Supporting Information

New dithienosilole and dithienogermole based BODIPY for solar cell applications

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1. Differential Pulse Voltametry (DPV) Studies

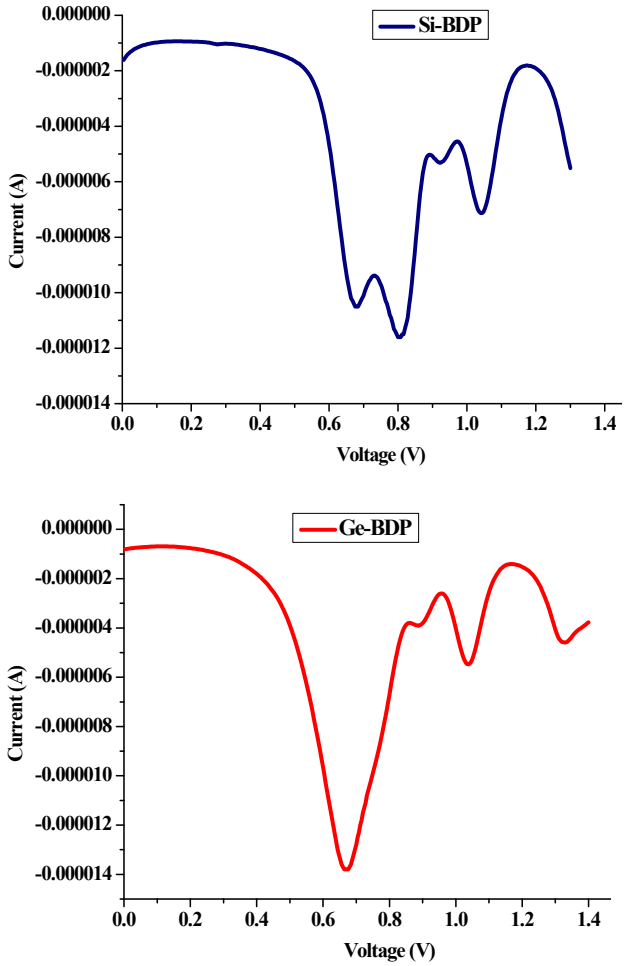


Figure S1 DPV oxidation potential curves of Si-BDP and Ge-BDP dyes in CH_2Cl_2 solution

2. DFT calculations:

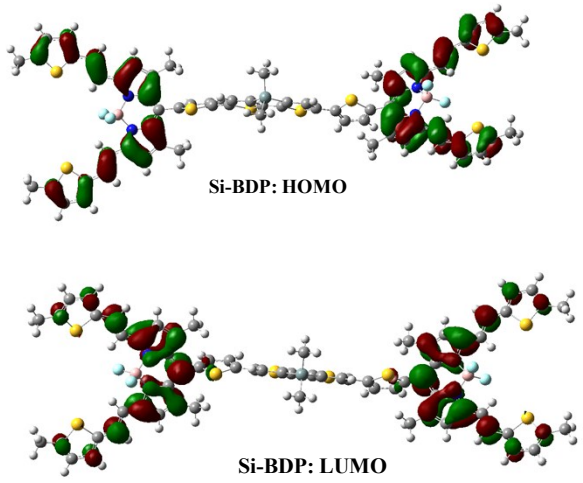


Figure S2 Distribution of frontier molecular orbitals (HOMO and LUMO) of Si-BDP

Table S1: Major allowed transitions for the dye Si-BDP calculated by B3LYP/6-311g (d,p) level of theory in DCM solvent.

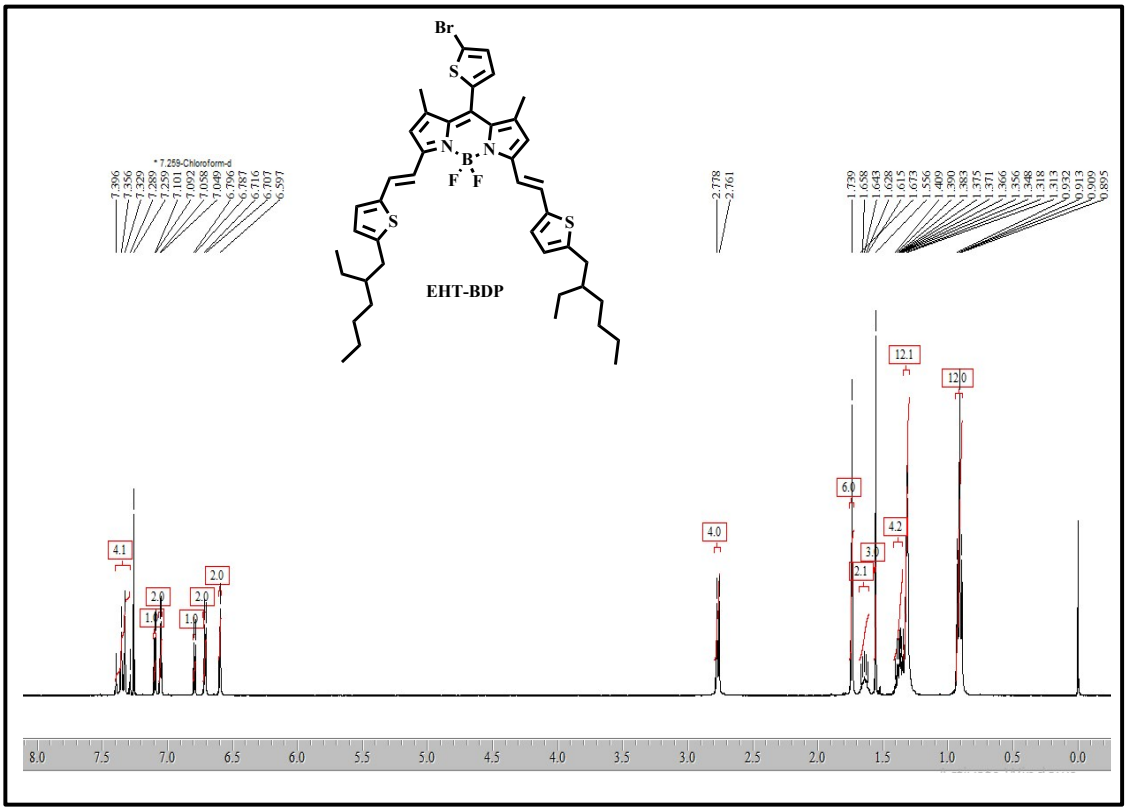
Excited state	Wavelength (nm)	Osc. strength	Major contributions
S_1	667.18	0.2404	H-2->LUMO (79%), HOMO->LUMO (18%)
S_2	665.78	0.0864	H-2->L+1 (64%), HOMO->L+1 (29%)
S_3	661.98	0.229	H-2->L+1 (25%), H-1->LUMO (56%), HOMO->L+1 (18%)
S_4	661.06	1.4855	H-2->LUMO (13%), H-1->L+1 (50%), HOMO->LUMO (37%)
S_5	653.33	0.0027	H-1->L+1 (49%), HOMO->LUMO (45%)
S_6	653.16	0.0027	H-1->LUMO (38%), HOMO->L+1 (53%)
S_7	488.81	1.2195	H-2->L+2 (23%), HOMO->L+2 (65%)
S_8	487.22	0.0003	H-1->L+2 (98%)
S_9	485.10	1.5445	H-4->LUMO (13%), H-3->L+1 (13%), H-2->L+2 (38%), HOMO->L+2 (33%)
S_{10}	468.94	0.0069	H-4->L+1 (39%), H-3->LUMO (41%), H-1->L+4 (10%), HOMO->L+3 (10%)

Table S2: Major allowed transitions for the dye Ge-BDP calculated by B3LYP/6-311g (d,p) level of theory in DCM solvent.

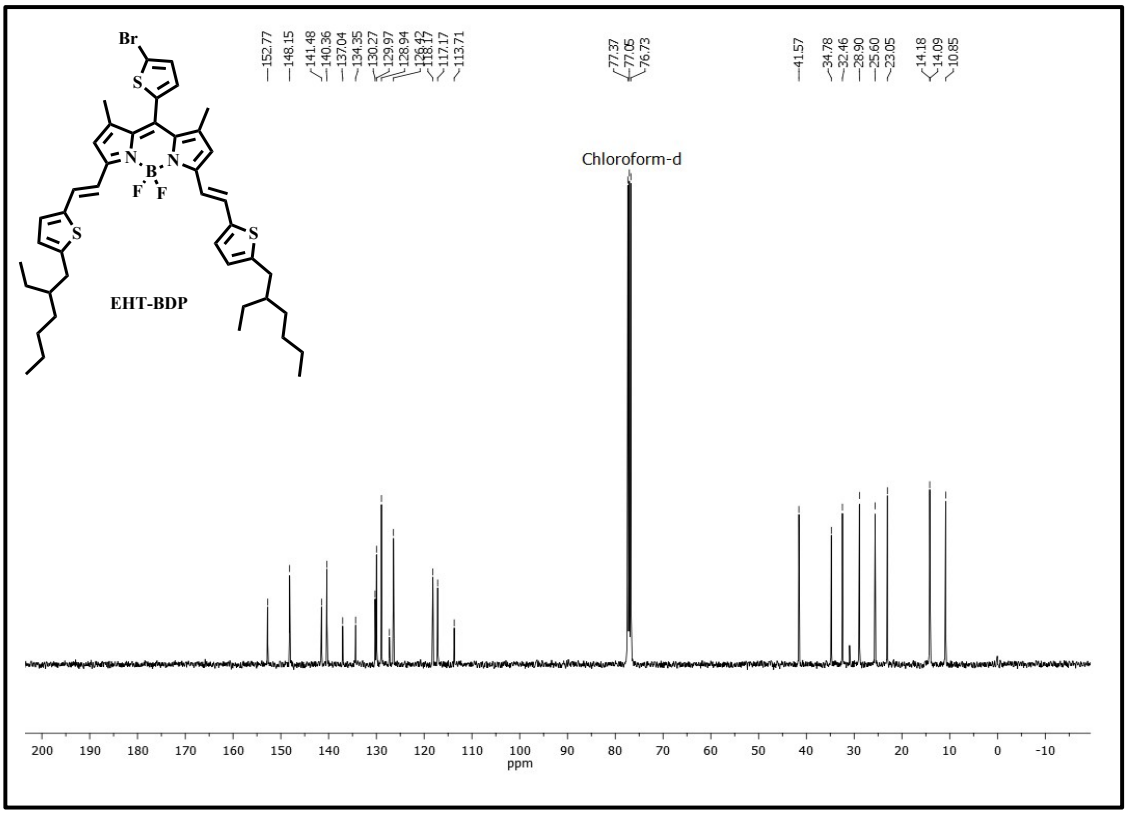
Excited state	Wavelength (nm)	Osc. strength	Major contributions
S_1	672.72	0.1083	H-2->LUMO (90%)
S_2	670.97	0.0133	H-2->L+1 (88%), HOMO->L+1 (10%)
S_3	662.55	0.2916	H-1->LUMO (59%), HOMO->L+1 (36%)
S_4	661.35	1.6273	H-1->L+1 (49%), HOMO->LUMO (48%)
S_5	653.43	0.0023	H-1->L+1 (52%), HOMO->LUMO (45%)
S_6	653.36	0.0018	H-1->LUMO (41%), HOMO->L+1 (55%)
S_7	486.72	2.2472	H-4->LUMO (13%), H-3->L+1 (13%), H-2->L+2 (44%), HOMO->L+2 (29%)
S_8	483.57	0.0003	H-1->L+2 (98%)
S_9	482.80	0.5367	H-2->L+2 (15%), HOMO->L+2 (70%)
S_{10}	468.90	0.0054	H-4->L+1 (39%), H-3->LUMO (41%), H-1->L+4 (10%), HOMO->L+3 (10%)

3. NMR spectra

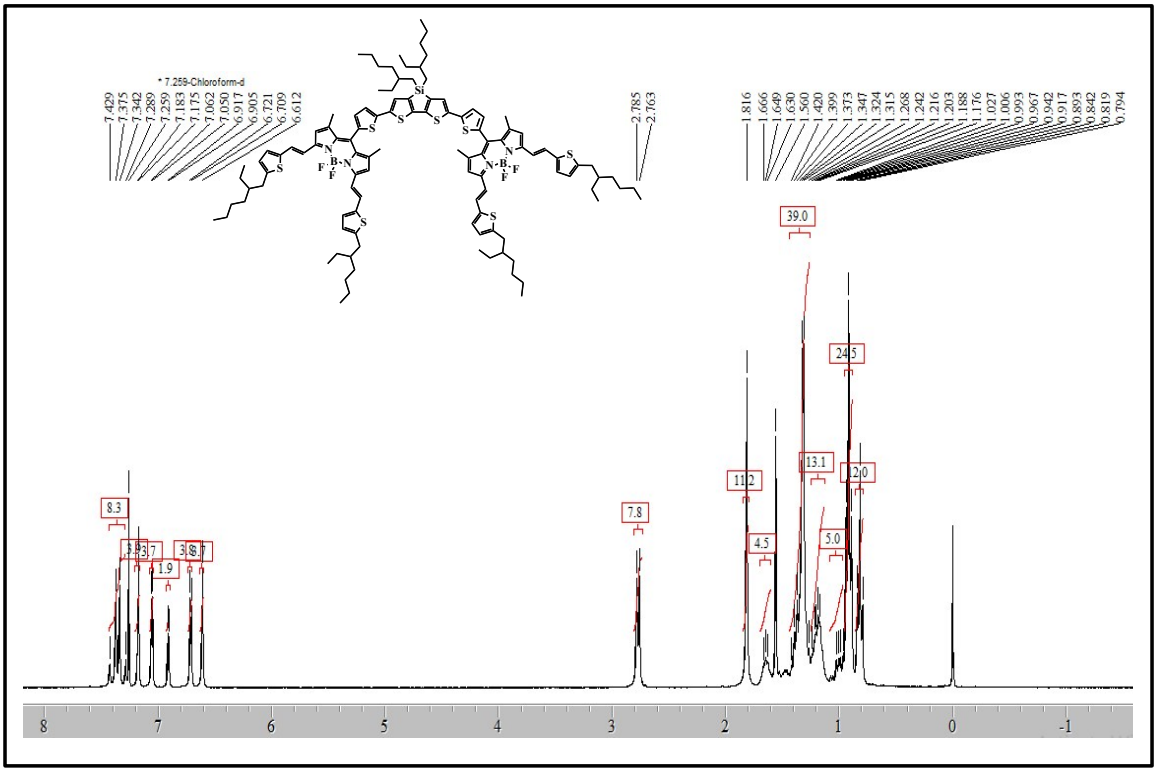
^{1}H NMR Spectrum of EHT-BDP in $CDCl_3$



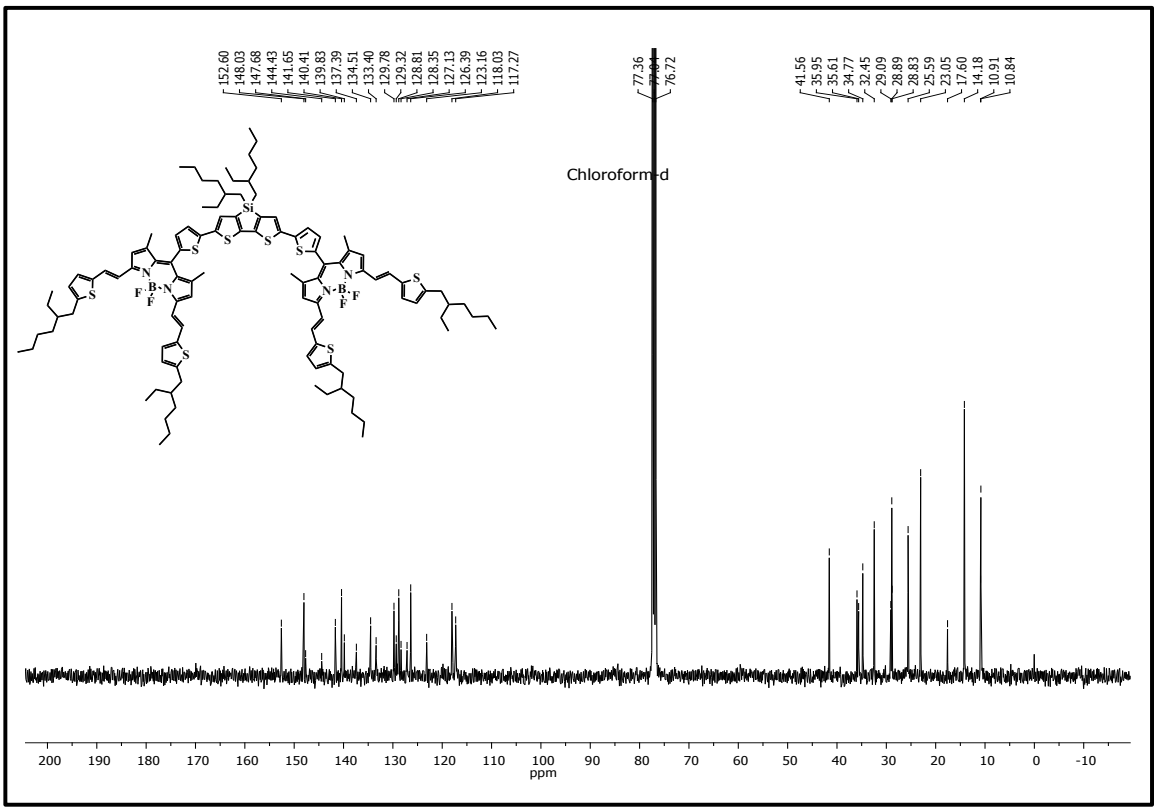
^{13}C NMR Spectrum of EHT-BDP in $CDCl_3$



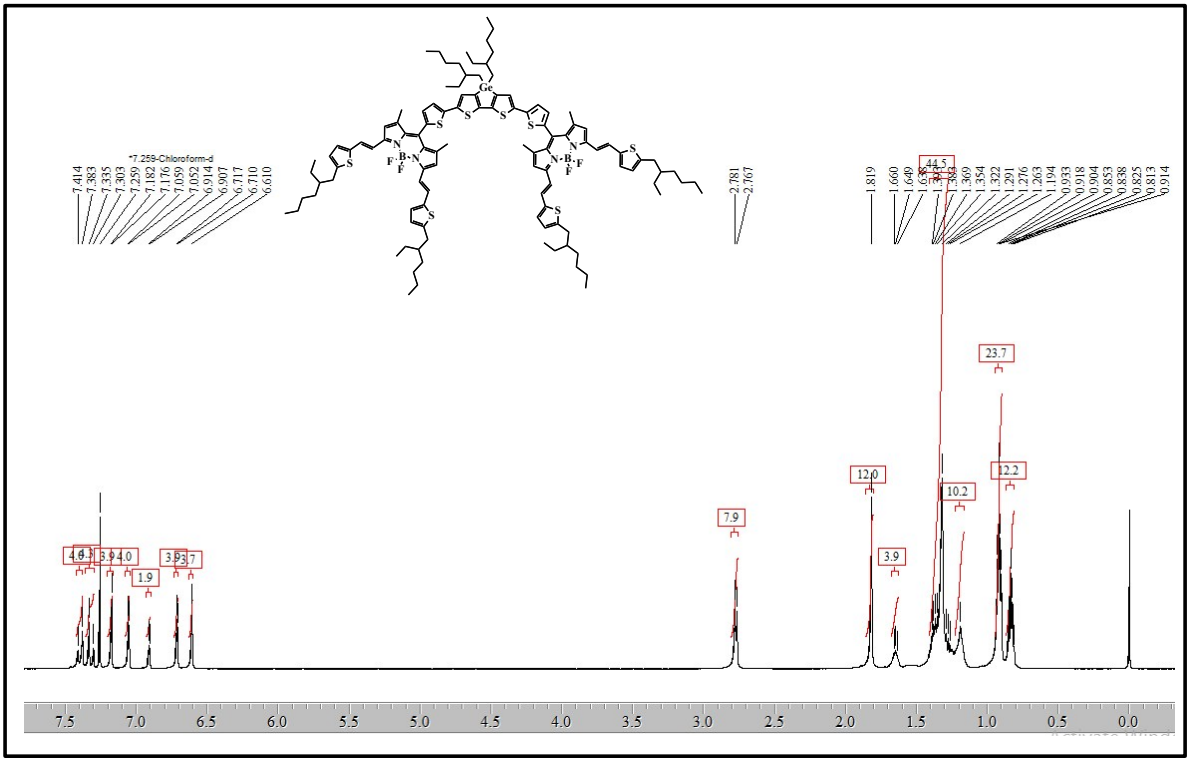
^{1}H NMR Spectrum of Si-BDP in $CDCl_3$



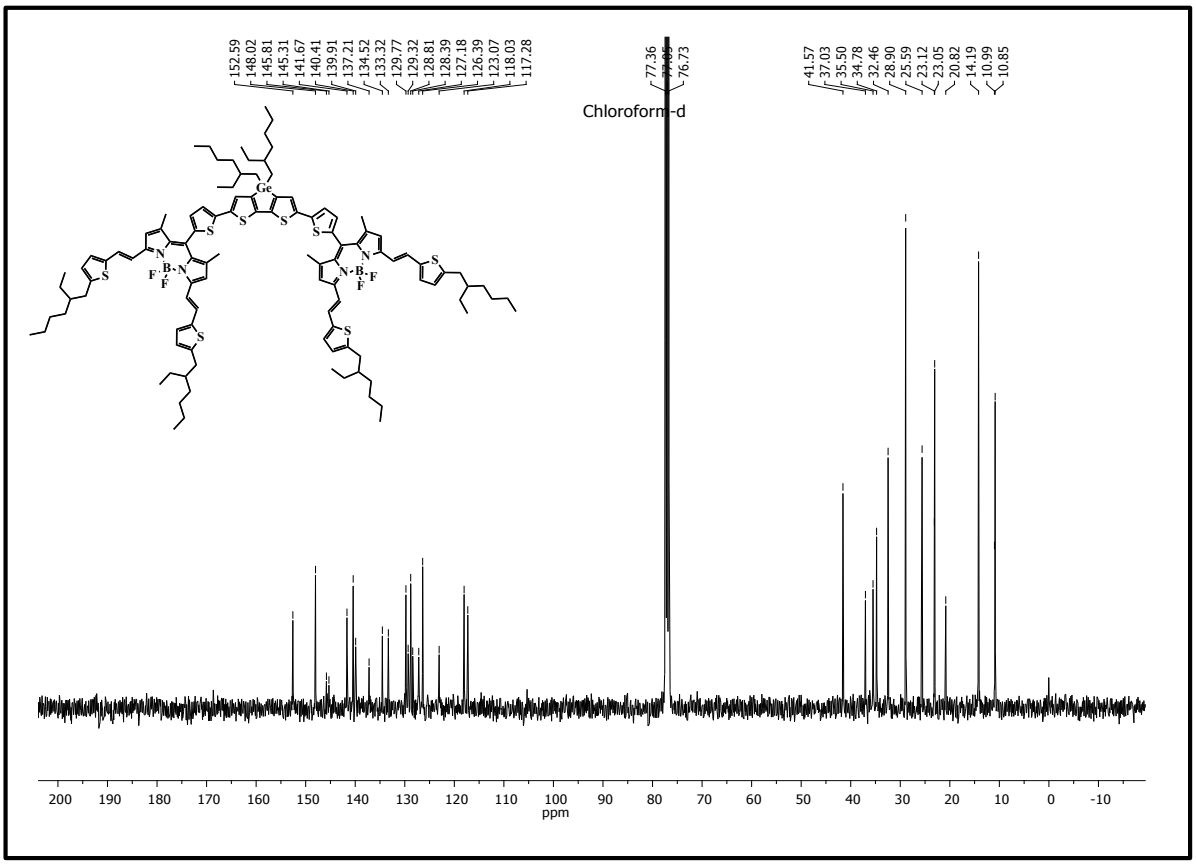
^{13}C NMR Spectrum of Sl-BDP in $CDCl_3$



^{1} H NMR Spectrum of Ge-BDP in $CDCl_3$



^{13} C NMR Spectrum of Ge-BDP in $CDCl_3$



4. Mass Spectra