Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Redox induced color changes between red-violet and blue by redox in hetero-metal complexes of type $[Co^{II}(4'\text{-ferrocenyl-}2,2';6'2''\text{-terpyridine})_2]X_2$ (X = counter anion)

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Table S1 Selected Co- N bond length for **1** and **5** (Å)

	1·2MeCN	**5·H_2O·1.5Acetone**
Co(1)-N(1)	2.175(4)	1.942(7)
Co(1)-N(2)	1.940(3)	1.839(7)
Co(1)-N(3)	2.167(4)	1.922(7)
Co(1)-N(4)	1.981(4)	1.937(5)
Co(1)-N(5)	1.870(3)	1.848(7)
Co(1)-N(6)	1.996(4)	1.959(5)

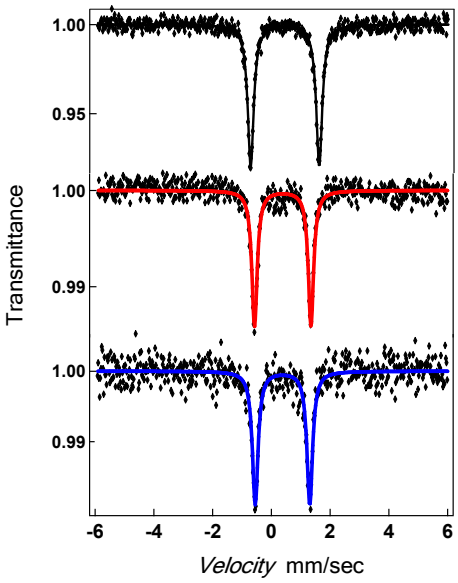


Fig. S1 Mössbaure spectra of Fctpy (black), **1** (red) and **5** (blue) measured at room temperature.

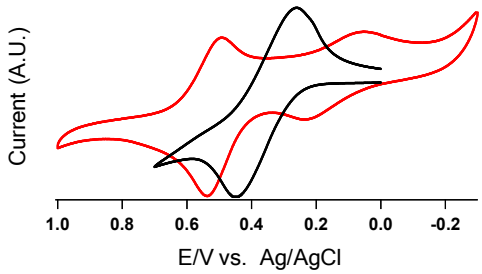


Fig. S2 Cyclic voltammogram of **1** (red) and ferrocene (black) in the solid state.

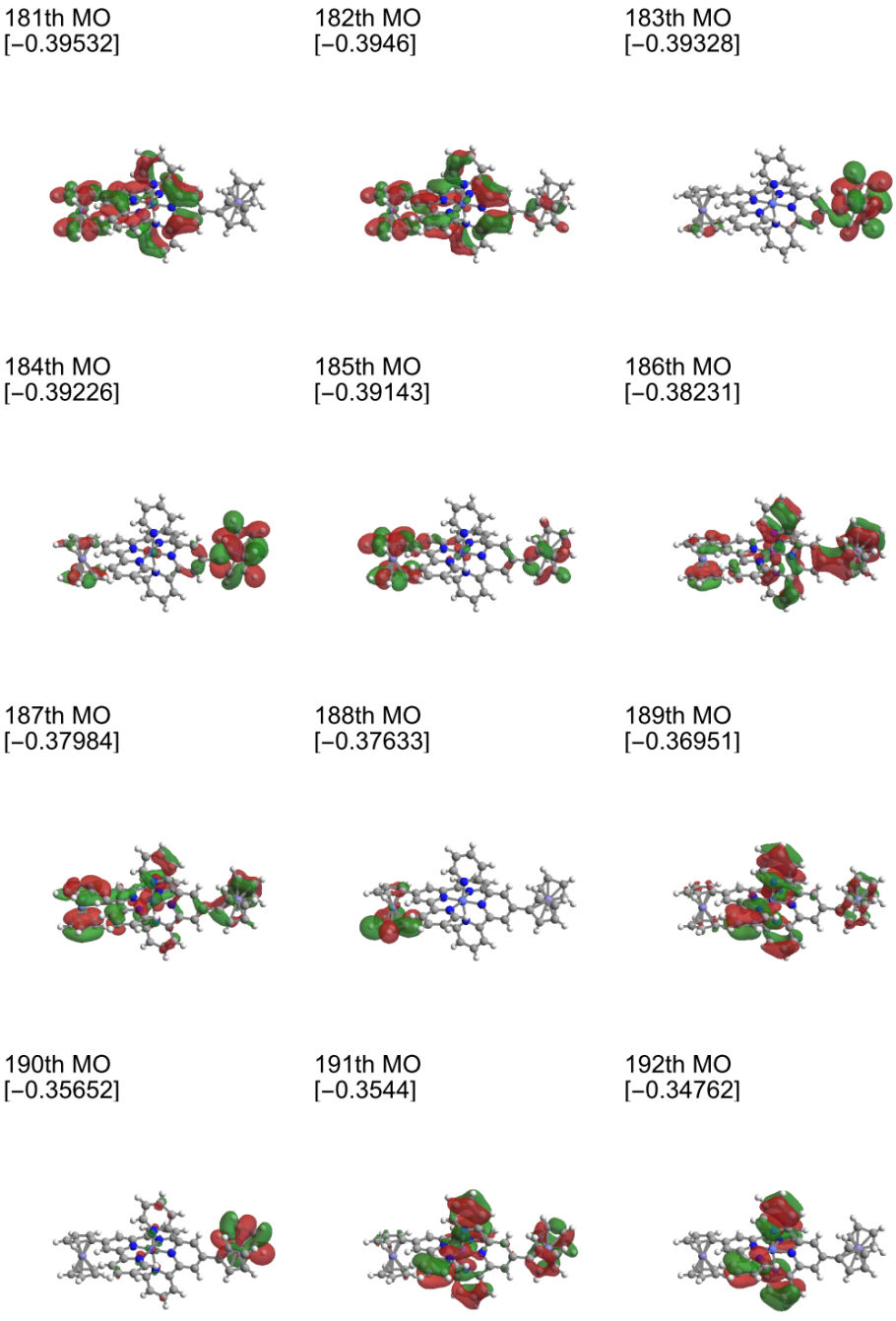
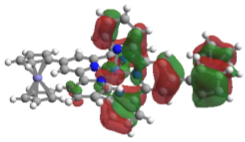
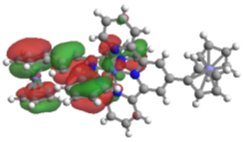


Fig. S3 Molecular orbitals of **5** in CH_3CN solution (Continued: 1/5).

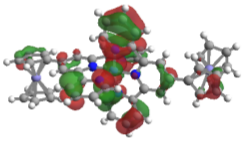
193th MO
[−0.3472]



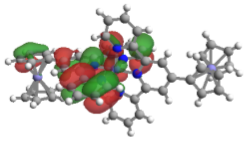
194th MO
[−0.34551]



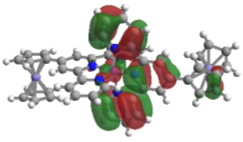
195th MO
[−0.33563]



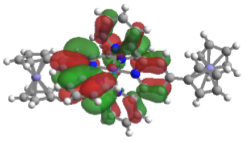
196th MO
[−0.32399]



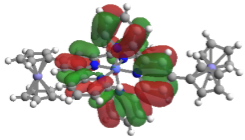
197th MO
[−0.32263]



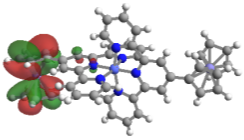
198th MO
[−0.30704]



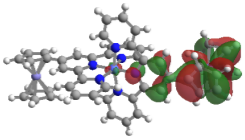
199th MO
[−0.30384]



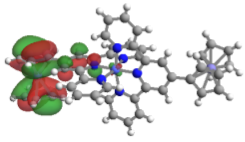
200th MO
[−0.30136]



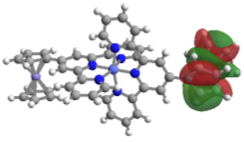
201th MO
[−0.3006]



202th MO
[−0.29553]



203th MO
[−0.29512]



204th MO
[−0.28038]

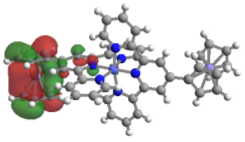
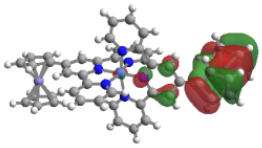
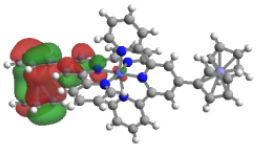


Fig. S3 (Continued: 2/5).

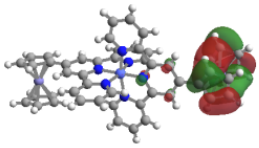
205th MO
[−0.27914]



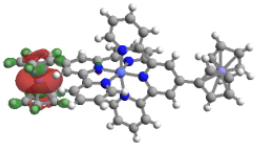
206th MO
[−0.27421]



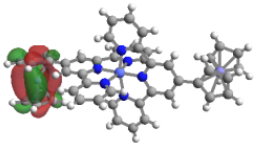
207th MO
[−0.27008]



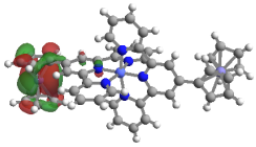
208th MO
[−0.23756]



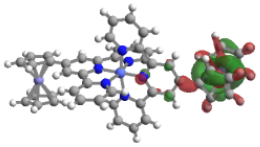
209th MO
[−0.23396]



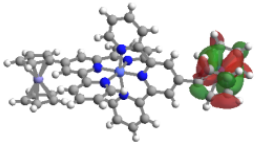
210th MO
[−0.2326]



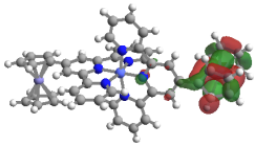
211th MO
[−0.2323]



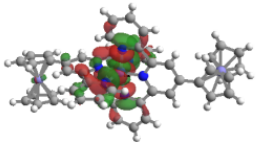
212th MO
[−0.23118]



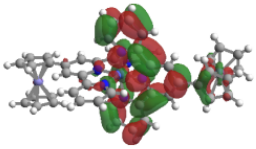
213th MO (HOMO)
[−0.22798]



214th MO (LUMO)
[−0.11809]



215th MO
[−0.11705]



216th MO
[−0.11584]

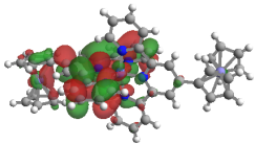
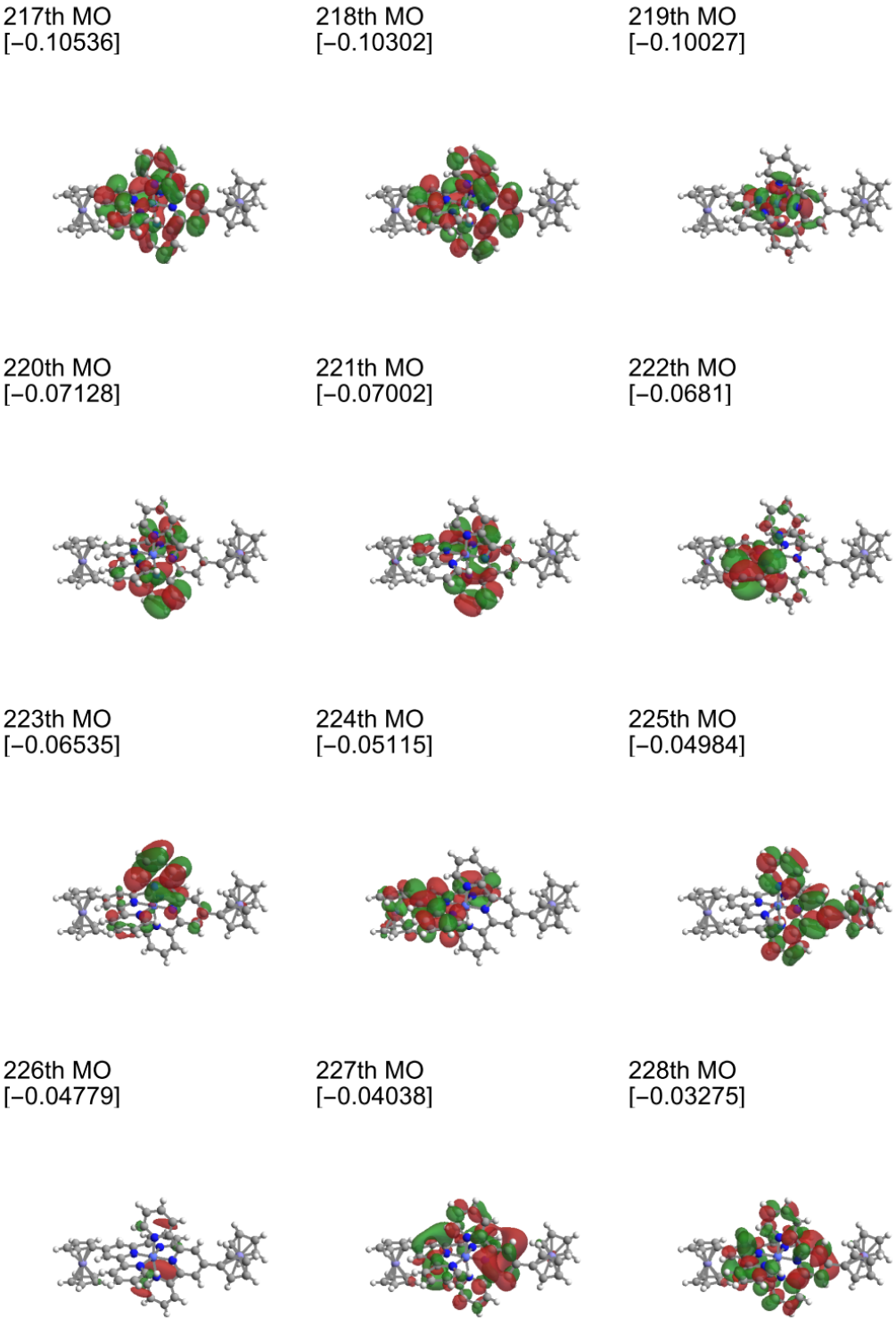


Fig. S3 (Continued: 3/5).



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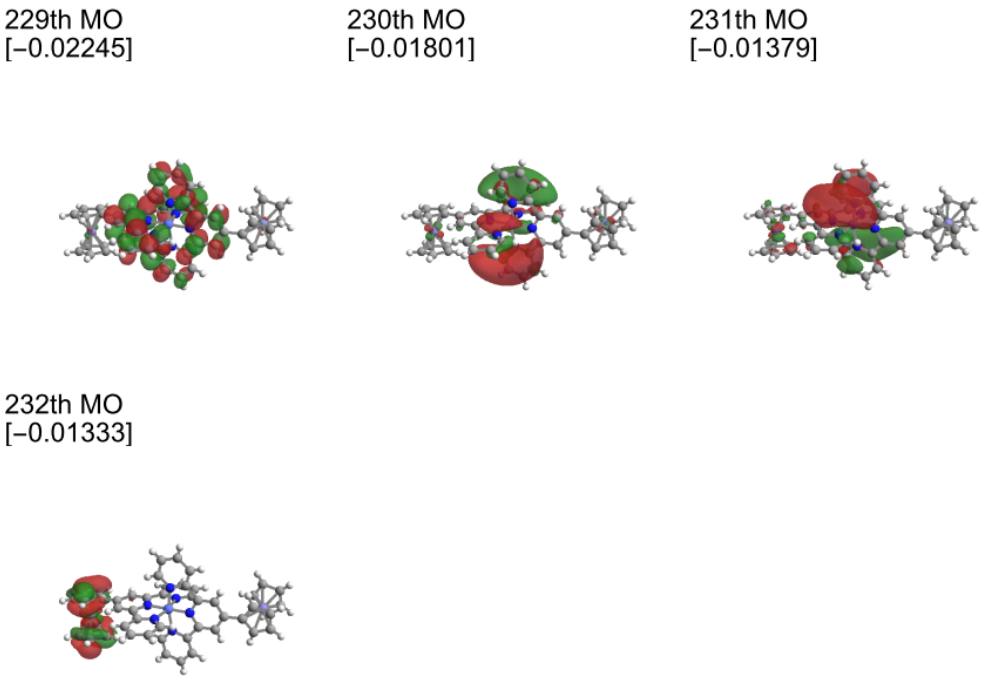


Fig. S3 (Continued: 5/5).

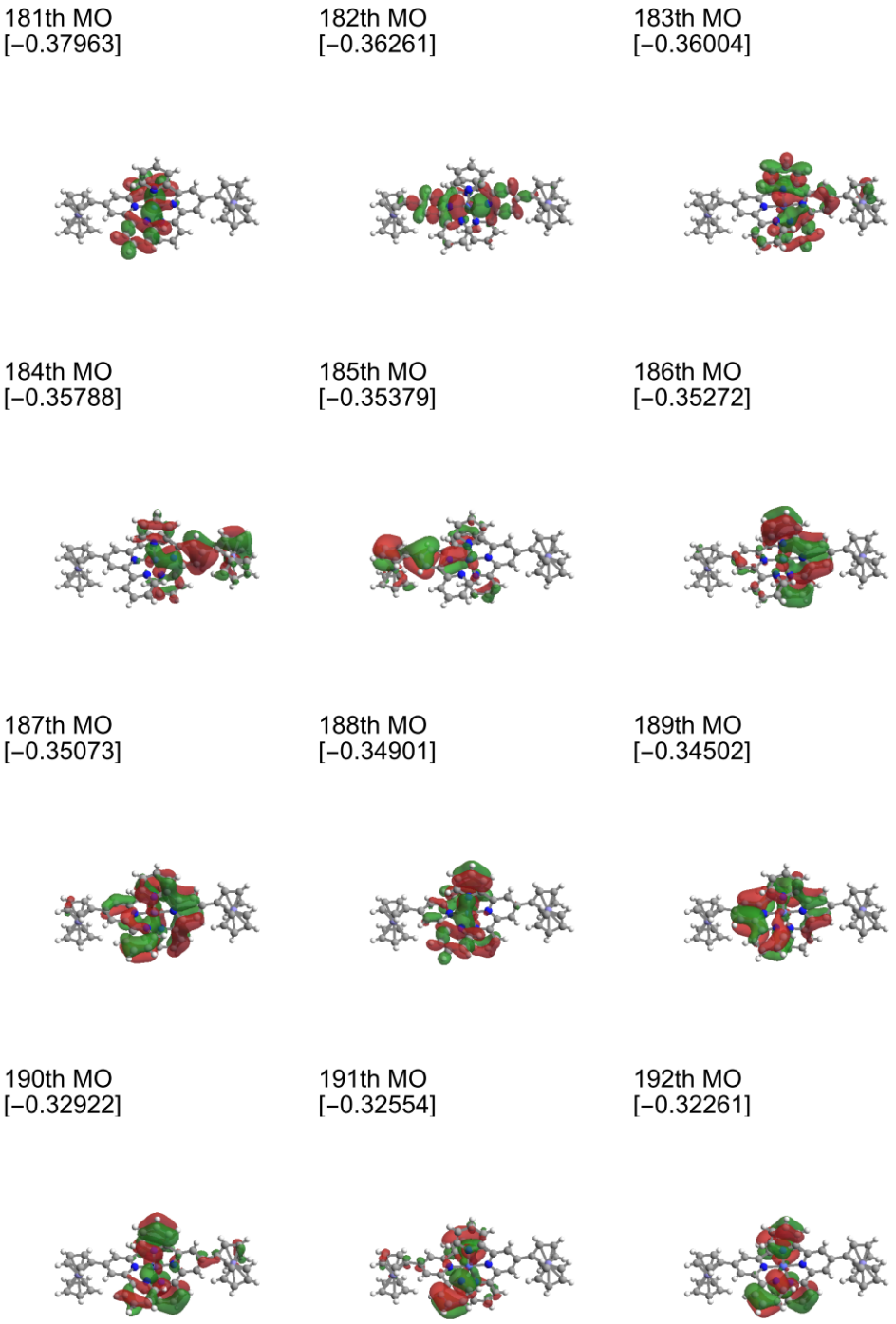


Fig. S4 Alpha molecular orbitals of **1** in the CH_3CN solution (Continued: 1/6).

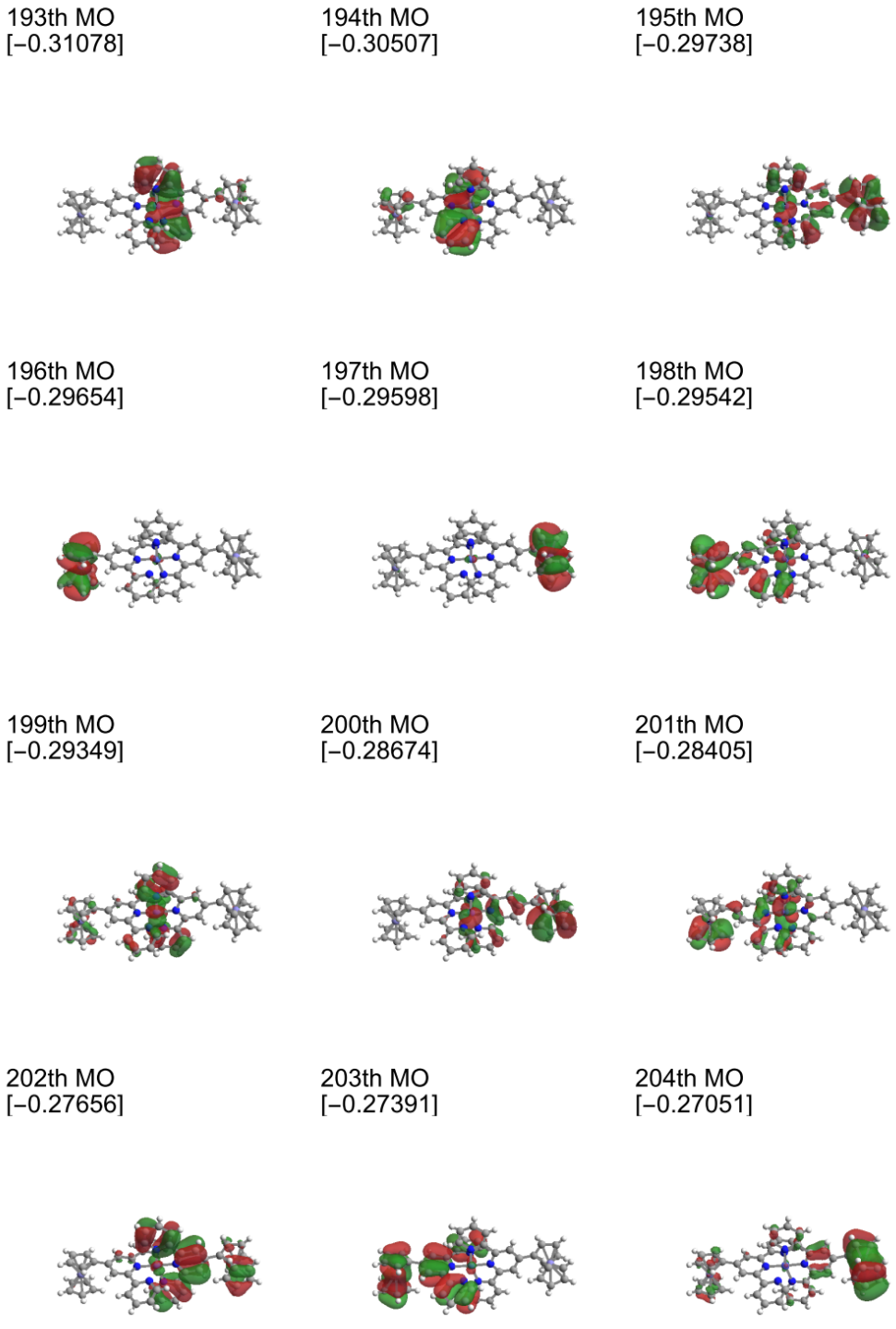


Fig. S4 (Continued: 2/6).

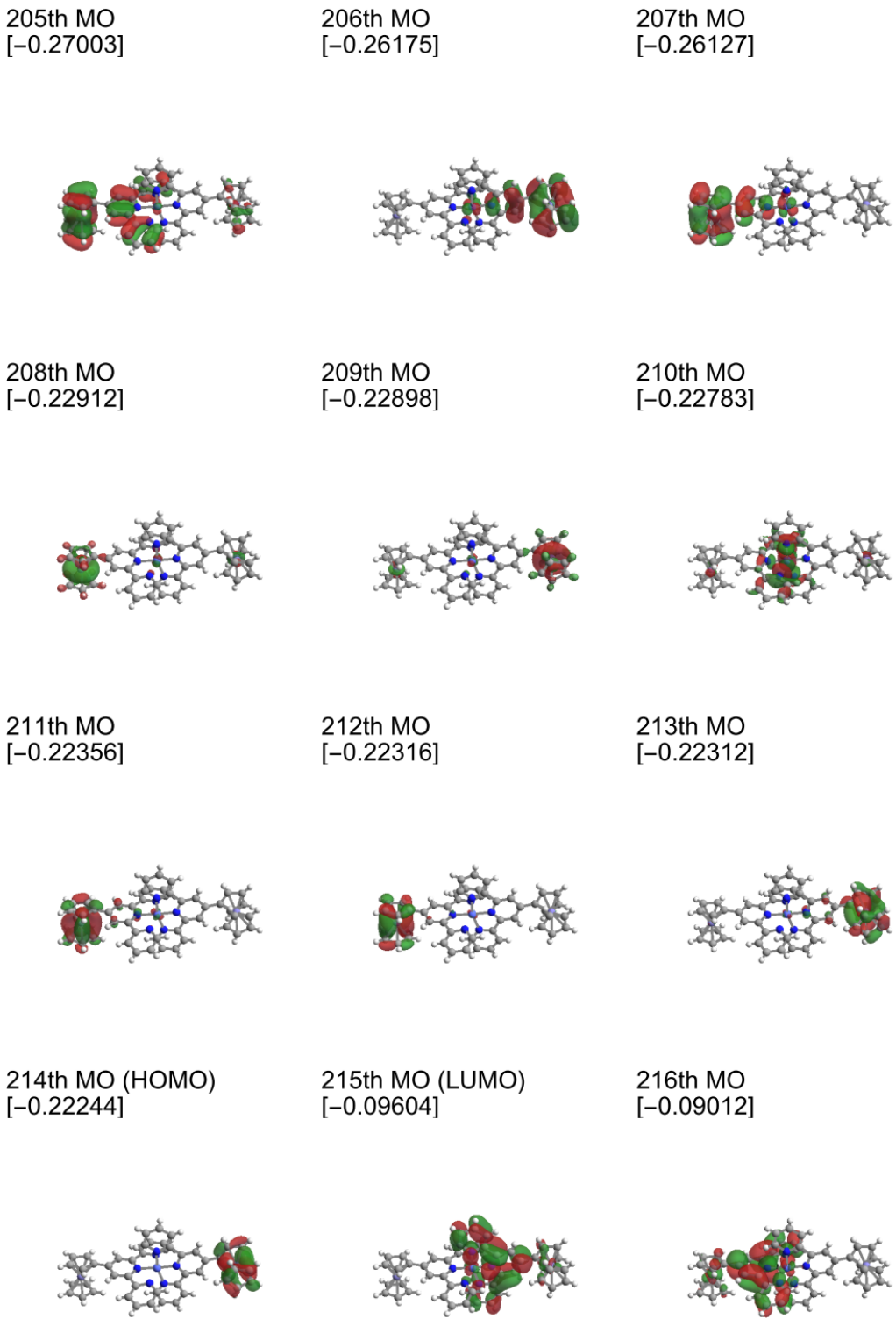
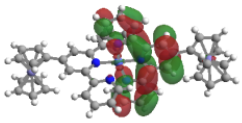
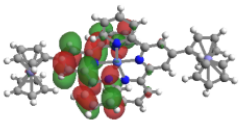


Fig. S4 (Continued: 3/6).

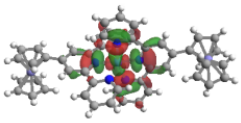
217th MO
[−0.08384]



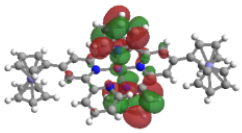
218th MO
[−0.0779]



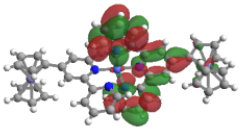
219th MO
[−0.06474]



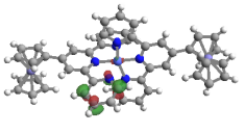
220th MO
[−0.05014]



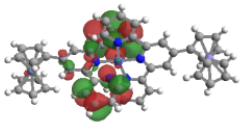
221th MO
[−0.04984]



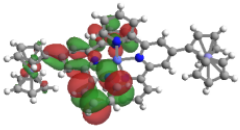
222th MO
[−0.04512]



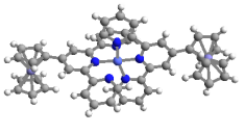
223th MO
[−0.04294]



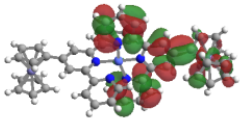
224th MO
[−0.04193]



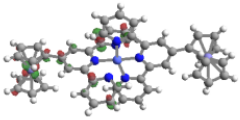
225th MO
[−0.03867]



226th MO
[−0.03374]



227th MO
[−0.0307]



228th MO
[−0.0304]

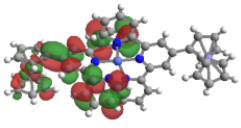
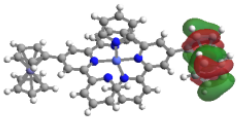
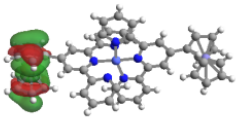


Fig. S4 (Continued: 4/6).

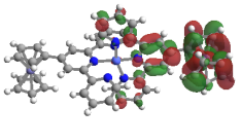
229th MO
[−0.01538]



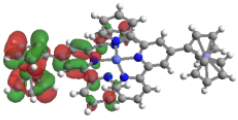
230th MO
[−0.01433]



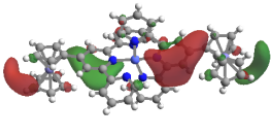
231th MO
[−0.00747]



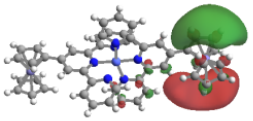
232th MO
[−0.00723]



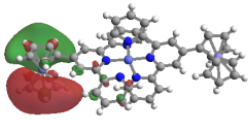
233th MO
[0.00265]



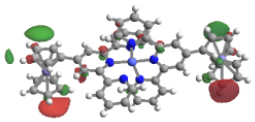
234th MO
[0.0042]



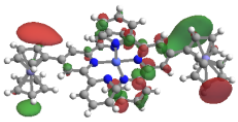
235th MO
[0.00448]



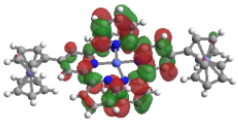
236th MO
[0.01169]



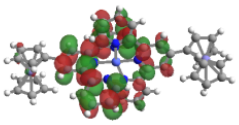
237th MO
[0.01486]



238th MO
[0.01556]



239th MO
[0.01965]



240th MO
[0.02626]

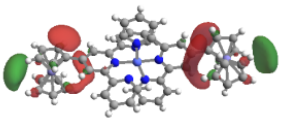
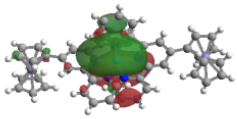
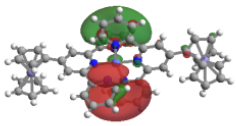


Fig. S4 (Continued: 5/6).

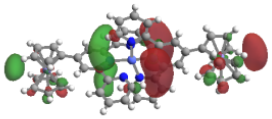
241th MO
[0.03084]



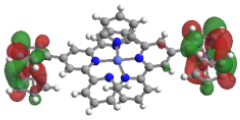
242th MO
[0.03291]



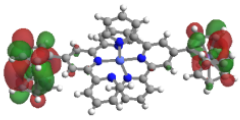
243th MO
[0.04809]



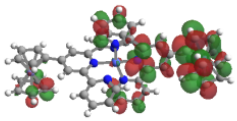
244th MO
[0.05888]



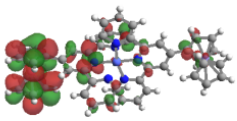
245th MO
[0.05909]



246th MO
[0.06106]



247th MO
[0.06227]



248th MO
[0.06466]

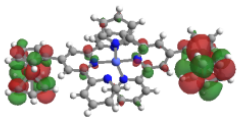


Fig. S4 (Continued: 6/6).

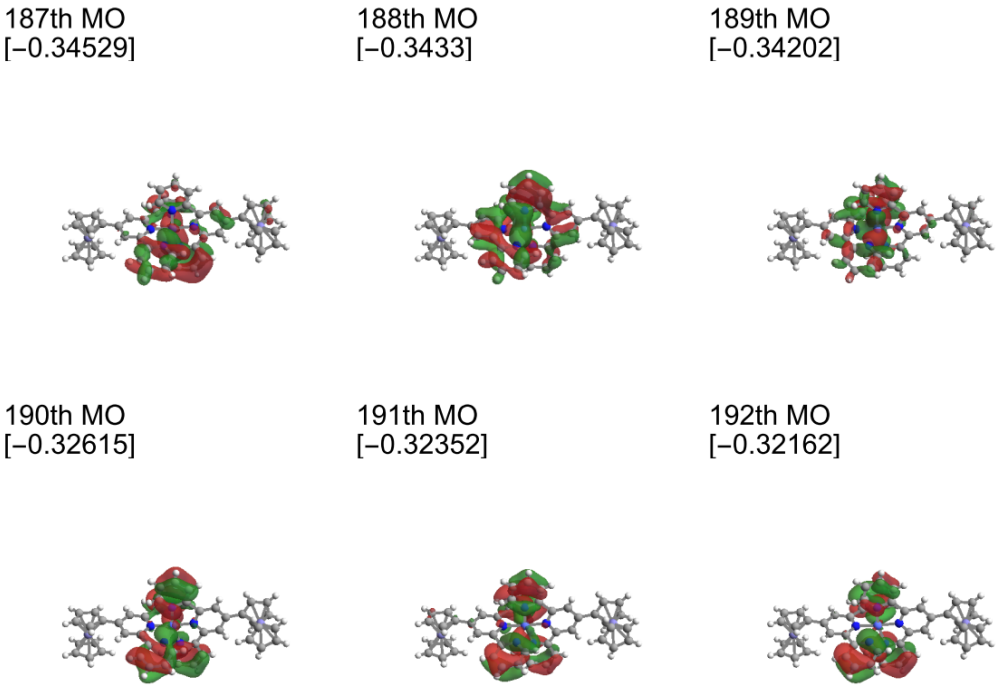


Fig. S5 Beta molecular orbitals of **1** in the CH_3CN solution (Continued: 1/6).

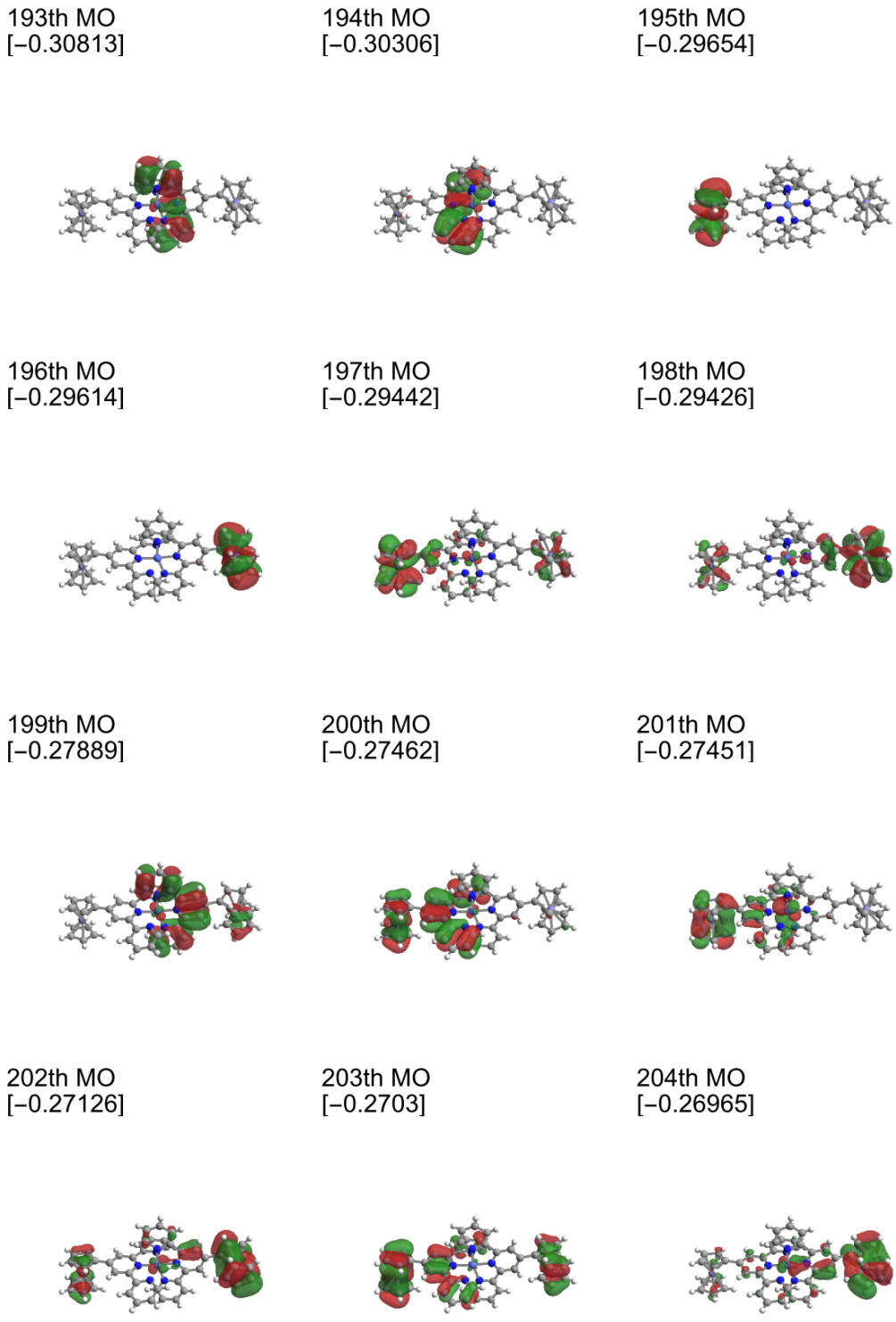
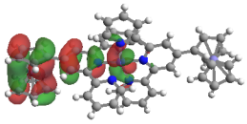
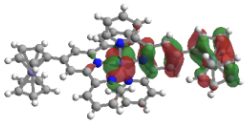


Fig. S5 (Continued: 2/6).

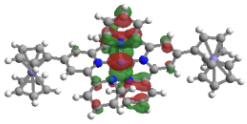
205th MO
[−0.2571]



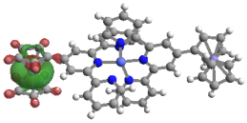
206th MO
[−0.24504]



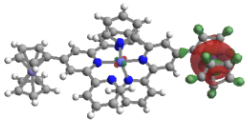
207th MO
[−0.23854]



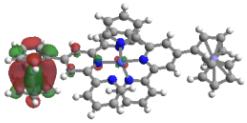
208th MO
[−0.22911]



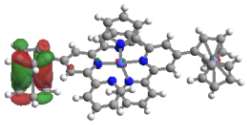
209th MO
[−0.22901]



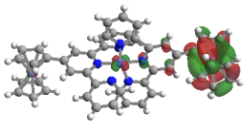
210th MO
[−0.22359]



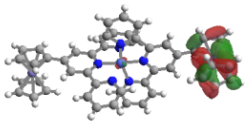
211th MO
[−0.22319]



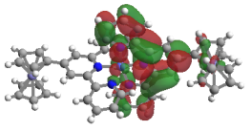
212th MO
[−0.22303]



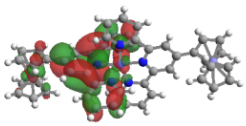
213th MO (HOMO)
[−0.22267]



214th MO (LUMO)
[−0.09483]



215th MO
[−0.08949]



216th MO
[−0.08312]

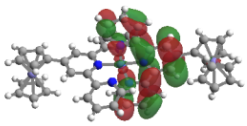
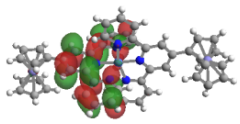
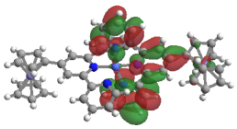


Fig. S5 (Continued: 3/6).

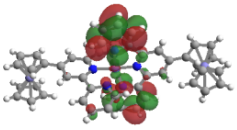
217th MO
[−0.07726]



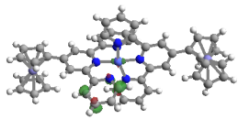
218th MO
[−0.05085]



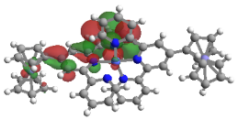
219th MO
[−0.04967]



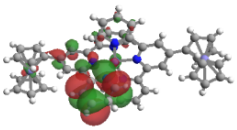
220th MO
[−0.04527]



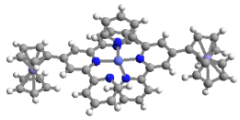
221th MO
[−0.04227]



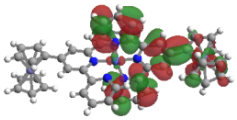
222th MO
[−0.04159]



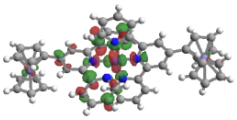
223th MO
[−0.03867]



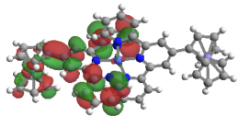
224th MO
[−0.03437]



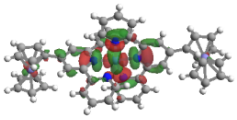
225th MO
[−0.03115]



226th MO
[−0.03067]



227th MO
[−0.02817]



228th MO
[−0.01554]

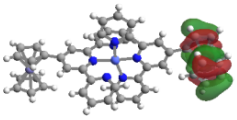
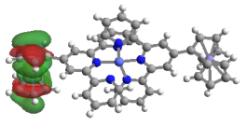
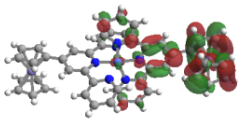


Fig. S5 (Continued: 4/6).

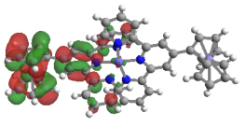
229th MO
[−0.01435]



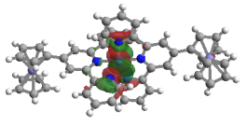
230th MO
[−0.00771]



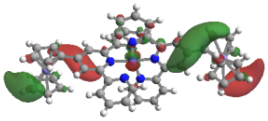
231th MO
[−0.00724]



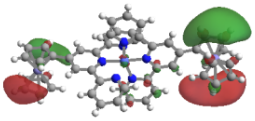
232th MO
[−0.00415]



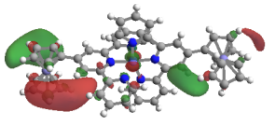
233th MO
[0.00329]



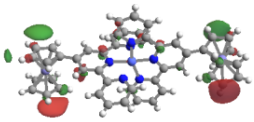
234th MO
[0.00427]



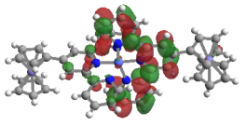
235th MO
[0.00482]



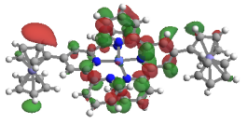
236th MO
[0.01172]



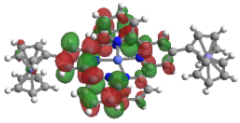
237th MO
[0.01474]



238th MO
[0.01529]



239th MO
[0.01934]



240th MO
[0.02627]

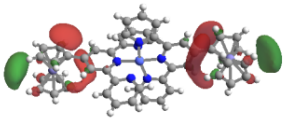
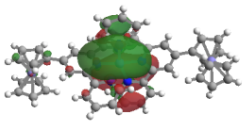
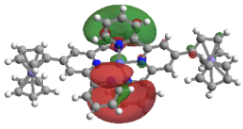


Fig. S5 (Continued: 5/6).

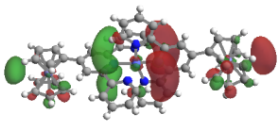
241th MO
[0.03114]



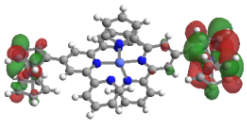
242th MO
[0.03311]



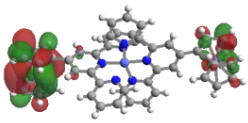
243th MO
[0.04881]



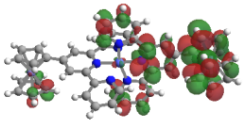
244th MO
[0.0588]



245th MO
[0.05906]



246th MO
[0.06104]



247th MO
[0.06229]

248th MO
[0.06462]

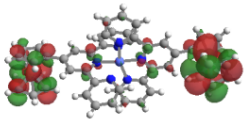


Fig. S5 (Continued: 6/6).

Table S2 Spin-singlet excited states of **$Co^{II}(Fctpy)_2$** in CH_3CN calculated by using the TDDFT method. The solvent effect was taken into account by the PCM method. ΔE, λ, and f are excitation energy, excitation wavelength, and oscillator strength, respectively.

State	ΔE (eV)	λ (nm)	f	Configuration			Coefficient
				Occ. MO		Unocc. MO	
1	0.519	2390.0	0.0002	130A	→	135A	0.953
				130A	←	135A	-0.241
				111A	→	135A	0.219
				130A	→	132A	0.207
				109A	→	135A	-0.109
				110A	→	135A	0.102
2	0.881	1408.0	0.0000	129B	→	139B	0.790
				125A	→	135A	-0.420
				129B	→	138B	-0.182
				115A	→	135A	-0.138
				128A	→	135A	-0.127
				129B	→	140B	0.120
				116A	→	135A	-0.111
				125A	←	135A	-0.102
3	1.025	1210.2	0.0000	128B	→	139B	0.762
				126A	→	135A	-0.425
				128B	→	138B	-0.188
				123A	→	135A	-0.163
				117A	→	135A	-0.133
				128B	→	140B	0.126
				114A	→	135A	-0.121
				128B	→	142B	-0.107
				128B	→	131B	0.105
4	1.283	966.1	0.0000	127A	→	135A	0.651
				127B	→	139B	-0.470
				129B	→	142B	-0.328
				124A	→	135A	0.252
				118A	→	135A	-0.148
				128A	→	135A	-0.137
				127A	→	132A	0.135
				119A	→	135A	-0.117
				113A	→	135A	0.111
				127B	→	138B	0.107
5	1.298	954.9	0.0000	129B	→	142B	0.869
				127A	→	135A	0.235
				127B	→	139B	-0.182
				129B	→	145B	0.156
				125A	→	135A	0.132
				124A	→	135A	0.106
				125B	→	142B	-0.105
6	1.520	815.5	0.0001	128B	→	142B	0.646
				126A	→	135A	-0.535

				128B	→	139B	-0.262
				123A	→	135A	-0.196
				117A	→	135A	-0.153
				114A	→	135A	-0.142
				128B	→	145B	0.115
				126A	→	132A	-0.112
				128B	→	138B	0.111
				128B	→	131B	-0.110
				128B	←	139B	0.104
7	1.733	715.3	0.0004	127B	→	139B	0.716
				127A	→	135A	0.502
				124A	→	135A	0.187
				127B	→	138B	-0.158
				127B	→	142B	0.154
				124B	→	139B	-0.141
				127A	←	135A	-0.140
				128A	→	135A	-0.117
				118A	→	135A	-0.111
				116B	→	139B	-0.110
				127B	→	140B	0.103
				127A	→	132A	0.102
				127B	←	139B	-0.100
8	2.116	586.0	0.0001	125A	→	135A	0.725
				129B	→	139B	0.485
				128A	→	135A	0.214
				115A	→	135A	0.207
				129B	←	139B	-0.197
				116A	→	135A	0.165
				129A	→	135A	0.156
				125A	→	132A	0.155
				129B	→	131B	0.138
				125A	←	135A	-0.133
				129B	→	138B	-0.125
9	2.246	552.1	0.0002	128B	→	142B	0.592
				126A	→	135A	0.442
				128B	→	139B	0.411
				130A	→	131A	-0.393
				123A	→	135A	0.159
				117A	→	135A	0.117
				114A	→	135A	0.110
				128B	←	139B	-0.105
				128B	→	145B	0.104
10	2.367	523.9	0.0030	130A	→	131A	0.901
				128B	→	142B	0.289
				128B	→	139B	0.169
				126A	→	135A	0.162
				130A	→	132A	0.114
11	2.400	516.6	0.0020	130A	→	132A	0.863

				127B	→	142B	0.351
				130A	→	135A	-0.184
				129B	→	130B	-0.161
				130A	→	131A	-0.108
12	2.468	502.4	0.0044	129B	→	130B	0.956
				130A	→	132A	0.151
13	2.628	471.8	0.0007	127B	→	142B	0.764
				130A	→	132A	-0.354
				128B	→	130B	0.284
				127B	→	131B	-0.154
				124B	→	142B	-0.148
				127B	→	145B	0.133
				116B	→	142B	-0.110
				127B	→	139B	-0.101
				126B	→	142B	-0.101
14	2.646	468.6	0.0080	128B	→	130B	0.730
				127B	→	142B	-0.266
				125B	→	132B	0.244
				129B	→	132B	0.235
				126A	→	131A	-0.231
				128A	→	133A	-0.221
				130A	→	132A	0.181
				128A	→	131A	-0.140
15	2.795	443.7	0.0008	129B	→	131B	0.944
				129B	→	139B	-0.134
				130A	→	133A	0.111
				129A	→	132A	-0.104
				126B	→	131B	0.101
				129B	→	142B	0.101
16	2.840	436.6	0.0006	130A	→	133A	0.900
				130A	→	134A	-0.362
				129B	→	131B	-0.122
17	2.937	422.1	0.0004	129A	→	134A	0.476
				126B	→	133B	-0.465
				127B	→	131B	-0.359
				127A	→	132A	0.273
				129B	→	133B	-0.255
				124B	→	131B	-0.167
				129A	→	132A	0.129
				124A	→	132A	-0.122
				121A	→	132A	0.116
				124A	→	142A	0.109
				121B	→	131B	-0.106
				124B	→	141B	0.105
18	2.966	418.1	0.0005	130A	→	134A	0.899
				130A	→	133A	0.374
19	2.994	414.1	0.0135	129B	→	132B	0.592
				128B	→	130B	-0.479

				128A	→	133A	-0.368
				125B	→	132B	0.262
				123A	→	131A	0.146
				128A	→	131A	-0.134
				123B	→	130B	-0.131
				125B	→	130B	0.126
20	3.083	402.2	0.0001	128B	→	131B	0.957
				127B	→	130B	0.145
				128B	→	139B	-0.101
21	3.163	392.0	0.0003	128A	→	131A	0.556
				129B	→	132B	0.453
				125B	→	130B	-0.406
				128B	→	132B	-0.319
				127B	→	130B	0.171
				129B	→	130B	0.128
				123A	→	133A	-0.125
				123B	→	132B	0.125
				128B	→	130B	0.117
22	3.232	383.6	0.0002	129A	→	132A	0.607
				126B	→	131B	-0.553
				124B	→	133B	-0.194
				124A	→	134A	-0.180
				129B	→	131B	0.170
				127B	→	130B	-0.148
				129B	→	133B	0.129
				129A	→	134A	-0.128
				126B	→	133B	0.120
				127A	→	134A	0.119
23	3.281	377.9	0.0001	127B	→	130B	0.834
				129B	→	132B	-0.273
				128A	→	133A	-0.187
				125B	→	132B	0.180
				129B	→	133B	0.132
				128B	→	131B	-0.131
				126A	→	131A	-0.122
				128B	→	130B	-0.104
24	3.299	375.8	0.0016	127B	→	130B	0.405
				128B	→	132B	0.387
				129B	→	132B	0.372
				128A	→	133A	0.312
				125B	→	132B	-0.308
				129B	→	133B	-0.227
				128A	→	131A	-0.214
				126A	→	131A	0.205
				128B	→	130B	0.158
				125B	→	130B	0.154
				126A	→	133A	-0.102
25	3.363	368.6	0.0129	128B	→	132B	0.809

				125B	→	130B	-0.278
				128A	→	131A	0.275
				128B	→	133B	-0.173
				123B	→	132B	0.124
				128B	→	134B	0.111
				123A	→	133A	-0.108
				127B	→	130B	-0.107
				128A	→	133A	-0.105
26	3.390	365.8	0.0122	129B	→	133B	0.771
				127B	→	131B	-0.372
				129B	→	132B	0.271
				127A	→	132A	0.231
				125B	→	132B	-0.123
				128A	→	133A	0.122
27	3.518	352.4	0.0015	127B	→	131B	0.643
				129B	→	133B	0.435
				129A	→	134A	0.341
				126B	→	133B	-0.288
				127A	→	132A	-0.159
				124A	→	132A	-0.145
				124B	→	131B	-0.144
				128B	→	133B	0.102
28	3.653	339.4	0.0003	128B	→	133B	0.942
				128B	→	132B	0.173
				128B	→	136B	0.103
29	3.739	331.6	0.0024	130A	→	136A	0.842
				127A	→	131A	-0.415
				130A	→	138A	-0.157
				125B	→	130B	0.131
				128A	→	131A	0.120
				130A	→	133A	0.108
30	3.775	328.4	0.0157	127A	→	131A	0.629
				130A	→	136A	0.433
				125B	→	130B	-0.365
				125A	→	131A	-0.242
				128A	→	131A	-0.241
				130A	→	138A	-0.132
				129A	→	131A	-0.117
				124A	→	131A	0.109
				129B	→	135B	-0.109
31	3.801	326.2	0.0107	126A	→	131A	0.475
				129B	→	135B	-0.408
				129B	→	134B	0.251
				128A	→	131A	0.215
				129B	→	132B	-0.164
				129A	→	131A	-0.149
				127A	→	132A	0.137
				130A	→	137A	-0.137

				128B	→	133B	-0.131
				128B	→	130B	0.129
				123A	→	131A	0.127
				114B	→	130B	0.126
				127A	→	131A	-0.123
				120B	→	135B	0.123
				125A	→	131A	-0.119
				125B	→	135B	0.109
				125B	→	132B	0.104
				120A	→	137A	-0.101
32	3.809	325.5	0.0001	130A	→	137A	0.933
				130A	→	138A	-0.158
				127B	→	132B	0.128
				129B	→	135B	-0.109
33	3.831	323.7	0.0071	130A	→	138A	0.552
				129B	→	134B	-0.307
				125A	→	131A	-0.261
				127A	→	131A	-0.253
				126A	→	131A	-0.245
				125B	→	130B	-0.197
				128B	→	134B	-0.135
				129B	→	135B	-0.131
				125A	→	137A	0.109
				122B	→	134B	-0.106
				120A	→	136A	-0.102
34	3.836	323.2	0.0016	130A	→	138A	0.704
				130A	→	137A	0.269
				130A	→	136A	0.220
				127A	→	131A	0.217
				129B	→	134B	0.205
				125A	→	131A	0.165
				126A	→	131A	0.153
				129B	→	135B	0.125
				128A	→	131A	-0.122
35	3.873	320.1	0.0035	127B	→	132B	0.840
				127B	→	133B	-0.281
				129A	→	132A	0.123
				130A	→	137A	-0.115
				127B	→	134B	0.114
				130A	→	139A	0.111
				125B	→	130B	0.101
36	3.881	319.5	0.0686	125B	→	130B	0.449
				127A	→	131A	0.418
				128A	→	131A	0.407
				130A	→	139A	-0.371
				129A	→	131A	0.219
				129B	→	134B	-0.206
				125A	→	131A	0.206

				129B	→	135B	-0.168
				126B	→	130B	-0.101
37	3.892	318.5	0.0154	130A	→	139A	0.827
				130A	→	140A	-0.211
				127B	→	132B	-0.186
				125B	→	130B	0.180
				128A	→	131A	0.176
				129B	→	135B	-0.153
				127A	→	131A	0.139
				129A	→	131A	0.125
				126A	→	131A	-0.103
38	3.905	317.5	0.0233	126A	→	131A	0.404
				129B	→	134B	-0.367
				127A	→	132A	0.357
				125B	→	132B	0.229
				129B	→	135B	0.222
				127B	→	131B	0.195
				128A	→	133A	-0.175
				120A	→	131A	-0.154
				128A	→	132A	-0.146
				130A	→	139A	0.139
				129A	→	131A	-0.132
				128B	→	135B	-0.114
				125A	→	136A	-0.111
				125A	→	133A	0.108
				120B	→	130B	0.103
39	3.946	314.2	0.159	126B	→	131B	0.687
				129A	→	132A	0.420
				127B	→	133B	-0.244
				125A	→	132A	0.176
				130A	→	138A	-0.135
				124A	→	134A	-0.113
				126B	→	141B	0.110
				127B	→	132B	-0.105
				115B	→	131B	0.104
				121A	→	138A	0.103
40	3.955	313.5	0.0576	129A	→	132A	0.503
				127B	→	132B	-0.235
				124B	→	133B	0.205
				129A	→	142A	0.200
				129B	→	137B	0.188
				121B	→	136B	0.181
				126B	→	141B	-0.173
				121A	→	138A	-0.152
				129B	→	136B	0.145
				124A	→	134A	0.145
				126B	→	131B	0.131
				115B	→	131B	-0.125

				119A	→	132A	0.125
				122B	→	137B	-0.122
				124B	→	131B	0.122
				122A	→	139A	0.120
				124A	→	138A	-0.112
				124A	→	132A	0.108
				122A	→	132A	0.105
				121A	→	134A	-0.104
				127A	→	134A	-0.102
				126A	→	131A	-0.102
				125A	→	132A	-0.100
41	3.999	310.0	0.0145	127A	→	132A	0.498
				127B	→	131B	0.357
				129A	→	131A	0.288
				126A	→	131A	-0.198
				129B	→	136B	0.194
				125B	→	132B	-0.145
				128A	→	132A	-0.133
				126B	→	130B	0.116
				124A	→	132A	0.116
				127B	→	133B	0.114
				126B	→	133B	0.103
				128B	→	135B	0.100
42	4.044	306.6	0.0268	129A	→	131A	0.628
				126A	→	131A	0.246
				127A	→	132A	-0.241
				125B	→	130B	-0.211
				125A	→	131A	0.194
				128A	→	131A	-0.168
				127B	→	133B	-0.166
				125B	→	132B	0.152
				124B	→	131B	0.143
				128B	→	134B	-0.127
				126B	→	133B	-0.109
				127B	→	131B	-0.106
				128A	→	132A	0.102
				126B	→	130B	-0.100
43	4.050	306.1	0.0109	129A	→	131A	0.374
				124B	→	131B	-0.241
				129B	→	136B	-0.213
				124A	→	132A	-0.211
				126B	→	130B	0.210
				126B	→	133B	0.196
				129A	→	134A	-0.190
				115B	→	133B	0.182
				127A	→	132A	0.176
				125A	→	131A	0.175
				121A	→	132A	0.134

				122A	→	138A	-0.133
				122B	→	136B	0.126
				125B	→	130B	-0.121
				126B	→	144B	0.120
				121B	→	131B	-0.119
				119A	→	134A	-0.118
				129A	→	145A	0.117
				121A	→	139A	0.115
				129B	→	135B	0.111
				118A	→	134A	0.110
				130A	→	139A	-0.108
44	4.080	303.9	0.0363	127B	→	133B	0.789
				127B	→	132B	0.257
				129A	→	132A	0.218
				126B	→	130B	-0.195
				125A	→	132A	0.176
				128A	→	132A	0.161
				127A	→	134A	-0.144
				126B	→	133B	-0.118
				126A	→	132A	-0.108
45	4.094	302.8	0.0084	126B	→	130B	0.575
				123A	→	131A	-0.324
				123B	→	130B	0.311
				129B	→	135B	-0.218
				128A	→	136A	-0.197
				127B	→	133B	0.196
				128B	→	135B	0.194
				125B	→	134B	-0.172
				126A	→	131A	0.155
				129A	→	131A	0.112
				113B	→	132B	0.110
				126B	→	133B	-0.102
46	4.113	301.5	0.0023	126B	→	130B	0.688
				123A	→	131A	0.254
				123B	→	130B	-0.233
				129A	→	131A	-0.215
				125B	→	134B	0.163
				128B	→	135B	-0.160
				128A	→	136A	0.149
				129B	→	135B	0.141
				128B	→	134B	-0.138
				129B	→	134B	0.135
				125A	→	131A	0.110
				126B	→	133B	-0.103
47	4.120	300.9	0.001	129B	→	135B	0.487
				128B	→	135B	0.338
				125B	→	135B	0.270
				129A	→	131A	-0.257

				125A	→	131A	0.245
				129B	→	134B	0.221
				128A	→	137A	-0.191
				128A	→	136A	-0.175
				123B	→	135B	-0.166
				126A	→	133A	-0.162
				128B	→	134B	-0.141
				126B	→	130B	-0.135
				123A	→	136A	0.134
				128A	→	131A	0.123
				123B	→	132B	-0.122
				125B	→	130B	-0.121
				123A	→	131A	-0.116
				123A	→	133A	0.115
				123B	→	130B	0.112
48	4.174	297.0	0.0029	126A	→	132A	0.836
				128A	→	132A	0.333
				125A	→	132A	0.156
				123A	→	132A	0.150
				126A	→	135A	-0.143
				129B	→	134B	-0.135
				130A	→	138A	0.129
49	4.180	296.6	0.0241	129B	→	134B	0.553
				125A	→	131A	-0.269
				123A	→	131A	-0.231
				128B	→	134B	-0.223
				126A	→	132A	0.218
				125B	→	134B	0.172
				128A	→	133A	-0.162
				123B	→	130B	0.162
				123A	→	137A	-0.136
				128A	→	136A	0.130
				123B	→	134B	0.117
				127A	→	132A	0.114
				129A	→	131A	0.111
				123B	→	135B	0.107
				125B	→	130B	0.101
50	4.199	295.3	0.1175	125A	→	131A	0.627
				129B	→	135B	-0.463
				129A	→	131A	-0.299
				125B	→	130B	-0.191
				126A	→	133A	0.170
				128A	→	131A	-0.149
				128B	→	134B	-0.146
				128A	→	132A	0.110
				125B	→	134B	0.106
51	4.216	294.1	0.0464	128A	→	132A	0.637
				125A	→	132A	0.426

				126A	→	132A	-0.329
				127B	→	133B	-0.204
				127A	→	132A	0.165
				126B	→	131B	-0.159
				125A	→	135A	-0.130
				125A	→	131A	-0.125
				124A	→	134A	0.119
				124A	→	132A	0.102
				124B	→	133B	0.102
52	4.229	293.2	0.0041	124A	→	132A	0.371
				124B	→	131B	0.342
				129A	→	138A	-0.302
				126B	→	136B	0.299
				129B	→	136B	-0.268
				124B	→	137B	0.174
				124A	→	139A	0.162
				121A	→	132A	0.156
				129A	→	133A	0.148
				127A	→	139A	-0.147
				127B	→	137B	0.143
				121B	→	131B	-0.133
				122A	→	138A	-0.121
				122B	→	136B	0.118
				126B	→	132B	-0.116
				121A	→	139A	0.101
				127B	→	131B	0.101
53	4.270	290.4	0.0049	128B	→	134B	0.388
				128B	→	135B	-0.312
				123A	→	133A	0.300
				123B	→	132B	-0.276
				126A	→	133A	-0.249
				128A	→	141A	0.212
				128A	→	137A	0.202
				125B	→	140B	-0.169
				129B	→	134B	0.169
				113B	→	130B	-0.160
				129B	→	140B	-0.149
				115A	→	131A	0.144
				125B	→	135B	-0.141
				125B	→	130B	-0.132
				116A	→	131A	-0.123
				128A	→	133A	-0.122
				123A	→	131A	-0.116
				113B	→	132B	0.115
54	4.315	287.4	0.0191	127A	→	133A	0.577
				129B	→	136B	-0.337
				129A	→	133A	-0.266
				128A	→	133A	-0.206

				127A	→	134A	-0.199
				129B	→	134B	-0.151
				129A	→	138A	0.144
				126B	→	136B	-0.138
				125B	→	132B	-0.121
				125A	→	133A	-0.119
				124B	→	137B	-0.116
				129A	→	139A	-0.109
				124B	→	133B	0.108
				129B	→	135B	0.106
				129B	→	137B	-0.106
				124A	→	134A	0.101
55	4.337	285.9	0.0077	129B	→	137B	0.419
				128A	→	132A	0.379
				127A	→	133A	0.338
				125A	→	132A	-0.265
				125B	→	131B	-0.214
				128A	→	133A	-0.175
				127A	→	134A	0.171
				124A	→	134A	-0.148
				124B	→	133B	-0.145
				122A	→	132A	0.134
				128A	→	135A	0.125
				129A	→	142A	-0.121
				127A	→	132A	0.117
				129A	→	133A	0.116
				129B	→	134B	-0.110
				129B	→	138B	-0.103
				122B	→	131B	-0.102
56	4.342	285.5	0.0071	129B	→	136B	0.480
				127A	→	133A	0.365
				129A	→	133A	0.306
				129B	→	137B	-0.288
				127A	→	134A	-0.219
				129A	→	138A	-0.163
				126B	→	136B	0.153
				126A	→	133A	-0.150
				125B	→	131B	0.128
				124B	→	137B	0.128
				125A	→	133A	0.125
				128B	→	134B	-0.121
				124A	→	139A	0.116
				129B	→	138B	0.113
57	4.369	283.8	0.002	125B	→	131B	0.748
				129B	→	137B	0.370
				126B	→	137B	0.218
				129A	→	139A	-0.210
				124B	→	136B	0.166

				124A	→	138A	0.141
				128B	→	134B	0.119
58	4.378	283.2	0.03	128B	→	134B	0.421
				125B	→	131B	-0.355
				126A	→	133A	0.338
				128B	→	135B	0.305
				127A	→	133A	0.237
				125A	→	133A	0.186
				125B	→	132B	0.176
				128A	→	133A	0.163
				123B	→	130B	-0.162
				129A	→	139A	-0.133
				126B	→	137B	0.115
				129B	→	134B	0.114
				128A	→	132A	0.109
				125A	→	132A	-0.109
59	4.380	283.1	0.0542	126A	→	133A	0.566
				129A	→	133A	-0.280
				125B	→	131B	0.264
				129B	→	136B	0.235
				128B	→	135B	-0.201
				126B	→	137B	-0.192
				129A	→	139A	0.190
				129B	→	135B	0.154
				124A	→	138A	-0.116
				124B	→	136B	-0.113
				128B	→	134B	0.111
				128A	→	137A	-0.111
				129B	→	137B	-0.108
				126B	→	132B	-0.107
60	4.394	282.2	0.0077	125B	→	131B	0.348
				128B	→	135B	0.299
				129A	→	139A	0.260
				126B	→	137B	-0.249
				126A	→	133A	-0.238
				127A	→	133A	0.221
				129B	→	136B	-0.213
				124B	→	136B	-0.182
				124A	→	138A	-0.172
				125A	→	132A	-0.169
				128B	→	134B	0.159
				124A	→	134A	-0.153
				124B	→	133B	-0.143
				127B	→	136B	-0.129
				129A	→	133A	0.126
				123B	→	130B	-0.123
				115B	→	131B	0.123
				124A	→	133A	0.112

				127A	→	138A	0.111
				129B	→	137B	-0.103
61	4.420	280.5	0.0262	125A	→	132A	0.518
				129B	→	137B	0.417
				127A	→	133A	0.295
				128A	→	132A	-0.280
				128A	→	135A	-0.234
				128B	→	135B	0.196
				127A	→	134A	0.164
				128B	→	134B	-0.152
				126A	→	133A	0.137
				127A	→	132A	-0.128
				125B	→	135B	-0.112
				129B	→	136B	0.110
				129B	→	138B	-0.104
				129A	→	135A	-0.102
				125B	→	131B	-0.101
62	4.429	279.9	0.0162	128B	→	134B	0.481
				128B	→	135B	-0.288
				128A	→	137A	-0.274
				125B	→	135B	0.245
				125A	→	132A	0.244
				123B	→	134B	0.210
				125B	→	134B	0.194
				129A	→	133A	0.177
				128A	→	132A	-0.172
				126A	→	133A	-0.172
				123A	→	136A	0.166
				123A	→	133A	-0.151
				123B	→	132B	0.145
				129B	→	140B	0.131
				129B	→	137B	0.125
				113B	→	130B	0.122
				126A	→	136A	-0.114
				128B	→	132B	-0.105
				129B	→	134B	-0.101
63	4.433	279.7	0.0072	126B	→	132B	0.276
				125A	→	133A	0.266
				120A	→	131A	-0.255
				128B	→	135B	-0.240
				126A	→	131A	-0.228
				120B	→	130B	0.206
				128A	→	136A	-0.173
				129B	→	134B	0.169
				121A	→	132A	0.162
				125B	→	134B	-0.150
				122A	→	133A	0.143
				127A	→	133A	0.141

				119B	→	130B	-0.137
				121B	→	131B	-0.136
				123B	→	135B	-0.134
				125A	→	134A	0.131
				122B	→	132B	-0.131
				125B	→	135B	0.122
				123A	→	137A	0.121
				128B	→	140B	-0.115
				125B	→	133B	0.106
				114A	→	131A	-0.105
				121B	→	130B	0.103
64	4.460	278.0	0.0004	130A	→	140A	0.932
				130A	→	139A	0.248
				129B	→	136B	0.103
65	4.480	276.8	0.0596	127A	→	134A	0.428
				129A	→	133A	0.371
				129B	→	136B	-0.368
				128A	→	134A	-0.240
				126A	→	133A	0.236
				129B	→	137B	-0.222
				121B	→	131B	0.203
				121A	→	132A	-0.199
				127A	→	132A	0.175
				130A	→	140A	0.173
				122B	→	133B	-0.132
				126B	→	132B	0.127
				122A	→	134A	0.113
				126B	→	133B	-0.102
66	4.484	276.5	0.0241	129A	→	133A	0.592
				127A	→	134A	-0.426
				126A	→	133A	0.310
				129A	→	135A	-0.229
				128A	→	134A	0.183
				127A	→	133A	-0.138
				120A	→	131A	0.132
				128B	→	134B	-0.129
				126B	→	132B	0.128
				128B	→	135B	-0.124
				120B	→	130B	-0.106
67	4.502	275.4	0.0492	127A	→	134A	0.418
				126B	→	132B	0.355
				129B	→	136B	0.307
				129B	→	137B	-0.248
				121A	→	132A	0.209
				121B	→	131B	-0.203
				120A	→	131A	0.171
				127A	→	132A	-0.152
				126A	→	131A	0.145

				120B	→	130B	-0.126
				128A	→	134A	-0.123
				125A	→	132A	-0.118
				122B	→	133B	0.116
				122A	→	134A	-0.116
				129A	→	134A	-0.114
				130A	→	140A	-0.110
68	4.517	274.5	0.0179	126B	→	132B	0.727
				130A	→	142A	0.344
				126A	→	134A	0.181
				129B	→	137B	0.162
				128B	→	136B	-0.141
				129A	→	133A	-0.120
				129A	→	138A	-0.115
				127A	→	134A	-0.108
				127A	→	132A	0.108
				118A	→	132A	-0.105
				126B	→	136B	0.103
				116B	→	131B	0.102
69	4.534	273.5	0.0069	130A	→	142A	0.658
				126A	→	134A	0.330
				129A	→	134A	-0.262
				126B	→	132B	-0.248
				128B	→	136B	-0.192
				130A	→	141A	-0.156
				126B	→	133B	-0.155
				116B	→	131B	-0.144
				124B	→	131B	-0.130
				118A	→	132A	0.124
				118B	→	131B	-0.109
				119A	→	132A	0.104
70	4.554	272.2	0.0062	128A	→	135A	0.394
				129A	→	135A	-0.292
				126B	→	132B	-0.217
				128A	→	133A	-0.206
				127A	→	134A	0.189
				129A	→	134A	0.189
				122B	→	131B	0.177
				116B	→	131B	0.166
				128B	→	135B	0.161
				122A	→	132A	-0.158
				121B	→	133B	-0.151
				125B	→	132B	-0.146
				118A	→	132A	-0.139
				124B	→	131B	0.139
				130A	→	142A	0.136
				121A	→	134A	0.134
				129A	→	138A	0.127

				121B	→	131B	-0.125
				129A	→	133A	0.120
				124A	→	134A	0.119
				125A	→	134A	0.115
				124B	→	133B	0.114
				126B	→	136B	-0.103
71	4.564	271.7	0.0361	129A	→	135A	0.659
				129A	→	133A	0.218
				129A	→	134A	0.199
				128B	→	135B	-0.175
				128A	→	133A	0.172
				128A	→	135A	-0.171
				130A	→	142A	0.152
				126B	→	132B	-0.124
				122B	→	131B	0.122
				122A	→	132A	-0.121
				125A	→	132A	-0.118
				129B	→	137B	0.116
				116B	→	131B	0.114
				125B	→	132B	0.110
72	4.583	270.5	0.0164	128B	→	136B	0.522
				129A	→	135A	-0.328
				128A	→	133A	0.279
				128B	→	135B	-0.275
				125B	→	132B	0.179
				128A	→	135A	0.173
				129A	→	133A	-0.148
				129A	→	134A	-0.147
				122B	→	131B	0.120
				128A	→	134A	-0.119
				122A	→	132A	-0.118
				125A	→	132A	-0.116
				114B	→	130B	-0.114
				126B	→	133B	-0.113
				126A	→	133A	-0.107
				128B	→	137B	-0.106
				119B	→	130B	0.102
73	4.587	270.3	0.0025	128B	→	136B	0.542
				130A	→	142A	0.319
				129A	→	134A	0.223
				128A	→	135A	-0.193
				122B	→	131B	-0.174
				130A	→	141A	-0.167
				129B	→	137B	-0.166
				122A	→	132A	0.163
				125A	→	132A	0.153
				128A	→	134A	0.148
				118B	→	131B	0.143

				128B	→	134B	0.129
				121A	→	134A	-0.122
				121B	→	133B	0.119
				126B	→	133B	0.119
				128B	→	137B	-0.118
				119A	→	132A	-0.113
				125A	→	134A	0.113
				124B	→	131B	0.106
				128A	→	133A	-0.103
74	4.590	270.1	0.0442	128B	→	136B	0.473
				129A	→	135A	0.354
				128A	→	133A	-0.167
				122B	→	130B	-0.161
				122A	→	131A	0.159
				123B	→	132B	-0.147
				120A	→	133A	-0.147
				125A	→	131A	-0.144
				129A	→	134A	-0.140
				120B	→	132B	0.129
				119B	→	130B	-0.115
				118B	→	131B	-0.115
				125B	→	132B	-0.114
				129B	→	137B	0.114
				128A	→	137A	-0.114
				120B	→	130B	0.113
				128B	→	134B	0.112
				116A	→	131A	-0.110
				120A	→	131A	-0.100
				128A	→	135A	0.100
75	4.597	269.7	0.0693	128A	→	133A	0.259
				125B	→	132B	0.242
				129A	→	135A	-0.226
				122B	→	130B	-0.224
				128A	→	135A	-0.215
				120A	→	133A	-0.204
				122A	→	131A	0.204
				120B	→	132B	0.183
				125A	→	131A	-0.175
				128B	→	136B	-0.157
				128A	→	137A	-0.155
				116B	→	130B	0.150
				128B	→	135B	-0.148
				118B	→	130B	-0.146
				123B	→	132B	-0.138
				115A	→	131A	-0.135
				129A	→	134A	0.118
				116A	→	131A	-0.118
				128B	→	134B	-0.114

				130A	→	141A	-0.114
76	4.620	268.4	0.0014	130A	→	141A	0.930
				130A	→	142A	0.215
				128A	→	135A	-0.152
				127A	→	133A	0.114
77	4.634	267.5	0.0206	128A	→	135A	0.619
				125A	→	132A	0.263
				125A	→	135A	-0.224
				125A	→	133A	0.176
				128A	→	132A	-0.174
				129A	→	135A	0.171
				114A	→	131A	0.148
				127A	→	135A	0.146
				129A	→	134A	0.144
				126B	→	133B	0.143
				130A	→	141A	0.141
				128B	→	135B	-0.136
				122B	→	131B	-0.126
				122A	→	132A	0.122
				128B	→	134B	-0.106
				114B	→	130B	-0.106
78	4.645	266.9	0.0069	128B	→	137B	0.924
				128B	→	138B	-0.235
				128B	→	136B	0.195
79	4.661	266.0	0.0069	125B	→	132B	0.383
				126B	→	133B	-0.372
				129A	→	134A	-0.298
				114A	→	131A	-0.246
				128A	→	135A	0.225
				128A	→	133A	0.217
				125A	→	133A	-0.189
				126A	→	131A	-0.181
				114B	→	130B	0.160
				123B	→	130B	0.148
				129A	→	135A	0.134
				118A	→	132A	-0.129
				119A	→	132A	-0.120
				123A	→	131A	-0.119
				125A	→	132A	0.115
				125A	→	135A	-0.113
				128A	→	134A	0.101
				124A	→	132A	0.100
80	4.671	265.5	0.1971	126B	→	133B	0.443
				129A	→	134A	0.346
				125B	→	132B	0.328
				128A	→	133A	0.197
				114A	→	131A	-0.188
				118A	→	132A	0.187

				127A	→	132A	-0.168
				124B	→	131B	-0.161
				119A	→	132A	0.160
				123B	→	130B	0.158
				130A	→	142A	0.152
				125A	→	133A	-0.142
				126A	→	131A	-0.132
				114B	→	130B	0.124
				118B	→	131B	-0.112
				128A	→	135A	0.111
				124A	→	132A	-0.105
81	4.693	264.2	0.0052	128A	→	134A	0.759
				127A	→	134A	0.288
				126A	→	134A	0.254
				125A	→	134A	0.217
				130A	→	142A	-0.200
				125A	→	133A	0.189
82	4.747	261.2	0.0172	126A	→	134A	0.796
				130A	→	142A	-0.338
				125A	→	133A	-0.286
				128A	→	134A	-0.175
				126B	→	133B	0.111
				123A	→	134A	0.103
83	4.772	259.8	0.0068	125A	→	133A	0.631
				123B	→	130B	0.292
				128A	→	136A	0.267
				128A	→	134A	-0.256
				126A	→	134A	0.245
				120B	→	130B	-0.169
				123A	→	137A	-0.133
				120A	→	137A	-0.115
				122B	→	132B	0.107
				127B	→	134B	-0.101
84	4.780	259.4	0.0005	129B	→	138B	0.932
				129B	→	137B	0.248
				129B	→	139B	0.217
85	4.791	258.8	0.0021	127B	→	134B	0.754
				127B	→	135B	-0.551
				127B	→	132B	-0.161
				127B	→	136B	-0.133
86	4.797	258.5	0.0002	125B	→	133B	0.946
				128A	→	136A	0.126
				125A	→	134A	-0.106
87	4.825	257.0	0.0001	124A	→	131A	0.963
				127A	→	131A	-0.203
				125A	→	131A	-0.102
88	4.838	256.3	0.0003	124B	→	130B	0.979
89	4.845	255.9	0.0001	127B	→	135B	0.783

				127B	→	134B	0.549
				129B	→	140B	0.154
				124B	→	130B	0.102
90	4.885	253.8	0.0058	129B	→	140B	0.892
				125B	→	135B	-0.153
				129B	→	139B	-0.146
				123B	→	132B	-0.117
				127B	→	135B	-0.108
				127B	→	134B	-0.101
91	4.900	253.0	0.0295	124B	→	131B	0.571
				124A	→	132A	-0.568
				125A	→	134A	-0.337
				129A	→	138A	0.162
				128A	→	134A	0.149
				121B	→	131B	-0.136
				125B	→	133B	-0.113
				126B	→	136B	0.107
				123A	→	131A	0.100
92	4.933	251.3	0.044	123A	→	131A	0.618
				123B	→	130B	0.505
				125A	→	134A	0.334
				125A	→	133A	-0.252
				128A	→	134A	-0.132
				120A	→	131A	-0.129
				114A	→	131A	0.126
93	4.973	249.3	0.0428	125A	→	134A	0.729
				124A	→	132A	-0.366
				124B	→	131B	0.245
				123A	→	131A	-0.233
				128A	→	134A	-0.204
				123B	→	130B	-0.201
				129A	→	138A	-0.100
94	5.006	247.7	0.0004	129B	→	141B	0.937
				126B	→	137B	0.123
				129B	→	139B	0.117
95	5.044	245.8	0.0002	128B	→	138B	0.926
				128B	→	137B	0.263
				128B	→	139B	0.217
96	5.071	244.5	0.0012	123A	→	132A	0.482
				120B	→	131B	-0.473
				119B	→	131B	-0.295
				121B	→	131B	-0.258
				117B	→	133B	0.174
				128B	→	141B	0.170
				123A	→	135A	0.139
				120A	→	132A	0.131
				119B	→	133B	-0.130
				123B	→	131B	0.127

				128A	→	137A	-0.125
				123B	→	132B	-0.121
				114B	→	131B	-0.118
				126A	→	132A	-0.108
				117B	→	131B	-0.100
97	5.082	244.0	0.0032	128A	→	137A	0.432
				123B	→	132B	0.377
				125A	→	137A	0.257
				120A	→	133A	-0.250
				122A	→	131A	0.228
				114B	→	132B	0.167
				123B	→	131B	0.158
				119B	→	132B	-0.157
				120A	→	136A	-0.157
				120B	→	131B	-0.146
				129A	→	137A	0.138
				127A	→	137A	-0.129
				125B	→	135B	0.118
				122A	→	137A	0.118
				123A	→	133A	0.106
				123A	→	132A	0.105
				120B	→	132B	0.105
				122A	→	133A	-0.103
98	5.092	243.5	0.0006	123A	→	132A	0.723
				120B	→	131B	0.296
				127B	→	136B	-0.239
				123A	→	135A	0.233
				123B	→	131B	-0.225
				119B	→	131B	0.184
				121B	→	131B	0.167
				126A	→	135A	-0.135
				126A	→	132A	-0.128
				128B	→	141B	-0.119
				117B	→	133B	-0.118
99	5.094	243.4	0.0074	127B	→	136B	0.831
				123A	→	132A	0.237
				124B	→	133B	-0.154
				127B	→	134B	0.142
				127B	→	137B	-0.142
				129A	→	139A	0.139
				124B	→	136B	-0.108
100	5.124	242.0	0.0009	123B	→	131B	0.945
				120B	→	131B	0.167
				123A	→	132A	0.102

Table S3 Spin-singlet excited states of **$Co^{III}(Fctpy)_2$** in CH_3CN calculated by using the TDDFT method. The solvent effect was taken into account by the PCM method. ΔE,λ, and f are excitation energy, excitation wavelength, and oscillator strength, respectively.

State	ΔE (eV)	λ (nm)	f	Configuration			Coefficient
				Occ. MO		Unocc. MO	
1	1.751	708.0	0.0133	209	→	231	0.302
				209	→	215	-0.285
				213	→	215	0.256
				213	→	231	-0.247
				209	→	225	-0.210
				212	→	215	-0.206
				213	→	225	0.168
				212	→	231	0.140
				212	→	225	-0.122
2	1.756	706.1	0.0010	208	→	232	0.222
				210	→	232	0.220
				211	→	214	-0.214
				211	→	216	0.210
				210	→	214	0.200
				210	→	216	-0.197
				211	→	232	-0.184
				210	→	224	0.173
				208	→	214	0.171
				208	→	216	-0.169
				211	→	224	-0.168
				208	→	224	0.167
3	1.788	693.3	0.0054	208	→	232	0.300
				208	→	214	0.261
				208	→	216	-0.258
				208	→	224	0.244
				211	→	214	0.188
				211	→	216	-0.183
				211	→	232	0.181
				211	→	224	0.155
				211	→	229	0.138
				208	→	229	0.131
4	1.794	691.1	0.0004	209	→	215	0.313
				213	→	215	0.256
				209	→	231	-0.231
				209	→	225	0.211
				212	→	215	-0.209
				209	→	230	0.202
				212	→	230	-0.177
				213	→	231	-0.152
				213	→	225	0.137
				212	→	225	-0.129
				212	→	231	0.113
				209	→	214	-0.100

5	1.891	655.7	0.0281	212	→	215	0.365
				212	→	231	-0.298
				213	→	215	0.272
				213	→	230	0.222
				212	→	225	0.206
				213	→	231	-0.178
				213	→	225	0.162
				212	→	214	-0.117
6	1.917	646.7	0.0174	210	→	214	0.264
				210	→	216	-0.258
				210	→	232	0.258
				211	→	232	0.221
				210	→	224	0.203
				211	→	214	0.196
				211	→	216	-0.185
				210	→	229	0.170
				211	→	229	-0.157
				211	→	224	0.155
7	2.074	597.9	0.0000	195	→	216	0.413
				195	→	214	0.393
				181	→	216	0.249
				181	→	214	0.235
				195	→	215	0.105
				203	→	216	-0.105
				203	→	214	-0.103
8	2.126	583.1	0.0000	208	→	229	0.573
				210	→	229	-0.317
				211	→	229	-0.267
				208	←	229	-0.114
9	2.168	571.9	0.0004	209	→	230	0.482
				213	→	230	0.411
				212	→	230	0.177
				209	→	231	0.165
				213	→	231	0.147
10	2.277	544.4	0.0015	213	→	214	0.243
				213	→	216	0.213
				194	→	216	0.165
				194	→	214	0.156
				194	→	219	-0.154
				190	→	216	0.121
				197	→	216	0.116
				190	→	214	0.114
				190	→	219	-0.114
				209	→	214	-0.113
				197	→	214	0.109
				209	→	216	-0.105
				184	→	216	0.105
				186	→	216	0.104
				186	→	219	-0.103

				184	→	219	-0.103
				197	→	219	-0.102
				212	→	214	0.100
11	2.351	527.3	0.0032	211	→	229	0.491
				210	→	229	-0.357
				210	→	214	0.185
				208	→	216	0.147
				211	→	214	0.131
				208	→	214	-0.126
12	2.361	525.2	0.0010	210	→	216	0.191
				192	→	219	0.181
				211	→	216	0.160
				192	→	216	0.156
				187	→	219	0.151
				192	→	214	0.150
				207	→	214	0.138
				191	→	219	-0.135
				207	→	216	0.134
				196	→	219	-0.128
				207	→	219	0.126
				210	→	214	0.123
				187	→	216	0.121
				211	→	229	-0.118
				187	→	214	0.117
				185	→	219	-0.115
				211	→	214	0.115
				196	→	216	-0.114
				191	→	216	-0.114
				208	→	214	0.112
				196	→	214	-0.110
				191	→	214	-0.109
13	2.397	517.3	0.0062	212	→	230	0.495
				213	→	230	-0.278
				213	→	215	0.251
				209	→	215	0.174
				212	→	231	0.169
				212	→	215	0.105
14	2.485	498.9	0.0006	210	→	229	0.386
				208	→	229	0.320
				211	→	229	0.278
				211	→	214	-0.226
				210	→	232	-0.151
				210	→	214	0.142
				211	→	216	0.139
				210	→	216	-0.119
				211	→	232	0.111
15	2.486	498.8	0.0008	212	→	215	0.324
				209	→	230	0.312
				213	→	230	-0.261

				212	→	230	-0.224
				213	→	231	-0.218
				212	→	214	-0.138
				212	→	231	0.137
				213	→	215	-0.114
				213	→	214	0.107
				213	→	217	-0.104
16	2.516	492.8	0.0006	213	→	214	0.519
				213	→	216	0.276
				213	→	215	0.164
				194	→	219	0.112
17	2.586	479.5	0.0001	212	→	214	0.557
				212	→	216	0.341
				212	→	215	0.167
18	2.605	476.0	0.0022	213	→	216	0.412
				213	→	214	-0.256
				211	→	216	0.220
				211	→	214	0.195
				210	→	214	0.165
				210	→	216	0.153
				213	→	218	0.145
				213	→	217	-0.107
19	2.605	475.9	0.0008	213	→	216	0.359
				211	→	216	-0.259
				211	→	214	-0.230
				213	→	214	-0.214
				210	→	214	-0.188
				210	→	216	-0.177
				192	→	219	0.127
				213	→	218	0.124
20	2.619	473.5	0.0002	210	→	216	0.383
				210	→	214	0.350
				211	→	216	-0.331
				211	→	214	-0.313
21	2.621	473.1	0.0204	213	→	217	0.369
				213	→	218	-0.282
				213	→	215	-0.262
				213	→	216	0.240
				209	→	215	0.188
				213	→	231	-0.168
				209	→	231	0.110
22	2.651	467.7	0.0032	209	→	214	0.556
				209	→	216	0.330
				213	→	217	0.104
23	2.677	463.1	0.0351	209	→	215	0.346
				213	→	217	-0.299
				213	→	218	0.234
				209	→	231	0.218
				213	→	215	-0.212

				213	→	231	-0.148
				213	→	230	0.142
				209	→	216	0.113
24	2.702	458.8	0.0011	212	→	216	0.568
				212	→	214	-0.340
				212	→	218	0.132
25	2.704	458.6	0.0019	211	→	215	0.442
				210	→	215	0.344
				211	→	217	0.209
				210	→	217	0.204
				210	→	218	0.140
				211	→	218	0.136
26	2.718	456.2	0.0032	211	→	215	0.434
				210	→	217	-0.328
				210	→	218	-0.254
				210	→	215	-0.195
				211	→	214	-0.158
				208	→	214	-0.111
				211	→	216	0.104
27	2.721	455.7	0.0012	212	→	217	0.405
				212	→	218	-0.328
				213	→	231	-0.172
				212	→	216	0.164
				209	→	215	-0.162
				212	→	215	-0.147
				212	→	231	-0.134
				209	→	231	-0.133
				209	→	230	0.113
28	2.725	455.1	0.0035	210	→	215	0.489
				211	→	217	-0.296
				211	→	218	-0.235
				210	→	214	-0.183
				210	→	218	-0.140
				210	→	217	-0.124
29	2.736	453.3	0.0002	211	→	217	0.325
				211	→	218	0.287
				211	→	215	-0.217
				210	→	215	0.215
				208	→	214	-0.203
				210	→	217	-0.150
				210	→	216	0.147
				210	→	229	0.139
				210	→	218	-0.139
				211	→	214	0.138
				210	→	214	-0.135
				210	→	232	0.125
30	2.744	451.8	0.0003	208	→	214	0.445
				208	→	216	0.409
				210	→	217	-0.153

				210	→	218	-0.137
				211	→	215	-0.124
				208	→	215	0.100
31	2.774	447.0	0.0013	209	→	216	0.570
				209	→	214	-0.349
				209	→	215	-0.154
32	2.802	442.5	0.0497	209	→	217	0.273
				208	→	216	0.273
				208	→	232	0.248
				209	→	218	-0.221
				208	→	217	-0.181
				208	→	218	-0.155
				210	→	217	0.153
				208	→	214	-0.143
				210	→	218	0.119
				212	→	217	-0.116
				208	→	224	0.113
33	2.805	442.0	0.0029	209	→	217	0.341
				209	→	218	-0.278
				208	→	216	-0.223
				208	→	232	-0.202
				208	→	217	0.157
				212	→	217	-0.135
				208	→	218	0.134
				208	→	214	0.117
				210	→	217	-0.114
				212	→	215	-0.107
34	2.836	437.2	0.0003	209	→	231	0.308
				212	→	230	-0.289
				213	→	231	0.220
				212	→	231	-0.209
				209	→	215	0.192
				213	→	230	-0.180
				213	→	215	0.176
				213	→	225	-0.162
				209	→	230	0.126
				212	→	217	0.126
				209	→	225	-0.123
35	2.852	434.7	0.0108	212	→	231	0.312
				209	→	217	0.241
				209	→	230	-0.237
				212	→	215	0.230
				212	→	217	0.213
				213	→	230	0.201
				209	→	218	-0.192
				212	→	225	-0.181
				212	→	218	-0.152
				213	→	231	0.121
				212	→	230	-0.117

36	2.856	434.1	0.001	208	→	215	0.576
				208	→	214	-0.194
				208	→	217	0.168
				211	→	232	-0.106
				210	→	232	0.104
37	2.864	432.9	0	211	→	232	0.323
				208	→	215	0.292
				210	→	229	-0.189
				211	→	217	0.185
				211	→	216	0.178
				211	→	224	0.172
				210	→	232	-0.159
				208	→	229	-0.155
				211	→	218	0.148
				211	→	214	-0.119
				210	→	216	-0.118
				208	→	218	-0.111
				208	→	217	-0.103
38	2.881	430.3	0.0007	213	→	219	0.528
				213	→	218	0.161
				209	→	216	0.127
				212	→	219	0.120
				209	→	219	-0.111
				194	→	216	0.109
				194	→	214	0.105
39	2.893	428.6	0.0224	208	→	217	0.355
				208	→	218	0.295
				211	→	232	0.229
				210	→	232	0.164
				208	→	215	-0.158
				211	→	216	0.155
				211	→	224	0.143
				211	→	214	-0.134
				210	→	216	0.126
				210	→	214	-0.117
				210	→	217	0.109
				210	→	229	-0.109
				210	→	224	0.108
40	2.931	423.0	0.0024	210	→	219	0.257
				211	→	219	0.226
				207	→	214	-0.171
				207	→	216	-0.163
				210	→	216	0.156
				192	→	216	-0.142
				192	→	214	-0.135
				208	→	216	0.123
				207	→	219	0.122
				196	→	216	0.115
				211	→	216	0.114

				208	→	214	0.109
				196	→	214	0.108
				187	→	216	-0.107
				210	→	218	0.106
				192	→	219	0.103
				187	→	214	-0.101
				191	→	216	0.100
41	2.946	420.9	0.0001	213	→	218	0.507
				213	→	217	0.451
				213	→	219	-0.148
42	2.958	419.2	0.0055	208	→	232	0.276
				210	→	232	-0.273
				208	→	217	0.254
				208	→	218	0.211
				208	→	216	0.193
				210	→	224	-0.177
				211	→	229	-0.168
				210	→	216	-0.154
				210	→	214	0.141
				208	→	224	0.137
				210	→	217	-0.132
43	3.003	412.9	0.0001	212	→	219	0.534
				213	→	219	-0.301
				212	→	218	0.191
				209	→	219	-0.180
44	3.041	407.7	0.0003	212	→	218	0.504
				212	→	217	0.440
				212	→	219	-0.152
45	3.052	406.2	0.0001	211	→	219	0.435
				210	→	219	-0.347
				211	→	218	0.319
				211	→	217	-0.221
				210	→	218	-0.158
46	3.065	404.5	0	210	→	218	0.378
				211	→	218	0.335
				210	→	217	-0.309
				211	→	217	-0.291
				211	→	219	-0.160
				209	→	219	0.106
47	3.067	404.3	0	209	→	219	0.486
				212	→	219	0.359
				209	→	218	0.164
				213	→	219	0.164
48	3.084	402.0	0	210	→	218	0.341
				211	→	219	0.322
				210	→	217	-0.299
				211	→	218	-0.267
				211	→	217	0.249
				210	→	219	-0.230

49	3.112	398.4	0	209	→	218	0.503
				209	→	217	0.451
				209	→	219	-0.150
50	3.120	397.4	0.0005	210	→	219	0.468
				211	→	219	0.319
				208	→	219	-0.193
				192	→	219	-0.132
				187	→	219	-0.109
				207	→	219	-0.102
51	3.188	389.0	0.002	209	→	219	0.392
				194	→	219	0.216
				213	→	219	-0.168
				197	→	219	0.156
				190	→	219	0.148
				212	→	219	-0.144
				186	→	219	0.140
				184	→	219	0.125
				206	→	219	-0.119
				192	→	219	0.110
				200	→	219	-0.105
52	3.201	387.3	0.0001	208	→	218	0.433
				208	→	219	0.405
				208	→	217	-0.318
53	3.223	384.7	0.0001	208	→	219	0.522
				208	→	218	-0.321
				208	→	217	0.317
54	3.276	378.5	0	195	→	219	0.556
				181	→	219	0.296
				203	→	219	-0.193
				195	→	218	0.119
				202	→	219	0.116
55	3.413	363.3	0.5426	207	→	214	0.491
				207	→	216	-0.449
				207	→	215	0.145
				206	→	215	-0.117
56	3.541	350.2	0.1116	206	→	215	0.642
				206	→	214	-0.217
57	3.642	340.5	0.0418	204	→	214	0.397
				204	→	216	-0.311
				207	→	217	0.247
				207	→	218	0.195
				203	→	214	0.183
				207	→	215	0.138
				205	→	215	0.124
				204	→	215	0.115
				207	→	214	-0.109
58	3.650	339.7	0.0876	205	→	215	0.626
				205	→	214	-0.215
59	3.666	338.2	0.0007	207	→	215	0.554

				207	→	214	-0.270
				204	→	214	-0.198
				204	→	216	0.175
				207	→	216	-0.130
60	3.693	335.8	0.0032	207	→	215	0.340
				207	→	216	0.285
				207	→	217	-0.248
				204	→	214	0.216
				207	→	218	-0.201
				204	→	216	-0.189
				207	→	214	0.141
				203	→	214	-0.124
61	3.713	333.9	0.0084	207	→	216	0.330
				207	→	217	0.302
				207	→	218	0.250
				207	→	214	0.250
				203	→	214	0.150
				204	→	214	-0.144
				204	→	216	0.134
				203	→	216	-0.120
62	3.738	331.7	0.0007	202	→	214	0.345
				202	→	216	0.306
				206	→	214	0.253
				203	→	214	0.220
				203	→	216	0.215
				204	→	216	0.164
				206	→	216	0.144
				205	→	214	-0.113
				205	→	216	-0.108
63	3.745	331.1	0.0048	213	→	220	0.674
				213	→	221	0.158
64	3.769	328.9	0.0009	206	→	214	0.416
				203	→	214	-0.311
				203	→	216	-0.273
				204	→	216	-0.153
				206	→	216	0.145
				213	→	221	-0.145
				206	→	215	0.142
65	3.773	328.6	0.0043	213	→	221	0.629
				213	→	220	-0.178
				213	→	222	0.126
66	3.801	326.2	0.0458	202	→	214	0.302
				202	→	215	-0.298
				206	→	214	-0.239
				206	→	217	0.203
				203	→	214	-0.203
				202	→	216	0.161
				206	→	218	-0.161
				203	→	216	-0.139

				205	→	215	-0.117
				205	→	214	-0.113
67	3.813	325.2	0.0363	202	→	215	0.370
				206	→	214	-0.303
				205	→	214	-0.188
				206	→	218	0.186
				206	→	217	-0.179
				202	→	216	0.178
				206	→	216	0.146
				203	→	215	-0.133
				206	→	215	-0.125
				203	→	214	-0.106
				203	→	216	-0.103
68	3.824	324.2	0.0015	211	→	220	0.458
				211	→	221	-0.345
				211	→	232	-0.220
				210	→	220	-0.169
				211	→	222	0.156
				210	→	221	0.139
				210	→	222	-0.110
				210	→	232	0.107
69	3.832	323.6	0.0019	212	→	220	0.580
				212	→	221	0.278
				213	→	223	-0.139
				212	→	231	0.135
70	3.850	322.1	0.0046	206	→	216	0.619
				202	→	215	-0.142
				206	→	214	-0.120
				202	→	216	-0.111
				205	→	216	0.108
71	3.862	321.0	0.0111	210	→	220	0.578
				211	→	220	0.317
				210	→	221	-0.159
				210	→	232	-0.131
72	3.863	321.0	0.0001	212	→	221	0.489
				212	→	220	-0.364
				213	→	223	-0.260
				213	→	222	-0.125
73	3.881	319.4	0.014	213	→	223	0.508
				212	→	221	0.322
				213	→	222	0.299
				213	→	231	0.109
74	3.891	318.6	0.0049	211	→	221	0.531
				211	→	220	0.352
				210	→	221	0.232
				210	→	220	-0.113
75	3.898	318.1	0.005	209	→	220	0.559
				209	→	221	0.330
				209	→	231	0.146

				209	→	222	0.116
				209	→	223	0.113
76	3.902	317.8	0.0021	210	→	221	0.557
				210	→	220	0.311
				211	→	220	-0.201
				211	→	222	0.145
77	3.913	316.8	0.1515	203	→	216	0.424
				203	→	214	-0.346
				207	→	217	0.286
				207	→	218	0.144
				204	→	214	0.114
				210	→	222	-0.103
78	3.928	315.7	0.001	213	→	222	0.578
				213	→	223	-0.335
				205	→	214	0.128
				213	→	221	-0.108
79	3.930	315.5	0.0006	205	→	214	0.533
				205	→	216	0.214
				202	→	216	0.198
				202	→	214	0.187
				205	→	215	0.178
				213	→	222	-0.135
80	3.934	315.2	0.0013	209	→	221	0.544
				209	→	220	-0.391
				209	→	222	0.116
81	3.937	315.0	0.0097	211	→	222	0.595
				210	→	222	0.262
				211	→	221	0.146
				210	→	221	-0.120
				211	→	223	-0.108
82	3.938	314.9	0.004	210	→	222	0.589
				210	→	221	0.205
				211	→	222	-0.190
				211	→	221	-0.163
				210	→	223	-0.119
83	3.949	314.0	0.0287	212	→	223	0.466
				206	→	217	-0.281
				206	→	218	0.219
				202	→	215	-0.211
				212	→	222	0.176
				212	→	221	-0.164
				212	→	231	0.101
84	3.957	313.3	0.0204	208	→	220	0.320
				212	→	223	-0.278
				206	→	217	-0.252
				208	→	221	-0.252
				202	→	215	-0.200
				206	→	218	0.192
				208	→	232	-0.163

				208	→	222	0.141
				212	→	222	-0.127
85	3.957	313.3	0.0342	208	→	220	0.348
				208	→	221	-0.275
				206	→	217	0.247
				212	→	223	0.230
				202	→	215	0.196
				206	→	218	-0.188
				208	→	232	-0.177
				208	→	222	0.154
				212	→	222	0.108
86	3.968	312.5	0.0038	204	→	216	0.478
				204	→	214	0.410
				203	→	216	-0.261
				203	→	214	-0.100
87	3.991	310.7	0.0007	205	→	216	0.606
				205	→	214	-0.238
				202	→	214	0.173
88	4.008	309.3	0.0011	204	→	215	0.612
				203	→	215	0.266
				204	→	214	-0.110
				203	→	214	-0.100
89	4.022	308.3	0.0019	209	→	223	0.586
				209	→	222	0.240
				209	→	221	-0.224
				209	→	231	0.131
90	4.024	308.1	0.0003	212	→	222	0.631
				212	→	223	-0.280
91	4.030	307.6	0.0018	207	→	218	0.491
				207	→	217	-0.357
				208	→	220	0.235
				208	→	221	0.226
92	4.033	307.4	0.0006	208	→	220	0.434
				208	→	221	0.406
				207	→	218	-0.264
				207	→	217	0.193
				208	→	222	-0.162
93	4.070	304.6	0.0599	205	→	217	0.522
				205	→	218	-0.414
				202	→	215	0.138
94	4.071	304.6	0.0002	208	→	222	0.593
				208	→	221	0.313
				208	→	223	-0.129
95	4.076	304.2	0.0005	207	→	219	0.632
				192	→	219	-0.131
				187	→	219	-0.129
96	4.095	302.8	0.0001	209	→	222	0.632
				209	→	223	-0.283
				209	→	221	-0.101

97	4.103	302.2	0.0158	211	→	223	0.473
				210	→	223	0.314
				204	→	217	-0.300
				204	→	218	-0.233
98	4.104	302.1	0.024	204	→	217	0.425
				204	→	218	0.327
				210	→	223	0.288
				211	→	223	0.276
				203	→	215	-0.144
99	4.118	301.1	0.0003	210	→	223	0.537
				211	→	223	-0.410
				210	→	222	0.118
100	4.123	300.7	0.0045	203	→	215	0.505
				204	→	215	-0.290
				202	→	215	0.165
				203	→	214	-0.163
				204	→	217	0.144
				202	→	219	-0.131
				204	→	218	0.127
				203	→	219	-0.124
101	4.141	299.4	0.0012	202	→	216	0.490
				202	→	214	-0.399
				205	→	216	0.160
				202	→	215	-0.128
				203	→	216	-0.115
102	4.175	297.0	0.0004	206	→	218	0.474
				206	→	217	0.362
				202	→	219	0.218
				206	→	219	0.211
103	4.179	296.7	0.0509	201	→	214	0.467
				201	→	216	-0.407
				201	→	215	0.141
				200	→	215	0.108
104	4.186	296.2	0.0035	202	→	219	0.379
				206	→	219	0.356
				206	→	218	-0.244
				206	→	217	-0.233
				203	→	219	0.140
				205	→	219	-0.131
				203	→	215	0.130
				204	→	219	0.107
105	4.194	295.6	0.0026	213	→	225	0.446
				212	→	225	-0.253
				200	→	215	0.249
				213	→	231	0.230
				199	→	215	0.121
				212	→	223	0.114
106	4.209	294.6	0.0169	211	→	224	0.453
				210	→	224	-0.283

				211	→	232	-0.218
				200	→	215	-0.158
				210	→	232	0.141
				211	→	222	-0.116
				211	→	221	0.114
107	4.212	294.4	0.0259	200	→	215	0.422
				199	→	215	0.250
				213	→	225	-0.190
				200	→	214	-0.152
				211	→	224	0.142
				212	→	225	0.141
				206	→	219	0.126
				210	→	224	-0.114
108	4.219	293.9	0.0022	206	→	219	0.484
				203	→	219	-0.244
				202	→	219	-0.232
				199	→	215	-0.159
				204	→	219	-0.150
				200	→	215	-0.138
				205	→	219	0.100
109	4.252	291.6	0.0009	199	→	215	0.341
				212	→	225	-0.296
				213	→	226	-0.254
				213	→	227	-0.190
				203	→	219	-0.171
				200	→	215	-0.165
				212	→	231	-0.131
				199	→	214	-0.116
				213	→	225	-0.102
110	4.253	291.5	0.0004	208	→	223	0.681
				208	→	222	0.150
111	4.256	291.3	0.0102	213	→	226	0.362
				199	→	215	0.268
				213	→	227	0.262
				203	→	219	-0.224
				212	→	225	0.181
				200	→	215	-0.141
				205	→	219	-0.121
				204	→	219	-0.107
				202	→	219	0.101
112	4.259	291.1	0.0054	203	→	219	0.360
				199	→	215	0.285
				202	→	219	-0.229
				205	→	219	0.216
				200	→	215	-0.171
				204	→	219	0.166
				195	→	219	0.142
				206	→	219	0.133
113	4.288	289.2	0.0472	212	→	225	0.306

				213	→	226	-0.274
				213	→	225	0.234
				198	→	214	0.220
				198	→	216	-0.197
				213	→	227	-0.174
				213	→	231	0.157
				209	→	225	0.151
				212	→	231	0.144
114	4.291	288.9	0.0146	198	→	214	0.404
				198	→	216	-0.363
				212	→	225	-0.151
				209	→	225	-0.129
				198	→	215	0.129
				213	→	226	0.128
				213	→	225	-0.120
				198	→	224	0.111
115	4.313	287.5	0.1012	209	→	225	0.513
				209	→	231	0.229
				200	→	215	0.147
				209	→	223	-0.144
				210	→	224	-0.128
				199	→	215	-0.121
116	4.324	286.8	0.0436	210	→	224	0.410
				211	→	224	0.256
				210	→	232	-0.243
				205	→	218	0.149
				211	→	232	-0.147
				205	→	217	0.133
				203	→	217	0.129
				210	→	226	-0.124
117	4.327	286.5	0.0019	205	→	218	0.487
				205	→	217	0.386
				202	→	217	-0.140
				209	→	225	-0.121
				210	→	224	-0.117
118	4.346	285.3	0.0188	208	→	224	0.553
				208	→	232	-0.264
				208	→	222	-0.142
				208	→	221	0.131
119	4.354	284.8	0.011	212	→	226	0.535
				212	→	227	0.382
				212	→	228	-0.145
120	4.363	284.2	0.0062	204	→	218	0.465
				204	→	217	-0.345
				203	→	217	-0.318
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121	4.372	283.6	0.0024	205	→	219	0.597
				202	→	219	0.291
				203	→	219	-0.108

122	4.387	282.6	0.0023	211	→	226	0.527
				211	→	227	-0.393
				211	→	228	-0.157
				210	→	226	-0.114
123	4.398	281.9	0.0197	210	→	226	0.432
				210	→	227	-0.317
				203	→	217	0.251
				204	→	218	0.163
				204	→	217	-0.135
				210	→	228	-0.123
124	4.405	281.5	0.0097	203	→	217	0.274
				210	→	226	-0.270
				209	→	226	-0.259
				210	→	227	0.196
				209	→	227	-0.195
				202	→	217	-0.190
				204	→	219	0.189
				204	→	218	0.129
				210	→	224	-0.117
125	4.411	281.1	0.0148	204	→	219	0.464
				209	→	226	0.346
				209	→	227	0.256
				203	→	219	-0.207
				203	→	217	0.101
				209	→	228	-0.100
126	4.413	280.9	0.0001	213	→	224	0.682
				204	→	219	0.133
127	4.416	280.8	0.0191	204	→	219	0.344
				209	→	226	-0.310
				203	→	217	-0.263
				209	→	227	-0.227
				203	→	218	-0.148
				204	→	217	0.136
				213	→	224	-0.133
				203	→	219	-0.127
				202	→	217	0.103
				204	→	218	-0.102
128	4.450	278.6	0.4676	202	→	217	0.573
				203	→	217	0.194
				197	→	215	-0.120
129	4.477	276.9	0.0043	201	→	216	0.524
				201	→	214	0.435
130	4.488	276.2	0.0008	200	→	214	0.610
				200	→	215	0.212
				200	→	216	0.198
				194	→	216	0.102
131	4.508	275.1	0.0004	212	→	224	0.700
132	4.515	274.6	0.0111	208	→	226	0.475
				208	→	227	-0.368

				203	→	218	0.198
				208	→	228	-0.154
				197	→	214	0.146
				197	→	216	0.122
133	4.515	274.6	0.0008	197	→	214	0.457
				197	→	216	0.375
				208	→	226	-0.161
				194	→	216	-0.131
				208	→	227	0.124
				194	→	214	-0.117
134	4.528	273.8	0.1838	203	→	218	0.569
				208	→	226	-0.177
				203	→	219	-0.161
				202	→	218	-0.150
				208	→	227	0.133
				203	→	217	-0.110
135	4.535	273.4	0.0004	201	→	215	0.576
				196	→	214	-0.248
				196	→	216	-0.163
				201	→	214	-0.134
136	4.538	273.2	0.0322	202	→	218	0.597
				203	→	217	-0.147
				202	→	219	-0.146
				197	→	215	0.129
				203	→	218	0.114
137	4.545	272.8	0.0005	196	→	214	0.390
				196	→	216	0.365
				201	→	215	0.286
				196	→	215	0.161
				192	→	214	0.140
				192	→	216	0.135
138	4.550	272.5	0.0013	200	→	216	0.590
				199	→	214	0.195
				200	→	214	-0.156
				197	→	216	-0.154
				194	→	214	0.105
139	4.567	271.5	0	211	→	225	0.602
				210	→	225	0.357
140	4.569	271.4	0.0005	199	→	214	0.540
				199	→	216	0.360
				199	→	215	0.175
				200	→	216	-0.158
141	4.579	270.8	0	210	→	225	0.603
				211	→	225	-0.358
142	4.580	270.7	0	209	→	224	0.700
143	4.589	270.2	0	213	→	227	0.431
				213	→	226	-0.403
				213	→	228	-0.372
144	4.613	268.8	0.0121	201	→	217	0.530

				201	→	218	0.420
145	4.625	268.1	0.0144	200	→	217	0.522
				200	→	218	-0.415
				197	→	217	-0.101
146	4.653	266.5	0.0003	198	→	216	0.526
				198	→	214	0.453
147	4.677	265.1	0	212	→	227	0.423
				212	→	226	-0.413
				212	→	228	-0.371
148	4.683	264.8	0.0002	199	→	216	0.582
				199	→	214	-0.324
				199	→	215	-0.114
				200	→	216	0.111
149	4.706	263.5	0	211	→	227	0.416
				211	→	226	0.415
				211	→	228	0.374
150	4.708	263.3	0.0024	197	→	215	0.511
				199	→	217	0.199
				202	→	217	0.174
				196	→	216	0.170
				199	→	218	-0.155
				196	→	214	-0.139
				202	→	218	-0.138
				197	→	214	-0.124

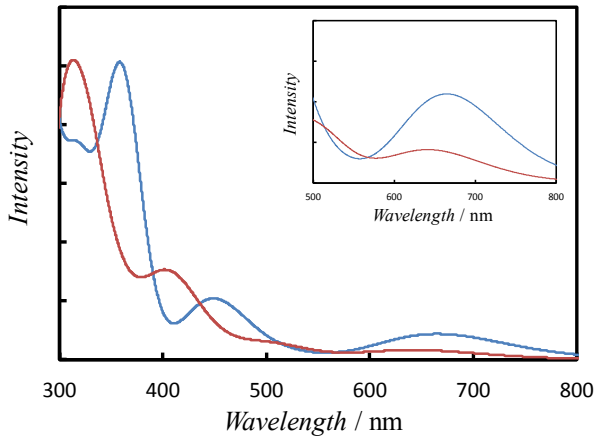

Fig. S6 Theoretical UV/Vis spectra for **1** (red) and **5** (blue) in CH_3CN calculated using the TDDFT method.