.905
	LUMO+2	0.0056	67.579	29.037	9.681
	LUMO+3	0.0120	61.602	37.221	12.184

Table S9. Contribution of different fragments of **DMA-BODIPY** to important frontier molecular orbitals in S_0, S_1, and T_2 states.

Compound	MO	E (au)	Main Contribution %		
			thiophene-fused BODIPY	Meso substitution	Atom S
S_0 State DMA-BODIPY	HOMO-3	-0.2797	99.392	0.607	17.470
	HOMO-2	-0.2746	99.699	0.300	16.560
	HOMO-1	-0.2463	99.019	0.980	1.989
	HOMO	-0.2452	8.476	91.517	0.052
	LUMO	-0.0879	92.262	7.736	1.556
	LUMO+1	0.0035	63.526	32.449	4.106
	LUMO+2	0.0086	77.154	21.714	5.425
	LUMO+3	0.0148	75.128	22.466	7.970
S_1 State DMA-BODIPY	HOMO-3	-0.2810	98.779	0.902	32.722
	HOMO-2	-0.2791	99.327	0.237	31.366
	HOMO-1	-0.2471	7.081	70.031	0.125
	HOMO	-0.2399	99.302	0.554	5. 151
	LUMO	-0.0906	93.870	4.527	3.773
	LUMO+1	0.0032	67.150	19.927	8.564
	LUMO+2	0.0061	79.802	12.501	11.451
	LUMO+3	0.0139	68.815	23.657	16.561
T_2 State DMA-BODIPY	HOMO-3	-0.2769	97.652	2.341	33.197
	HOMO-2	-0.2730	99.850	0.139	30.705
	HOMO-1	-0.2467	98.887	1.091	4.905
	HOMO	-0.2413	24.161	75.829	0.833
	LUMO	-0.0891	79.450	20.531	2.483
	LUMO+1	0.0031	57.360	39.381	6.603
	LUMO+2	0.0126	94.276	5.324	13.615
	LUMO+3	0.0163	54.064	42.558	5.193

Table S10. Contribution of different fragments of **SBDPiR690** to important frontier molecular orbitals in S_0, S_1, and T_2 states.

Compound	MO	E (au)	Main Contribution %			
			thiophene-fused BODIPY	phenyl substitution	$-CF_3$ Group	Atom S
S_0 State SBDPiR690	HOMO-3	-0.3001	54.760	44.744	0.488	19.754
	HOMO-2	-0.2902	82.925	16.347	0.721	22.708
	HOMO-1	-0.2872	98.311	1.607	0.082	37.717
	HOMO	-0.2437	80.302	19.186	0.511	2.815
	LUMO	-0.1119	85.435	10.361	4.201	2.784
	LUMO+1	-0.0274	54.450	45.299	0.186	7.976
	LUMO+2	-0.0122	50.806	47.920	1.047	8.125
	LUMO+3	0.0029	66.162	23.564	5.161	15.160
S_1 State SBDPiR690	HOMO-3	-0.2987	69.609	30.124	0.268	29.973
	HOMO-2	-0.2894	87.294	12.215	0.490	28.159
	HOMO-1	-0.2891	80.316	18.717	0.964	20.618
	HOMO	-0.2372	77.940	21.565	0.496	2.796
	LUMO	-0.1161	82.387	13.354	4.257	3.148
	LUMO+1	-0.0343	55.514	44.234	0.205	7.944
	LUMO+2	-0.0167	53.870	44.561	1.392	7.663
	LUMO+3	0.0037	72.954	15.331	5.500	15.941
T_2 State SBDPiR690	HOMO-3	-0.2985	46.225	52.982	0.487	10.133
	HOMO-2	-0.2897	92.579	6.960	0.455	30.767
	HOMO-1	-0.2827	98.680	1.242	0.076	34.353
	HOMO	-0.2496	78.606	20.932	0.463	3.188
	LUMO	-0.1189	86.229	8.986	4.782	2.477
	LUMO+1	-0.0268	53.592	46.179	0.170	8.123
	LUMO+2	-0.0140	49.620	49.228	0.958	8.544
	LUMO+3	0.0028	64.882	24.898	5.088	14.551

Table S11. Contribution of different fragments of **SBDPiR688** to important frontier molecular orbitals in S_0, S_1, and T_2 states.

Compound	MO	E (au)	Main Contribution %			
			thiophene-fused BODIPY	phenyl substitution	$-CF_3$ Group	Atom S
	HOMO-3	-0.3115	51.195	47.924	0.874	10.394
	HOMO-2	-0.2957	93.985	5.517	0.494	32.079
	HOMO-1	-0.2914	98.684	1.243	0.073	37.644
S_0 State	HOMO	-0.2512	83.387	16.078	0.534	2.932
SBDPiR688	LUMO	-0.1175	84.677	11.192	4.126	2.850
	LUMO+1	-0.0398	45.488	54.314	0.154	6.545
	LUMO+2	-0.0252	41.079	57.794	1.020	5.689
	LUMO+3	-0.0038	23.704	74.165	0.964	7.685
	HOMO-3	-0.3085	58.669	40.573	0.758	17.490
	HOMO-2	-0.2962	88.443	10.542	1.009	24.235
	HOMO-1	-0.2941	97.603	2.322	0.076	37.153
S_1 State	HOMO	-0.2450	80.709	18.773	0.518	3.030
SBDPiR688	LUMO	-0.1224	81.446	14.415	4.136	3.284
	LUMO+1	-0.0464	48.641	51.141	0.182	6.728
	LUMO+2	-0.0288	46.472	52.024	1.408	5.605
	LUMO+3	-0.0019	21.442	76.343	0.961	6.204
	HOMO-3	-0.3100	49.642	49.270	1.080	5.850
	HOMO-2	-0.2945	96.955	2.714	0.326	34.858
	HOMO-1	-0.2870	98.852	1.072	0.074	34.292
T_2 State	HOMO	-0.2567	81.690	17.824	0.486	3.258
SBDPiR688	LUMO	-0.1244	85.360	9.954	4.681	2.526
	LUMO+1	-0.0405	44.756	55.057	0.141	6.648
	LUMO+2	-0.0281	40.618	58.316	0.966	6.133
	LUMO+3	-0.0039	20.394	77.796	0.790	6.472

Table S12. Contribution of different fragments of **SBDPiR698** to important frontier molecular orbitals in S_0, S_1, and T_2 states.

Compound	MO	E (au)	Main Contribution %			
			thiophene-fused BODIPY	phenyl substitution	$-CF_3$ Group	Atom S
	HOMO-3	-0.3002	58.141	41.480	0.371	23.137
	HOMO-2	-0.2912	77.821	21.392	0.779	19.307
	HOMO-1	-0.2887	98.439	1.474	0.088	37.545
S_0 State	HOMO	-0.2448	79.770	19.720	0.508	2.797
SBDPiR698	LUMO	-0.1128	85.770	10.007	4.218	2.781
	LUMO+1	-0.0268	56.310	43.429	0.191	8.349
	LUMO+2	-0.0117	52.412	46.286	1.029	8.748
	LUMO+3	-0.0018	26.389	70.983	1.232	8.240
	HOMO-3	-0.2994	74.863	24.964	0.173	33.260
	HOMO-2	-0.2907	96.680	3.243	0.077	37.040
	HOMO-1	-0.2898	65.157	33.410	1.426	8.518
S_1 State	HOMO	-0.2380	77.371	22.137	0.492	2.758
SBDPiR698	LUMO	-0.1168	82.718	12.997	4.283	3.131
	LUMO+1	-0.0338	56.882	42.856	0.208	8.229
	LUMO+2	-0.0165	54.955	43.472	1.362	8.074
	LUMO+3	-0.0001	24.576	72.707	1.204	7.061
	HOMO-3	-0.2985	46.430	52.885	0.680	11.936
	HOMO-2	-0.2911	90.345	9.145	0.504	28.852
	HOMO-1	-0.2842	98.788	1.134	0.077	34.203
T_2 State	HOMO	-0.2509	78.095	21.446	0.459	3.178
SBDPiR698	LUMO	-0.1200	86.558	8.635	4.803	2.474
	LUMO+1	-0.0260	55.533	44.227	0.174	8.518
	LUMO+2	-0.0134	51.269	47.557	0.938	9.162
	LUMO+3	-0.0020	23.548	74.146	1.042	7.228

Table S13. Contribution of different fragments of **SBDPiR710** to important frontier molecular orbitals in S_0, S_1, and T_2 states.

Compound	MO	E (au)	Main Contribution %			
			thiophene-fused BODIPY	phenyl substitution	$-CF_3$ Group	Atom S
	HOMO-3	-0.2945	75.659	24.199	0.136	34.677
	HOMO-2	-0.2861	89.957	9.841	0.200	32.272
	HOMO-1	-0.2854	63.777	35.387	0.824	12.909
S_0 State	HOMO	-0.2400	76.851	22.660	0.486	2.700
SBDPiR710	LUMO	-0.1103	85.146	10.655	4.194	2.752
	LUMO+1	-0.0252	55.146	44.594	0.190	8.096
	LUMO+2	-0.0102	51.270	47.423	1.036	8.335
	LUMO+3	0.0036	66.250	23.350	5.088	14.820
	HOMO-3	-0.2947	85.104	14.791	0.101	38.533
	HOMO-2	-0.2877	96.146	3.782	0.070	37.623
	HOMO-1	-0.2828	49.658	48.873	1.453	2.249
S_1 State	HOMO	-0.2326	74.233	25.293	0.469	2.588
SBDPiR710	LUMO	-0.1143	81.588	14.175	4.232	3.060
	LUMO+1	-0.0328	55.794	43.943	0.203	7.916
	LUMO+2	-0.0153	54.365	44.034	1.394	7.659
	LUMO+3	0.0046	75.226	12.314	5.652	16.022
	HOMO-3	-0.2928	67.290	32.447	0.259	27.719
	HOMO-2	-0.2867	64.978	34.185	0.829	13.339
	HOMO-1	-0.2815	98.299	1.616	0.084	33.999
T_2 State	HOMO	-0.2460	74.918	24.644	0.437	3.089
SBDPiR710	LUMO	-0.1173	86.113	9.096	4.788	2.458
	LUMO+1	-0.0240	54.320	45.444	0.173	8.290
	LUMO+2	-0.0115	49.937	48.897	0.934	8.812
	LUMO+3	0.0035	64.566	25.242	4.976	14.221

Table S14. Contribution of different fragments of **SBDPiR731** to important frontier molecular orbitals in S_0, S_1, and T_2 states.

Compound	MO	E (au)	Main Contribution %			
			thiophene-fused BODIPY	phenyl substitution	$-CF_3$ Group	Atom S
	HOMO-3	-0.2913	93.183	6.670	0.145	40.346
	HOMO-2	-0.2843	97.840	2.079	0.081	38.185
	HOMO-1	-0.2740	31.165	67.991	0.834	0.724
S_0 State	HOMO	-0.2338	69.996	29.563	0.438	2.477
SBDPiR731	LUMO	-0.1083	84.361	11.467	4.167	2.674
	LUMO+1	-0.0225	58.395	41.328	0.201	8.493
	LUMO+2	-0.0069	56.257	42.325	1.088	9.375
	LUMO+3	0.0041	66.196	23.229	5.194	15.256
	HOMO-3	-0.2920	93.513	6.262	0.221	39.439
	HOMO-2	-0.2856	93.593	6.300	0.105	37.306
	HOMO-1	-0.2716	34.830	63.960	1.195	0.638
S_1 State	HOMO	-0.2267	68.690	30.876	0.429	2.342
SBDPiR731	LUMO	-0.1116	81.092	14.658	4.247	2.917
	LUMO+1	-0.0284	58.203	41.521	0.213	8.308
	LUMO+2	-0.0111	57.857	40.485	1.398	8.629
	LUMO+3	0.0050	74.186	13.825	5.393	16.723
	HOMO-3	-0.2888	94.637	5.200	0.159	38.645
	HOMO-2	-0.2808	97.721	2.198	0.079	34.589
	HOMO-1	-0.2759	29.320	69.897	0.768	1.083
T_2 State	HOMO	-0.2411	67.892	31.714	0.390	2.895
SBDPiR731	LUMO	-0.1157	85.977	9.220	4.799	2.428
	LUMO+1	-0.0196	58.137	41.595	0.187	8.998
	LUMO+2	-0.0071	54.216	44.540	0.932	10.264
	LUMO+3	0.0035	59.519	31.393	4.447	13.874

Table S15. Electron excitation characteristics of **PY-BODIPY, PH-BODIPY, MeO-BODIPY** in different transition states.

[a] Sr: the geometric mean function of the overlap between electrons and hole distributions. [b] D_{HE}: the distance of centroid between the hole and the electron. [c] Δσ: the difference in the overall spatial distribution breadth of electrons and holes. [d] H_{CT}: mean ductility of holes and electrons in the CT direction. [e] H: the overall average distribution breadth of electrons and holes. [f] t: the separated degree of holes and electrons. The t >0 implies that the holes and electrons are sufficiently separated by CT, and the t <0 can be considered that the holes and electrons are not significantly separated in the CT direction. The small $D_{HE,}$ large S_r and negative t suggest that the electron excited character belongs to local exite (LE). The proportion of LE state (Figure S10，S11，S12) also illustrates this fact.

	PY-BODIPY			PH-BODIPY		
Transition Process	$S_0 \rightarrow S_1$	$S_1 \rightarrow T_1$	$S_1 \rightarrow T_2$	$S_0 \rightarrow S_1$	$S_1 \rightarrow T_1$	$S_1 \rightarrow T_2$
Sr[a]/a.u.	0.759	--	--	0.764	--	--
D_{HE}[b]/Å	0.399	0.665	0.163	0.389	0.686	0.171
Δσ[c]/Å	-0.011	--	--	0.009	--	--
H_{CT}[d]/Å	1.528	1.702	1.449	1.530	1.750	1.427
H[e]/Å	3.283	2.816	3.719	3.270	2.856	3.720
t[f] /Å	-1.129	-1.037	-1.286	-1.141	-1.063	-1.256
LE/%	97.426	97.146	97.183	97.198	97.695	96.458
CT/%	2.574	2.854	2.817	2.802	2.305	3.542
	MeO-BODIPY					
Transition Process	$S_0 \rightarrow S_1$	$S_1 \rightarrow T_1$	$S_1 \rightarrow T_2$			
Sr/a.u.	0.755	--	--			
D_{HE}/Å	0.434	0.782	0.185			
Δσ/Å	0.018	--	--			
H_{CT}/Å	1.591	1.883	1.633			
H/Å	3.280	2.935	3.725			
t/Å	-1.157	-1.100	-1.448			
LE/%	96.506	97.475	94.759			
CT/%	3.494	2.525	5.241			

Table S16. Electron excitation characteristics of **SBDPiR690** in different transition states.

SBDPiR690					
Transition Process	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_4$	$S_1 \rightarrow T_1$	$S_1 \rightarrow T_2$	$S_2 \rightarrow T_2$
Sr/a.u.	0.770	0.712	--	--	--
D_{HE}/Å	0.693	1.709	0.638	1.265	2.879
Δσ/Å	- 0.319	-1.697	--	--	--
H_{CT}/Å	2.312	2.200	2.576	3.567	3.109
H/Å	4.119	4.940	3.495	4.498	3.787
t/Å	-1.619	-0.490	-1.938	-2.302	-0.230
LE/%	77.977	51.904	82.030	80.805	94.342
CT/%	22.023	48.096	17.970	19.195	5.989

Table S17. Electron excitation characteristics of **SBDPiR688** in different transition states.

SBDPiR688					
Transition Process	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_4$	$S_1 \rightarrow T_1$	$S_1 \rightarrow T_2$	$S_2 \rightarrow T_2$
Sr/a.u.	0.764	0.738	--	--	--
D_{HE}/Å	0.563	1.437	0.801	1.127	2.816
Δσ/Å	-0.139	-1.410	--	--	--
H_{CT}/Å	2.468	2.185	2.229	3.659	3.161
H/Å	4.104	4.845	3.325	4.436	3.847
t/Å	-1.906	-0.748	-1.428	-2.532	-0.345
LE/%	78.509	42.951	88.539	88.032	93.856
CT/%	21.491	57.049	11.429	11.968	6.732

Table S18. Electron excitation characteristics of **SBDPiR698** in different transition states.

SBDPiR698					
Transition Process	$S_0 \rightarrow S_1$	$S_0 \rightarrow S_4$	$S_1 \rightarrow T_1$	$S_1 \rightarrow T_2$	$S_2 \rightarrow T_2$
Sr/a.u.	0.764	0.694	--	--	--
D_{HE}/Å	0.711	1.815	0.681	1.246	0.307
Δσ/Å	-0.365	-1.833	--	--	--
H_{CT}/Å	2.273	2.190	2.483	3.578	3.115
H/Å	4.105	4.957	3.449	4.480	3.796
t/Å	-1.562	-0.375	-1.802	-2.332	-0.246
LE/%	77.722	50.990	82.214	79.205	94.355
CT/%	22.278	49.010	17.786	20.795	5.951

Table S19. Electron excitation characteristics of **SBDPiR710, SBDPiR731 and DMA-BODIPY** in different transition states. It is important to note that the $S_0 \rightarrow S_2$ processes of DMA-BODIPY are attributed to CT excitation.

	Sr/a.u.	D_{HE}/Å	Δσ/Å	H_{CT}/Å	H/Å	t/Å	LE	CT
SBDPiR710 $S_0 \rightarrow S_1$	0.760	0.803	-0.477	2.296	4.252	-1.493	74.192	25.808
SBDPiR731 $S_0 \rightarrow S_1$	0.759	1.006	-0.702	2.388	4.444	-1.382	70.182	29.818
DMA-BODIPY $S_0 \rightarrow S_1$	0.752	0.536	0.062	1.635	3.301	-1.099	94.415	5.585
DMA-BODIPY $S_0 \rightarrow S_2$	0.400	4.108	0.594	2.063	2.962	2.064	14.89	85.12

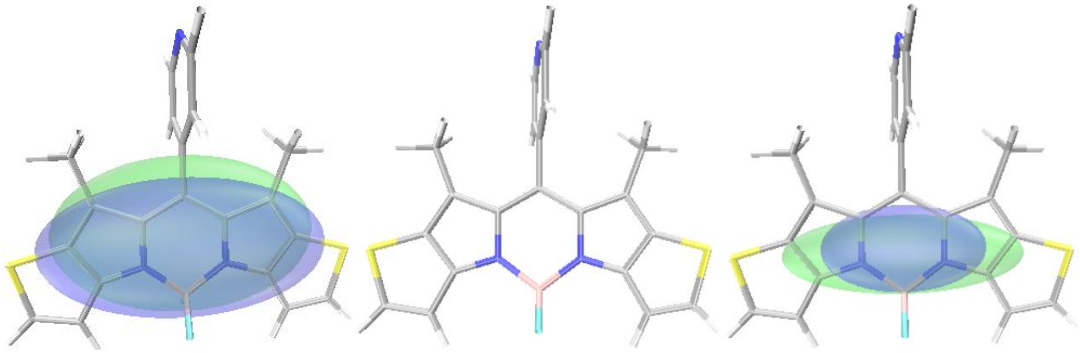


Figure S10. cele&chole graph in $S_0 \rightarrow S_1$ transition and difference map for electron density in $S_1 \rightarrow T_1$, $S_1 \rightarrow T_2$ transition of **PY-BODIPY.** The figure S10-S12, S14-S17 can visually represent the electron excitation characteristics of LE.

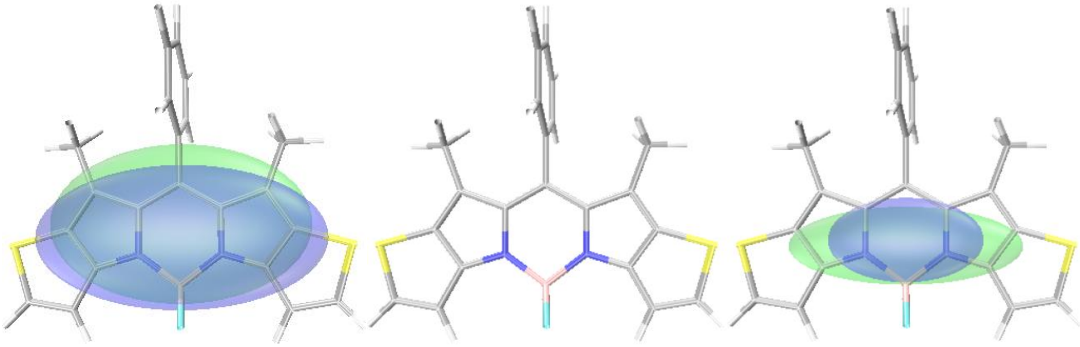


Figure S11. cele&chole graph in $S_0 \rightarrow S_1$ transition and difference map for electron density in $S_1 \rightarrow T_1$, $S_1 \rightarrow T_2$ transition of **PH-BODIPY.**

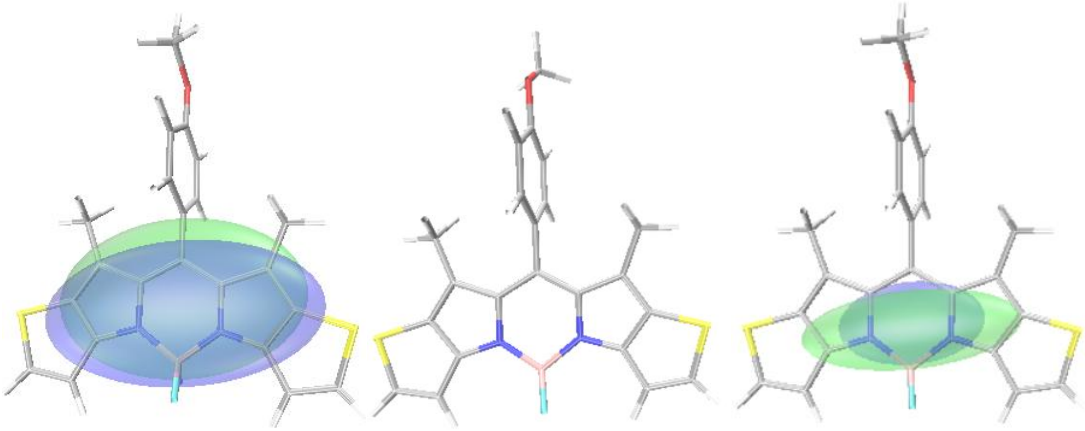


Figure S12. cele&chole graph in $S_0 \rightarrow S_1$ transition and difference map for electron density in $S_1 \rightarrow T_1$, $S_1 \rightarrow T_2$ transition of **MeO-BODIPY.**

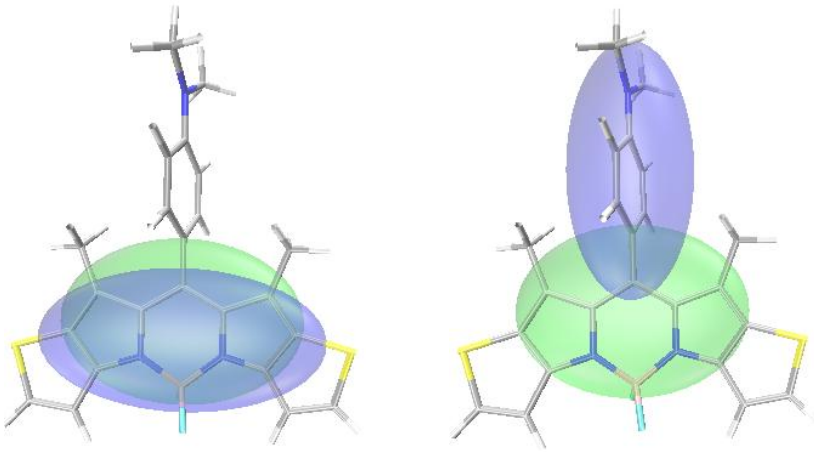


Figure S13. cele&chole graph in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transition of **DMA-BODIPY.**

It is evident that $S_0 \rightarrow S_1$ is LE excitation, while $S_0 \rightarrow S_2$ is attributed to CT excitation.

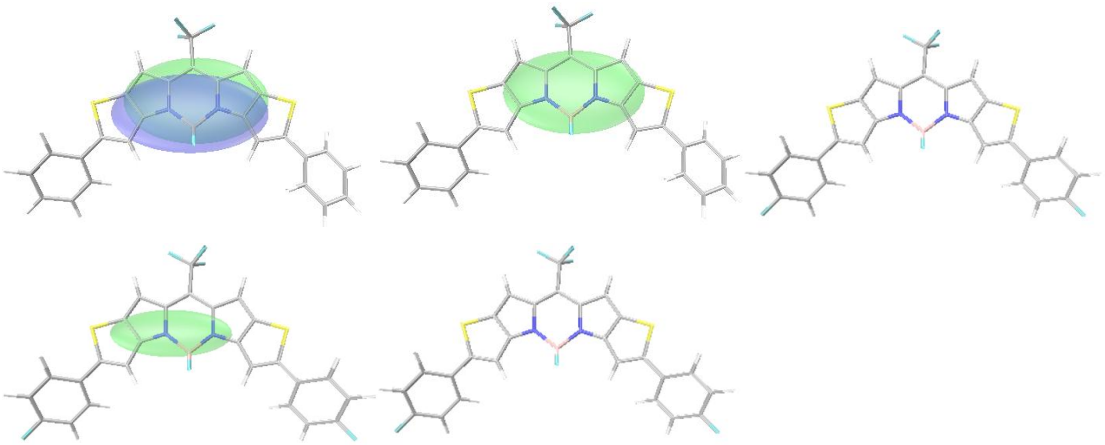


Figure S14. cele&chole graph in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_4$ transition, difference map for electron density in $S_1 \rightarrow T_1$, $S_1 \rightarrow T_2$ and $S_2 \rightarrow T_2$ transition of **SBDPiR690.**

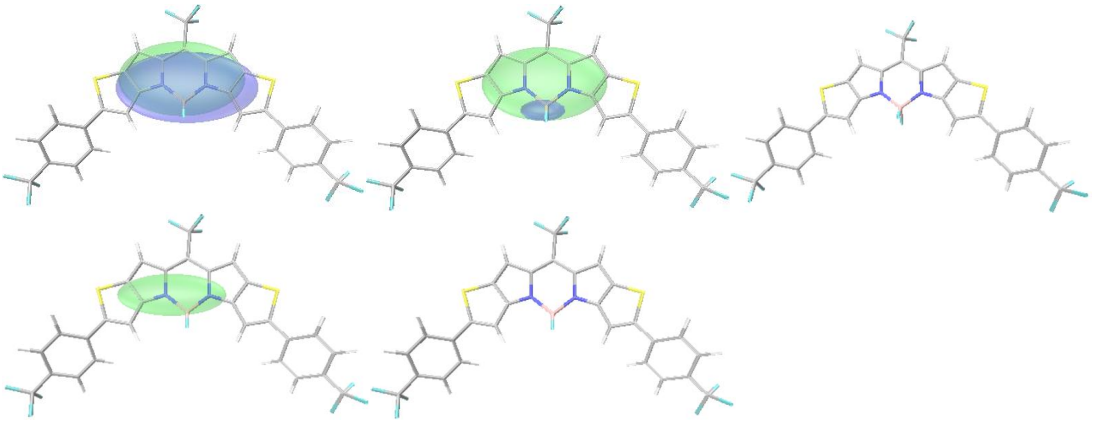


Figure S15. cele&chole graph in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_4$ transition, difference map for electron density in $S_1 \rightarrow T_1$, $S_1 \rightarrow T_2$ and $S_2 \rightarrow T_2$ transition of **SBDPiR688.**

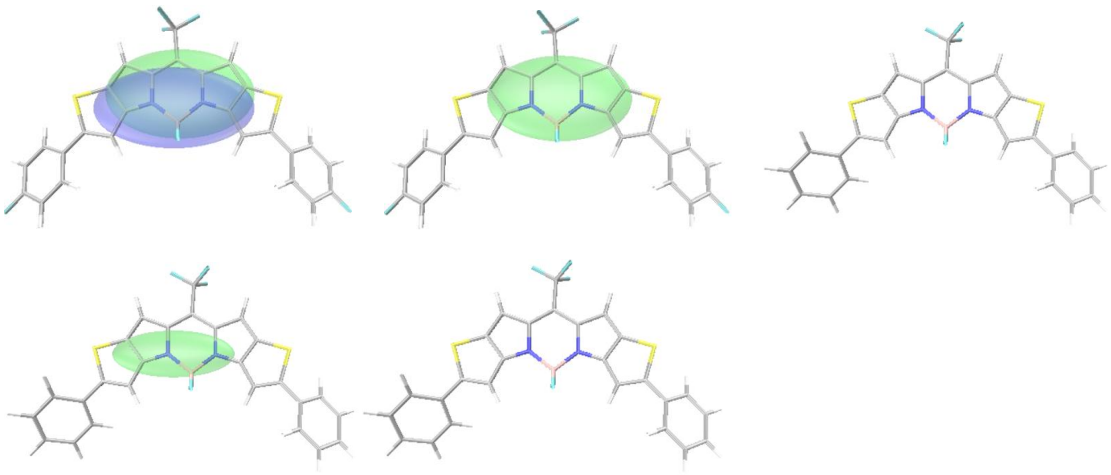


Figure S16. cele&chole graph in $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_4$ transition, difference map for electron density in $S_1 \rightarrow T_1$, $S_1 \rightarrow T_2$ and $S_2 \rightarrow T_2$ transition of **SBDPiR698.**

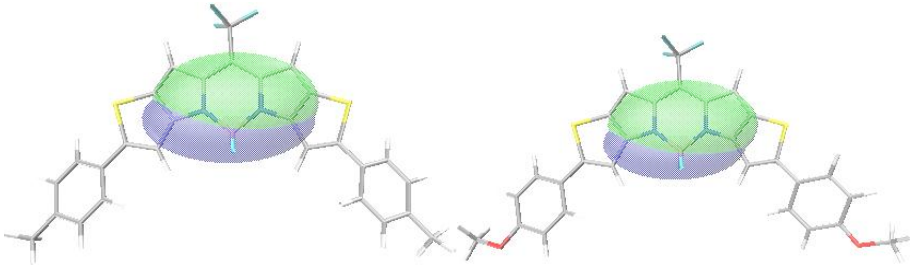


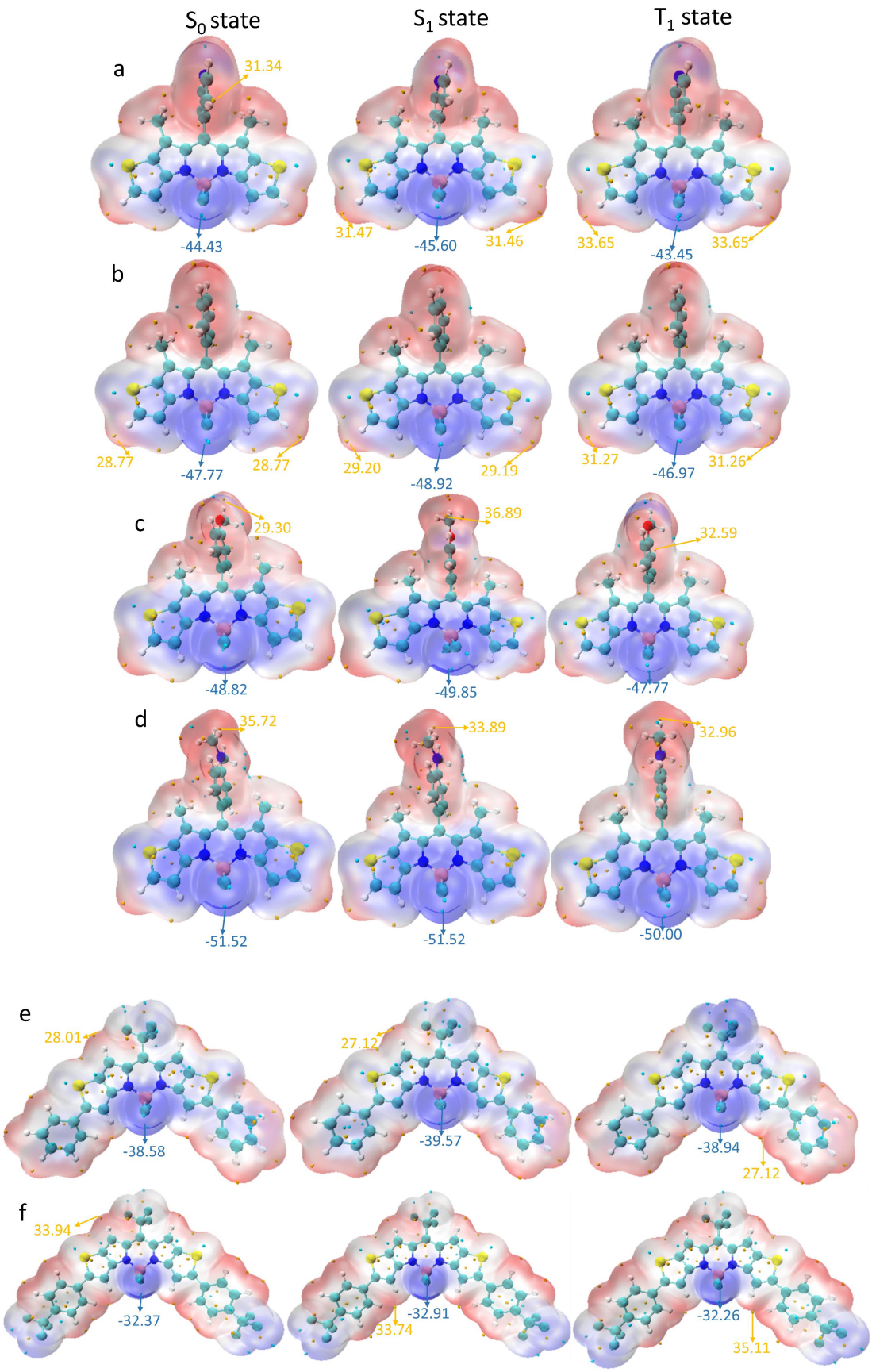
Figure S17. cele&chole graph in $S_0 \rightarrow S_1$ transition of **SBDPiR710** (left) and **SBDPiR731**(right).

Table S20. The adiabatic energy of the ground state, singlet and triplet excited-states at their optimized geometries, along with SOC between the involved T_1 and S_1 states, T_2 and S_1 states.

	PY-BODIPY	PH-BODIPY	MeO-BODIPY	DMA-BODIPY
S_0 (hartree)	-1955.47574	-1939.44251	-2053.92751	-2073.36165
S_1 (hartree)	-1955.39420	-1939.36001	-2053.84472	-2073.27827
T_1(hartree)	-1955.42397	-1939.38947	-2053.87414	-2073.30745
T_2(hartree)	-1955.39243	-1939.35793	-2053.84252	-2073.29009
S_0-T_1 (hartree)	0.0518	0.0530	0.0534	0.0542
S_0-T_1(eV)	1.409	1.443	1.452	1.475
S_1-T_1(hartree)	0.0298	0.0295	0.0294	0.0292
S_1-T_1(eV)	0.810	0.802	0.801	0.794
S_1-T_2(hartree)	0.0018	0.0021	0.0022	0.0118
S_1-T_2(eV)	0.048	0.056	0.060	0.322
SOC S_1-T_1(cm^{-1})	0.18	0.13	0.14	0.35
SOC S_1-T_2(cm^{-1})	2.19	2.18	2.17	0.97

Table S21. The adiabatic energy of the ground state, singlet and triplet excited-states at their optimized geometries, along with SOC between the involved T_1 and S_1 states, T_2 and S_1 states, T_2 and S_2 states.

	SBDPiR690	SBDPiR688	SBDPiR698	SBDPiR710	SBDPiR731
S_0 (hartree)	-2428.76630	-3102.67417	-2627.18827	-2507.36699	-2657.73652
S_1 (hartree)	-2428.69940	-3102.60604	-2627.12119	-2507.30150	-2657.67332
S_2 (hartree)	-2428.67110	-3102.58005	-2627.09289	-2507.27148	-2657.63988
T_1 (hartree)	-2428.72968	-3102.63667	-2627.15155	-2507.33091	-2657.70158
T_2 (hartree)	-2428.68840	-3102.59756	-2627.11009	-2507.28840	-2657.65683
S_0-T_1 (hartree)	0.0366	0.0375	0.0367	0.0361	0.0349
S_0-T_1 (eV)	0.996	1.020	0.999	0.982	0.951
S_1-T_1 (hartree)	0.0303	0.0306	0.0304	0.0294	0.0283
S_1-T_1 (eV)	0.824	0.834	0.826	0.800	0.769
S_1-T_2 (hartree)	0.0110	0.0085	0.0111	0.0131	0.0165
S_1-T_2 (eV)	0.299	0.231	0.302	0.357	0.449
S_2-T_2 (hartree)	0.0173	0.0175	0.0172	0.0169	0.0169
S_2-T_2 (eV)	0.471	0.476	0.468	0.460	0.461
SOC S_1-T_1(cm^{-1})	0.03	0.09	0.10	0.04	0.02
SOC S_1-T_2(cm^{-1})	0.57	0.62	0.50	0.38	0.35
SOC S_2-T_2(cm^{-1})	2.42	2.04	2.10	1.94	1.84


S0 state
S1 state
T1 state
a
31.34
-44.43
31.47
-45.60
31.46
33.65
-43.45
33.65
b
28.77
-47.77
28.77
29.20
-48.92
29.19
31.27
-46.97
31.26
c
29.30
-48.82
36.89
-49.85
32.59
-47.77
d
35.72
-51.52
33.89
-51.52
32.96
-50.00
e
28.01
-38.58
27.12
-39.57
-38.94
27.12
f
33.94
-32.37
-32.91
33.74
-32.26
35.11

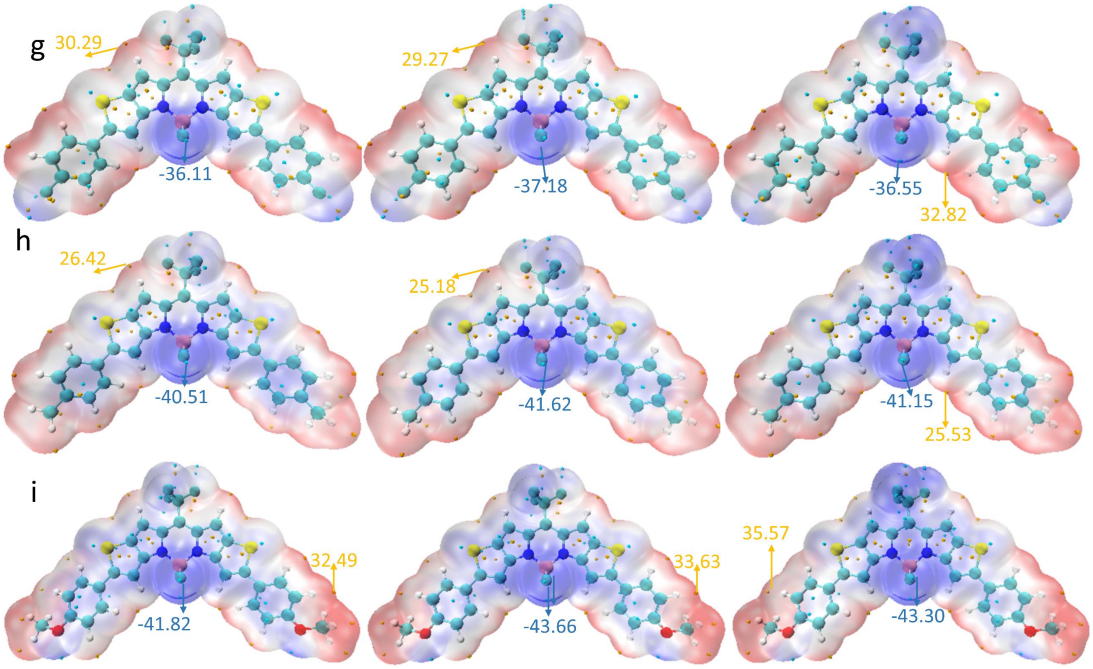


Figure S18. (a) Electrostatic potential surface plots of **PY-BODIPY** at the S_0 state(left), S_1 (middle) state and T_1 (right) state. (b)**PH-BODIPY**, (c)**MeO-BODIPY**, (d)**DMA-BODIPY**, (e)**SBDPiR690**, (f) **SBDPiR688**, (g) **SBDPiR698**, (h) **SBDPiR710**, (i) **SBDPiR731**. The blue font indicates the electrostatic potential value at the minimum value point, while the yellow font corresponds to the electrostatic potential value at the maximum value point (The unit of the value is Kcal/mol). Among all compounds, the average value of the molecular surface electrostatic potential near the fluorine atom on the parent nucleus of BODIPY is the most negative (-51.52 to -32.26 kcal/mol). This is attributed to the fact that the lone electron pairs in the 2p orbital of the fluorine atom after forming σ-bond can still be transferred to the empty orbital of other atoms and participate in the formation of π bonds, large π bonds, and d-p π bonds. From PY-BODIPY, PH-BODIPY, MeO-BODIPY to DAM-BODIPY, with the increase of the electron donor ability at the meso substituents, the minimum value of the surface electrostatic potential decreases gradually. For SBDPiR710 and SBDPiR731, the electron-donor group positioned para to the phenyl group exhibits a significantly lower surface electrostatic potential minimum compared to that of the molecules (SBDPiR690, SBDPiR688, SBDPiR698) where the electron-withdrawing group is para-linked to the phenyl group. The distribution of the surface electrostatic potential maximum of S_0 and S_1 states was consistent for all compounds except PH-BODIPY and SBDPiR688. Even for PH-BODIPY, MeO-BODIPY and DAM-BODIPY, the distribution of the surface electrostatic potential maxima is the same in the S_0, S_1, T_1 states. The maximum surface potential of PH-BODIPY is on the thiophene ring, whereas for MeO-BODIPY and DAM-BODIPY, the maximum surface potential is concentrated on the substituent group of the meso position.

XYZcoordinates(angstrom)

Note: upper case letters before the atomic coordinates indicate the atomic symbol of the atominvolved inthe calculations.

PY-BODIPY in S_0 State

C	1.22010500	0.20432300	0.00691700
N	1.23092300	-1.19429700	0.01245500
B	-0.00001000	-2.12055400	0.00012800
N	-1.23093400	-1.19428700	-0.01245500
C	-1.22010600	0.20433300	-0.00690100
C	0.00000200	0.89482900	0.00001500
C	-2.51757500	-1.58437200	-0.00359600
C	-3.35557900	-0.44678100	0.00812600
C	-2.56971300	0.69762300	0.00947000
C	2.56971400	0.69760400	-0.00950800
C	3.35557200	-0.44680600	-0.00821700
C	2.51756000	-1.58439100	0.00353600
C	-3.22525000	-2.82595300	0.00223000
C	-4.56780200	-2.59496000	0.01746600
S	-5.03559500	-0.90842400	0.02495400
S	5.03558400	-0.90845900	-0.02513100
C	4.56778100	-2.59499300	-0.01762700
C	3.22522800	-2.82597700	-0.00232700
C	-3.08022700	2.10458400	0.02103900
F	-0.01265300	-2.94083100	1.13811200
F	0.01262200	-2.94115300	-1.13761900
C	3.08023500	2.10456200	-0.02108600
C	0.00001100	2.38278900	0.00001900
C	0.16778500	3.09401500	1.18738100
C	0.15708500	4.48581400	1.13288700
C	-0.15702800	4.48582300	-1.13283700
C	-0.16774900	3.09402500	-1.18733900
H	-2.77579400	-3.81085800	-0.00389300
H	-5.35188300	-3.34302800	0.02451700
H	5.35185600	-3.34306600	-0.02472000
H	2.77576500	-3.81087800	0.00381300
H	-4.15465800	2.10098700	0.22024000
H	-2.91784900	2.59453000	-0.94391400
H	-2.59234000	2.71176400	0.78740800
H	4.15466400	2.10096200	-0.22029400
H	2.91786200	2.59451300	0.94386500
H	2.59234400	2.71174000	-0.78745500
H	0.30202300	2.57902800	2.13376400
H	0.28234200	5.06733400	2.04255700
H	-0.28227600	5.06735100	-2.04250300
H	-0.30199300	2.57904600	-2.13372600

N	0.00003300	5.17926500	0.00002800

PY-BODIPY in S_1 State

C	1.22139200	0.20142100	0.01113000
N	1.22368700	-1.18026900	0.04922100
B	0.00020200	-2.10513700	0.00002700
N	-1.22342800	-1.18047100	-0.04921900
C	-1.22134000	0.20121300	-0.01115200
C	-0.00004200	0.92114500	-0.00000200
C	-2.52516600	-1.59548400	-0.03714900
C	-3.36847300	-0.45922100	0.01079600
C	-2.59904700	0.68840400	0.04263600
C	2.59904400	0.68879600	-0.04275400
C	3.36862600	-0.45872200	-0.01084400
C	2.52548200	-1.59509800	0.03716900
C	-3.21077600	-2.82702600	-0.04119000
C	-4.57070100	-2.61242600	-0.00207300
S	-5.04704000	-0.93825800	0.04263800
S	5.04726100	-0.93752700	-0.04269500
C	4.57115700	-2.61175800	0.00213100
C	3.21126300	-2.82654400	0.04126700
C	-3.10291400	2.08986300	0.14508400
F	-0.04747600	-2.93148400	1.13584500
F	0.04800900	-2.93154000	-1.13574500
C	3.10277300	2.09029400	-0.14535800
C	-0.00022800	2.40479500	0.00002100
C	0.34947700	3.12648000	1.14435200
C	0.33131500	4.51786000	1.09373900
C	-0.33247700	4.51780600	-1.09358800
C	-0.35021300	3.12642200	-1.14426100
H	-2.75607900	-3.80958800	-0.06984800
H	-5.34403100	-3.37207000	0.00052400
H	5.34459200	-3.37129500	-0.00043400
H	2.75670200	-3.80916800	0.06997800
H	-4.15922500	2.07729300	0.42656500
H	-3.01494600	2.62599100	-0.80680700
H	-2.55503300	2.66691400	0.89563000
H	4.15907400	2.07778300	-0.42688200
H	3.01480700	2.62650500	0.80648400
H	2.55481900	2.66722600	-0.89593900
H	0.62539800	2.61413200	2.06128800
H	0.59466800	5.09887700	1.97404300
H	-0.59603100	5.09878000	-1.97386000

H	-0.62600700	2.61402900	-2.06120900
N	-0.00068200	5.21370400	0.00008900

PY-BODIPY in T_1 State

C	1.21324300	0.19188900	0.00922200
N	1.21973700	-1.17743900	0.03134100
B	0.00000800	-2.10497100	0.00000200
N	-1.21972700	-1.17744700	-0.03133900
C	-1.21324100	0.19188200	-0.00922200
C	-0.00000200	0.91757300	0.00000100
C	-2.53474500	-1.59625200	-0.02094700
C	-3.37329200	-0.46067800	0.01013000
C	-2.60040100	0.68461200	0.02846600
C	2.60040100	0.68462700	-0.02846900
C	3.37329800	-0.46065900	-0.01013200
C	2.53475600	-1.59623800	0.02094800
C	-3.21408600	-2.82590200	-0.02097300
C	-4.57668900	-2.61306800	0.00705900
S	-5.04950400	-0.93618900	0.03498900
S	5.04951200	-0.93616200	-0.03499400
C	4.57670600	-2.61304400	-0.00706000
C	3.21410400	-2.82588400	0.02097500
C	-3.09477800	2.09123500	0.09740700
F	-0.03092600	-2.93273800	1.13605700
F	0.03094600	-2.93274200	-1.13605000
C	3.09477200	2.09125100	-0.09741500
C	-0.00000800	2.40490200	0.00000100
C	0.28123900	3.12926100	1.16123200
C	0.26945200	4.52104600	1.11032500
C	-0.26949500	4.52104400	-1.11032100
C	-0.28126700	3.12925900	-1.16122800
H	-2.75710000	-3.80740200	-0.03891800
H	-5.35029000	-3.37130200	0.01130900
H	5.35031100	-3.37127300	-0.01130900
H	2.75712300	-3.80738700	0.03892200
H	-4.16378400	2.09057500	0.32530600
H	-2.95196000	2.61849300	-0.85188500
H	-2.57980700	2.66672700	0.87183400
H	4.16377800	2.09059400	-0.32531700
H	2.95195500	2.61851200	0.85187600
H	2.57979800	2.66673900	-0.87184200
H	0.50359100	2.61737100	2.09302000
H	0.48441700	5.10197000	2.00383300

H	-0.48446700	5.10196600	-2.00382800
H	-0.50361300	2.61736700	-2.09301700
N	-0.00002500	5.21741400	0.00000200

PY-BODIPY in T_2 State

C	1.22804700	0.21021100	-0.00241300
N	1.21339800	-1.18948400	0.04755800
B	0.00208200	-2.09970500	0.04622400
N	-1.24588400	-1.15711900	-0.02278300
C	-1.22555300	0.27126200	-0.00008000
C	-0.00994600	0.93657500	0.00013900
C	-2.52360000	-1.58702300	-0.03828900
C	-3.37140700	-0.46399200	-0.00593600
C	-2.57760400	0.73738900	0.03897400
C	2.55853600	0.67277500	-0.06781200
C	3.34547900	-0.50098600	-0.03609800
C	2.50786800	-1.61575000	0.02831700
C	-3.20824900	-2.84185500	-0.05054600
C	-4.55562800	-2.64080400	-0.03311700
S	-4.99135700	-0.93249200	0.00656900
S	5.01135900	-0.98012300	-0.07734900
C	4.54322400	-2.66917500	-0.01173100
C	3.19558700	-2.86901900	0.04042600
C	-3.11768700	2.11913700	0.12142000
F	-0.09097300	-2.87218500	1.21189000
F	-0.02167000	-2.95625400	-1.06170800
C	3.10921200	2.06546000	-0.16638600
C	0.01357700	2.42250700	0.00758200
C	0.36768100	3.13010900	1.15852700
C	0.37172700	4.52172600	1.11716400
C	-0.27585100	4.54687500	-1.07483300
C	-0.31426700	3.15564000	-1.13462200
H	-2.73565000	-3.81593500	-0.07225800
H	-5.34986800	-3.37513200	-0.04125300
H	5.32044200	-3.42274300	-0.01348300
H	2.72939700	-3.84587300	0.08511200
H	-4.16401100	2.09559500	0.43598100
H	-3.07096800	2.62240100	-0.85301100
H	-2.55415600	2.73240900	0.82948700
H	4.13740200	2.02156300	-0.53755500
H	3.13149500	2.56871900	0.80642500
H	2.53563600	2.69396400	-0.85123100
H	0.63361500	2.60650300	2.07204900
H	0.63898300	5.09321400	2.00252800

H	-0.52427500	5.13774000	-1.95298400
H	-0.58783800	2.65286300	-2.05749200
N	0.05766800	5.23012600	0.02569200

PH-BODIPY in S_0 State

C	1.21931300	0.20220000	-0.01030700
N	1.23034300	-1.19677200	-0.02672000
B	-0.00000600	-2.12214100	0.00002100
N	-1.23035300	-1.19676700	0.02674300
C	-1.21931500	0.20220500	0.01033200
C	0.00000000	0.89686300	0.00001200
C	-2.51695900	-1.58767300	0.01421400
C	-3.35469400	-0.45104200	-0.01091800
C	-2.56841900	0.69412300	-0.02023900
C	2.56841900	0.69411200	0.02024700
C	3.35468900	-0.45105800	0.01090600
C	2.51694900	-1.58768400	-0.01421500
C	-3.22446900	-2.82975400	0.01128500
C	-4.56700100	-2.59971900	-0.01397700
S	-5.03437100	-0.91310500	-0.03460300
S	5.03436400	-0.91312800	0.03456300
C	4.56698600	-2.59974000	0.01394300
C	3.22445200	-2.82976900	-0.01129800
C	-3.08248900	2.09929000	-0.05956600
F	0.02660800	-2.94402500	1.13758600
F	-0.02662300	-2.94404700	-1.13752900
C	3.08250200	2.09927400	0.05957300
C	0.00000400	2.38435300	0.00000500
C	-0.23333600	3.08250900	1.18785500
C	-0.22711600	4.47628800	1.18701200
C	0.22715200	4.47627400	-1.18702000
C	0.23335200	3.08249500	-1.18785100
H	-2.77465400	-3.81443800	0.02612500
H	-5.35087700	-3.34794100	-0.02080500
H	5.35085900	-3.34796600	0.02075700
H	2.77463300	-3.81445000	-0.02613300
H	-4.14361700	2.09107600	-0.32156400
H	-2.55102200	2.70995000	-0.79325600
H	-2.97892500	2.58807500	0.91412200
H	4.14361200	2.09105300	0.32164500
H	2.55099300	2.70996300	0.79320600
H	2.97901300	2.58802900	-0.91413900
H	-0.41500500	2.53293500	2.10782300

H	-0.40298000	5.01611100	2.11250500
H	0.40302400	5.01608700	-2.11251800
H	0.41501500	2.53291100	-2.10781300
C	0.00002300	5.17418900	-0.00000700
H	0.00003100	6.26003500	-0.00001200

PH-BODIPY in S_1 State

C	1.21950000	0.19612900	-0.00767000
N	1.22378100	-1.18680900	-0.03575600
B	0.00000200	-2.11121900	0.00002500
N	-1.22378000	-1.18681100	0.03575500
C	-1.21950000	0.19612700	0.00767300
C	0.00000000	0.91845800	0.00000500
C	-2.52597200	-1.59962900	0.02408200
C	-3.36767500	-0.46131000	-0.01192300
C	-2.59661800	0.68547800	-0.03342400
C	2.59661700	0.68548100	0.03341700
C	3.36767600	-0.46130600	0.01190500
C	2.52597400	-1.59962500	-0.02409400
C	-3.21431100	-2.83006600	0.02424800
C	-4.57381900	-2.61361500	-0.00695400
S	-5.04744000	-0.93744000	-0.03811400
S	5.04744200	-0.93743400	0.03808100
C	4.57382200	-2.61360900	0.00692200
C	3.21431400	-2.83006200	-0.02426800
C	-3.09659500	2.09030300	-0.10358700
F	0.03471900	-2.93884400	1.13619300
F	-0.03471100	-2.93890700	-1.13609600
C	3.09659500	2.09030700	0.10358000
C	-0.00000200	2.40448400	0.00000400
C	-0.28945400	3.11165100	1.17268000
C	-0.28724000	4.50560800	1.17324400
C	0.28723100	4.50560800	-1.17323700
C	0.28944800	3.11165000	-1.17267200
H	-2.76116500	-3.81355800	0.04492200
H	-5.34837200	-3.37192700	-0.01129500
H	5.34837600	-3.37192000	0.01125400
H	2.76116900	-3.81355500	-0.04494000
H	-4.16053700	2.08687700	-0.35533900
H	-2.56499300	2.67576600	-0.85934500
H	-2.97723800	2.61183400	0.85291400
H	4.16053500	2.08688100	0.35533800
H	2.56498800	2.67577100	0.85933400

H	2.97724300	2.61183500	-0.85292300
H	-0.51286600	2.56403900	2.08485100
H	-0.50951000	5.04523700	2.08906600
H	0.50949900	5.04523600	-2.08906000
H	0.51286200	2.56403800	-2.08484200
C	-0.00000600	5.20490000	0.00000300
H	-0.00000700	6.29083600	0.00000300

PH-BODIPY in T_1 State

C	1.21082700	0.18648800	-0.00579300
N	1.21966200	-1.18371300	-0.01665400
B	0.00000000	-2.11095000	0.00003100
N	-1.21966200	-1.18371300	0.01665700
C	-1.21082700	0.18648700	0.00579800
C	0.00000000	0.91452200	0.00000600
C	-2.53551500	-1.60022900	0.00765800
C	-3.37230200	-0.46292000	-0.00883700
C	-2.59765200	0.68146600	-0.01494300
C	2.59765200	0.68146700	0.01493300
C	3.37230100	-0.46292000	0.00881600
C	2.53551500	-1.60022800	-0.00767000
C	-3.21732600	-2.82882000	0.00344000
C	-4.57965000	-2.61430800	-0.01478200
S	-5.04957700	-0.93591100	-0.02714400
S	5.04957700	-0.93591000	0.02710100
C	4.57965000	-2.61430800	0.01474400
C	3.21732600	-2.82881900	-0.00346100
C	-3.08620400	2.09135600	-0.04137300
F	0.01662300	-2.94011900	1.13630700
F	-0.01662000	-2.94019100	-1.13619200
C	3.08620500	2.09135600	0.04135800
C	-0.00000100	2.40440100	0.00000600
C	-0.18713400	3.11438000	1.19147800
C	-0.18777700	4.50877900	1.19286700
C	0.18777600	4.50877900	-1.19285500
C	0.18713200	3.11438000	-1.19146500
H	-2.76181000	-3.81115100	0.01217000
H	-5.35443900	-3.37125700	-0.02069600
H	5.35443900	-3.37125700	0.02064800
H	2.76181000	-3.81115100	-0.01218600
H	-4.16559200	2.10118400	-0.21391600
H	-2.60463200	2.67475100	-0.83137800
H	-2.88881000	2.60375500	0.90628900

H	4.16559200	2.10118400	0.21391000
H	2.60462600	2.67475800	0.83135300
H	2.88882200	2.60374800	-0.90631100
H	-0.33154800	2.56723400	2.11989000
H	-0.33313600	5.04812700	2.12424500
H	0.33313500	5.04812700	-2.12423300
H	0.33154600	2.56723400	-2.11987700
C	-0.00000100	5.20850000	0.00000600
H	0.00000000	6.29452200	0.00000600

PH-BODIPY in T_2 State

C	-1.22608300	0.20384400	-0.00360500
N	-1.21045900	-1.19674300	0.03975800
B	0.00215700	-2.10464700	0.03677200
N	1.24850000	-1.16055800	-0.01843800
C	1.22399700	0.26898100	0.00381900
C	0.00951000	0.93502400	0.00174300
C	2.52791900	-1.58708600	-0.03053200
C	3.37216200	-0.46110900	0.00072900
C	2.57527800	0.73807600	0.04012500
C	-2.55723100	0.66529100	-0.06043600
C	-3.34327600	-0.50939900	-0.03288600
C	-2.50468300	-1.62408100	0.02291300
C	3.21632500	-2.83941400	-0.04246200
C	4.56355400	-2.63498400	-0.02565700
S	4.99392000	-0.92515500	0.01214000
S	-5.00917800	-0.98962200	-0.06872000
C	-4.53996500	-2.67895600	-0.01285000
C	-3.19182200	-2.87770000	0.03246800
C	3.10962700	2.12287900	0.10754300
F	0.03272300	-2.95349800	-1.07797000
F	0.08973800	-2.88794500	1.19642900
C	-3.10898500	2.05878200	-0.14064000
C	-0.01618400	2.42282200	0.00675200
C	0.27659200	3.13998000	-1.15807100
C	0.24662800	4.53432000	-1.15315100
C	-0.36510300	4.51184400	1.18373300
C	-0.33960100	3.11819400	1.17715500
H	2.74648500	-3.81487900	-0.06339500
H	5.35974500	-3.36709300	-0.03290500
H	-5.31661200	-3.43308300	-0.01479000
H	-2.72487000	-3.85451800	0.07071600
H	4.15983500	2.10730700	0.40973600

H	2.54897200	2.73820800	0.81628300
H	3.04673900	2.61902700	-0.86959100
H	-4.13822800	2.01948700	-0.50992200
H	-2.53503200	2.69670500	-0.81625600
H	-3.12849300	2.54862100	0.83914200
H	0.52132500	2.60042300	-2.06957500
H	0.47193800	5.08238500	-2.06326500
H	-0.61378400	5.04304900	2.09775200
H	-0.57092900	2.56131200	2.08173900
C	-0.07307000	5.22246100	0.01798000
H	-0.09570900	6.30817100	0.02237500

MeO-BODIPY in S_0 State

C	0.15575700	1.22908100	0.01445000
N	1.54239700	1.39643000	-0.06678700
B	2.60011700	0.27869800	-0.07526700
N	1.82333900	-1.04605700	0.02602000
C	0.43223800	-1.19429800	0.04375500
C	-0.39806100	-0.06137600	0.05219400
C	2.35837000	-2.27989700	0.00161400
C	1.32488000	-3.24134700	0.00143500
C	0.09707300	-2.59040700	0.01687900
C	-0.47983700	2.51477700	0.09118100
C	0.56977500	3.42389700	0.03599200
C	1.78898500	2.71842000	-0.05523600
C	3.67268500	-2.84074400	-0.03729600
C	3.59701400	-4.20072200	-0.06301400
S	1.97439200	-4.85713700	-0.04264400
S	0.84400000	5.14388000	0.06849300
C	2.56946700	4.86742000	-0.03781300
C	2.94446900	3.55902400	-0.09662300
C	-1.23904400	-3.26470200	-0.00990300
F	3.47873300	0.42419000	1.00969000
F	3.35346500	0.31790900	-1.25994300
C	-1.92690600	2.87386500	0.22550000
C	-1.87177300	-0.22699500	0.10407100
C	-2.49977800	-0.62169900	1.29305800
C	-3.87764400	-0.76175900	1.34632200
C	-4.03494900	-0.14133200	-0.99383900
C	-2.64852700	0.01305100	-1.02757000
H	4.59945500	-2.28108600	-0.04513400
H	4.42965400	-4.89358800	-0.09112200
H	3.22606000	5.72934700	-0.05168400

H	3.97090700	3.22121300	-0.16403700
H	-1.11583700	-4.30002800	-0.33905300
H	-1.93633800	-2.76657000	-0.68739800
H	-1.69773100	-3.28068500	0.98384200
H	-2.01288400	3.91059700	0.56195900
H	-2.44322800	2.23303800	0.94392700
H	-2.45018600	2.78623100	-0.73187900
H	-1.90236200	-0.81120500	2.18099400
H	-4.37611200	-1.05702300	2.26437900
H	-4.61336700	0.04273000	-1.89142500
H	-2.16887000	0.31914300	-1.95372600
C	-4.65282700	-0.52511900	0.20111800
O	-5.98870300	-0.69352100	0.34635100
C	-6.81670900	-0.45343200	-0.78443100
H	-6.72308600	0.58296500	-1.12657800
H	-6.57141700	-1.13786600	-1.60365100
H	-7.83776900	-0.63615800	-0.45087100

MeO-BODIPY in S_1 State

C	0.16962100	1.22907600	0.02326500
N	1.54174800	1.38582300	-0.05863800
B	2.59520300	0.27153600	-0.06738800
N	1.81489000	-1.04559700	0.02440800
C	0.43940800	-1.19400800	0.03673600
C	-0.41436200	-0.06242200	0.05274700
C	2.36840400	-2.29440400	0.00148700
C	1.32922600	-3.25662200	-0.00218600
C	0.10418300	-2.61660400	0.00871000
C	-0.46578600	2.54382600	0.09347700
C	0.58783800	3.43649900	0.03308500
C	1.80930400	2.72520500	-0.05409000
C	3.66680100	-2.84301600	-0.03445700
C	3.60056700	-4.21812200	-0.06068900
S	1.98640100	-4.87346700	-0.04476800
S	0.87756900	5.15798400	0.05636300
C	2.59357700	4.87168000	-0.04474200
C	2.95617300	3.54428700	-0.09599500
C	-1.23825600	-3.26872600	-0.02456700
F	3.47495100	0.40985700	1.02079400
F	3.35949400	0.31549600	-1.24767700
C	-1.91279500	2.88687600	0.22448400
C	-1.88870800	-0.22457400	0.10425600
C	-2.52654200	-0.60540200	1.29460900

C	-3.90483600	-0.74774900	1.34932000
C	-4.06089000	-0.13930700	-0.99200400
C	-2.67243100	0.00401800	-1.02695900
H	4.59441800	-2.28398700	-0.04099000
H	4.43930600	-4.90409900	-0.08642200
H	3.26178100	5.72493900	-0.06244500
H	3.98174100	3.20170700	-0.15881700
H	-1.12561100	-4.32306200	-0.29190500
H	-1.90375900	-2.79583000	-0.75250000
H	-1.73806500	-3.21955100	0.94967700
H	-2.01471100	3.94186300	0.49372400
H	-2.40771700	2.28407000	0.99147900
H	-2.45487900	2.72396300	-0.71413100
H	-1.93196900	-0.78604400	2.18659700
H	-4.40359800	-1.03684700	2.26937300
H	-4.63882700	0.04231600	-1.89056200
H	-2.19373200	0.29728800	-1.95802700
C	-4.68028200	-0.51495800	0.20415800
O	-6.01852100	-0.67861000	0.35110200
C	-6.84460000	-0.43999200	-0.78046500
H	-6.74640200	0.59436200	-1.12788700
H	-6.60257300	-1.12893800	-1.59704400
H	-7.86693600	-0.61634900	-0.44702600

MeO-BODIPY in T_1 State

C	0.27274400	1.21584100	0.03621500
N	1.64039700	1.27395200	-0.02924700
B	2.60924200	0.08767000	-0.05706000
N	1.72749800	-1.16380100	-0.00076100
C	0.35835600	-1.20296700	0.04035100
C	-0.41271300	-0.01924500	0.06541100
C	2.18929300	-2.46414800	-0.02474000
C	1.08241200	-3.34083600	0.00171300
C	-0.08794600	-2.60648100	0.03855100
C	-0.27031300	2.58403500	0.07801600
C	0.84426700	3.39966600	0.02557600
C	2.00938700	2.60394600	-0.03730400
C	3.44046700	-3.10138600	-0.07361900
C	3.27450100	-4.47057300	-0.08234500
S	1.61471600	-5.00025700	-0.03211800
S	1.25763500	5.09287300	0.02225600
C	2.94971400	4.68305600	-0.05934500
C	3.21193300	3.32929900	-0.08484300

C	-1.48090000	-3.14127700	0.06730600
F	3.48924500	0.13235300	1.03979200
F	3.38618800	0.10067800	-1.23036400
C	-1.69531400	3.01885300	0.16414900
C	-1.89971700	-0.07247800	0.11589100
C	-2.57245200	-0.26588100	1.33151500
C	-3.95782100	-0.31930300	1.38240200
C	-4.05655000	0.01740700	-1.01539600
C	-2.66082000	0.06736000	-1.04454700
H	4.40516500	-2.61032200	-0.10149100
H	4.05823500	-5.21728600	-0.11632700
H	3.67790000	5.48436400	-0.08600700
H	4.20874900	2.90910900	-0.13370600
H	-1.46190300	-4.22279300	-0.08993900
H	-2.10634400	-2.68967500	-0.70819500
H	-1.96737100	-2.94608700	1.02902200
H	-1.73982800	4.09907800	0.32555800
H	-2.22225900	2.52485100	0.98559500
H	-2.24303100	2.78887200	-0.75599700
H	-1.99788900	-0.37592500	2.24799600
H	-4.48063200	-0.46876700	2.32224100
H	-4.61405500	0.12917900	-1.93804100
H	-2.15766500	0.21756700	-1.99672800
C	-4.70802600	-0.17770800	0.20628300
O	-6.05551900	-0.24333600	0.35053300
C	-6.85472500	-0.10920300	-0.81662400
H	-6.69886900	0.86598500	-1.29095400
H	-6.63991700	-0.90840400	-1.53448500
H	-7.88878800	-0.18943800	-0.48220500

MeO-BODIPY in T_2 State

C	0.16222300	1.22502200	0.03806000
N	1.58609100	1.33508500	-0.03793900
B	2.60141100	0.14545600	-0.06363900
N	1.76910700	-1.11731700	0.02063900
C	0.37122500	-1.21608800	0.02366700
C	-0.43217000	-0.02642700	0.05241500
C	2.27198800	-2.38408600	0.00122900
C	1.20797000	-3.28776400	-0.00995600
C	-0.01174700	-2.57266500	-0.00652000
C	-0.38411100	2.54549900	0.10810000
C	0.76363200	3.41291400	0.03784000
C	1.93576400	2.63778500	-0.04659300

C	3.56400900	-2.99515400	-0.02665300
C	3.44478800	-4.35319400	-0.05372900
S	1.78538700	-4.92249800	-0.04777900
S	1.13108700	5.05952800	0.05047400
C	2.86070100	4.73245400	-0.05837900
C	3.14355600	3.39987400	-0.09942800
C	-1.37213800	-3.20599900	-0.03442500
F	3.47883600	0.28123700	1.02074400
F	3.34477300	0.22070100	-1.25053200
C	-1.79517200	2.99415400	0.23334200
C	-1.91389200	-0.13669900	0.10442700
C	-2.56248700	-0.50424000	1.29255000
C	-3.94480900	-0.60035400	1.34766800
C	-4.08267200	0.02711900	-0.98936600
C	-2.68925300	0.12348400	-1.02458300
H	4.51164500	-2.47010100	-0.02572600
H	4.24401800	-5.08287800	-0.07468900
H	3.54388100	5.57072900	-0.08246600
H	4.14372500	2.98964000	-0.16341200
H	-1.28501400	-4.23363900	-0.40030500
H	-2.06615300	-2.67391800	-0.68875000
H	-1.82510800	-3.24851600	0.96229700
H	-1.83271400	4.04177500	0.54252100
H	-2.34711100	2.39233400	0.96036600
H	-2.32413400	2.90580700	-0.72441800
H	-1.97279100	-0.71433400	2.18135000
H	-4.45249500	-0.87963300	2.26592400
H	-4.65446400	0.23317300	-1.88663100
H	-2.20101700	0.40243900	-1.95509400
C	-4.71317200	-0.33453600	0.20463700
O	-6.05675600	-0.45409500	0.35227200
C	-6.87409900	-0.18270100	-0.77780800
H	-6.74193300	0.84973400	-1.11999400
H	-6.65466200	-0.87484900	-1.59814500
H	-7.90193100	-0.32695700	-0.44568600

DMA-BODIPY in S_0 State

C	-0.49135700	1.22447800	0.02559700
N	-1.88874100	1.27884400	0.07094900
B	-2.85244400	0.08274800	-0.01536400
N	-1.96989800	-1.17590200	-0.07082200
C	-0.57241600	-1.21488900	-0.01640800
C	0.16887200	-0.01872800	0.00675800

C	-2.40983300	-2.44702900	-0.04135400
C	-1.30806900	-3.32398700	0.03461600
C	-0.13396000	-2.57909800	0.06806100
C	0.03798700	2.55627900	-0.05216900
C	-1.08391500	3.37832000	-0.02393400
C	-2.24239800	2.57691300	0.04184700
C	-3.67814500	-3.10683200	-0.04579900
C	-3.50081800	-4.45583000	0.02254800
S	-1.83324500	-4.98375200	0.09577100
S	-1.49641900	5.06972800	-0.08465600
C	-3.19607400	4.65449100	-0.02547200
C	-3.46379900	3.32030100	0.03816700
C	1.24172400	-3.15185700	0.21044000
F	-3.65376300	0.18034200	-1.16521800
F	-3.69785300	0.04089600	1.10535100
C	1.45035200	3.03512700	-0.18282100
C	1.64584300	-0.06894100	0.01124200
C	2.35147300	-0.51968500	-1.10947700
C	3.73818600	-0.55390400	-1.12162700
C	3.76088800	0.28342400	1.15100500
C	2.37485100	0.33915100	1.13323800
H	-4.64417100	-2.62050500	-0.09585200
H	-4.27840400	-5.21031300	0.03240400
H	-3.92089500	5.45978100	-0.03907700
H	-4.46078600	2.90010700	0.07954700
H	1.16956900	-4.16979300	0.60346900
H	1.86171000	-2.56091600	0.88835900
H	1.75927200	-3.20032200	-0.75274400
H	1.45093900	4.05243100	-0.58404100
H	2.03782500	2.39863800	-0.84836100
H	1.95848500	3.05725300	0.78641500
H	1.80522000	-0.83178900	-1.99641100
H	4.24232800	-0.88600200	-2.02090800
H	4.28200800	0.59867100	2.04668500
H	1.84702400	0.69798500	2.01359000
C	4.48473900	-0.16934000	0.01992400
C	6.56392300	-0.49701000	-1.21101700
H	6.35954700	0.27034000	-1.97127900
H	7.63456600	-0.50861900	-1.00914000
H	6.28914900	-1.47342100	-1.62256100
N	5.85490000	-0.23720100	0.03052600
C	6.58838100	0.35263600	1.13736400
H	7.65421800	0.19045700	0.97924300
H	6.40697600	1.43349100	1.22479400

H	6.31437400	-0.12211000	2.08471300

DMA-BODIPY in S_1 State

C	-0.50435600	1.22436000	0.01152000
N	-1.88696300	1.27708200	0.04261000
B	-2.85215800	0.08626500	0.00467500
N	-1.97150600	-1.16796100	-0.03998000
C	-0.58888400	-1.21163500	0.00244100
C	0.17864800	-0.01883900	0.01118100
C	-2.43003900	-2.45436100	-0.02599900
C	-1.32277500	-3.33558000	0.02632600
C	-0.14957800	-2.60490700	0.05730200
C	0.03117600	2.58341700	-0.04640500
C	-1.08848900	3.39425100	-0.02972900
C	-2.25487100	2.59229100	0.01819000
C	-3.68440000	-3.09828600	-0.03288700
C	-3.51735000	-4.46431800	0.00847300
S	-1.85891100	-4.99685300	0.05865500
S	-1.50786600	5.08872700	-0.07631700
C	-3.19940500	4.67278800	-0.03665700
C	-3.46148300	3.32201900	0.01137700
C	1.23476000	-3.15500300	0.15492900
F	-3.68330100	0.15519300	-1.12825200
F	-3.67819300	0.07393100	1.14363500
C	1.45223200	3.03237300	-0.13240300
C	1.66027000	-0.07291900	0.01410700
C	2.37285100	-0.42711100	-1.13649800
C	3.76126300	-0.48053000	-1.14595800
C	3.78296700	0.17708800	1.17939100
C	2.39459400	0.23202700	1.16513400
H	-4.65042900	-2.60960900	-0.06558700
H	-4.30300200	-5.21085600	0.00986700
H	-3.93085800	5.47249200	-0.04922700
H	-4.45959400	2.90233700	0.03870600
H	1.18880600	-4.21161400	0.43310800
H	1.83213900	-2.62447500	0.90204600
H	1.77062200	-3.07978000	-0.79817600
H	1.48570300	4.09098700	-0.40424000
H	2.01420400	2.46407400	-0.87938900
H	1.97485200	2.91219400	0.82338400
H	1.83007000	-0.65834500	-2.05031100
H	4.26467800	-0.74764700	-2.06722300
H	4.30291800	0.42348200	2.09724700

H	1.86884800	0.51838800	2.07328200
C	4.50689000	-0.19475200	0.02203100
C	6.58738900	-0.39040000	-1.23298800
H	6.39133000	0.46851200	-1.89216600
H	7.65825700	-0.44088600	-1.03626200
H	6.30264400	-1.30456300	-1.76229400
N	5.88351200	-0.28414700	0.03413300
C	6.61000700	0.28250900	1.15802300
H	7.67687300	0.12204500	1.00271300
H	6.42921200	1.36209300	1.27044700
H	6.33161500	-0.21396400	2.09209300

DMA-BODIPY in T_1 State

C	0.51339600	1.21539500	0.00239400
N	1.88294700	1.27638100	-0.00900800
B	2.85407400	0.09222900	0.00359800
N	1.97327600	-1.16078100	0.01335600
C	0.60335000	-1.20173900	0.00277000
C	-0.17189200	-0.02017300	0.00285500
C	2.43768700	-2.46043800	0.00150800
C	1.33193800	-3.33861000	-0.01673000
C	0.15979400	-2.60618000	-0.02020500
C	-0.03304100	2.58277800	0.02376300
C	1.08139100	3.40038200	0.01672400
C	2.24947400	2.60688400	-0.00058600
C	3.69076000	-3.09604200	-0.00273100
C	3.52745100	-4.46541500	-0.02267800
S	1.86742000	-4.99716800	-0.03705700
S	1.49135100	5.09427100	0.03201100
C	3.18638200	4.68781300	0.01790800
C	3.45171200	3.33463200	0.00123300
C	-1.23230100	-3.14307100	-0.04409600
F	3.68179100	0.13396200	1.14124900
F	3.68625100	0.11144900	-1.13131500
C	-1.46096900	3.01508500	0.05183000
C	-1.65873400	-0.07779000	-0.00141100
C	-2.38179000	-0.26356600	1.18082400
C	-3.77096800	-0.32385800	1.18781400
C	-3.77554800	-0.00058600	-1.20546400
C	-2.38636800	0.05600600	-1.18794200
H	4.65511000	-2.60356600	0.00760100
H	4.31297600	-5.21096200	-0.02914400
H	3.91351400	5.49050800	0.02180400

H	4.45038900	2.91608500	-0.00844700
H	-1.20549300	-4.22555800	-0.19405100
H	-1.82681700	-2.69606400	-0.84621200
H	-1.75732500	-2.94166800	0.89573100
H	-1.51371500	4.09633900	0.20453900
H	-2.01820300	2.52406300	0.85493700
H	-1.97248100	2.77735100	-0.88697800
H	-1.84629500	-0.35973500	2.12288000
H	-4.28047800	-0.46106500	2.13391900
H	-4.28821400	0.11514600	-2.15267100
H	-1.85449000	0.21233300	-2.12397900
C	-4.50784500	-0.20943500	-0.01381500
C	-6.59734500	-0.22498600	1.24050100
H	-6.41328800	0.72654200	1.76200400
H	-7.66649300	-0.31554500	1.04807700
H	-6.30879500	-1.04492500	1.90437300
N	-5.88607800	-0.30813100	-0.02430500
C	-6.60355600	0.11285200	-1.21618600
H	-7.67132300	-0.03344400	-1.05269900
H	-6.42632000	1.17165000	-1.45880500
H	-6.31420500	-0.49287700	-2.07951600

DMA-BODIPY in T_2 State

C	-0.49539000	-1.24295100	-0.03989000
N	-1.87765600	-1.21792300	-0.17216200
B	-2.78497900	0.00030500	0.00023200
N	-1.87733200	1.21835200	0.17213800
C	-0.49506200	1.24298400	0.03983500
C	0.23602000	-0.00008800	-0.00000700
C	-2.32331800	2.51236600	0.12940800
C	-1.22959100	3.36023600	-0.04479100
C	-0.05703900	2.58729700	-0.14546900
C	-0.05773800	-2.58741800	0.14535000
C	-1.23048900	-3.36002700	0.04459500
C	-2.32398200	-2.51183000	-0.12953000
C	-3.58114000	3.17960000	0.18115300
C	-3.41104200	4.53033600	0.05260300
S	-1.73992300	5.02002800	-0.13639400
S	-1.74127000	-5.01969000	0.13607700
C	-3.41224900	-4.52950200	-0.05286200
C	-3.58198000	-3.17870400	-0.18130500
C	1.28813500	3.14157700	-0.50611200
F	-3.62790700	-0.16306700	1.12470500

F	-3.62847900	0.16381000	-1.12378000
C	1.28727300	-3.14209200	0.50598300
C	1.66755600	-0.00026300	0.00005300
C	2.41986300	0.80709100	0.92240100
C	3.78071000	0.79656600	0.94297600
C	3.78061700	-0.79739200	-0.94282200
C	2.41976800	-0.80776000	-0.92225100
H	-4.54559900	2.70144400	0.30363100
H	-4.17910700	5.29310000	0.06125900
H	-4.18053000	-5.29204800	-0.06156800
H	-4.54630800	-2.70026900	-0.30373100
H	1.15057500	4.07830000	-1.05597700
H	1.85377100	2.46397800	-1.15113900
H	1.90930600	3.36688900	0.36862500
H	1.14943900	-4.07877200	1.05585200
H	1.85311600	-2.46465900	1.15100000
H	1.90835900	-3.36759400	-0.36876400
H	1.87697500	1.39589200	1.65452200
H	4.30424700	1.37798400	1.69195100
H	4.30409000	-1.37894500	-1.69173700
H	1.87681800	-1.39652200	-1.65435600
C	4.52241600	-0.00041600	0.00004300
C	6.61503100	0.86246300	0.91219300
H	6.47431500	0.53202000	1.94529700
H	7.66972700	0.79997900	0.65740300
H	6.28342800	1.89756600	0.81058700
N	5.86107200	-0.00044800	-0.00001500
C	6.61486700	-0.86355100	-0.91218000
H	7.66966000	-0.80065600	-0.65789700
H	6.28357700	-1.89870200	-0.80997100
H	6.47359300	-0.53361300	-1.94536300

SBDPiR690 in S_0 State

C	-4.59503500	-0.78783000	-0.02054900
C	-3.23864600	-0.99869200	-0.01839500
C	-2.53866500	0.23511200	-0.02033900
C	-3.37974500	1.38181300	-0.02049000
S	-5.05570300	0.92093300	-0.03017500
N	-1.25112500	0.61935000	-0.01125500
C	-1.23332900	2.01629500	-0.00958200
C	-2.58220700	2.50332400	-0.01525700
B	-0.02936000	-0.33395000	-0.00587300
N	1.21456700	0.58144300	0.00668500

C	1.20610400	1.97172300	0.00744200
C	-0.00347600	2.67558600	-0.00101800
C	0.10475000	4.18552600	0.00058600
F	-1.07561000	4.81273700	-0.00986800
F	0.78760000	4.62085600	-1.07273700
F	0.76824800	4.61980200	1.08629800
F	-0.03794100	-1.13967200	-1.14696900
F	-0.05360100	-1.14808200	1.12897900
C	2.50372200	0.19193000	0.01834100
C	3.34656900	1.33560600	0.02301600
C	2.54715100	2.46044600	0.01757300
C	3.20063300	-1.04397200	0.01604100
C	4.55748800	-0.83792700	0.02216100
S	5.02063300	0.86963400	0.03589100
C	5.60503700	-1.86640200	0.02973700
C	5.33218800	-3.13729800	0.56068600
C	6.31215900	-4.12411500	0.56215400
C	7.57985600	-3.85776200	0.04235100
C	7.86175200	-2.59591500	-0.48028400
C	6.88299300	-1.60645700	-0.48765900
C	-5.64568200	-1.81253900	-0.02732300
C	-6.92240200	-1.54726700	0.49064900
C	-7.90481900	-2.53287400	0.48353600
C	-7.62777300	-3.79546000	-0.04003500
C	-6.36142800	-4.06688100	-0.56051700
C	-5.37734200	-3.08427700	-0.55856800
H	-2.77620900	-1.97726100	0.01172000
H	-2.88943900	3.53634100	-0.01424900
H	2.84450100	3.49926000	0.02021100
H	2.73576900	-2.02136100	-0.01706900
H	4.35716000	-3.34403000	0.99108800
H	6.08842500	-5.10079100	0.97997700
H	8.34413900	-4.62875700	0.04757300
H	8.84394000	-2.38146500	-0.88976300
H	7.11008200	-0.63511700	-0.91885700
H	-7.14568800	-0.57519400	0.92217300
H	-8.88596300	-2.31493800	0.89357300
H	-8.39512700	-4.56339100	-0.04541300
H	-6.14194100	-5.04424200	-0.97888300
H	-4.40320700	-3.29485700	-0.98905300

SBDPiR690 in S_1 State

C	-4.60983600	-0.79166100	-0.01445500

C	-3.23069600	-0.98832700	-0.01442100
C	-2.54692300	0.22963300	-0.01306700
C	-3.38668700	1.38064200	-0.01113400
S	-5.06226000	0.91979600	-0.01507100
N	-1.24466300	0.63163300	-0.00655500
C	-1.23542700	2.01659000	-0.00497300
C	-2.59491100	2.50507000	-0.00761100
B	-0.03122700	-0.31841700	-0.00335400
N	1.20861800	0.59276200	0.00293900
C	1.21055100	1.97088800	0.00353800
C	-0.00094700	2.69890900	-0.00066300
C	0.11092100	4.18932400	0.00021800
F	-1.07237500	4.81800900	-0.00630700
F	0.79528900	4.64571200	-1.07298500
F	0.78345800	4.64551100	1.08091300
F	-0.04136600	-1.13611400	-1.14104400
F	-0.04969600	-1.13958600	1.13171800
C	2.51037500	0.18375300	0.01060400
C	3.35574500	1.33223400	0.01144000
C	2.56597500	2.45931800	0.00882800
C	3.18817500	-1.03647000	0.01210200
C	4.56899100	-0.84622900	0.01513300
S	5.02890900	0.86262700	0.01770200
C	5.59522400	-1.87157200	0.01877300
C	5.26232400	-3.21263500	0.30763900
C	6.23970700	-4.19781300	0.30777900
C	7.56934900	-3.87457700	0.02531900
C	7.91446500	-2.55118500	-0.25697200
C	6.94213700	-1.56034100	-0.26083100
C	-5.64178500	-1.81168300	-0.01658400
C	-6.98583100	-1.49388400	0.26868600
C	-7.96378200	-2.47929300	0.26475100
C	-7.62699300	-3.80357300	-0.02313600
C	-6.30005400	-4.13323700	-0.31079900
C	-5.31714700	-3.15347300	-0.31051900
H	-2.75719600	-1.96185700	0.00723000
H	-2.89987400	3.53834800	-0.00540600
H	2.86366600	3.49746600	0.00922100
H	2.71006600	-2.00765900	-0.01153100
H	4.23970600	-3.47921200	0.55273000
H	5.96571000	-5.22291500	0.53669900
H	8.33099100	-4.64815000	0.02738100
H	8.94458500	-2.29205000	-0.48017900
H	7.23036800	-0.54069500	-0.50169800

H	-7.26740400	-0.47344600	0.51412000
H	-8.99170300	-2.21512500	0.49220600
H	-8.39298900	-4.57283900	-0.02556400
H	-6.03249100	-5.15907900	-0.54401900
H	-4.29666500	-3.42447900	-0.55973400

SBDPiR690 in S_2 State

C	-4.57721700	-0.82527300	-0.02286800
C	-3.21021200	-1.00594500	-0.02005100
C	-2.53278600	0.24606100	-0.02410600
C	-3.37486400	1.36657000	-0.02658200
S	-5.00595400	0.88585300	-0.03781300
N	-1.24608300	0.66979500	-0.01307300
C	-1.23933200	2.07566700	-0.01086000
C	-2.56989700	2.53032600	-0.01880300
B	-0.02011500	-0.29007500	-0.00497000
N	1.20659200	0.62136700	0.00685900
C	1.21730800	2.01723700	0.00706100
C	0.00693700	2.74705700	-0.00128900
C	0.11399600	4.23251800	0.00084000
F	-1.07688800	4.85448800	-0.00745700
F	0.79593500	4.70343500	-1.06999400
F	0.78001500	4.70146400	1.08241900
F	-0.05314200	-1.09976800	-1.14328300
F	-0.07081400	-1.10386700	1.12973800
C	2.50106500	0.19843700	0.01896400
C	3.34703600	1.32025800	0.02340900
C	2.55064400	2.47590800	0.01680900
C	3.17677900	-1.05011000	0.01688000
C	4.54037400	-0.87317800	0.02268500
S	4.99822200	0.83526000	0.03401700
C	5.58031800	-1.90776100	0.03099100
C	5.29505500	-3.18299400	0.54604000
C	6.26676400	-4.17820500	0.54535300
C	7.54316400	-3.91750200	0.04414300
C	7.83880800	-2.65148200	-0.46021600
C	6.86652200	-1.65524300	-0.47031400
C	-5.63027400	-1.84486100	-0.02609000
C	-6.89824400	-1.58537800	0.51549900
C	-7.88330600	-2.56859100	0.50574200
C	-7.61584100	-3.82543800	-0.03615800
C	-6.35597300	-4.09213600	-0.57412000
C	-5.37092900	-3.11018200	-0.57645200

H	-2.72917300	-1.97648000	0.00805900
H	-2.90354500	3.55510200	-0.01781000
H	2.86993800	3.50757500	0.01853400
H	2.69441200	-2.01975800	-0.01224400
H	4.31438600	-3.38695500	0.96503100
H	6.02963800	-5.15771800	0.94934500
H	8.30150100	-4.69426600	0.04958300
H	8.82727900	-2.43860200	-0.85558400
H	7.10701500	-0.68196200	-0.89008100
H	-7.11475800	-0.62106300	0.96860700
H	-8.85821400	-2.35389800	0.93212800
H	-8.38423800	-4.59216200	-0.04040800
H	-6.14208300	-5.06523200	-1.00524300
H	-4.40276400	-3.31648400	-1.02268100

SBDPiR690 in T_1 State

C	-4.61562400	-0.78600200	-0.02324600
C	-3.23496800	-0.98401700	-0.02058200
C	-2.55563100	0.23065800	-0.02438500
C	-3.39160800	1.38344700	-0.02957700
S	-5.06677400	0.92432800	-0.03750000
N	-1.24285000	0.63734400	-0.01318500
C	-1.23175100	2.00995100	-0.01366000
C	-2.59812500	2.50344800	-0.02454400
B	-0.03299200	-0.31544600	-0.00480600
N	1.20574900	0.59752900	0.00970500
C	1.20735900	1.96244700	0.01227700
C	0.00013500	2.69970300	-0.00129200
C	0.11506500	4.18157600	-0.00079100
F	-1.06875600	4.81329400	-0.01767200
F	0.81102100	4.64808900	-1.06735900
F	0.78164100	4.64999100	1.08345000
F	-0.03593700	-1.13057700	-1.14371600
F	-0.05691900	-1.13738300	1.12892200
C	2.51811300	0.18229600	0.02356700
C	3.36108300	1.33290600	0.03288100
C	2.57142300	2.45538700	0.02775400
C	3.18973000	-1.03404800	0.01933600
C	4.57348200	-0.84315200	0.02547400
S	5.03364400	0.86387700	0.04389600
C	5.60114300	-1.87463600	0.02044500
C	5.27180500	-3.20281900	0.35375600
C	6.24607500	-4.19284000	0.34663000

C	7.56562500	-3.88179300	0.01196800
C	7.90499200	-2.56856100	-0.31627200
C	6.93479600	-1.57367500	-0.31307300
C	-5.65044300	-1.81170700	-0.01831500
C	-6.98093200	-1.50383700	0.32009900
C	-7.95765000	-2.49265900	0.32275000
C	-7.62774100	-3.80687400	-0.01055300
C	-6.31103100	-4.12474100	-0.34986800
C	-5.33061600	-3.14058800	-0.35682300
H	-2.76522500	-1.95910700	0.00723800
H	-2.89700900	3.53805800	-0.02530600
H	2.86361000	3.49463500	0.03163500
H	2.71491400	-2.00655700	-0.01167000
H	4.25595300	-3.45681600	0.63810600
H	5.97651000	-5.21061300	0.61061600
H	8.32455800	-4.65792000	0.00863000
H	8.92751300	-2.31898100	-0.58119100
H	7.21565100	-0.56153000	-0.59174400
H	-7.25465100	-0.49077900	0.60250800
H	-8.97783300	-2.23723400	0.59124200
H	-8.39153300	-4.57822800	-0.00771200
H	-6.04835800	-5.14331100	-0.61783600
H	-4.31703800	-3.39972200	-0.64482000

SBDPiR690 in T_2 State

C	4.57381300	-0.83412300	0.02368900
C	3.21038600	-1.01068100	0.02253500
C	2.53865700	0.24388300	0.03019100
C	3.38732400	1.36160100	0.03467700
S	5.00505100	0.88336100	0.04183800
N	1.25524600	0.67204900	0.01775100
C	1.23707300	2.08937500	0.01544200
C	2.58632100	2.54553400	0.02630200
B	0.01071400	-0.29490300	0.00713300
N	-1.20885200	0.61153800	-0.00585300
C	-1.21758500	2.00219600	-0.00839700
C	0.00705800	2.73468500	0.00230600
C	-0.10291200	4.22632400	-0.00200400
F	1.08849200	4.84784000	0.00812200
F	-0.78369800	4.68900200	1.06783600
F	-0.76301000	4.68423000	-1.08665700
F	0.07140800	-1.09657900	1.14671100
F	0.09246400	-1.09909200	-1.12935800

C	-2.50965400	0.19650100	-0.01970500
C	-3.34638500	1.31897500	-0.02809800
C	-2.54077700	2.47133100	-0.02169600
C	-3.19443100	-1.05006000	-0.01626600
C	-4.55309500	-0.86423700	-0.02486800
S	-5.00952400	0.84438500	-0.04047400
C	-5.59727900	-1.89828800	-0.03261400
C	-5.32525300	-3.16614000	-0.57122000
C	-6.29915300	-4.15981100	-0.56850400
C	-7.56649300	-3.90383400	-0.04272400
C	-7.84988100	-2.64439000	0.48439900
C	-6.87421100	-1.65086700	0.49319600
C	5.63193000	-1.85041600	0.02631700
C	6.88686000	-1.59743800	-0.54611600
C	7.87456700	-2.57848800	-0.53842900
C	7.62098800	-3.82540100	0.03173200
C	6.37316400	-4.08502500	0.60018900
C	5.38619000	-3.10476600	0.60552300
H	2.72492700	-1.97886500	-0.00597100
H	2.93044600	3.56611800	0.02644300
H	-2.85249000	3.50516900	-0.02616400
H	-2.71973800	-2.02346400	0.01643400
H	-4.35198900	-3.36548000	-1.00962300
H	-6.07111200	-5.13388800	-0.99076300
H	-8.32700400	-4.67855900	-0.04712100
H	-8.83130100	-2.43446100	0.89876400
H	-7.10340400	-0.68264000	0.93050500
H	7.09172900	-0.64137800	-1.02187200
H	8.84010600	-2.36965100	-0.98837400
H	8.39122800	-4.59027300	0.03454900
H	6.17047000	-5.05061700	1.05303200
H	4.42713800	-3.30380000	1.07436900

SBDPiR688 in S_0 State

C	-4.59932400	0.22058900	-0.01339600
C	-3.24486500	0.00434100	-0.02763700
C	-2.54250100	1.23788900	-0.03995900
C	-3.38267500	2.38493000	-0.03522600
S	-5.05901300	1.92776000	-0.02420100
N	-1.25481600	1.62024900	-0.04391200
C	-1.23640100	3.01686500	-0.04565500
C	-2.58420100	3.50600900	-0.04091500
B	-0.03268400	0.66597800	-0.05288000

N	1.21137600	1.58233600	-0.03200900
C	1.20297400	2.97221200	-0.03148900
C	-0.00650200	3.67622800	-0.04235900
C	0.10217800	5.18707900	-0.04256000
F	-1.07767000	5.81381700	-0.07037000
F	0.79923500	5.61809300	-1.10768100
F	0.75137900	5.62137500	1.05109700
F	-0.04323300	-0.12408600	-1.20430600
F	-0.05442900	-0.16035000	1.07163700
C	2.50037200	1.19396000	-0.01765100
C	3.34292500	2.33758600	-0.00250000
C	2.54324100	3.46237500	-0.01271700
C	3.19839900	-0.04202400	-0.00582900
C	4.55356700	0.16825900	0.01696500
S	5.01696600	1.87414300	0.01883200
C	5.60178200	-0.86057100	0.02659000
C	5.34949400	-2.11737100	-0.54122800
C	6.32782400	-3.10525200	-0.53443900
C	7.56946900	-2.83722100	0.03645800
C	7.84038000	-1.59034600	0.60107100
C	6.85986000	-0.60803900	0.59640100
C	8.65693400	-3.87189000	0.03307700
F	8.23424900	-5.06875600	-0.40505600
F	9.17537500	-4.06394200	1.26274100
F	9.69106900	-3.51134500	-0.75608400
C	-5.65106600	-0.80430800	0.00382700
C	-6.90749800	-0.54089700	0.56502300
C	-7.89413500	-1.52166300	0.58434000
C	-7.62485700	-2.77320600	0.03915900
C	-6.37903000	-3.05299500	-0.52632000
C	-5.39891500	-2.07190100	-0.54698800
C	-8.65976100	-3.86039600	0.06135900
F	-9.85429300	-3.43154000	0.49975500
F	-8.29518100	-4.88425600	0.86136700
F	-8.85783700	-4.39348500	-1.16096800
H	-2.78440800	-0.97539000	0.00035100
H	-2.89041100	4.53931000	-0.03857400
H	2.84015700	4.50127400	-0.00536900
H	2.73441800	-1.02035500	0.01368300
H	4.39167100	-2.31852700	-1.00967200
H	6.12502000	-4.07300700	-0.98013200
H	8.80961600	-1.38971300	1.04806800
H	7.07010900	0.35184500	1.05914700
H	-7.11737500	0.42629700	1.01246200

H	-8.86157000	-1.31014900	1.02643000
H	-6.18040100	-4.02976000	-0.95765700
H	-4.44054700	-2.28142400	-1.01058600

SBDPiR688 in S_1 State

C	-4.61160400	0.21806100	-0.00843900
C	-3.23378500	0.01662300	-0.00513200
C	-2.54831700	1.23359200	-0.01354300
C	-3.38829300	2.38587700	-0.02331000
S	-5.06413500	1.92742200	-0.02636400
N	-1.24633500	1.63402500	-0.00866600
C	-1.23672600	3.01836400	-0.01960800
C	-2.59697100	3.50893500	-0.02875400
B	-0.03210500	0.68260700	0.00071900
N	1.20752700	1.59659100	0.00079900
C	1.20805200	2.97377900	-0.00981600
C	-0.00331400	3.70136800	-0.02025500
C	0.10863900	5.19326100	-0.03497200
F	-1.07450000	5.82073500	-0.04548700
F	0.79079200	5.63538300	-1.11425600
F	0.78320000	5.65710900	1.03986700
F	-0.04155100	-0.13936500	-1.13220100
F	-0.05008200	-0.12840500	1.14084500
C	2.50951700	1.19006700	0.00265900
C	3.35422400	2.34046700	-0.00158400
C	2.56400700	3.46553600	-0.01039300
C	3.18952000	-0.02856400	0.01165600
C	4.56908500	0.16736700	0.01307600
S	5.02807100	1.87414400	0.00194000
C	5.59714200	-0.85806100	0.01819700
C	5.26843000	-2.19607600	-0.27820500
C	6.24309500	-3.18386600	-0.27328600
C	7.56325200	-2.84918600	0.02411200
C	7.91427600	-1.52872600	0.31521800
C	6.94063400	-0.54379300	0.31340400
C	8.64319800	-3.89158100	0.01056000
F	8.15977600	-5.13759500	-0.11478300
F	9.38196900	-3.86630900	1.13783800
F	9.50916700	-3.70504300	-1.00815100
C	-5.64511200	-0.80228100	-0.00018800
C	-6.98500900	-0.48030300	0.28959200
C	-7.96861900	-1.45995700	0.29497700
C	-7.62494100	-2.77968500	0.01062600

C	-6.30172500	-3.12397900	-0.28034100
C	-5.32178800	-2.14594500	-0.28904100
C	-8.66081600	-3.86562000	0.02973000
F	-9.90952200	-3.38899800	0.15584400
F	-8.46741800	-4.72742300	1.05056500
F	-8.63356400	-4.60759600	-1.09546000
H	-2.76156900	-0.95731600	0.02658300
H	-2.90076800	4.54255900	-0.03620900
H	2.85962700	4.50430100	-0.01569200
H	2.71340900	-1.00067800	0.03980500
H	4.25026700	-2.46625200	-0.53494700
H	5.97575200	-4.20881500	-0.50635700
H	8.94397600	-1.27452300	0.54814800
H	7.22735900	0.47357700	0.56301900
H	-7.26722500	0.54005000	0.53191700
H	-8.99544900	-1.19584100	0.52304800
H	-6.04250800	-4.15369600	-0.50800700
H	-4.30438000	-2.42227700	-0.54227700

SBDPiR688 in S_2 State

C	-4.52724928	0.17597538	-0.03924832
C	-3.17215323	0.01899700	0.15222883
C	-2.50272471	1.26851519	0.08411093
C	-3.34158163	2.36944067	-0.15375690
S	-4.96959777	1.86535539	-0.30335283
N	-1.22603920	1.71345788	0.21761369
C	-1.23108455	3.10378802	0.05617251
C	-2.55230501	3.53659413	-0.16913387
B	-0.01184752	0.85067349	0.61448157
N	1.21109593	1.70743930	0.22573477
C	1.22211383	3.09787056	0.06585349
C	-0.00308146	3.80631083	0.06515660
C	0.00654414	5.28290509	-0.12860696
F	-1.08212881	5.88039312	0.39075406
F	0.04089440	5.64340823	-1.43591828
F	1.07487859	5.87115871	0.44298617
F	-0.01105238	-0.34969585	-0.09231944
F	-0.01515041	0.58900880	1.98583088
C	2.48606593	1.25689519	0.09827652
C	3.33053623	2.35478046	-0.13277325
C	2.54527770	3.52603801	-0.15025007
C	3.15005783	0.00394415	0.16632713
C	4.50676326	0.15600418	-0.01891928

S	4.95538737	1.84468575	-0.27550199
C	5.53526964	-0.88761586	-0.03114708
C	5.17682882	-2.21872452	-0.29354666
C	6.13683940	-3.22384095	-0.29713035
C	7.46932089	-2.90395827	-0.04719138
C	7.84601566	-1.58515310	0.20880836
C	6.88389871	-0.58542154	0.22052805
C	8.53375251	-3.96069059	-0.07083989
F	8.03257980	-5.20069786	-0.19034581
F	9.28514404	-3.94679473	1.04920741
F	9.39404152	-3.78786762	-1.09740888
C	-5.55821318	-0.86516907	-0.04658322
C	-6.90481444	-0.56118291	0.19767876
C	-7.87174410	-1.56154712	0.19680509
C	-7.49419640	-2.87924748	-0.04128968
C	-6.15774439	-3.20213661	-0.28705544
C	-5.19818964	-2.20183130	-0.29511565
C	-8.50796824	-3.98415052	-0.05262558
F	-9.74061515	-3.56228452	0.27250862
F	-8.18984572	-4.96987075	0.81185909
F	-8.60280104	-4.57002267	-1.26528183
H	-2.69398998	-0.93257711	0.34848869
H	-2.87418728	4.55250181	-0.33930447
H	2.87194003	4.54125895	-0.31654691
H	2.66721723	-0.94644423	0.35705541
H	4.14460306	-2.47099988	-0.51260215
H	5.84730377	-4.24868290	-0.50282673
H	8.88548626	-1.34076336	0.40690482
H	7.18821516	0.43257563	0.44610634
H	-7.20942353	0.45935402	0.41097231
H	-8.90954731	-1.31314003	0.39086887
H	-5.87163259	-4.23194393	-0.48060791
H	-4.16568717	-2.45639251	-0.50992223

SBDPiR688 in T_1 State

C	-4.61598700	0.22807900	-0.01144000
C	-3.23612800	0.02751500	-0.01074100
C	-2.55707300	1.24204300	-0.02057300
C	-3.39378800	2.39486800	-0.02898400
S	-5.06899900	1.93605600	-0.03158000
N	-1.24417700	1.64817100	-0.01559100
C	-1.23295700	3.01971500	-0.02355500
C	-2.60119800	3.51423000	-0.03223400

B	-0.03409800	0.69431100	-0.00775600
N	1.20397200	1.60979800	-0.00843600
C	1.20430600	2.97345700	-0.01494600
C	-0.00241300	3.71035200	-0.02173800
C	0.11221900	5.19358700	-0.02936300
F	-1.07185400	5.82388300	-0.03328900
F	0.79407700	5.65317500	-1.10672900
F	0.79243700	5.66359900	1.04448800
F	-0.04364200	-0.12703400	-1.14104400
F	-0.05020700	-0.11739600	1.13175600
C	2.51697500	1.19611600	-0.00800800
C	3.35978100	2.34739800	-0.00954500
C	2.57014600	3.46862600	-0.01487900
C	3.18905000	-0.01954300	-0.00040300
C	4.57182000	0.17505900	0.00406600
S	5.03281900	1.87971400	-0.00664400
C	5.59894000	-0.85907600	0.01059600
C	5.27123700	-2.17949100	-0.34456000
C	6.23991400	-3.17505000	-0.34096600
C	7.54902400	-2.85908600	0.01478300
C	7.89696100	-1.55366100	0.36707600
C	6.92869000	-0.56199400	0.36577400
C	8.62243500	-3.90832800	0.02170200
F	8.16300300	-5.12386600	-0.31411200
F	9.20082700	-4.02785000	1.23426400
F	9.61786700	-3.61309000	-0.83954900
C	-5.64945600	-0.80057400	0.00223200
C	-6.97557900	-0.49414800	0.35026400
C	-7.95374600	-1.48147900	0.36530600
C	-7.61143600	-2.78931400	0.03424400
C	-6.29926000	-3.11603400	-0.31700600
C	-5.32658800	-2.12979600	-0.33584600
C	-8.64068900	-3.88141800	0.03671600
F	-9.84542100	-3.45901400	0.45186000
F	-8.28441800	-4.90477400	0.83922700
F	-8.81397900	-4.41264500	-1.19149600
H	-2.76581800	-0.94724300	0.02017100
H	-2.89953100	4.54903300	-0.03787100
H	2.86106300	4.50827600	-0.01725200
H	2.71487100	-0.99257600	0.02416500
H	4.26010000	-2.43089400	-0.64510100
H	5.97582700	-4.18893500	-0.62098100
H	8.91946700	-1.31647700	0.64599100
H	7.20950500	0.44447900	0.66197100

H	-7.25232100	0.51738500	0.63258300
H	-8.97260000	-1.23222200	0.64079900
H	-6.04310600	-4.13809300	-0.58073400
H	-4.31607700	-2.38960200	-0.63139100

SBDPiR688 in T_2 State

C	-4.57806400	0.17937900	-0.01326900
C	-3.21469100	-0.00096800	-0.02348800
C	-2.54174400	1.25175300	-0.03835000
C	-3.39014500	2.37078700	-0.03987800
S	-5.00796300	1.89630700	-0.03160400
N	-1.25826900	1.67901300	-0.03934500
C	-1.24009700	3.09681700	-0.04293700
C	-2.58917300	3.55386800	-0.04446600
B	-0.01238500	0.71201000	-0.04169900
N	1.20631600	1.62045500	-0.02728300
C	1.21401500	3.01057900	-0.02747500
C	-0.01107700	3.74257600	-0.03994600
C	0.09859600	5.23528300	-0.04271500
F	-1.09280400	5.85566800	-0.06313000
F	0.78526700	5.69041500	-1.11105900
F	0.75209100	5.69721100	1.04353300
F	-0.07824000	-0.07942500	-1.18758400
F	-0.08792000	-0.09960100	1.08858800
C	2.50755700	1.20755600	-0.01410100
C	3.34294300	2.33173900	-0.00193500
C	2.53614800	3.48251400	-0.01167700
C	3.19412400	-0.03667300	-0.00356700
C	4.55249200	0.15375900	0.01622200
S	5.00643100	1.86225300	0.01945600
C	5.59598800	-0.87866200	0.02318000
C	5.32917300	-2.14915800	-0.50880900
C	6.30134400	-3.14285200	-0.49910000
C	7.55919800	-2.86984900	0.03364800
C	7.84761000	-1.60949800	0.55848200
C	6.87058600	-0.62361900	0.55583600
C	8.63944900	-3.90909400	0.03130100
F	8.20357300	-5.11307700	-0.37582200
F	9.18061300	-4.08237600	1.25527000
F	9.66445100	-3.57291800	-0.78208900
C	-5.63490000	-0.83703000	0.00366600
C	-6.88800200	-0.57402000	0.57198500
C	-7.87790700	-1.55176800	0.58630000

C	-7.61340900	-2.80219200	0.03673900
C	-6.36840100	-3.08244800	-0.53040900
C	-5.38709100	-2.10275100	-0.55330600
C	-8.65055400	-3.88673200	0.05750000
F	-9.84354400	-3.45538100	0.49798900
F	-8.28825000	-4.91348900	0.85477900
F	-8.85132500	-4.41670900	-1.16581900
H	-2.72928100	-0.96934500	0.00311400
H	-2.93314600	4.57451900	-0.04497700
H	2.84635800	4.51673600	-0.00685800
H	2.72015400	-1.01081000	0.01378600
H	4.36050000	-2.35658800	-0.95165100
H	6.08216600	-4.12005200	-0.91584800
H	8.82871000	-1.40126300	0.97558600
H	7.09770800	0.34583600	0.98967700
H	-7.09689600	0.38874400	1.03052700
H	-8.84349100	-1.33917000	1.03195500
H	-6.17157000	-4.05852000	-0.96423800
H	-4.43013200	-2.31201700	-1.02031300

SBDPiR698 in S_0 State

C	-4.59286700	-0.52063300	0.01290200
C	-3.23692800	-0.73190200	-0.00833300
C	-2.53744100	0.50232800	-0.02842400
C	-3.37885300	1.64870300	-0.01944500
S	-5.05456900	1.18730300	0.00061000
N	-1.25021700	0.88717900	-0.04093900
C	-1.23319300	2.28425300	-0.04464200
C	-2.58209600	2.77066000	-0.03101900
B	-0.02754500	-0.06500400	-0.05589800
N	1.21566300	0.85134400	-0.04190500
C	1.20622300	2.24169200	-0.04592800
C	-0.00390700	2.94455300	-0.05158400
C	0.10290100	4.45471800	-0.05509100
F	-1.07785300	5.08045000	-0.08659500
F	0.80121800	4.88583600	-1.11988900
F	0.74967100	4.89412400	1.03857500
F	-0.04343100	-0.85726400	-1.20676600
F	-0.04273200	-0.89234200	1.06904400
C	2.50493400	0.46275900	-0.02967900
C	3.34676700	1.60708200	-0.02139800
C	2.54677000	2.73142100	-0.03297100
C	3.20258500	-0.77287000	-0.00895700

C	4.55875000	-0.56486000	0.01215100
S	5.02111000	1.14242800	-0.00074400
C	5.60716400	-1.59139600	0.03199400
C	5.35752100	-2.85613700	-0.52502600
C	6.33058000	-3.84796700	-0.50392000
C	7.55663500	-3.55363600	0.07383900
C	7.84856900	-2.31743100	0.62805100
C	6.86319200	-1.33650200	0.60348400
F	8.50781300	-4.51214800	0.09418500
C	-5.64295400	-1.54478100	0.03240800
C	-6.90055000	-1.28466600	0.59831500
C	-7.88817200	-2.26306100	0.62219300
C	-7.59702700	-3.50144700	0.07217200
C	-6.36955000	-3.80063400	-0.50030000
C	-5.39371600	-2.81173900	-0.51991000
F	-8.55046500	-4.45711400	0.09129200
H	-2.77411800	-1.71043900	0.02029400
H	-2.88993400	3.80348700	-0.02735900
H	2.84373300	3.77032400	-0.02994500
H	2.73803900	-1.75065800	0.01998800
H	4.40164300	-3.06070600	-0.99660700
H	6.15511800	-4.82783000	-0.93468200
H	8.82124300	-2.13741900	1.07280500
H	7.07308300	-0.37191500	1.05708700
H	-7.11007000	-0.31819200	1.04805200
H	-8.86207500	-2.07959700	1.06277400
H	-6.19519800	-4.78209400	-0.92779400
H	-4.43651000	-3.02019500	-0.98699200

SBDPiR698 in S_1 State

C	-4.60673500	-0.52287300	-0.00007000
C	-3.22803100	-0.71905300	-0.00784700
C	-2.54513100	0.49978900	-0.01806000
C	-3.38558400	1.64999000	-0.01803400
S	-5.06089800	1.18761000	-0.01133200
N	-1.24334900	0.90279600	-0.01865100
C	-1.23514500	2.28799000	-0.02276100
C	-2.59481900	2.77531600	-0.02220000
B	-0.02929000	-0.04628300	-0.01944600
N	1.20988500	0.86561600	-0.01959800
C	1.21100000	2.24396500	-0.02387900
C	-0.00108100	2.97121300	-0.02610200
C	0.10975900	4.46165400	-0.02988100

F	-1.07402200	5.08941900	-0.03589200
F	0.79185800	4.91542500	-1.10554400
F	0.78400200	4.92133200	1.04835400
F	-0.04359000	-0.86559200	-1.15630800
F	-0.04244400	-0.86640800	1.11634700
C	2.51168800	0.45731700	-0.01926000
C	3.35621700	1.60611900	-0.01956500
C	2.56595300	2.73306100	-0.02386100
C	3.19027700	-0.76290600	-0.00909000
C	4.57033300	-0.57115400	-0.00144300
S	5.02977600	1.13721200	-0.01336400
C	5.59593000	-1.59634000	0.01420400
C	5.27025200	-2.93393700	-0.29955800
C	6.23743100	-3.92698200	-0.28254300
C	7.53986200	-3.57473700	0.04682300
C	7.91101000	-2.27391800	0.35755600
C	6.93388000	-1.28968600	0.33968700
F	8.48335300	-4.53624100	0.06314100
C	-5.63677400	-1.54406300	0.01503500
C	-6.97384300	-1.23150200	0.33795800
C	-7.95546400	-2.21139500	0.35451200
C	-7.58950800	-3.51390300	0.04505000
C	-6.28805300	-3.87190000	-0.28179500
C	-5.31643500	-2.88307100	-0.29754300
F	-8.53733600	-4.47135000	0.05986700
H	-2.75418900	-1.69236300	0.01966500
H	-2.90076000	3.80829500	-0.02269300
H	2.86325900	3.77131000	-0.02483100
H	2.71346600	-1.73473100	0.01910000
H	4.25621200	-3.19719900	-0.58012500
H	6.00052300	-4.95670700	-0.52741400
H	8.94106900	-2.05006600	0.61270100
H	7.21726300	-0.27482800	0.60368800
H	-7.25335800	-0.21523600	0.60063700
H	-8.98500400	-1.98277400	0.60753100
H	-6.05517800	-4.90275800	-0.52579400
H	-4.30299300	-3.15080800	-0.57605400

SBDPiR698 in S_2 State

C	-4.51250100	-0.59037600	0.05908200
C	-3.15991200	-0.74788200	-0.14284700
C	-2.49418600	0.50817100	-0.12149700
C	-3.33451300	1.61141200	0.09650000

S	-4.95981200	1.10567700	0.26222800
N	-1.21897700	0.95403200	-0.26412600
C	-1.22688500	2.34872300	-0.13161000
C	-2.54743200	2.78197800	0.08595600
B	0.00009400	0.08980900	-0.64539800
N	1.21850800	0.95342500	-0.26377400
C	1.22676100	2.34804900	-0.13169900
C	0.00020400	3.05365100	-0.15381800
C	0.00065100	4.53228000	0.01409100
F	-1.07910300	5.11713900	-0.53932500
F	1.07890300	5.11689900	-0.54236100
F	0.00257800	4.91704800	1.31596400
F	-0.00073100	-0.18941900	-2.01467000
F	-0.00087600	-1.10247800	0.07498000
C	2.49407400	0.50780900	-0.12168500
C	3.33442500	1.61123100	0.09586600
C	2.54759100	2.78143900	0.08541000
C	3.15991800	-0.74807000	-0.14261000
C	4.51241200	-0.59042400	0.05918700
S	4.96035800	1.10560900	0.26212100
C	5.54297200	-1.63213100	0.10921000
C	5.35426300	-2.83266200	-0.59492600
C	6.30699500	-3.84364600	-0.54841400
C	7.45557400	-3.63179800	0.19916900
C	7.68740400	-2.45974500	0.90077300
C	6.72003400	-1.46121400	0.85381800
F	8.38865500	-4.60855200	0.24319900
C	-5.54322500	-1.63186800	0.10917700
C	-6.72000000	-1.46095400	0.85422100
C	-7.68749300	-2.45935300	0.90111200
C	-7.45599300	-3.63123300	0.19909900
C	-6.30762100	-3.84306300	-0.54881700
C	-5.35476500	-2.83221300	-0.59532400
F	-8.38915500	-4.60784200	0.24311400
H	-2.67767700	-1.70993900	-0.26616400
H	-2.87159200	3.80019600	0.23750700
H	2.87156900	3.79975600	0.23664600
H	2.67790600	-1.71027400	-0.26561500
H	4.46247200	-2.97114600	-1.19800600
H	6.17543300	-4.77469900	-1.08911500
H	8.59933800	-2.34209900	1.47596900
H	6.88195600	-0.55051700	1.42386100
H	-6.88164600	-0.55047000	1.42469000
H	-8.59923600	-2.34178200	1.47662100

H	-6.17630400	-4.77401200	-1.08974900
H	-4.46310100	-2.97066700	-1.19859900

SBDPiR698 in T_1 State

C	-4.61226400	-0.51755400	0.00271100
C	-3.23176500	-0.71448800	-0.00524900
C	-2.55373000	0.50102600	-0.01860100
C	-3.39054800	1.65301600	-0.02041400
S	-5.06532900	1.19220600	-0.01327600
N	-1.24146000	0.90872700	-0.02015600
C	-1.23144800	2.28146900	-0.02604600
C	-2.59812800	2.77382000	-0.02572900
B	-0.03101900	-0.04319400	-0.02064400
N	1.20702100	0.87063000	-0.02033000
C	1.20781500	2.23571800	-0.02577700
C	0.00000500	2.97210300	-0.03018000
C	0.11386100	4.45413400	-0.03458800
F	-1.07051200	5.08489400	-0.04443000
F	0.80183300	4.91797700	-1.10724500
F	0.78792600	4.92566700	1.04374100
F	-0.04406600	-0.86141300	-1.15764700
F	-0.04372900	-0.86253500	1.11495700
C	2.51940900	0.45622800	-0.01854100
C	3.36167600	1.60719200	-0.01968300
C	2.57153400	2.72940000	-0.02490000
C	3.19141300	-0.76005900	-0.00548300
C	4.57471000	-0.56831500	0.00299600
S	5.03450100	1.13878000	-0.01209600
C	5.60177100	-1.59910800	0.01880000
C	5.27739500	-2.92625900	-0.32587400
C	6.24269000	-3.92281100	-0.31134800
C	7.53891100	-3.57986900	0.04740000
C	7.90679000	-2.28721300	0.38999600
C	6.93075800	-1.30008200	0.37387100
F	8.48095500	-4.54433300	0.06136500
C	-5.64508500	-1.54399200	0.01847700
C	-6.97215000	-1.23904100	0.37423200
C	-7.95330000	-2.22150500	0.39026300
C	-7.59199200	-3.51570400	0.04736100
C	-6.29759000	-3.86444700	-0.31193700
C	-5.32748800	-2.87228300	-0.32679200
F	-8.53891700	-4.47601200	0.06128900
H	-2.76037200	-1.68883200	0.02257200

H	-2.89796100	3.80814100	-0.02729200
H	2.86327600	3.76876400	-0.02607400
H	2.71631300	-1.73258400	0.02214900
H	4.26696700	-3.18093700	-0.62698400
H	6.00766300	-4.94699700	-0.57973300
H	8.93243600	-2.07013700	0.66742600
H	7.21036500	-0.29059900	0.66146800
H	-7.24678800	-0.22825600	0.66200800
H	-8.97777700	-1.99921900	0.66795800
H	-6.06736200	-4.88965600	-0.58065300
H	-4.31826600	-3.13144900	-0.62828800

SBDPiR698 in T_2 State

C	4.57129400	-0.56381600	-0.01414300
C	3.20823900	-0.73963500	-0.00360000
C	2.53795800	0.51549900	0.02522400
C	3.38742000	1.63224000	0.03293500
S	5.00473700	1.15292300	0.01948100
N	1.25477600	0.94480000	0.03039500
C	1.23756300	2.36214500	0.04309000
C	2.58703400	2.81733100	0.04456300
B	0.00965600	-0.02140200	0.02428300
N	-1.20935000	0.88581600	0.02923400
C	-1.21721500	2.27652900	0.03997400
C	0.00793100	3.00821500	0.04972800
C	-0.10110600	4.50000800	0.06035800
F	1.09070400	5.12045600	0.07635700
F	-0.78132900	4.95212600	1.13480700
F	-0.76118100	4.96885800	-1.01966600
F	0.08029600	-0.83122300	1.15782600
F	0.08064000	-0.81745900	-1.11826000
C	-2.51032700	0.47165600	0.02186900
C	-3.34629800	1.59460400	0.02520800
C	-2.54003400	2.74653600	0.03728100
C	-3.19583200	-0.77467700	-0.00184000
C	-4.55377200	-0.58690800	-0.01336900
S	-5.00989100	1.12108800	0.00961200
C	-5.59832200	-1.62029700	-0.02933100
C	-5.34973700	-2.87721600	0.54491800
C	-6.31569700	-3.87746500	0.52412000
C	-7.53918800	-3.59827000	-0.06499500
C	-7.83268800	-2.36965400	-0.63328200
C	-6.85117400	-1.38308100	-0.61444500

F	-8.48653700	-4.56477100	-0.08196900
C	5.62696900	-1.58229500	-0.03123900
C	6.86831400	-1.33698800	-0.63606900
C	7.85797400	-2.31440000	-0.65307500
C	7.58139700	-3.53838700	-0.06550200
C	6.36682600	-3.82327400	0.54012900
C	5.39165400	-2.83308000	0.56063600
F	8.53572700	-4.49377300	-0.08147200
H	2.72159700	-1.70699800	-0.03904100
H	2.93216000	3.83755400	0.05086300
H	-2.85122800	3.78051300	0.04302000
H	-2.72233400	-1.74871700	-0.03584900
H	-4.39691500	-3.06938700	1.02816400
H	-6.13640600	-4.85144700	0.96688100
H	-8.80313900	-2.19855100	-1.08669700
H	-7.06233100	-0.42505000	-1.08121900
H	7.06742100	-0.38550600	-1.12213800
H	8.82102500	-2.14131500	-1.12090800
H	6.20157000	-4.79404600	0.99486900
H	4.44481100	-3.02838000	1.05428500

SBDPiR710 in S_0 State

C	-4.59342500	-0.50279000	0.01569800
C	-3.23604600	-0.71084200	-0.00581000
C	-2.53801100	0.52312400	-0.02266400
C	-3.37977200	1.66941900	-0.01078800
S	-5.05526600	1.20651600	0.00992900
N	-1.25067500	0.90871300	-0.03611200
C	-1.23368800	2.30578600	-0.03845600
C	-2.58316500	2.79140500	-0.02238900
B	-0.02858200	-0.04328000	-0.05351500
N	1.21466100	0.87216100	-0.03972200
C	1.20587500	2.26256200	-0.04362200
C	-0.00417000	2.96582400	-0.04756700
C	0.10269400	4.47540200	-0.05152500
F	-1.07818400	5.10138500	-0.08490000
F	0.80227700	4.90716500	-1.11561200
F	0.74809400	4.91659300	1.04262500
F	-0.04606400	-0.83506100	-1.20520400
F	-0.04281300	-0.87271500	1.07045100
C	2.50390200	0.48227800	-0.02853000
C	3.34656900	1.62615800	-0.02065400
C	2.54716800	2.75089000	-0.03179300

C	3.19974900	-0.75339200	-0.00968300
C	4.55735800	-0.54899600	0.00889900
S	5.02051700	1.15936700	-0.00148700
C	5.60355700	-1.57607400	0.02557700
C	5.34110000	-2.85657500	-0.48247900
C	6.32285200	-3.84166600	-0.45766100
C	7.59467800	-3.58479000	0.06515400
C	7.85509500	-2.30185900	0.56391300
C	6.88052900	-1.31251400	0.54663800
C	8.65895200	-4.64878300	0.09964800
C	-5.64140200	-1.52712600	0.03124300
C	-6.91843700	-1.25985000	0.54250000
C	-7.89689800	-2.24962300	0.55850700
C	-7.63608300	-3.53136100	0.06596100
C	-6.35806000	-3.79344100	-0.44823600
C	-5.37640800	-2.81303100	-0.47045100
C	-8.69075100	-4.60503300	0.07249100
H	-2.77113400	-1.68830900	0.01728100
H	-2.89120600	3.82418100	-0.01744700
H	2.84489600	3.78958100	-0.02927700
H	2.73317200	-1.73008000	0.01732500
H	4.37157000	-3.07697900	-0.91887500
H	6.09998300	-4.82568600	-0.86160700
H	8.83533500	-2.07831700	0.97779200
H	7.10994800	-0.33470000	0.96217700
H	8.32184000	-5.56194300	-0.39634600
H	8.92278600	-4.89966700	1.13252300
H	9.57199600	-4.30496700	-0.39655300
H	-7.14973600	-0.28081800	0.95400100
H	-8.87796900	-2.02240500	0.96686100
H	-6.13531900	-4.78067600	-0.84570000
H	-4.40368200	-3.03665700	-0.89784500
H	-8.94502900	-4.90471000	-0.94969300
H	-9.60380800	-4.26031700	0.56331200
H	-8.33500300	-5.49828800	0.59566300

SBDPiR710 in S_1 State

C	-4.60757900	-0.50434100	0.00565300
C	-3.22682800	-0.69600500	0.00872900
C	-2.54577600	0.52234700	0.00277800
C	-3.38643600	1.67202300	-0.00410100
S	-5.06141700	1.20882500	-0.00628600
N	-1.24389300	0.92618800	0.00371100

C	-1.23583800	2.31139300	-0.00415700
C	-2.59528000	2.79763600	-0.00894100
B	-0.03060900	-0.02244200	0.01011400
N	1.20848900	0.88803000	0.00181200
C	1.21062400	2.26651300	-0.00607200
C	-0.00127500	2.99383200	-0.00774200
C	0.10965500	4.48368400	-0.01559300
F	-1.07414300	5.11217500	-0.01446300
F	0.78411400	4.93667000	-1.09702600
F	0.79155000	4.94703600	1.05671800
F	-0.04565200	-0.85225700	-1.11990000
F	-0.04381000	-0.83500400	1.15241900
C	2.51010500	0.47807800	-0.00081600
C	3.35552300	1.62590200	-0.00903500
C	2.56557700	2.75362800	-0.01291900
C	3.18624900	-0.74197800	0.00471800
C	4.56845200	-0.55551400	0.00015900
S	5.02838600	1.15531400	-0.01284400
C	5.58889600	-1.58162600	0.00338200
C	5.23721500	-2.94428800	-0.09864300
C	6.21220800	-3.93075700	-0.09446900
C	7.57223900	-3.60986600	0.00908600
C	7.92425700	-2.25467300	0.10822000
C	6.96020600	-1.26091000	0.10661700
C	8.63224600	-4.67497500	0.01861000
C	-5.63279300	-1.52616100	0.00754900
C	-7.00007100	-1.20171900	0.11241100
C	-7.97051800	-2.19392100	0.11122000
C	-7.62417000	-3.54650300	0.00673400
C	-6.26190700	-3.87256900	-0.09710600
C	-5.28511700	-2.89229100	-0.09835000
C	-8.66853100	-4.62695500	0.00164300
H	-2.75048800	-1.66792400	0.02192900
H	-2.90169100	3.83044100	-0.01513700
H	2.86402300	3.79151900	-0.01951600
H	2.70661600	-1.71225400	0.01920300
H	4.19523100	-3.23278700	-0.18921700
H	5.91485900	-4.97273600	-0.17650000
H	8.97319000	-1.98113600	0.19060200
H	7.27659400	-0.22487300	0.19376000
H	8.19798900	-5.66908200	-0.10849100
H	9.18661800	-4.66068200	0.96329400
H	9.35713500	-4.50934100	-0.78529100
H	-7.31354900	-0.16515700	0.20381700

H	-9.01745300	-1.91548500	0.19550100
H	-5.96961200	-4.91636000	-0.18170400
H	-4.24384600	-3.18331800	-0.18892000
H	-8.63346300	-5.19501800	-0.93425200
H	-9.67210400	-4.21033900	0.11257700
H	-8.49720900	-5.33651200	0.81806800

SBDPiR710 in S_2 State

C	4.51392000	-0.57306500	-0.05822400
C	3.16079200	-0.72880400	0.14330000
C	2.49474600	0.52710900	0.11855300
C	3.33498700	1.63020100	-0.10175500
S	4.96056600	1.12374500	-0.26671100
N	1.21968300	0.97277300	0.26127700
C	1.22731300	2.36782800	0.12721100
C	2.54785000	2.80051400	-0.09195300
B	0.00131700	0.10917400	0.64393000
N	-1.21780900	0.97189800	0.26266500
C	-1.22654400	2.36696700	0.12946500
C	0.00012400	3.07255100	0.15015900
C	-0.00112300	4.55052300	-0.01979200
F	1.07952700	5.13716100	0.53054400
F	-1.07847900	5.13608800	0.53815000
F	-0.00600200	4.93467300	-1.32217100
F	0.00235300	-0.16936100	2.01381800
F	0.00145100	-1.08425600	-0.07497900
C	-2.49294200	0.52564800	0.12187300
C	-3.33420600	1.62850200	-0.09600200
C	-2.54773000	2.79912700	-0.08701300
C	-3.15795700	-0.73079300	0.14518400
C	-4.51145100	-0.57576500	-0.05438700
S	-4.95968700	1.12102400	-0.26017300
C	-5.54207200	-1.61626100	-0.10165900
C	-5.34540000	-2.83032000	0.57196800
C	-6.30904000	-3.83272400	0.51886100
C	-7.50074000	-3.65761300	-0.19201600
C	-7.69716700	-2.43935000	-0.85462200
C	-6.73726200	-1.43572800	-0.81586700
C	-8.54557800	-4.74006300	-0.25370400
C	5.54515600	-1.61287800	-0.10601600
C	6.73753400	-1.43451500	-0.81953200
C	7.69933000	-2.44094400	-0.85747400
C	7.50304200	-3.65496400	-0.19410200

C	6.30882100	-3.82860400	0.51948900
C	5.34764000	-2.82834700	0.57118800
C	8.53368300	-4.75160400	-0.23873300
H	2.67792400	-1.69012500	0.26902600
H	2.87165200	3.81856600	-0.24513900
H	-2.87224800	3.81715700	-0.23891800
H	-2.67430700	-1.69202300	0.26848600
H	-4.44239800	-2.98437200	1.15540400
H	-6.13638300	-4.76492600	1.05042600
H	-8.61384200	-2.27858300	-1.41694000
H	-6.91342800	-0.51350300	-1.36400300
H	-8.26885700	-5.59213800	0.37169800
H	-8.67346100	-5.09902500	-1.28042000
H	-9.51706100	-4.36672300	0.08548300
H	6.91470900	-0.51379000	-1.36983500
H	8.61496400	-2.28075500	-1.42059800
H	6.13701300	-4.76047700	1.05299200
H	4.44431600	-2.98015200	1.15471300
H	8.83632400	-5.04487200	0.77160900
H	9.42536000	-4.43420200	-0.78454000
H	8.13195900	-5.64341900	-0.73122100

SBDPiR710 in T_1 State

C	4.61521500	-0.50150100	-0.01128900
C	3.23368500	-0.69777200	0.00024100
C	2.55502200	0.51706400	0.01171100
C	3.39119300	1.66962300	0.00862600
S	5.06609900	1.21023200	-0.00230900
N	1.24256200	0.92466500	0.01758500
C	1.23231500	2.29790600	0.02281900
C	2.59793000	2.79024800	0.01662000
B	0.03216100	-0.02680500	0.02397600
N	-1.20640600	0.88582400	0.01854500
C	-1.20776200	2.25130900	0.02433400
C	0.00031800	2.98779700	0.03063200
C	-0.11386200	4.46918400	0.03956200
F	1.07022500	5.10076600	0.06153900
F	-0.81046000	4.92953000	1.10864900
F	-0.77956500	4.94653900	-1.04201300
F	0.04577700	-0.83949500	1.16555000
F	0.04480800	-0.85339300	-1.10699000
C	-2.51884300	0.47074900	0.01378900
C	-3.36097700	1.62195800	0.01223100

C	-2.57050400	2.74436700	0.02001400
C	-3.19076900	-0.74500300	0.00248500
C	-4.57548300	-0.55472700	-0.00722900
S	-5.03364100	1.15430300	0.00253700
C	-5.60306100	-1.58206000	-0.01882100
C	-5.28194800	-2.91585700	0.29447200
C	-6.26087200	-3.90097400	0.28243200
C	-7.59019500	-3.60081100	-0.03762000
C	-7.91022000	-2.27057000	-0.34533800
C	-6.94152500	-1.27905200	-0.33781000
C	-8.65236600	-4.66539800	-0.05883300
C	5.64908800	-1.52426500	-0.02236900
C	6.98139000	-1.21859400	-0.34967500
C	7.95716000	-2.20831400	-0.35680300
C	7.64528000	-3.53434200	-0.03953200
C	6.31530400	-3.83870800	0.28832000
C	5.33427600	-2.85997400	0.30022200
C	8.69649800	-4.61015300	-0.03829900
H	2.76256600	-1.67236500	-0.02209600
H	2.89762300	3.82459400	0.01601900
H	-2.86254100	3.78363600	0.02052200
H	-2.71533100	-1.71745000	-0.02134500
H	-4.26651400	-3.18209700	0.56941800
H	-5.99014800	-4.92289000	0.53384400
H	-8.93541200	-2.01351600	-0.59962900
H	-7.22692400	-0.26371200	-0.60038000
H	-8.25657700	-5.62712500	0.27514500
H	-9.05150000	-4.79282800	-1.07077600
H	-9.49067200	-4.39289300	0.59018900
H	7.26161900	-0.20412800	-0.62105800
H	8.97882600	-1.94727500	-0.61903000
H	6.05089100	-4.86144700	0.54553100
H	4.32052400	-3.12772400	0.58009500
H	8.82018700	-5.02913200	0.96601700
H	9.66270200	-4.22070800	-0.36694400
H	8.41266500	-5.43321800	-0.70192800

SBDPiR710 in T_2 State

C	-4.57206700	-0.54834300	0.01880800
C	-3.20827600	-0.72279400	0.00791600
C	-2.53822600	0.53262800	-0.01829800
C	-3.38780500	1.64939100	-0.02376900
S	-5.00521800	1.16889000	-0.01067900

N	-1.25505700	0.96212500	-0.02529100
C	-1.23803100	2.37926800	-0.03772000
C	-2.58782100	2.83404700	-0.03631900
B	-0.01004700	-0.00368400	-0.02279700
N	1.20914400	0.90314000	-0.02759800
C	1.21691300	2.29394700	-0.03931600
C	-0.00823000	3.02545000	-0.04745400
C	0.10075800	4.51677000	-0.05934600
F	-1.09107500	5.13757600	-0.07548000
F	0.78064300	4.96881200	-1.13439100
F	0.76131800	4.98750900	1.01994900
F	-0.08229100	-0.81173600	-1.15784100
F	-0.07900900	-0.80256900	1.11824200
C	2.51027000	0.48867700	-0.02143500
C	3.34633800	1.61153600	-0.02655400
C	2.54002800	2.76353500	-0.03843700
C	3.19544100	-0.75775300	0.00188200
C	4.55410300	-0.57182400	0.01060300
S	5.00980700	1.13720500	-0.01263600
C	5.59910600	-1.60399900	0.02464200
C	5.34486600	-2.87410000	-0.51138000
C	6.32236700	-3.86501900	-0.48532900
C	7.58698700	-3.62311100	0.06014500
C	7.84138600	-2.34977000	0.58435900
C	6.86811100	-1.35751400	0.57178700
C	8.64932000	-4.69061900	0.08919500
C	-5.62897300	-1.56416200	0.03315500
C	-6.88065300	-1.31340000	0.60845900
C	-7.86571700	-2.29789900	0.61530400
C	-7.63240100	-3.55809200	0.05876000
C	-6.37610200	-3.80373800	-0.51282200
C	-5.39051100	-2.82634400	-0.53449000
C	-8.69208400	-4.62749000	0.06178200
H	-2.72123500	-1.69001800	0.04013700
H	-2.93284000	3.85431900	-0.04167200
H	2.85121800	3.79753500	-0.04514300
H	2.72110200	-1.73128300	0.03615900
H	4.38177000	-3.08214100	-0.96832900
H	6.10158100	-4.84133300	-0.90944800
H	8.81574400	-2.13527100	1.01729200
H	7.09225600	-0.38831300	1.01009200
H	8.30455300	-5.60442600	-0.40083900
H	8.92359200	-4.94037400	1.11958500
H	9.55874800	-4.35312800	-0.41831200

H	-7.08948300	-0.35494900	1.07802000
H	-8.82872400	-2.08361600	1.07098200
H	-6.17374000	-4.77436500	-0.95923600
H	-4.43507800	-3.03315500	-1.00780100
H	-8.95903900	-4.91312400	-0.96099100
H	-9.59800700	-4.28546500	0.56757000
H	-8.33507400	-5.52887400	0.57011000

SBDPiR731 in S_0 State

C	1.23329300	2.52855400	-0.03605400
N	1.24888300	1.13140000	-0.03365500
B	0.02679200	0.18070900	-0.00731600
N	-1.21511200	1.09652300	0.02681500
C	-1.20536400	2.48697600	0.03286800
C	0.00476700	3.18962100	-0.00096500
C	-2.50436300	0.70664800	0.05746300
C	-3.34584200	1.85081100	0.08382000
C	-2.54638800	2.97528400	0.06938000
C	2.58367500	3.01182300	-0.06759900
C	3.37832900	1.88881900	-0.08237500
C	2.53561300	0.74352400	-0.06137600
C	-3.19941000	-0.52832100	0.05331300
C	-4.55866400	-0.32742100	0.07929600
S	-5.01942900	1.38325600	0.11961700
S	5.05265700	1.42229700	-0.11420400
C	4.59012600	-0.28873400	-0.07899300
C	3.23037500	-0.49078100	-0.05794600
F	0.06976600	-0.63527600	1.12676600
F	0.01459600	-0.62674300	-1.14826200
C	-0.10112800	4.69849700	0.00255700
F	1.08026500	5.32433000	-0.02677300
F	-0.74646100	5.13572700	1.09859200
F	-0.80050600	5.13733900	-1.05942500
C	5.63387100	-1.31307600	-0.07849500
C	-5.60254800	-1.35299100	0.08020900
C	6.95244300	-1.01910800	0.28933100
C	7.94181900	-1.99858000	0.30326000
C	7.61531100	-3.30976000	-0.05664600
C	6.29942400	-3.62150000	-0.43356800
C	5.32818300	-2.63894700	-0.44579500
C	-5.29739000	-2.67640900	0.45568500
C	-6.26746300	-3.66054000	0.44387500
C	-7.58191400	-3.35246300	0.05994800

C	-7.90811500	-2.04362700	-0.30762500
C	-6.91960700	-1.06267900	-0.29465700
O	8.49448900	-4.33601700	-0.07410500
O	-8.46040000	-4.38031600	0.07893900
C	9.83932400	-4.07034000	0.30207400
C	-9.80361800	-4.11746400	-0.30385700
H	-2.84346200	4.01413100	0.08173200
H	2.89321500	4.04411600	-0.07569900
H	-2.72928200	-1.50222100	0.00654300
H	2.76007000	-1.46466700	-0.01491300
H	7.22509100	-0.01201500	0.59370400
H	8.94861700	-1.73138200	0.60020500
H	6.06664600	-4.64190600	-0.72058600
H	4.32178300	-2.89743300	-0.75939400
H	-4.29200500	-2.93168300	0.77523200
H	-6.03455300	-4.67918900	0.73709800
H	-8.91400400	-1.77883900	-0.60989900
H	-7.19155300	-0.05729300	-0.60524000
H	10.36489700	-5.02104600	0.21942100
H	9.89335300	-3.71040100	1.33515300
H	10.29769300	-3.33897500	-0.37215300
H	-10.32899100	-5.06815100	-0.21912500
H	-9.85404400	-3.76218800	-1.33878600
H	-10.26556500	-3.38334700	0.36501900

SBDPiR731 in S_1 State

C	1.23585900	2.53169000	-0.00727900
N	1.24211900	1.14590100	-0.00474800
B	0.02798700	0.19989100	0.00010800
N	-1.21011300	1.11015500	0.00575400
C	-1.21123300	2.48943600	0.00768200
C	0.00156300	3.21502500	-0.00031200
C	-2.51198600	0.70035900	0.01298200
C	-3.35582400	1.84824100	0.01927400
C	-2.56456900	2.97628700	0.01677300
C	2.59472100	3.01497300	-0.01583200
C	3.38490000	1.88746200	-0.01771600
C	2.54360700	0.73938100	-0.01137300
C	-3.18830100	-0.51976500	0.01214600
C	-4.57127600	-0.33464500	0.01835600
S	-5.02887800	1.37894100	0.02800200
S	5.05911400	1.42217200	-0.02629700
C	4.60435800	-0.29267200	-0.01638000

C	3.22226200	-0.48024600	-0.01020000
F	0.04616700	-0.62376800	1.13582800
F	0.03655700	-0.62301700	-1.13628200
C	-0.10744200	4.70409800	-0.00124500
F	1.07716700	5.33202800	-0.01020200
F	-0.77768800	5.16651900	1.07959500
F	-0.79253800	5.16402500	-1.07389000
C	5.62505000	-1.31343900	-0.01670200
C	-5.58901000	-1.35783200	0.01815400
C	6.99398800	-0.99445400	0.07777600
C	7.97583300	-1.97453800	0.07866800
C	7.60329800	-3.32300700	-0.01560800
C	6.24211500	-3.66622500	-0.11119400
C	5.27635500	-2.68380300	-0.11282000
C	-5.23650100	-2.72743700	0.11363200
C	-6.19940100	-3.71247800	0.11092100
C	-7.56156900	-3.37295500	0.01474300
C	-7.93789500	-2.02534400	-0.07878500
C	-6.95896200	-1.04254400	-0.07668600
O	8.47174500	-4.35087300	-0.02343800
O	-8.42684600	-4.40316800	0.02123700
C	9.86238700	-4.06104200	0.06658200
C	-9.81847400	-4.11791900	-0.06988600
H	-2.86298900	4.01416300	0.01998700
H	2.90329700	4.04708700	-0.01916300
H	-2.70819900	-1.48985800	-0.00075500
H	2.74376500	-1.45114900	0.00274700
H	7.30975300	0.04204700	0.16025800
H	9.01662500	-1.68394100	0.15451400
H	5.97423400	-4.71519000	-0.18694700
H	4.23470500	-2.97518000	-0.19600200
H	-4.19412200	-3.01604400	0.19710400
H	-5.92870600	-4.76075400	0.18612000
H	-8.97945900	-1.73768500	-0.15510500
H	-7.27753800	-0.00686300	-0.15865300
H	10.36822600	-5.02530900	0.04232200
H	10.09325100	-3.54783300	1.00581500
H	10.18875400	-3.45252300	-0.78316800
H	-10.32093300	-5.08397400	-0.04700000
H	-10.05003700	-3.60471200	-1.00891500
H	-10.14765700	-3.51132000	0.78011500

SBDPiR731 in S_2 State

C	1.24094300	2.59629600	-0.01970400
N	1.24516400	1.18878100	-0.02191500
B	0.01725000	0.23081900	0.00602700
N	-1.20709100	1.14280100	0.02280100
C	-1.21602100	2.53930800	0.01926000
C	-0.00462700	3.26813500	0.00104900
C	-2.50191300	0.72116200	0.04419400
C	-3.34632000	1.84393100	0.05079900
C	-2.54866800	2.99886000	0.03560800
C	2.57240500	3.04667100	-0.04114400
C	3.37449800	1.88061100	-0.05867700
C	2.52970600	0.76227700	-0.04730200
C	-3.17849400	-0.52744400	0.04747100
C	-4.54188400	-0.35101100	0.06048600
S	-4.99883500	1.35931800	0.07382800
S	5.00345800	1.39288500	-0.08921600
C	4.57128300	-0.31845000	-0.06467600
C	3.20296400	-0.49292000	-0.04757400
F	0.08099600	-0.57470300	1.14663100
F	0.04000000	-0.58878400	-1.12600300
C	-0.10974300	4.75291500	0.00185900
F	1.08229600	5.37346200	-0.01199800
F	-0.77069000	5.22557800	1.08538800
F	-0.79534600	5.22522200	-1.06670600
C	5.61801700	-1.34020400	-0.07959500
C	-5.58162200	-1.38263300	0.07869700
C	6.89269500	-1.09881400	0.44383300
C	7.88222200	-2.07982700	0.43019300
C	7.59645300	-3.33694000	-0.11054900
C	6.32201700	-3.59443900	-0.63805500
C	5.35153900	-2.60985000	-0.62675500
C	-5.30109300	-2.66008500	0.60046300
C	-6.26419200	-3.65285300	0.61026300
C	-7.54808800	-3.39685000	0.10680800
C	-7.85052100	-2.13281900	-0.40591200
C	-6.86779000	-1.14386000	-0.41719000
O	8.47912200	-4.36053600	-0.17063700
O	-8.42421700	-4.42949200	0.16316000
C	9.78332600	-4.14797100	0.35148500
C	-9.73682000	-4.21434600	-0.33382100
H	-2.86681100	4.03088100	0.03645700
H	2.90885700	4.07051100	-0.04407700
H	-2.69688100	-1.49743500	0.01630000

H	2.71840200	-1.46143800	-0.01205500
H	7.12726700	-0.13815700	0.89578000
H	8.85499300	-1.85637500	0.85138900
H	6.12116500	-4.57247600	-1.06354100
H	4.37888400	-2.81702200	-1.06271400
H	-4.32086300	-2.86766500	1.01884100
H	-6.04956900	-4.63615100	1.01685500
H	-8.83227900	-1.90776400	-0.80505700
H	-7.11667400	-0.17539200	-0.84334700
H	10.32150000	-5.08292800	0.19896300
H	9.74473400	-3.91909700	1.42208200
H	10.29405800	-3.34054000	-0.18431700
H	-10.26858200	-5.15459100	-0.19041500
H	-9.71737800	-3.96520300	-1.40057300
H	-10.24370500	-3.41942800	0.22422100

SBDPiR731 in T_1 State

C	1.23273900	2.52206900	-0.01607600
N	1.24078000	1.14788900	-0.01721900
B	0.02976300	0.19870000	-0.00286300
N	-1.20764300	1.11129500	0.01427100
C	-1.20883200	2.47777600	0.01469200
C	0.00075700	3.21277800	-0.00074600
C	-2.51926900	0.69602800	0.03225900
C	-3.36093900	1.84699300	0.04030200
C	-2.56980700	2.97003500	0.03131900
C	2.59783600	3.01113000	-0.03065800
C	3.38957700	1.88845500	-0.04044500
C	2.55181800	0.73763100	-0.03439500
C	-3.18970900	-0.52003300	0.03787200
C	-4.57593800	-0.33343800	0.05042600
S	-5.03322700	1.37871000	0.05935400
S	5.06331300	1.42530300	-0.05868700
C	4.61022600	-0.28827600	-0.05064900
C	3.22689700	-0.47870800	-0.03969900
F	0.05645900	-0.62390000	1.13200700
F	0.02791400	-0.62102100	-1.14016100
C	-0.11162300	4.69358400	0.00032500
F	1.07323300	5.32454100	-0.01695700
F	-0.77698300	5.16527200	1.08504000
F	-0.80766400	5.16430700	-1.06551700
C	5.63821000	-1.31103900	-0.05678500
C	-5.59903400	-1.35866500	0.05646200

C	6.98376100	-1.00625300	0.20862400
C	7.96854000	-1.98685800	0.21386400
C	7.61723700	-3.31575400	-0.05150500
C	6.27825200	-3.64127800	-0.32682300
C	5.31004500	-2.65858000	-0.33045500
C	-5.26437500	-2.70861000	0.31338500
C	-6.22966000	-3.69350600	0.30989200
C	-7.57248100	-3.36893600	0.05083000
C	-7.93036300	-2.03814700	-0.19826800
C	-6.94879500	-1.05519500	-0.19263500
O	8.48996300	-4.34416700	-0.06758400
O	-8.44137900	-4.39932700	0.06539400
C	9.85641300	-4.06894200	0.21516500
C	-9.81210700	-4.12651600	-0.20021700
H	-2.86230000	4.00913800	0.03412400
H	2.90001000	4.04471400	-0.03170000
H	-2.70999300	-1.49021200	0.01179300
H	2.75055400	-1.45062600	-0.01411500
H	7.27945000	0.01459700	0.43517500
H	8.99315100	-1.70949100	0.42954500
H	6.02711500	-4.67503300	-0.54132200
H	4.28698500	-2.93364000	-0.56439600
H	-4.23852900	-2.98408000	0.53376000
H	-5.97378700	-4.72865300	0.51152900
H	-8.95789700	-1.76180700	-0.40095500
H	-7.24983900	-0.03298000	-0.40530500
H	10.37192800	-5.02635600	0.15015600
H	9.97110700	-3.65800200	1.22380300
H	10.27629000	-3.37578300	-0.52126600
H	-10.32304900	-5.08657700	-0.13915700
H	-9.93860200	-3.70625600	-1.20351200
H	-10.22630900	-3.44225700	0.54756500

SBDPiR731 in T_2 State

C	1.23893800	2.61021200	-0.02656100
N	1.25432400	1.19333400	-0.02958800
B	0.00949400	0.22822900	-0.00040300
N	-1.20884100	1.13536300	0.02318100
C	-1.21598600	2.52641000	0.02211500
C	0.00944400	3.25719500	-0.00063800
C	-2.50950200	0.72077900	0.04898800
C	-3.34538100	1.84342000	0.06180900
C	-2.53910900	2.99568400	0.04516300

C	2.58942800	3.06278600	-0.05280900
C	3.38756400	1.87678200	-0.07232400
C	2.53659400	0.76171900	-0.05781400
C	-3.19400000	-0.52652300	0.05109200
C	-4.55274100	-0.34211900	0.06939300
S	-5.00885600	1.36743900	0.08969900
S	5.00430700	1.39140700	-0.09886400
C	4.56800100	-0.32547000	-0.06931900
C	3.20346000	-0.49564600	-0.05351900
F	0.10418500	-0.57190500	1.13842900
F	0.05578100	-0.57901600	-1.13718400
C	-0.09828400	4.74826000	0.00356700
F	1.09405600	5.36829200	-0.01630400
F	-0.74936100	5.20916900	1.09284700
F	-0.78688000	5.21255500	-1.06118200
C	5.61942700	-1.34488500	-0.08536700
C	-5.59575600	-1.37486400	0.08711700
C	6.87919300	-1.11458200	0.47572600
C	7.86998000	-2.09502900	0.46360000
C	7.59857300	-3.33900100	-0.11299700
C	6.33823500	-3.58452600	-0.67835000
C	5.36717500	-2.60010900	-0.66934000
C	-5.32691300	-2.64293100	0.63528800
C	-6.29044200	-3.63633800	0.64233000
C	-7.56392500	-3.38856400	0.11057700
C	-7.85571700	-2.13314000	-0.42759800
C	-6.87162500	-1.14444100	-0.43661400
O	8.48331900	-4.36101900	-0.17488300
O	-8.44236100	-4.42124800	0.16653500
C	9.77307100	-4.16086800	0.38636900
C	-9.74387100	-4.21275800	-0.35999800
H	-2.85037100	4.02969400	0.04986400
H	2.93578300	4.08260600	-0.05733700
H	-2.71940500	-1.49987200	0.01472200
H	2.71476600	-1.46185900	-0.01670400
H	7.10122100	-0.16500100	0.95685400
H	8.83199400	-1.88121200	0.91363800
H	6.14874400	-4.55253200	-1.13112800
H	4.40516400	-2.79619800	-1.13344400
H	-4.35465800	-2.84307300	1.07567800
H	-6.08375500	-4.61296600	1.06883000
H	-8.82976800	-1.91418800	-0.84865200
H	-7.11007500	-0.18251100	-0.88297300
H	10.31500300	-5.09271400	0.22822200

H	9.70602900	-3.95483300	1.46019200
H	10.29814400	-3.34252200	-0.11817500
H	-10.27937600	-5.15071200	-0.21480600
H	-9.70304100	-3.97803900	-1.42953000
H	-10.26213900	-3.41007100	0.17627000