

## $\beta$ 位取代基对卟咯锰(V)氧配合物电子吸收光谱的影响

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## Effect of $\beta$ -Substituents on the Electronic Absorption Spectra of Manganese(V)-oxo Corrole Complexes

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表 S1 配合物 **1-7** 的部分几何结构参数Table S1 Selected optimized structural parameters of compound **1-7**

Compound	$d_{\text{Mn-O}}/\text{nm}$	$d_{\text{Mn-N}}^{\text{a}}/\text{nm}$	$D_{1,2,3,4}$	$D_{5,6,7,8}$	$D_{9,10,11,12}$	$D_{\text{N,N,N,N}}$
<b>1</b>	0.1568	0.1916	5.30	-5.30	-0.02	-0.01
<b>2</b>	0.1570	0.1916	11.41	-17.56	7.02	-0.51
<b>3</b>	0.1555	0.1914	8.10	-9.94	2.15	-0.08
<b>4</b>	0.1552	0.1914	8.04	-9.95	2.16	-0.05
<b>5</b>	0.1556	0.1918	-10.94	-19.78	27.09	4.66
<b>6</b>	0.1551	0.1916	9.33	-12.10	2.92	-0.02
<b>7</b>	0.1552	0.1918	-16.07	-25.46	25.15	4.60

a: representing average values

## Cartesian Coordinates of Optimized Geometries

Complex **1**

Number	Atomic Type	X	Y	Z
1	Mn	-0.007633	-0.000028	0.45242
2	C	2.664245	-0.700398	-0.155208
3	C	3.574831	-1.789668	-0.258286
4	H	4.650422	-1.710362	-0.347711
5	C	2.819543	-2.957705	-0.240662
6	H	3.189145	-3.973399	-0.304019
7	C	1.436114	-2.594645	-0.13247
8	C	0.276216	-3.354898	-0.134268
9	C	-0.986817	-2.766478	-0.13304
10	C	-2.241782	-3.460335	-0.217875
11	H	-2.338959	-4.537977	-0.259521
12	C	-3.24496	-2.521604	-0.258628
13	H	-4.312119	-2.690411	-0.327466
14	C	-2.63198	-1.225327	-0.191758
15	C	-3.280744	0.000895	-0.216542
16	C	-2.631291	1.226761	-0.191908
17	C	-3.243611	2.523326	-0.259181
18	H	-4.310663	2.692608	-0.328468
19	C	-2.239968	3.461563	-0.21822

20	H	-2.336588	4.539248	-0.260102
21	C	-0.985377	2.767114	-0.132816
22	C	0.277975	3.354857	-0.133963
23	C	1.437456	2.59397	-0.131969
24	C	2.821062	2.956316	-0.24041
25	H	3.191167	3.971812	-0.303923
26	C	3.575726	1.787888	-0.258128
27	H	4.651238	1.708065	-0.34788
28	C	2.664618	0.699078	-0.154916
29	N	1.370127	-1.20423	-0.063218
30	N	-1.2386	-1.378501	-0.106957
31	N	-1.237862	1.379267	-0.106581
32	N	1.370785	1.203585	-0.062586
33	O	-0.091575	-0.000643	2.018322
34	H	0.342111	-4.438341	-0.178432
35	H	-4.365469	0.001223	-0.284234
36	H	0.344449	4.438259	-0.178435

Complex 2

Number	Atomic Type	X	Y	Z
1	Mn	-0.000733	-0.68256	0.539751
2	C	-0.700244	-3.329169	-0.150417
3	C	-1.779621	-4.24098	-0.304248
4	H	-1.692167	-5.311067	-0.439598
5	C	-2.950659	-3.49353	-0.274521
6	H	-3.959402	-3.867634	-0.375996
7	C	-2.597129	-2.112876	-0.099533
8	C	-3.382811	-0.959665	-0.086371
9	C	-2.773741	0.30695	-0.040827
10	C	-3.460943	1.566091	-0.071852
11	H	-4.533886	1.681173	-0.101827
12	C	-2.522288	2.567481	-0.073268
13	H	-2.703209	3.631167	-0.103175
14	C	-1.226345	1.955708	-0.015498
15	C	0.001705	2.626411	0.004636
16	C	1.227792	1.953451	0.00779
17	C	2.525294	2.562553	0.049492
18	H	2.707653	3.625533	0.094137
19	C	3.462166	1.559471	0.046684
20	H	4.535277	1.672947	0.080439

21	C	2.773741	0.3018	-0.00529
22	C	3.383322	-0.964366	-0.06427
23	C	2.595914	-2.116706	-0.09754
24	C	2.946409	-3.495831	-0.289681
25	H	3.953759	-3.870678	-0.401371
26	C	1.774235	-4.241993	-0.319532
27	H	1.684926	-5.310295	-0.46708
28	C	0.697197	-3.330838	-0.149103
29	N	-1.208549	-2.041736	-0.013182
30	N	-1.382278	0.5581	0.009431
31	N	1.380722	0.553785	-0.003801
32	N	1.208505	-2.045612	-0.00143
33	C	-4.867844	-1.086076	-0.162268
34	C	-5.572101	-1.767288	0.850217
35	C	-6.96291	-1.905878	0.779922
36	C	-7.670094	-1.371271	-0.304557
37	C	-6.9786	-0.697621	-1.319914
38	C	-5.588354	-0.555263	-1.25055
39	C	0.002426	4.123977	0.005365
40	C	-0.496104	4.838306	1.11185
41	C	-0.494931	6.237878	1.113946
42	C	-0.000257	6.943449	0.009438
43	C	0.495243	6.241944	-1.097241
44	C	0.498439	4.8423	-1.099505
45	C	4.868293	-1.089516	-0.123021
46	C	5.556657	-1.828526	0.859939
47	C	6.948092	-1.965679	0.803462
48	C	7.672859	-1.371892	-0.237765
49	C	6.998084	-0.639276	-1.223171
50	C	5.607302	-0.498003	-1.167087
51	O	-0.004637	-0.637673	2.108713
52	H	0.877163	4.301239	-1.963288
53	H	0.876443	6.782744	-1.960146
54	H	-0.001116	8.030767	0.011071
55	H	-0.877416	6.775335	1.978358
56	H	-0.875059	4.294375	1.973815
57	H	5.087282	0.058352	-1.942875
58	H	7.55301	-0.182455	-2.039093
59	H	8.75391	-1.479649	-0.281743
60	H	7.464914	-2.532444	1.57419

61	H	4.998947	-2.282678	1.675311
62	H	-7.519861	-0.287593	-2.169191
63	H	-8.75057	-1.479968	-0.359148
64	H	-7.492751	-2.427764	1.573189
65	H	-5.027357	-2.176379	1.697686
66	H	-5.055031	-0.044554	-2.048539

Complex 3

Number	Atomic Type	X	Y	Z
1	Mn	-0.003947	-0.793314	0.521049
2	C	-0.696977	-3.416594	-0.255498
3	C	-1.777695	-4.320777	-0.443261
4	H	-1.692751	-5.383997	-0.609685
5	C	-2.946817	-3.573534	-0.392415
6	H	-3.955245	-3.941015	-0.503351
7	C	-2.590052	-2.201053	-0.176468
8	C	-3.370537	-1.046933	-0.117842
9	C	-2.7697	0.215788	-0.022166
10	C	-3.458596	1.474497	-0.020378
11	H	-4.530116	1.587698	-0.058712
12	C	-2.521471	2.47356	0.014474
13	H	-2.698775	3.537099	0.01363
14	C	-1.226447	1.858175	0.051708
15	C	0.000944	2.522014	0.09148
16	C	1.228255	1.857466	0.081896
17	C	2.524826	2.470546	0.099585
18	H	2.703901	3.533178	0.134556
19	C	3.461048	1.470304	0.074817
20	H	4.533512	1.581758	0.073699
21	C	2.770731	0.213132	0.032081
22	C	3.372358	-1.049477	-0.05876
23	C	2.591939	-2.202596	-0.136875
24	C	2.951074	-3.574818	-0.350126
25	H	3.960829	-3.942727	-0.446713
26	C	1.782426	-4.321505	-0.418632
27	H	1.699396	-5.384379	-0.588179
28	C	0.699611	-3.417044	-0.245049
29	N	-1.207828	-2.135768	-0.077595
30	N	-1.382115	0.465117	0.037437
31	N	1.382225	0.463983	0.055535

32	N	1.208558	-2.13671	-0.058337
33	C	-4.851823	-1.167296	-0.19791
34	C	-5.603492	-1.791864	0.807415
35	C	-6.985636	-1.939349	0.760403
36	C	-7.67533	-1.441032	-0.349579
37	C	-6.979387	-0.810433	-1.386202
38	C	-5.597331	-0.69294	-1.28613
39	C	-0.000554	4.014299	0.126659
40	C	-0.389002	4.735959	1.262691
41	C	-0.40263	6.125357	1.327294
42	C	-0.006316	6.851641	0.199378
43	C	0.392392	6.185483	-0.964216
44	C	0.383847	4.7945	-0.971275
45	C	4.854776	-1.170217	-0.108441
46	C	5.584916	-1.804038	0.906974
47	C	6.967731	-1.951255	0.888232
48	C	7.68093	-1.442653	-0.202081
49	C	7.00727	-0.802239	-1.247354
50	C	5.623338	-0.685488	-1.175947
51	O	-0.015618	-0.80682	2.075816
52	H	0.700048	6.720519	-1.853467
53	H	-0.008291	7.935209	0.227104
54	H	-0.712614	6.612924	2.242653
55	H	7.530749	-0.404507	-2.107281
56	H	8.759343	-1.545527	-0.237517
57	H	7.460916	-2.448032	1.71385
58	H	-7.484319	-0.420959	-2.260877
59	H	-8.752746	-1.544345	-0.407094
60	H	-7.496397	-2.428586	1.57981
61	F	4.890248	-2.30926	1.998711
62	F	4.967242	-0.05531	-2.226175
63	F	0.778302	4.143409	-2.13293
64	F	-0.781626	4.024461	2.389014
65	F	-4.918742	-0.072313	-2.328105
66	F	-4.932246	-2.287741	1.917779

Complex 4

Number	Atomic Type	X	Y	Z
1	Mn	0.014729	-0.67935	-0.535713
2	C	0.723173	-3.352512	-0.000917

3	C	1.799486	-4.275474	-0.199276
4	C	2.967746	-3.519227	-0.346339
5	C	2.606514	-2.124131	-0.180655
6	C	3.360105	-0.963465	0.001764
7	C	2.750656	0.284917	0.254281
8	C	3.398909	1.495175	0.70518
9	C	2.452372	2.509049	0.715915
10	C	1.191927	1.937065	0.283783
11	C	-0.027613	2.60188	0.044388
12	C	-1.247374	1.960012	-0.218537
13	C	-2.52661	2.539645	-0.594092
14	C	-3.449552	1.507191	-0.65573
15	C	-2.773022	0.282856	-0.284201
16	C	-3.345819	-0.975947	-0.02665
17	C	-2.557796	-2.106545	0.211903
18	C	-2.900303	-3.470069	0.563696
19	C	-1.727535	-4.231086	0.501604
20	C	-0.668287	-3.340982	0.152175
21	N	1.226466	-2.058949	-0.05041
22	N	1.37465	0.55888	0.067622
23	N	-1.401602	0.565742	-0.112024
24	N	-1.184919	-2.052764	0.006866
25	C	4.847977	-1.072913	-0.032649
26	C	5.579379	-0.687004	-1.160083
27	C	6.968504	-0.770639	-1.209358
28	C	7.666867	-1.25834	-0.108524
29	C	6.969411	-1.667297	1.025236
30	C	5.581089	-1.580582	1.044259
31	C	-0.027938	4.096091	0.073606
32	C	0.477302	4.851451	-0.988376
33	C	0.471044	6.242947	-0.981784
34	C	-0.057184	6.923223	0.111333
35	C	-0.568987	6.203135	1.186947
36	C	-0.544626	4.812663	1.157036
37	C	-4.829492	-1.129312	-0.000381
38	C	-5.533341	-1.664135	-1.083915
39	C	-6.916866	-1.813811	-1.071181
40	C	-7.637534	-1.437745	0.059358
41	C	-6.968071	-0.915299	1.162511
42	C	-5.584672	-0.767034	1.118985

43	O	0.059573	-0.629793	-2.090123
44	F	4.917047	-0.221766	-2.275801
45	F	7.651891	-0.383717	-2.33684
46	F	9.036138	-1.344284	-0.143096
47	F	7.654455	-2.159585	2.110652
48	F	4.919726	-2.006836	2.179395
49	F	-4.950367	-0.260185	2.234407
50	F	-7.674972	-0.554015	2.284311
51	F	-9.001724	-1.585516	0.087317
52	F	-7.574683	-2.331265	-2.16138
53	F	-4.849444	-2.047718	-2.220184
54	F	-1.058053	4.13396	2.243567
55	F	-1.100871	6.867061	2.266419
56	F	-0.071903	8.29553	0.129591
57	F	0.991981	6.946187	-2.041264
58	F	1.011588	4.213522	-2.088785
59	C	-4.845485	1.682149	-1.210324
60	H	-5.58464	1.101213	-0.657941
61	H	-5.149956	2.724399	-1.084551
62	C	-2.901572	3.966629	-0.937268
63	H	-3.527679	3.947042	-1.838377
64	H	-2.028928	4.554264	-1.216949
65	C	-3.683849	4.698077	0.182617
66	H	-4.648143	4.214917	0.371094
67	H	-3.137037	4.694189	1.128432
68	H	-3.880041	5.738031	-0.10304
69	C	-4.930992	1.325632	-2.715495
70	H	-4.248991	1.952518	-3.300482
71	H	-4.65909	0.282597	-2.899215
72	H	-5.948372	1.487687	-3.090453
73	C	-4.212373	-4.017076	1.071253
74	H	-4.234156	-5.098562	0.898698
75	H	-5.062417	-3.617858	0.514215
76	C	-1.632649	-5.706216	0.789829
77	H	-0.622964	-5.955967	1.126023
78	H	-2.29378	-5.955241	1.629203
79	C	-4.422788	-3.752556	2.583112
80	H	-5.377959	-4.173021	2.918741
81	H	-3.622046	-4.21401	3.171638
82	H	-4.420343	-2.68137	2.807225



83	C	1.723064	-5.77825	-0.265657
84	H	2.389395	-6.139742	-1.058899
85	H	0.717544	-6.086587	-0.563217
86	C	4.292042	-4.101018	-0.774706
87	H	5.125116	-3.671372	-0.214012
88	H	4.302545	-5.170068	-0.537124
89	C	4.550451	-3.927579	-2.291974
90	H	4.537273	-2.872257	-2.583319
91	H	5.522373	-4.351218	-2.570213
92	H	3.775982	-4.437525	-2.875529
93	C	2.109404	-6.474888	1.060512
94	H	1.463283	-6.150088	1.8836
95	H	2.023492	-7.563458	0.965537
96	H	3.14095	-6.237295	1.342522
97	C	2.79639	3.915075	1.162817
98	H	1.909536	4.46279	1.475397
99	H	3.415513	3.843231	2.066151
100	C	3.573617	4.743099	0.107901
101	H	3.04587	4.782864	-0.847773
102	H	3.729511	5.767991	0.464149
103	H	4.557172	4.306122	-0.092326
104	C	-2.011178	-6.594233	-0.419263
105	H	-1.371715	-6.382431	-1.28331
106	H	-1.908735	-7.656044	-0.167338
107	H	-3.046689	-6.415508	-0.728766
108	C	4.785277	1.674144	1.284683
109	H	5.540017	1.117186	0.730171
110	H	5.076047	2.722863	1.182879
111	C	4.859541	1.291353	2.783935
112	H	4.15844	1.893386	3.372465
113	H	4.608107	0.239878	2.945304
114	H	5.86882	1.467274	3.17437

Complex 5

Number	Atomic Type	X	Y	Z
1	Mn	0.004255	-1.040002	-0.526438
2	C	0.695491	-3.657612	0.269352
3	C	1.775936	-4.561549	0.463853
4	H	1.690891	-5.623188	0.638768
5	C	2.944645	-3.816059	0.40611

6	H	3.951549	-4.186646	0.520657
7	C	2.58836	-2.444095	0.179001
8	C	3.367057	-1.28976	0.11009
9	C	2.77	-0.0256	0.006574
10	C	3.459598	1.232525	-0.003011
11	H	4.530639	1.35063	0.033594
12	C	2.522672	2.231406	-0.043799
13	H	2.705045	3.294052	-0.047926
14	C	1.227924	1.615738	-0.078311
15	C	-0.000961	2.276145	-0.124914
16	C	-1.229969	1.615011	-0.113648
17	C	-2.526188	2.228092	-0.139564
18	H	-2.710175	3.289483	-0.184618
19	C	-3.462338	1.228064	-0.109211
20	H	-4.534303	1.344121	-0.113166
21	C	-2.771497	-0.028177	-0.054245
22	C	-3.369607	-1.291957	0.046362
23	C	-2.591253	-2.44511	0.13676
24	C	-2.950488	-3.816551	0.362092
25	H	-3.958919	-4.187191	0.462184
26	C	-1.782593	-4.561721	0.438426
27	H	-1.699897	-5.622896	0.617214
28	C	-0.699665	-3.657894	0.25805
29	N	1.207131	-2.378063	0.080486
30	N	1.38313	0.223019	-0.055135
31	N	-1.383684	0.221996	-0.077071
32	N	-1.208796	-2.378827	0.059051
33	C	4.848235	-1.410644	0.185458
34	C	5.578348	-2.048828	-0.825881
35	C	6.962186	-2.188998	-0.767385
36	C	7.660098	-1.682402	0.324788
37	C	6.967532	-1.043159	1.348806
38	C	5.583177	-0.919232	1.271981
39	C	0.000631	3.768052	-0.169285
40	C	0.402301	4.46661	-1.313905
41	C	0.411612	5.85779	-1.368299
42	C	0.006937	6.592544	-0.257639
43	C	-0.400576	5.930362	0.896736
44	C	-0.39685	4.538416	0.929738
45	C	-4.851814	-1.412948	0.092189

46	C	-5.561117	-2.062049	-0.927
47	C	-6.945806	-2.202075	-0.895225
48	C	-7.665853	-1.684078	0.17704
49	C	-6.994436	-1.033444	1.207962
50	C	-5.608805	-0.909669	1.158074
51	O	0.01822	-1.066105	-2.078535
52	F	-4.882622	-2.578339	-2.009701
53	F	-7.60441	-2.841269	-1.917655
54	F	-9.030889	-1.814463	0.218198
55	F	-7.70052	-0.526844	2.272243
56	F	-4.977339	-0.27265	2.20464
57	F	0.811607	6.507574	-2.510883
58	F	0.80282	3.769482	-2.43295
59	F	-0.79947	3.914531	2.090328
60	F	-0.797324	6.651843	1.996694
61	F	0.009816	7.963826	-0.300714
62	F	4.930267	-0.293442	2.312554
63	F	7.65149	-0.547743	2.432708
64	F	9.024059	-1.812834	0.39234
65	F	7.641666	-2.817427	-1.78271
66	F	4.922074	-2.554378	-1.927035

Complex 6

Number	Atomic Type	X	Y	Z
1	Mn	0.003706	-0.834237	-0.581609
2	C	0.696841	-3.478134	0.102312
3	C	1.777033	-4.377056	0.265084
4	C	2.938519	-3.632374	0.238383
5	C	2.599408	-2.252731	0.05816
6	C	3.388251	-1.107292	0.028207
7	C	2.779417	0.152183	-0.042646
8	C	3.450017	1.415899	-0.033637
9	C	2.517576	2.40828	-0.029288
10	C	1.218917	1.809341	-0.067217
11	C	-0.003521	2.479138	-0.09709
12	C	-1.224423	1.806864	-0.104465
13	C	-2.525337	2.401275	-0.136595
14	C	-3.454077	1.405357	-0.140257
15	C	-2.779752	0.144661	-0.090578
16	C	-3.38644	-1.11532	-0.011159

17	C	-2.594345	-2.257954	0.041779
18	C	-2.931027	-3.637205	0.228749
19	C	-1.768198	-4.379674	0.261993
20	C	-0.689398	-3.479498	0.098626
21	N	1.215911	-2.194565	-0.041705
22	N	1.390047	0.415245	-0.083388
23	N	-1.390596	0.411608	-0.094409
24	N	-1.210534	-2.197314	-0.052072
25	C	4.869288	-1.244568	0.114661
26	C	5.600511	-1.850779	-0.911268
27	C	6.979731	-2.01153	-0.838749
28	C	7.664211	-1.56279	0.287141
29	C	6.964954	-0.958972	1.328961
30	C	5.586499	-0.810629	1.233587
31	C	-0.004024	3.974341	-0.108152
32	C	0.325556	4.691743	-1.25981
33	C	0.330307	6.081629	-1.2854
34	C	-0.002188	6.789378	-0.133545
35	C	-0.335438	6.102742	1.030804
36	C	-0.332094	4.712539	1.030631
37	C	-4.868083	-1.253999	0.05288
38	C	-5.580591	-1.889147	-0.968958
39	C	-6.960699	-2.049317	-0.917144
40	C	-7.665966	-1.569764	0.182926
41	C	-6.986216	-0.935799	1.219694
42	C	-5.606315	-0.788536	1.145409
43	O	0.010851	-0.80584	-2.132183
44	F	-4.901776	-2.376338	-2.06527
45	F	-7.627556	-2.674248	-1.941232
46	F	-9.026362	-1.721367	0.246036
47	F	-7.679063	-0.464929	2.307047
48	F	-4.953279	-0.158136	2.182507
49	F	0.660682	6.755952	-2.434663
50	F	0.668925	4.006968	-2.406271
51	F	-0.675953	4.049029	2.188911
52	F	-0.6648	6.798033	2.167749
53	F	-0.001474	8.159952	-0.145968
54	F	4.91321	-0.211137	2.276173
55	F	7.63726	-0.518803	2.441837
56	F	9.023429	-1.715155	0.370852

57	F	7.665797	-2.607492	-1.867365
58	F	4.941613	-2.308944	-2.031838
59	F	1.671377	-5.725942	0.443879
60	F	4.207811	-4.124974	0.379733
61	F	4.805878	1.603049	-0.016927
62	F	2.787412	3.750442	-0.001621
63	F	-2.799048	3.741971	-0.187348
64	F	-4.81021	1.58634	-0.183779
65	F	-4.199535	-4.131952	0.368807
66	F	-1.660632	-5.727427	0.448144

Complex 7

Number	Atomic Type	X	Y	Z
1	Mn	-0.01235	-0.461107	0.569019
2	C	-0.761217	-3.121671	0.047513
3	C	-1.849807	-4.011386	0.258732
4	C	-2.994815	-3.242888	0.403522
5	C	-2.635373	-1.859076	0.242121
6	C	-3.381335	-0.689115	0.100828
7	C	-2.746911	0.540017	-0.164357
8	C	-3.355609	1.753387	-0.638671
9	C	-2.382306	2.713235	-0.757117
10	C	-1.138909	2.150685	-0.305171
11	C	0.068276	2.819469	-0.04651
12	C	1.259161	2.154162	0.256221
13	C	2.531599	2.701542	0.649269
14	C	3.453044	1.68512	0.645267
15	C	2.788306	0.465647	0.267062
16	C	3.353825	-0.793996	0.016527
17	C	2.542001	-1.91241	-0.188158
18	C	2.845527	-3.274534	-0.532869
19	C	1.674208	-4.014836	-0.481245
20	C	0.625769	-3.128396	-0.128567
21	N	-1.252817	-1.823089	0.096564
22	N	-1.36072	0.790737	-0.027936
23	N	1.415644	0.76254	0.122602
24	N	1.166813	-1.849766	0.017594
25	C	-4.866456	-0.765052	0.194138
26	C	-5.534403	-0.353218	1.349164
27	C	-6.918311	-0.431362	1.464729

28	C	-7.667069	-0.931629	0.403386
29	C	-7.028405	-1.35234	-0.760726
30	C	-5.64528	-1.269102	-0.849664
31	C	0.080629	4.309653	-0.091402
32	C	-0.486657	5.069396	0.93388
33	C	-0.475592	6.45864	0.911319
34	C	0.109767	7.121242	-0.164326
35	C	0.680139	6.391233	-1.203968
36	C	0.662574	5.003067	-1.154602
37	C	4.833332	-0.956844	-0.038768
38	C	5.542775	-1.527707	1.020119
39	C	6.921173	-1.695281	0.975647
40	C	7.623831	-1.293931	-0.157717
41	C	6.944134	-0.727553	-1.232643
42	C	5.565406	-0.564969	-1.161418
43	O	-0.043386	-0.40549	2.1198
44	F	4.864306	-1.932637	2.148715
45	F	7.592053	-2.254187	2.035721
46	F	8.984138	-1.457148	-0.215167
47	F	7.637137	-0.333183	-2.35072
48	F	4.911252	0.001756	-2.233231
49	F	-1.036987	7.179087	1.936755
50	F	-1.07377	4.431416	2.004669
51	F	1.234886	4.298251	-2.190666
52	F	1.255742	7.045799	-2.265275
53	F	0.124572	8.491873	-0.199894
54	F	-5.030384	-1.688938	-2.008344
55	F	-7.767705	-1.847173	-1.807261
56	F	-9.032153	-1.011857	0.504191
57	F	-7.547299	-0.018806	2.613381
58	F	-4.81134	0.149041	2.408906
59	Br	1.541138	-5.859499	-0.933829
60	Br	4.522217	-4.026418	-1.062899
61	Br	5.277231	1.941048	1.170558
62	Br	2.959209	4.476148	1.233441
63	Br	-2.724547	4.434659	-1.528239
64	Br	-5.17055	2.064085	-1.16939
65	Br	-4.704321	-3.991409	0.820926
66	Br	-1.794341	-5.90679	0.424547

表 S2 配合物 **1-7** 的前线轨道能级 (eV)Table S2 Frontier orbital energy of complexes **1-7** (eV)

	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>
$E_{L+4}$	-0.06887	-0.07256	-0.07860	-0.09084	-0.08566	-0.10939	-0.11612
$E_{L+3}$	-0.08765	-0.08999	-0.09612	-0.10688	-0.09886	-0.12593	-0.13221
$E_{L+2}$	-0.09797	-0.09806	-0.10075	-0.11082	-0.10174	-0.13211	-0.13250
$E_{L+1}$	-0.12780	-0.12641	-0.13146	-0.14151	-0.13333	-0.16458	-0.16493
$E_L$	-0.12866	-0.12804	-0.13240	-0.14237	-0.13465	-0.16519	-0.16652
$E_H$	-0.19799	-0.19813	-0.20169	-0.21163	-0.20137	-0.23441	-0.23382
$E_{H-1}$	-0.20271	-0.19847	-0.20658	-0.21791	-0.20795	-0.23651	-0.23781
$E_{H-2}$	-0.25515	-0.25059	-0.25801	-0.26725	-0.24618	-0.28026	-0.26736
$E_{H-3}$	-0.26185	-0.25515	-0.26406	-0.27411	-0.25171	-0.28130	-0.27177
$E_{H-4}$	-0.26245	-0.25611	-0.26429	-0.27438	-0.25289	-0.28141	-0.27290
$\Delta E_{L+4-H-1}$	0.13384	0.12591	0.12798	0.12707	0.12229	0.12712	0.12169