Supporting Information for

Ferrocene-Isocoumarin Conjugated Molecules: Synthesis, Structural Characterization, Electronic Properties, and DFT-TDDFT Computational Study

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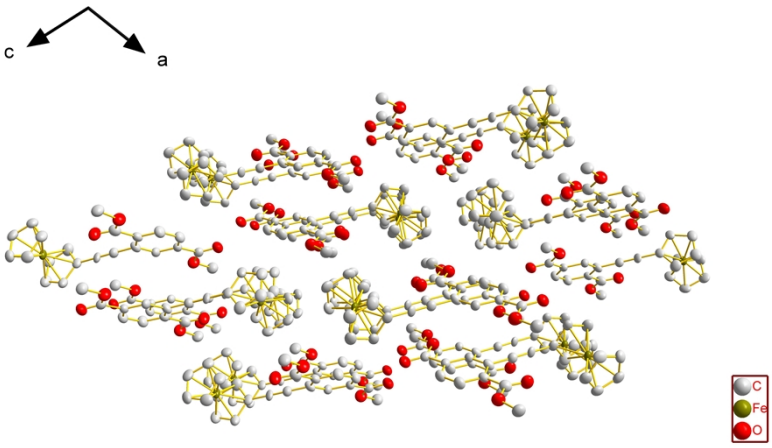


Fig. S1 (a) Packing structure of **Fc-TP** along the *b* axis.

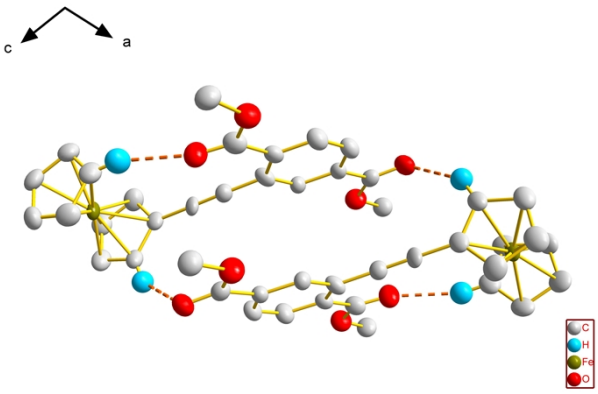


Fig. S2 Hydrogen-bonding interactions in **Fc-TP**.

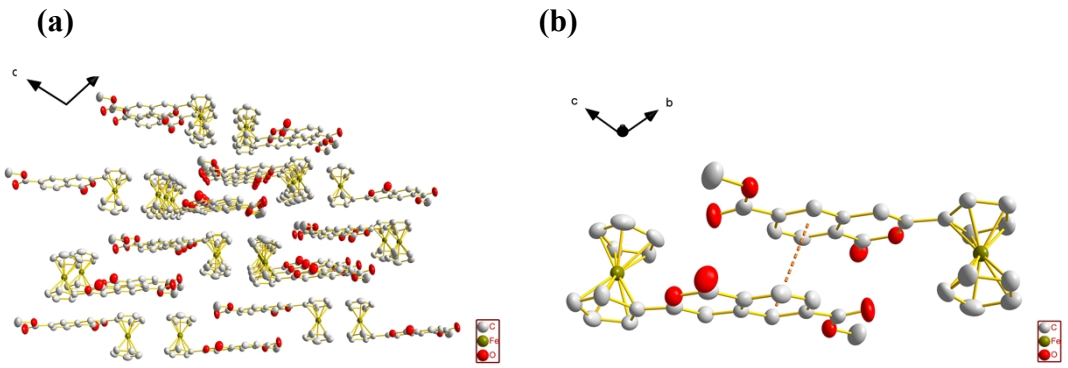


Fig. S3 (a) Packing structure of **Fc-Icm** along the *a* axis; (b) π-π interactions in **Fc-Icm**.

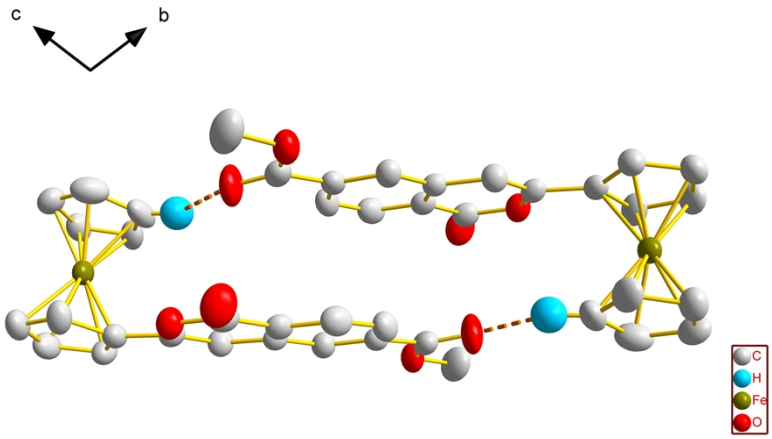


Fig. S4 Hydrogen-bonding interactions in **Fc-Icm**.

Table S1 Hydrogen bond distances (Å) and angles (º) for **Fc-TP** and **Fc-Icm**.

	D-H/ Å	H···A/ Å	D···A/ Å	Angle/ º
		Fc-TP		
C6-H6···O2	0.98 (4)	2.39 (29)	3.336 (51)	162.4 (219)
C2-H2···O4	0.98 (26)	2.45 (25)	3.315 (38)	147.7 (180)
		Fc-Icm		
C2-H2···O4	0.98 (44)	2.47 (30)	3.320 (52)	145.3 (235)

Table S2 Selected bond lengths (Å) and angles (deg) of **Fc-TP** and **Fc-Icm** predicted by DFT calculation.

		Fc-TP	
C1-C11	1.422	C11-C12	1.226
C12-C13	1.431	C13-C14	1.430
C14-C19	1.493	C19-O1	1.244
C19-O2	1.387	C21-O3	1.245
C21-O4	1.382		
C1-C11-C12	178.9	C11-C12-C13	176.7
C2-C1-C11	126.3	C5-C1-C11	126.3
C12-C13-C14	124.1	C12-C13-C18	117.8
		Fc-Icm	
C10-C11	1.456	C11-C12	1.366
C12-C13	1.446	C13-C14	1.426
C14-C15	1.474	C15-O1	1.237
C15-O2	1.420	C11-O2	1.404
C20-O3	1.380	C20-O4	1.245
C11-C12-C13	120.7	C12-C13-C14	119.4
C13-C14-C15	120.3	C14-C15-O2	115.9
O2-C11-C12	120.3	C15-O2-C11	123.5
C10-C11-C12	127.4	C9-C10-C11	125.5
C6-C10-C11	126.8		

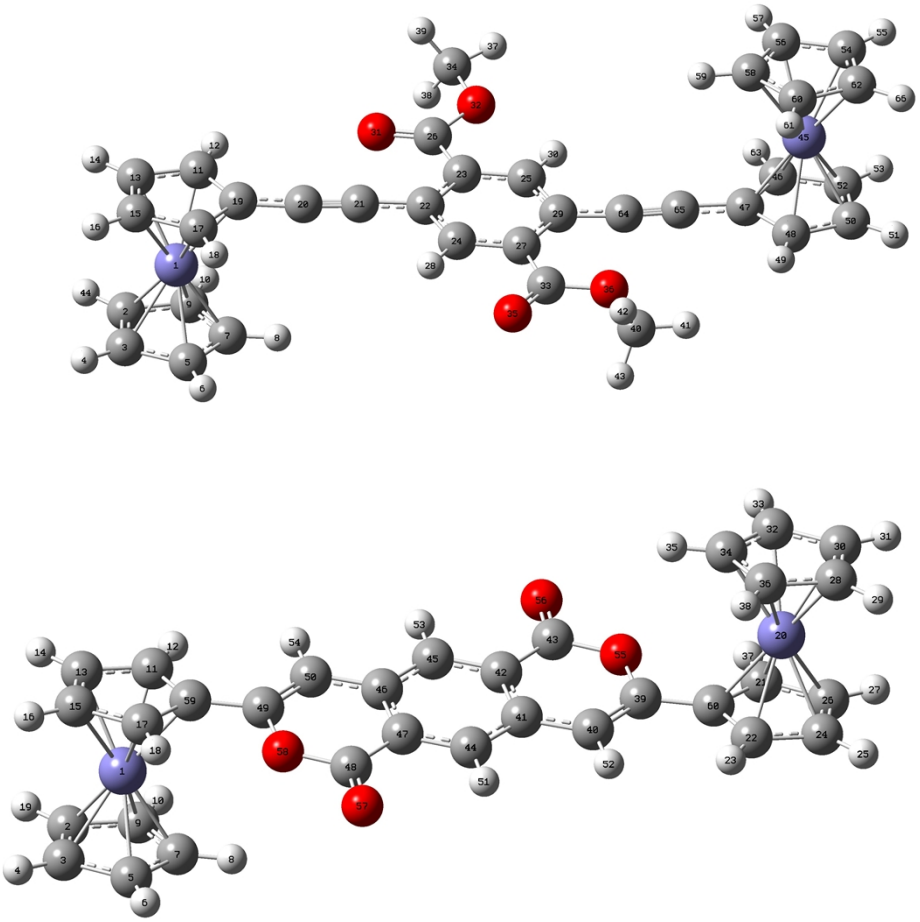


Fig. S5 Optimized ground-state geometries of **BFc-TP** and **BFc-PIcm** with *trans*-structure as predicted by DFT calculations.

Table S3 Selected bond lengths (Å), angles (°) and torsion angles (°) of *trans*-**BFc-TP** and *trans*-**BFc-PIcm** predicted by DFT calculations

		trans-**BFc-TP**	
C19-C20	1.418	C20-C21	1.227
C21-C22	1.425	C29-C64	1.428
C64-C65	1.227	C65-C47	1.420
C19-C20-C21	176.4	C20-C21-C22	176.9
C29-C64-C65	174.0	C64-C65-C47	178.2
C27-C29-C47-C48	-4.7	C27-C29-C47-C46	175.3
C11-C19-C22-C24	-176.6	C11-C19-C22-C23	4.2
		trans-**BFc-PIcm**	
C49-C59	1.455	C49-C50	1.366
C46-C50	1.445	C39-C60	1.455
C39-C40	1.366	C40-C41	1.445
C21-C60-C39-C40	168.1	C43-C42-C41-C44	-179.8
C45-C46-C47-C48	179.8	C17-C59-C49-C50	-168.08

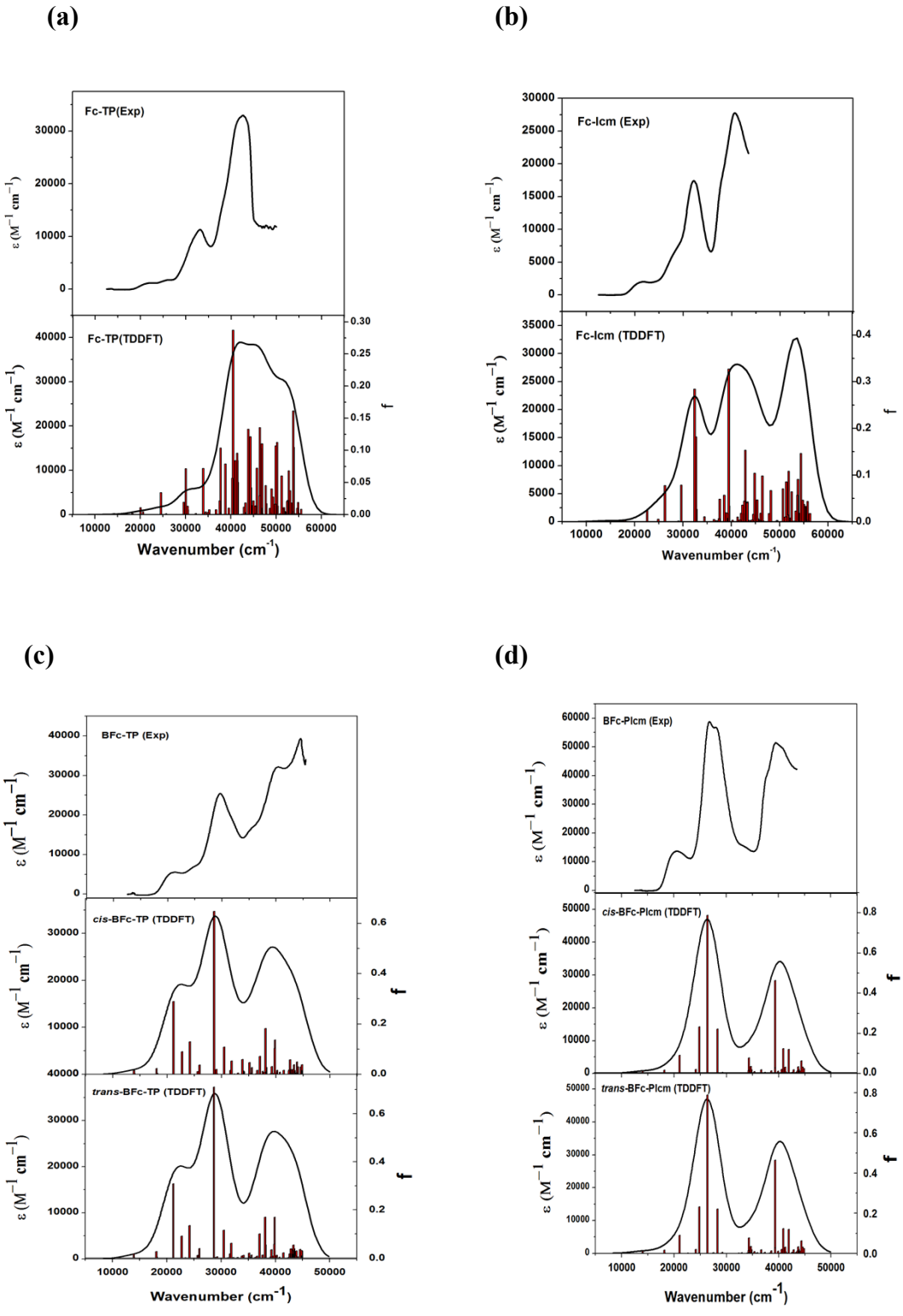
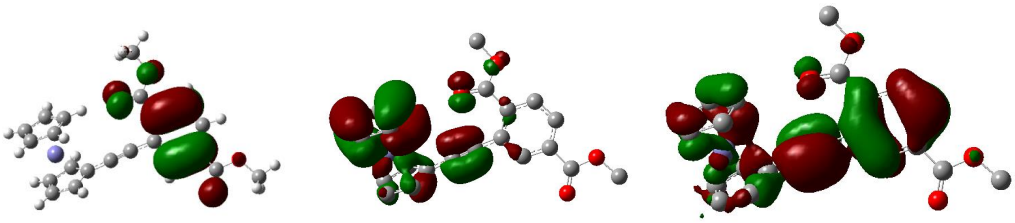


Fig. S6 Experimental (top) and TDDFT predicted (bottom) UV-vis spectra of (a) **Fc-TP**, (b) **Fc-Icm**, (c) **BFc-TP** and (d) **BFc-PIcm**.



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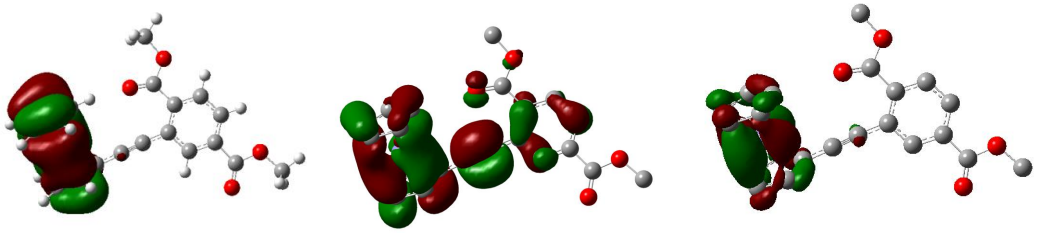

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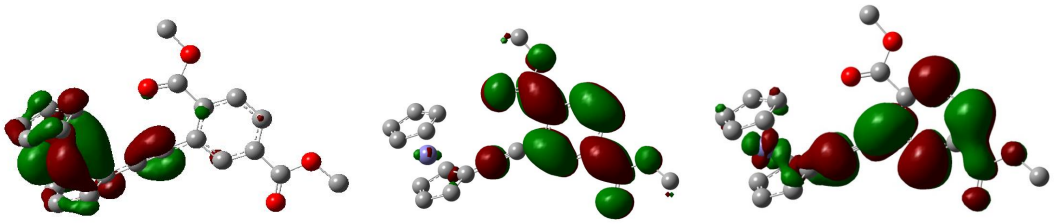

HOMO LUMO LUMO+1

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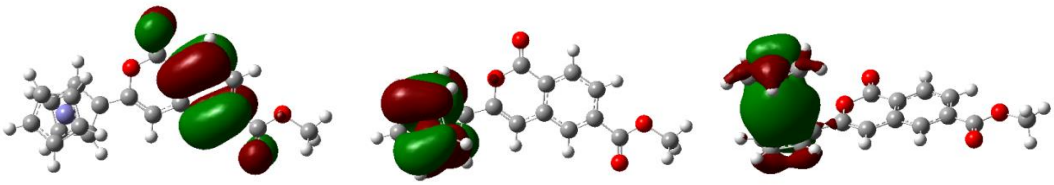

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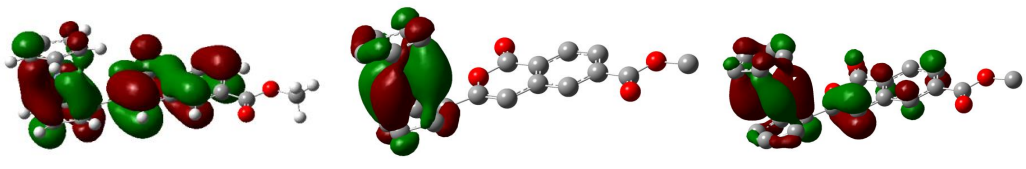
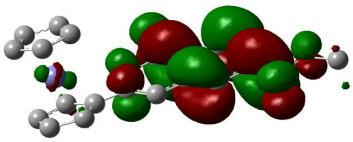


HOMO-2 HOMO-1 HOMO



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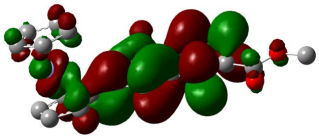

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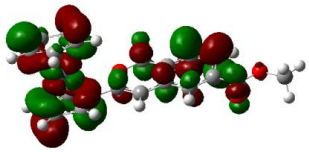

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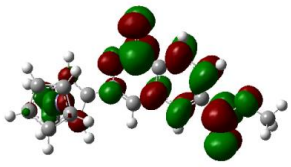

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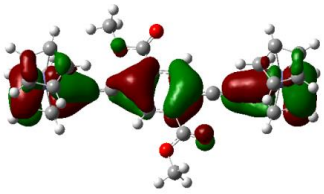

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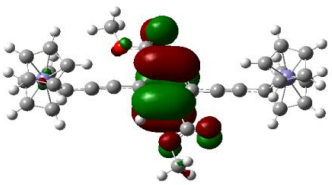

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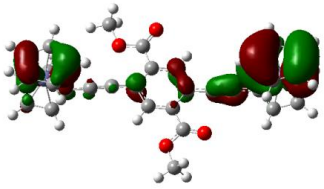

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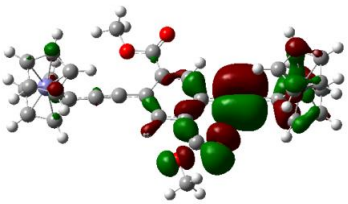

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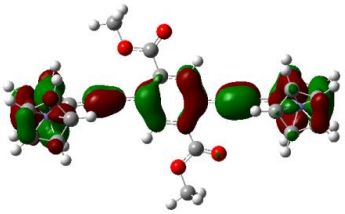

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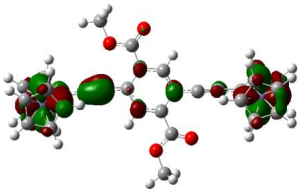

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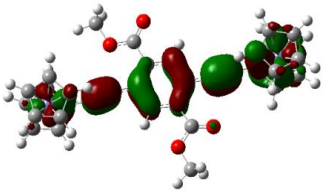

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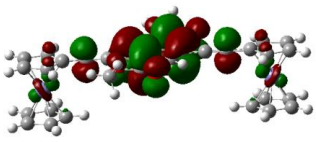

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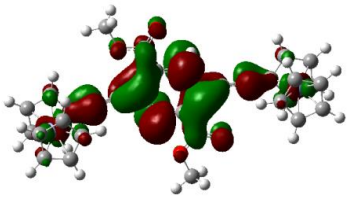

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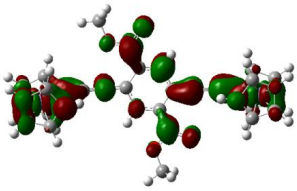

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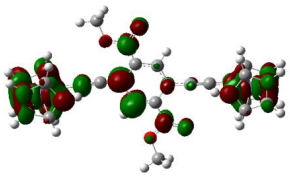

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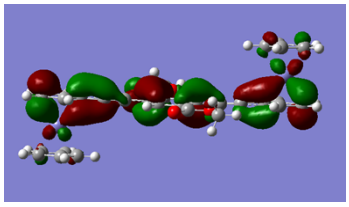

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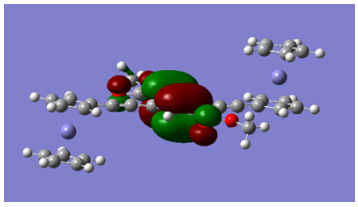

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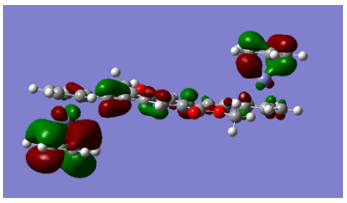

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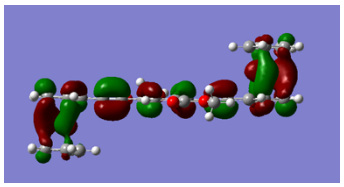

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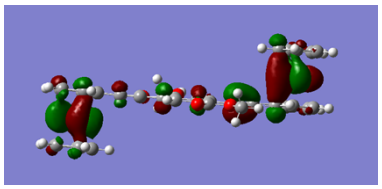

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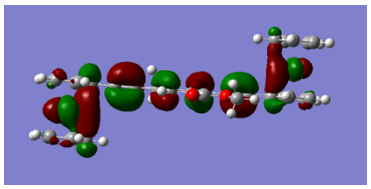

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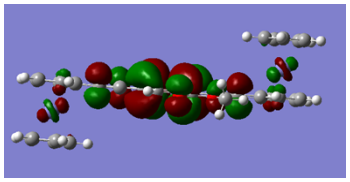

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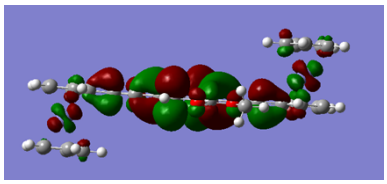

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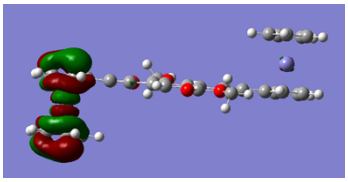

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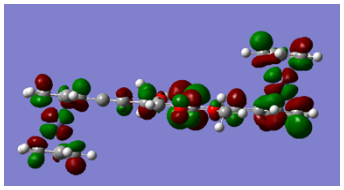

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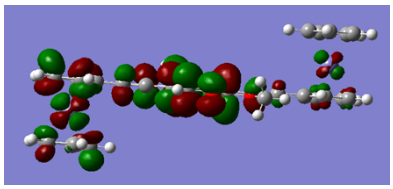

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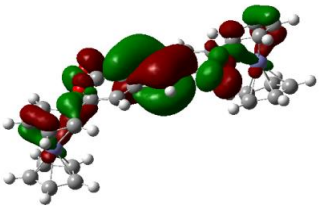

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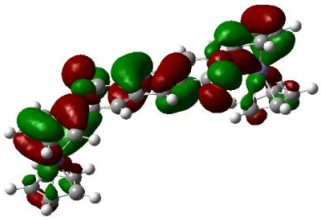

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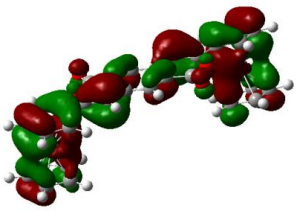

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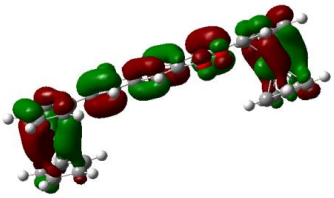

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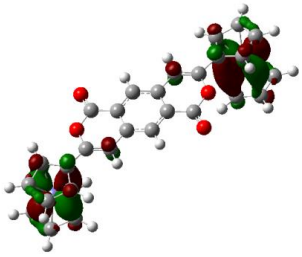

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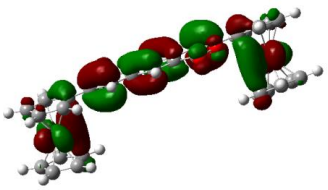

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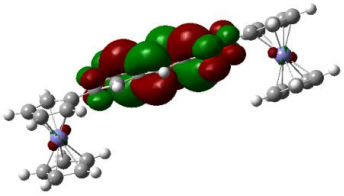

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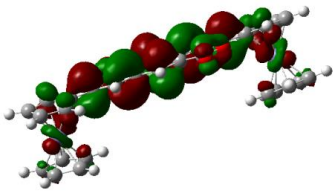

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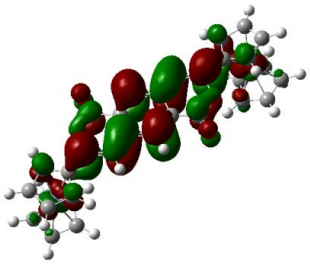

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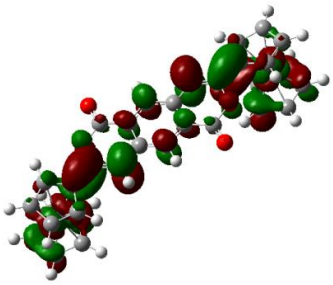

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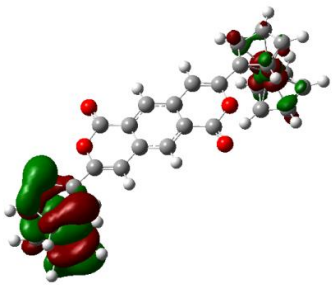
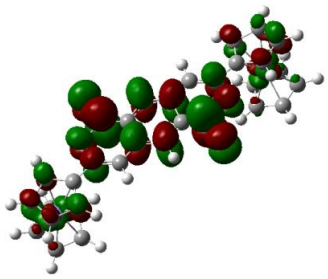
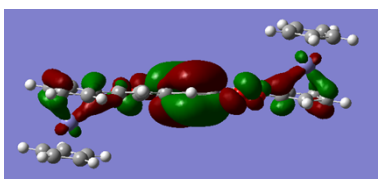


LUMO+5

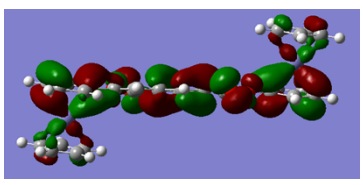


LUMO+7

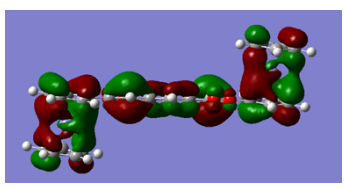
(e)



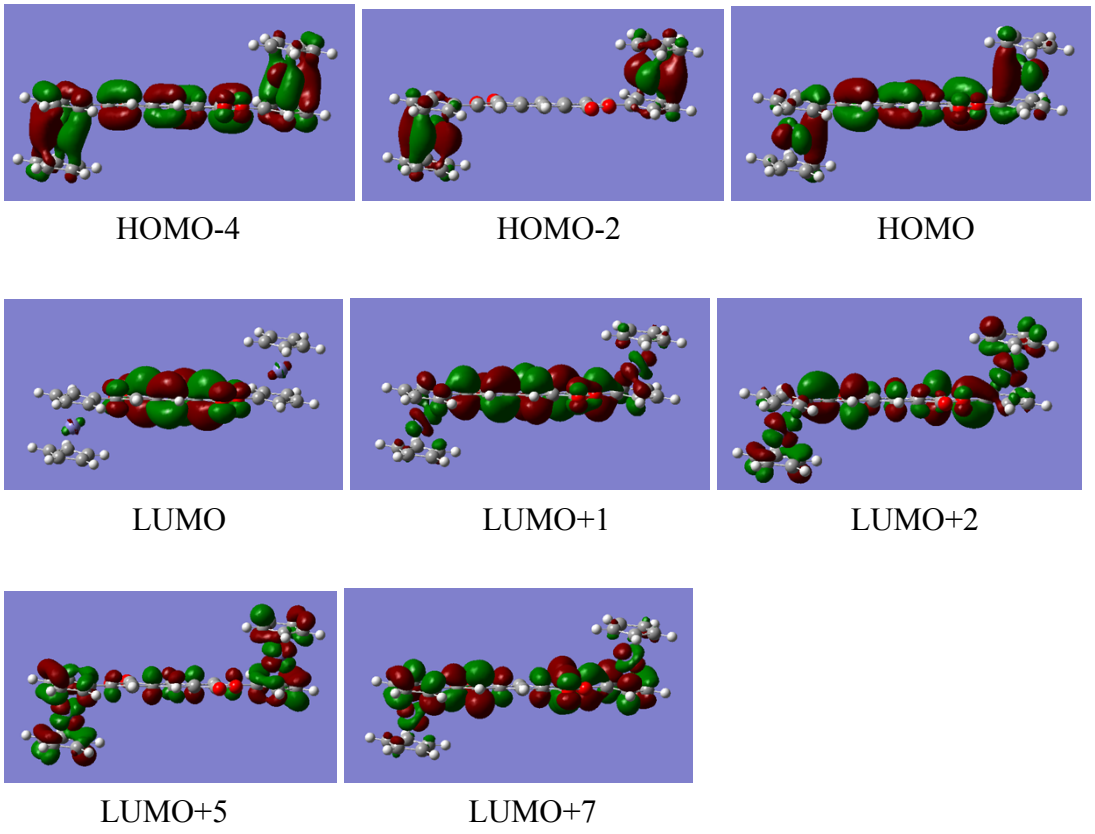
HOMO-15



HOMO-14



HOMO-5



(f)

Fig. S7 Main frontier orbitals of (a) **Fc-TP**, (b) **Fc-Icm**, (c) *cis*-**BFc-TP**, (d) *trans*-**BFc-TP**, (e) *cis*-**BFc-PIcm** and (f) *trans*-**BFc-PIcm**.

Table S4 Molecular Orbital Compositions of **Fc-TP**, **Fc-Icm**, **BFc-TP** and **BFc-PIcm** [a]

Fc-TP

		Composition(%)			
MO	E(eV)	Cp	Fe	−C≡C−	$Ph(COOMe)_2$
90	-7.806	15.79	3.70	3.98	76.53
91	-7.602	0.62	0.17	0.35	98.86
92	-7.292	71.84	25.64	0.92	1.60
93	-7.021	62.43	22.51	9.11	5.95
94	-6.770	17.48	3.30	38.88	40.34
95	-6.699	85.23	13.36	0.78	0.63
96	-6.640	19.04	80.70	0.21	0.05
97	-6.120	48.30	11.04	27.49	13.17
98	-5.480	18.75	80.33	0.63	0.29
99	**-5.434**	**17.19**	**76.41**	**4.65**	**1.75**
100	**-2.488**	**1.33**	**0.39**	**4.67**	**93.61**
101	-1.232	6.05	4.27	14.83	74.85
102	-0.598	32.31	52.45	7.84	7.40
103	-0.500	21.69	33.35	0.24	44.72
104	-0.473	17.22	26.83	0.53	55.42
105	0.441	57.98	11.94	21.37	8.71

Fc-Icm

		Composition(%)			
MO	E(eV)	Cp	Fe	−C=C−	rest
86	-7.893	23.62	7.34	2.47	66.57
87	-7.792	34.06	10.08	3.36	52.50
88	-7.713	0.34	0.11	0.30	99.25

89	-7.640	73.09	26.44	0.20	0.27
90	-7.240	69.92	15.06	3.67	11.35
91	-7.047	75.67	23.76	0.23	0.34
92	-7.014	27.98	71.43	0.27	0.32
93	-6.245	29.35	14.16	24.01	32.48
94	-5.856	18.20	81.52	0.17	0.11
95	**-5.774**	**16.26**	**71.15**	**6.09**	**6.50**
96	**-2.537**	**1.39**	**0.98**	**3.86**	**93.77**
97	-1.765	13.52	13.25	25.23	48.00
98	-0.875	38.79	60.63	0.26	0.32
99	-0.769	31.49	44.60	1.61	22.30
100	-0.481	6.04	4.37	2.37	87.22

cis-**BFc-TP**

		Composition(%)			
MO	E(eV)	Cp	Fe	−C≡C−	$Ph(COOMe)_2$
129	-7.851	51.47	13.21	10.18	25.14
132	-7.534	1.70	0.60	0.66	97.04
136	-7.146	70.95	19.65	4.74	4.66
137	-7.003	14.00	2.37	49.61	34.02
138	-6.995	86.69	10.25	1.89	1.17
139	-6.955	15.17	84.29	0.24	0.30
140	-6.816	87.75	11.48	0.56	0.21
141	-6.786	16.98	82.70	0.28	0.04
142	-6.533	55.74	10.39	23.66	10.21
143	-5.937	30.79	44.41	13.81	10.99
144	-5.788	18.54	80.47	0.71	0.28
145	-5.687	19.02	70.65	6.06	4.27
146	-5.619	18.65	80.47	0.72	0.16

147	**-5.440**	**17.61**	**50.16**	**18.83**	**13.40**
148	**-2.480**	**5.44**	**4.10**	**11.70**	**78.76**
149	-1.517	9.91	11.17	14.31	64.61
150	-0.949	25.62	41.78	9.63	22.97
151	-0.802	38.34	60.27	0.50	0.89
152	-0.631	39.13	60.18	0.53	0.16
153	-0.598	32.77	43.57	3.67	19.99
154	-0.424	21.08	24.06	3.25	51.61

trans-**BFc-TP**

		Composition (%)			
MO	E (eV)	Cp	Fe	−C≡C−	$Ph(COOMe)_2$
129	-7.839	49.18	12.64	10.26	27.93
132	-7.537	0.74	0.26	0.60	98.40
136	-7.143	70.66	19.35	5.21	4.78
137	-7.001	15.88	2.65	48.40	33.07
138	-6.993	85.59	9.96	2.72	1.73
139	-6.958	15.28	84.31	0.32	0.09
140	-6.814	88.99	10.21	0.59	0.21
141	-6.786	15.70	84.00	0.27	0.03
142	-6.531	55.64	10.61	23.64	10.11
143	-5.935	30.85	44.28	13.92	10.95
144	-5.788	18.69	80.46	0.73	0.12
145	-5.685	19.09	70.75	6.00	4.16
146	-5.620	18.67	80.45	0.73	0.15

147	**-5.437**	**17.66**	**50.20**	**18.80**	**13.34**
148	**-2.481**	**5.45**	**4.10**	**11.70**	**78.75**
149	-1.512	9.91	11.16	14.32	64.61
150	-0.947	25.71	41.80	9.63	22.86
151	-0.800	39.09	60.28	0.50	0.13
152	-0.628	39.11	60.11	0.55	0.23
153	-0.596	32.83	43.57	3.69	19.91
154	-0.422	21.11	24.10	3.27	51.52

cis-**BFc-PIcm**

		Composition(%)			
MO	E(eV)	Cp	Fe	−C=C−	rest
124	-7.907	8.22	3.14	1.94	86.70
125	-7.863	25.18	10.16	3.13	61.53
130	-7.091	75.66	23.81	0.23	0.30
131	-7.088	78.34	21.10	0.23	0.33
132	-7.066	25.67	73.71	0.32	0.30
133	-7.066	28.46	70.97	0.30	0.27
134	-6.791	52.09	9.03	24.08	14.80
135	-6.103	27.61	41.19	14.33	16.87
136	-5.921	18.47	81.26	0.16	0.11
137	-5.921	18.51	81.24	0.16	0.09
138	-5.894	18.34	78.67	1.92	1.07
139	**-5.682**	**16.12**	**44.57**	**19.67**	**19.64**
140	**-2.646**	**1.77**	**1.21**	**5.84**	**91.18**
141	-2.216	13.82	11.58	29.64	44.96

142	-1.213	26.74	40.95	20.82	11.49
143	-0.911	38.95	60.22	0.28	0.55
144	-0.908	39.08	60.40	0.27	0.25
145	-0.783	38.36	52.08	2.74	6.82
146	-0.514	14.20	10.36	5.25	70.19
147	-0.408	29.63	15.00	24.85	30.52

trans-**BFc-PIcm**

		Composition (%)			
MO	E (eV)	Cp	Fe	−C=C−	rest
124	-7.904	11.90	3.25	2.01	82.84
125	-7.858	37.50	11.04	3.48	47.98
130	-7.083	72.29	27.13	0.24	0.34
131	-7.083	73.66	25.77	0.24	0.33
132	-7.061	32.44	66.91	0.37	0.28
133	-7.058	29.48	69.92	0.30	0.31
134	-6.789	52.24	9.34	23.81	14.61
135	-6.098	27.53	40.39	14.74	17.34
136	-5.913	18.49	81.25	0.16	0.10
137	-5.913	18.52	81.23	0.16	0.10
138	-5.886	18.34	78.72	1.89	1.05
139	**-5.679**	**16.16**	**45.41**	**19.25**	**19.18**
140	**-2.644**	**1.77**	**1.21**	**5.85**	**91.16**
141	-2.214	13.78	11.49	29.65	45.08
142	-1.205	26.73	40.88	20.81	11.57

143	-0.903	38.91	60.18	0.30	0.60
144	-0.903	39.09	60.46	0.27	0.18
145	-0.775	38.31	52.14	2.75	6.80
146	-0.509	13.33	9.90	5.01	71.76
147	-0.405	30.41	15.48	25.17	28.87

[a] The HOMO and LUMO are given in bold.

Table S5 TDDFT predicted main vertical excitation energies for **Fc-TP**, **Fc-Icm**, **BFc-TP** and **BFc-PIcm**.

Fc-TP

##	Symmetry	*f*	eV	nm	Transition	Expansion codfficients
5	Singlet-A	0.0112	2.4831	499.30		
					96 ->102	0.12302
					98 ->100	-0.11228
					99 ->100	0.65888
					99 ->102	0.13266
7	Singlet-A	0.0345	3.0444	407.25		
					97 ->100	0.67518
10	Singlet-A	0.0193	3.6682	338.00		
					93 ->100	0.11953
					94 ->100	-0.43893
					96 ->100	0.10820
					97 ->101	0.12644
					99 ->101	0.44033
					99 ->102	0.14323
12	Singlet-A	0.0716	3.7242	332.91		
					93 ->100	-0.11101
					94 ->100	0.42502
					95 ->100	0.12598
					98 ->101	-0.20072
					99 ->101	0.43106
					99 ->102	0.14952
13	Singlet-A	0.0132	3.7722	328.68		

					95 ->100	0.31157
					98 ->101	0.55665
					98 ->102	0.18025
					99 ->101	0.15885
16	Singlet-A	0.0721	4.1995	295.24		
					90 ->100	-0.15699
					97 ->101	0.63402
25	Singlet-A	0.1038	4.6779	265.04		
					88 ->100	-0.17534
					90 ->100	-0.14996
					91 ->100	0.50221
					94 ->101	-0.36187
31	Singlet-A	f=0.2873	5.0172	247.12		
					90 ->100	-0.10001
					91 ->100	0.26865
					92 ->101	-0.10301
					92 ->102	0.18161
					93 ->101	-0.21137
					93 ->103	-0.19171
					93 ->104	0.17614
					94 ->101	0.32536
					94 ->102	-0.19489
					97 ->103	0.13892
					97 ->104	0.17768

Fc-Icm

##	Symmetry	*f*	eV	nm	Transition	Expansion codfficients
5	Singlet-A	0.0255	2.7969	443.29		

					92 -> 99	0.10658
					95 -> 96	0.67522
9	Singlet-A	0.0779	3.2541	381.01		
					93 -> 96	0.66822
11	Singlet-A	0.0790	3.6742	337.45		
					93 -> 97	0.11157
					95 -> 97	0.47865
					95 -> 99	-0.42585
					95 ->100	-0.12934
12	Singlet-A	0.2840	4.0165	308.68		
					92 -> 96	-0.45434
					93 -> 97	0.48775
					95 -> 97	-0.14431
13	Singlet-A	0.1821	4.0483	306.26		
					91 -> 96	-0.32008
					91 -> 97	-0.10808
					92 -> 96	0.43324
					93 -> 97	0.39253
					95 -> 97	-0.10827
14	Singlet-A	0.0271	4.0606	305.34		
					91 -> 96	0.60869
					92 -> 96	0.24623
					92 -> 99	-0.12037
					93 -> 97	0.16897
27	Singlet-A	0.3273	4.8911	253.49		
					86 -> 96	0.10716
					87 -> 97	-0.13224
					88 -> 96	0.42919
					90 -> 97	0.14060

					90 -> 99	0.10746
					91 -> 98	0.18375
					93 ->100	-0.11508
					94 ->100	-0.21000
					95 ->100	-0.21738

cis-**BFc-TP**

##	Symmetry	*f*	eV	nm	Transition	Expansion codfficients
9		0.2897	2.6287	471.66		
					147->148	0.64202
					147->149	-0.12245
13		0.1289	3.0000	413.28		
					139->150	0.14574
					139->153	0.12157
					143->148	0.61710
					144->151	0.13515
18		0.6470	3.5527	348.99		
					143->149	0.12333
					145->150	0.10658
					147->149	0.62725
					147->153	-0.14277
22		0.1088	3.7785	328.13		
					141->148	-0.10761
					142->148	-0.10092
					143->149	0.60523
					145->153	-0.14221
					147->150	0.19151
					147->154	0.11397

49	0.1826	4.7233	262.50		
				128 ->148	0.10429
				129 ->148	-0.14561
				132 ->148	0.38356
				136 ->149	-0.11019
				137 ->149	0.19425
				140 ->149	-0.14649
				143 ->153	-0.19891
				145 ->150	0.12539
				145 ->154	-0.22131
				147 ->153	-0.12227
57	0.1033	4.9377	251.10		
				129 ->148	0.33601
				132 ->148	0.15944
				133 ->148	-0.11976
				133 ->149	0.17399
				133 ->150	-0.15244
				133 ->153	0.13106
				133 ->154	-0.13147
				134 ->152	0.12660
				140 ->149	-0.10450
				145 ->152	0.10739
58	0.1369	4.9398	250.99		
				129 ->148	0.38780
				132 ->148	0.19085
				133 ->149	-0.14186
				133 ->150	0.13080
				133 ->153	-0.11017
				133 ->154	0.10614

					134 ->152	-0.11251
					136 ->152	-0.27922
					138 ->151	-0.10804
					139 ->149	-0.12556

trans-**BFc-TP**

##	Symmetry	*f*	eV	nm	Transition	Expansion codfficients
9		0.3091	2.6297	471.47		
					147->148	0.64181
					147->149	-0.12306
13		0.1347	3.0004	413.23		
					139->150	-0.14599
					139->153	-0.12114
					143->148	0.61715
					144->151	-0.13542
18		0.7103	3.5551	348.75		
					143->149	-0.12306
					145->150	0.10608
					147->149	0.62723
					147->153	0.14364
22		0.1162	3.7799	328.01		
					141->148	0.10809
					143->149	-0.10540
					145->149	0.60562
					145->153	0.14364
					147->150	0.18974
					147->154	0.11532
49		0.1691	4.7228	262.52		

					128 ->148	-0.11797
					129 ->148	0.21598
					132 ->148	0.38503
					136 ->149	-0.10435
					137 ->149	0.19540
					141 ->149	0.10483
					143 ->153	0.20309
					145 ->150	-0.12954
					145 ->154	0.22916
					147 ->153	-0.12423
58		0.1701	4.9434	250.81		
					128 ->148	0.19740
					129 ->148	0.38607
					131 ->148	-0.10470
					132 ->149	0.21145
					133 ->149	-0.10610
					134 ->149	0.10769
					134 ->150	-0.11419
					136 ->152	0.21493
					138 ->151	-0.12766
					139 ->149	0.14492
					141 ->149	0.10193

cis-**BFc-PIcm**

##	Symmetry	*f*	eV	nm	Transition	Expansion codfficients
9		0.0897	2.6081	475.37		
					139->140	0.68742
15		0.2321	3.0808	402.45		

				132->141	0.11223
				132->142	0.12941
				132->145	0.12511
				133->141	-0.12231
				133->142	0.15478
				133->145	-0.13657
				135->140	-0.35493
				135->141	0.18126
				136->143	0.16178
				137->144	0.14424
				139->141	0.38166
18		0.7887	3.2679	379.40	
				135->141	-0.24189
				135->145	-0.13459
				136->143	-0.12462
				137->144	-0.12557
				138->142	-0.19974
				139->141	0.49927
				139->145	-0.16379
22		0.2213	3.5063	353.61	
				135->141	0.58636
				138->142	-0.14506
				138->147	-0.11702
				139->145	-0.21481
58		0.4638	4.8735	254.40	
				124->140	0.39434
				125->140	0.30448
				125->141	0.36729
73		0.1226	5.0671	244.68	

					124->140	-0.14658
					124->141	0.16859
					125->141	0.12220
					129->141	-0.16040
					129->145	0.12846
					130->143	-0.10608
					131->144	0.10255
					134->142	0.38234
					135->145	0.32359
					138->147	-0.23139

trans-**BFc-PIcm**

##	Symmetry	*f*	eV	nm	Transition	Expansion codfficients
9		0.0927	2.6076	475.47		
					139->140	0.68711
15		0.2454	3.0793	402.64		
					130->142	-0.10188
					132->142	0.19440
					133->141	0.16262
					133->145	0.18201
					135->140	-0.35324
					135->141	0.18276
					136->143	-0.15403
					137->144	-0.15523
					139->141	0.38077
18		0.8445	3.2699	379.17		
					132->142	-0.10376
					135->141	-0.23694

				135->145	-0.13406
				136->143	0.12498
				137->144	0.12577
				138->142	-0.20071
				139->141	0.50011
				139->145	-0.16863
22		0.2490	3.5060	353.63	
				135->141	0.58948
				138->142	-0.14246
				138->147	-0.11719
				139->145	-0.21238
57		0.4929	4.8721	254.48	
				124->140	0.41292
				125->140	0.28935
				125->141	0.37920
73		0.1326	5.0695	244.57	
				122->141	0.11407
				124->140	0.16094
				124->141	-0.14530
				125->141	-0.12784
				128->142	0.10094
				129->141	0.16649
				129->145	-0.13518
				130->143	-0.11161
				131->144	-0.11290
				134->142	0.37629
				135->145	-0.32237
				138->147	0.22024

Table S6 Main Calculated Optical Transitions for **Fc-TP, Fc-Icm, BFc-TP** and **BFc-PIcm**

calcd (nm)	*f*	composition (%)	character	exptl (nm)
Fc-TP[a]				
499.30	0.0112	90 (HOMO→LUMO)	MLCT	464
407.25	0.0345	100 (HOMO-2→LUMO)	ICT	382
338.00	0.0193	43(HOMO-5→LUMO)	π-π*	302
		43(HOMO→LUMO+1)	MLCT	
332.91	0.0716	40(HOMO-5→LUMO)	π-π*	
		41(HOMO→LUMO+1)	MLCT	
328.68	0.0132	67 (HOMO-1→LUMO+1)	MLCT	
		21(HOMO-4→LUMO)	ICT	
295.24	0.0721	94 (HOMO-2→LUMO+1)	ICT	
265.04	0.1038	58 (HOMO-8→LUMO)	π-π*	235
		30 (HOMO-5→LUMO+1)	π-π*	
247.12	0.2873	24 (HOMO-5→LUMO+1)	π-π*	
		17 (HOMO-8→LUMO)	π-π*	
		10 (HOMO-6→LUMO+1)	ICT	
Fc-Icm[b]				
443.29	0.0255	98 (HOMO→LUMO)	MLCT	445
381.01	0.0779	100 (HOMO-2→LUMO)	ICT	357
337.45	0.0790	52 (HOMO→LUMO+1)	MLCT	
		41 (HOMO→LUMO+3)	d-d	

308.68	0.2840	44 (HOMO-3→LUMO)	MLCT	311
			π-π*	
		51 (HOMO-2→LUMO+1)		
306.26	0.1821	40 (HOMO-3→LUMO)	MLCT	
			π-π*	
		33 (HOMO-2→LUMO+1)	ICT	
		22 (HOMO-4→LUMO)		
305.34	0.0271	78 (HOMO-4→LUMO)	ICT	
			MLCT	
		13 (HOMO-3→LUMO)		
253.49	0.3273	48 (HOMO-7→LUMO)	π-π*	246
			MLCT	
		12 (HOMO-1→LUMO+4)	MLCT	
		12 (HOMO→LUMO+4)		
cis-**BFc-TP**[c]				
471.66	0.2897	96 (HOMO→LUMO)	ICT	473
413.28	0.1289	88 (HOMO-4→LUMO)	ICT	408
348.99	0.6470	89 (HOMO→LUMO+1)	ICT	336
328.13	0.1088	78 (HOMO-2→LUMO+1)	MLCT	
262.50	0.1826	40 (HOMO-15→LUMO)	π-π*	247
			d-d	
		13 (HOMO→LUMO+5)	d-d	
		11 (HOMO-4→LUMO+5)	π-π*	
		10 (HOMO-10→LUMO+1)		
251.10	0.1033	29 (HOMO-18→LUMO)	ICT	
			LMCT	
		28 (HOMO-11→LUMO+4)		
250.99	0.1369	41 (HOMO-18→LUMO)	ICT	
			LMCT	

trans-**BFc-TP**[c]				
		21 (HOMO-11→LUMO+4)		
471.47	0.3091		ICT	473
413.23	0.1347	96 (HOMO→LUMO)	ICT	408
348.75	0.7103	85 (HOMO-4→LUMO)	ICT	336
328.01	0.1162	89 (HOMO→LUMO+1)	MLCT	
262.52	0.1691	80 (HOMO-2→LUMO+1)	π-π*	247
		38 (HOMO-15→LUMO)	ICT	
		12 (HOMO-18→LUMO)	ICT	
		13 (HOMO-2→LUMO+6)	π-π*	
250.81	0.1701	10 (HOMO-4→LUMO+5)	ICT	
		40 (HOMO-18→LUMO)	LMCT	
		12 (HOMO-11→LUMO+4)	π-π*	
		12 (HOMO-15→LUMO)		
cis-**BFc-PIcm**[d]				
475.37	0.0897	100 (HOMO→LUMO)	ICT	483
402.45	0.2321	28 (HOMO-4→LUMO+1)	ICT	
		32 (HOMO→LUMO+1)	ICT	
379.40	0.7887	59 (HOMO→LUMO+1)	ICT	372
		14 (HOMO-4→LUMO+1)	ICT	
353.61	0.2213	81 (HOMO-4→LUMO+1)	ICT	358
		11 (HOMO→LUMO+5)	d-d	
254.40	0.4638	41 (HOMO-15→LUMO)	π-π*	247
		24 (HOMO-14→LUMO)	π-π*	
		35 (HOMO-14→LUMO+1)	π-π*	
244.68		34 (HOMO-5→LUMO+2)	LMCT	
			d-d	

		24 (HOMO-4→LUMO+3)	MLCT	
		12 (HOMO-1→LUMO+7)		
trans-**BFc-PIcm**[d]				
475.47	0.0927	100 (HOMO→LUMO)	ICT	483
402.64	0.2454	27 (HOMO-4→LUMO)	ICT	
		32 (HOMO→LUMO+1)	ICT	
379.40	0.8445	57 (HOMO→LUMO+1)	ICT	372
		13 (HOMO-4→LUMO+1)	ICT	
353.63	0.2490	81 (HOMO-4→LUMO+1)	ICT	358
		11 (HOMO→LUMO+5)	d-d	
254.48	0.4929	43 (HOMO-15→LUMO)	π-π*	247
		21 (HOMO-14→LUMO)	π-π*	
		36 (HOMO-14→LUMO+1)	π-π*	
244.57	0.1326	31 (HOMO-5→LUMO+2)	LMCT	
		23 (HOMO-4→LUMO+5)	d-d	
		11 (HOMO-2→LUMO+7)	MLCT	

[a] Only transitions (wavelength > 300 nm, f > 0.01; 240 nm < wavelength < 300 nm, f > 0.07) are listed in the table.

[b] Only transitions (wavelength > 300 nm, f > 0.02; 240 nm < wavelength < 300 nm, f > 0.1) are listed in the table.

[c] Only transitions (wavelength > 240 nm, f > 0.1) are listed in the table.

[d] Only transitions (wavelength > 300 nm, f > 0.08; 240 nm < wavelength < 300 nm , f > 0.1) are listed in the table.