

卟咯锰(III)与锰(V)-氧配合物与含氮配体的轴向配位性质

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Axial Coordination Behavior of Corrole Mn^{III} and Mn^VO Complexes with N-Based Ligands

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表 S1 在 B3LYP 方法下五重态(TPFC)Mn^{III}(L)的优化几何结构参数、结合能(ΔE)、NPA 电荷及配位键的 Wiberg 键级(WI)

Table S1 Selected optimized geometrical parameters, binding energy (ΔE), NPA charge and wiberg bond order (WI) of coordination bond of (TPFC)Mn^{III}(L) in the quintet state at B3LYP

	level			(TPFC)Mn ^{III}
	(TPFC)Mn ^{III} (L)			
	Im	4-MI	Py	
$d_{\text{Mn-N}}^{\text{a}}/\text{nm}$	0.1924	0.1928	0.1923	0.1903
$\Delta d(\text{N4})^{\text{b}}/\text{nm}$	0.0256	0.0274	0.0246	0.0005
$d_{\text{Mn-L}}^{\text{c}}/\text{nm}$	0.2283	0.2316	0.2331	
$D_{\text{L-NNNN}}^{\text{d}}/(\text{°})$	89.23	89.12	88.77	
$D_{\text{NNNN}}^{\text{e}}/(\text{°})$	-2.162	-0.487	0.438	0.672
$\Delta E^{\text{f}}/(\text{kJ}\cdot\text{mol}^{-1})$	-66.696	-64.700	-54.975	
Q_{L}^{g}	0.101	0.096	0.094	
Q_{N}^{h}	-0.494	-0.501	-0.452	
Q_{N}^{g}	-0.589	-0.593	-0.534	
$Q_{\Delta\text{N}}$	-0.095	-0.092	-0.082	
Q_{Mn}	1.418	1.444	1.417	1.455
$Q_{4\text{N}}$	-2.406	-2.412	-2.422	-2.520
Q_{Corrole}	-1.519	-1.540	-1.511	-1.455
WI	0.29	0.29	0.27	

^a average bonding lengths of four Mn-N bonds; ^b distances of coordination bond between ligands with (TPFC)Mn^{III}; ^c distances between Mn atom and the mean plane of the four nitrogen atoms in pyrrole; ^d dihedral angle between the plane of ligand and the mean plane of the four nitrogen atoms in pyrrole; ^e dihedral angle of four nitrogen atoms in pyrrole; ^f after zero-point energy correction; ^g after coordination; ^h before coordinating; Q_{L} is the natural charge of ligands; Q_{N} is the natural charge of coordinating N atom; $Q_{\Delta\text{N}}$ is the difference natural charge between Q_{N}^{g} and Q_{N}^{h} ; $Q_{4\text{N}}$ is the sum natural charge of four pyrrole nitrogen atom; Q_{Corrole} is the sum natural charge corrole skeleton.

表 S2 五重态的(TPFC)Mn^{III}(L)在 BP86 方法下优化的部分几何参数

Table S2 Selected optimized parameters of (TPFC)Mn^{III}(L) in the quintet state at BP86 level

Parameter	2-MI	5-MI	4-IPI	2-IPI	5-IPI
$d_{\text{Mn-N1}}/\text{nm}$	0.1922	0.1921	0.1923	0.1922	0.1922
$d_{\text{Mn-N2}}/\text{nm}$	0.1923	0.1921	0.1924	0.1924	0.1922
$d_{\text{Mn-N3}}/\text{nm}$	0.1933	0.1932	0.1935	0.1936	0.1931
$d_{\text{Mn-N4}}/\text{nm}$	0.1934	0.1933	0.1935	0.1932	0.1934
$d_{\text{Mn-N}}^{\text{a}}/\text{nm}$	0.1928	0.1927	0.1929	0.1929	0.1927
$d_{\text{Mn-L}}^{\text{b}}/\text{nm}$	0.2277	0.2257	0.2284	0.2304	0.2251
$\Delta d(\text{N4})^{\text{c}}/\text{nm}$	0.0281	0.0264	0.0289	0.0289	0.0261
$D_{\text{NNNN}}^{\text{d}}/(\text{°})$	-0.435	-0.922	-0.117	-0.121	-1.186

^a average bonding lengths of four Mn-N bonds; ^b distances of coordination bond between ligands with (TPFC)Mn^{III}; ^c distances between Mn atom and the mean plane of the four nitrogen atoms in pyrrole; ^d dihedral angle of four nitrogen atoms in pyrroles

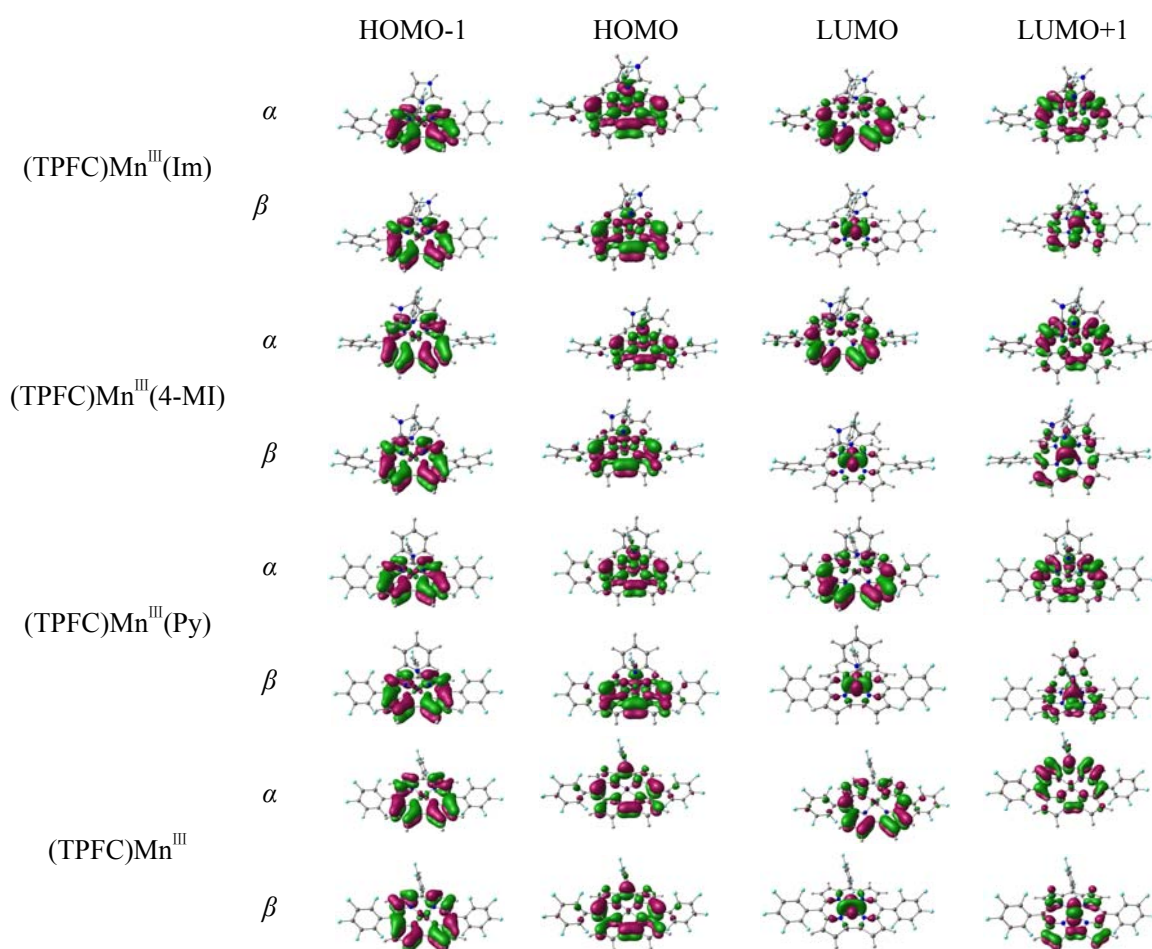


图 S1 五重态下(TPFC)Mn^{III}(L)和(TPFC)Mn^{III}的前线分子轨道的分布图(BP86 方法)

Fig.S1 Frontier molecular orbitals of (TPFC)Mn^{III}(L) and (TPFC)Mn^{III} in the quintet at BP86 level

表 S3 在 B3LYP 方法下单、三重态 (TPFC)Mn^VO(L)的结合能(ΔE)和结构数据

Table S3 Selected optimized geometrical parameters and binding energy (ΔE) of (TPFC)Mn^VO(L) in the singlet and triplet at B3LYP level

L	$\Delta E^a/(\text{kJ}\cdot\text{mol}^{-1})$		$d_{\text{Mn-O}}/\text{nm}$		$d_{\text{Mn-N(L)}}/\text{nm}$	
	Singlet	Triplet	Singlet	Triplet	Singlet	Triplet
Im	5.122	-8.457	0.1535	0.158	0.3945	0.2499
4-MI	3.166	0.055	0.1535	0.1575	0.4104	0.2973
Py	5.821	-0.751	0.1535	0.1578	0.3913	0.2678

^a with zero-point energy correction; ^b distance of manganese atom and nitrogen atom of ligand.

Cartesian Coordinates of Optimized Geometries

(TPFC)Mn^{III}(Im)

1	25	0	-0.019707	-0.924280	-0.151391
2	7	0	-1.273554	-2.342160	-0.447183
3	7	0	1.423865	0.344808	-0.308137
4	7	0	1.202425	-2.347235	-0.563603
5	9	0	-4.767054	-2.413258	1.866792
6	7	0	-1.455107	0.358601	-0.289086
7	9	0	-5.216765	-0.247735	-2.367957
8	9	0	-7.468539	-2.708811	1.992596
9	9	0	-7.917527	-0.521704	-2.211368
10	9	0	-9.055910	-1.759705	-0.039746
11	9	0	4.966928	-2.152880	-2.688546
12	9	0	9.010745	-1.740835	-0.254713
13	9	0	-0.912954	4.079625	-2.346802
14	9	0	7.669545	-2.409503	-2.557163
15	9	0	-0.896210	6.795110	-2.208685
16	9	0	7.618241	-0.828833	1.932678
17	9	0	0.047938	8.056126	0.042459
18	9	0	0.927481	3.857986	2.054509
19	9	0	4.913345	-0.598350	1.831866
20	6	0	2.555839	2.336031	-0.366100
21	1	0	2.743816	3.408686	-0.397386
22	6	0	-2.646318	-2.386078	-0.459473
23	9	0	0.964410	6.574401	2.167316
24	6	0	4.842872	-1.359976	-0.438072
25	6	0	-3.026443	-3.760705	-0.662589
26	1	0	-4.049894	-4.129124	-0.734407
27	6	0	-4.896762	-1.323715	-0.258498

28	6	0	0.034455	6.712951	-0.019930
29	6	0	-5.516844	-1.952728	0.840303
30	6	0	-1.268494	1.733281	-0.212366
31	6	0	5.589233	-1.829555	-1.537945
32	6	0	-2.828339	0.093465	-0.254116
33	6	0	-3.413823	-1.196611	-0.326398
34	6	0	0.006043	3.871931	-0.151231
35	6	0	-5.741854	-0.846721	-1.281059
36	6	0	6.985465	-1.964655	-1.486637
37	6	0	6.961140	-1.148197	0.800864
38	6	0	-0.759273	-3.614754	-0.652358
39	6	0	5.566188	-1.030533	0.726384
40	6	0	-0.004637	2.379482	-0.218644
41	6	0	-1.856519	-4.518156	-0.782657
42	1	0	-1.789261	-5.591793	-0.958298
43	6	0	-2.566343	2.356519	-0.118266
44	1	0	-2.743741	3.428275	-0.037230
45	6	0	0.667058	-3.620302	-0.695959
46	6	0	-7.137187	-0.983378	-1.216125
47	6	0	-6.907890	-2.108935	0.924743
48	6	0	-3.516425	1.354951	-0.138367
49	1	0	-4.597716	1.475379	-0.081848
50	6	0	7.673291	-1.619436	-0.313166
51	6	0	-7.720639	-1.620000	-0.109871
52	6	0	0.505789	5.954332	1.062516
53	6	0	3.359405	-1.233200	-0.479792
54	6	0	-0.455419	4.664426	-1.222061
55	6	0	-0.451073	6.066783	-1.167144
56	6	0	1.748572	-4.544002	-0.818806
57	1	0	1.662449	-5.623056	-0.946739
58	6	0	3.494802	1.323784	-0.419116
59	1	0	4.575483	1.434302	-0.505244
60	6	0	2.791765	0.065742	-0.392907
61	6	0	0.482327	4.553619	0.986850
62	6	0	2.574726	-2.413835	-0.589705
63	6	0	2.931226	-3.801275	-0.746258
64	1	0	3.946938	-4.191940	-0.806707
65	6	0	1.252419	1.723365	-0.291234
66	6	0	1.192651	-0.956844	2.827470
67	6	0	-0.944589	-1.369143	2.986814
68	6	0	-0.446859	-1.402026	4.272857
69	7	0	0.910784	-1.139349	4.150389
70	1	0	1.582129	-1.086123	4.912727
71	1	0	2.187631	-0.743174	2.440442

72	1	0	-1.963200	-1.530235	2.639144
73	1	0	-0.916978	-1.581754	5.236028
74	7	0	0.083693	-1.090738	2.099541

(TPFC)Mn^{III}(4-MI)

1	25	0	-0.011900	-0.914117	-0.090304
2	7	0	-1.262250	-2.323920	-0.473187
3	7	0	1.437922	0.347829	-0.266508
4	7	0	1.217258	-2.345493	-0.453804
5	9	0	-4.868777	-2.423307	1.631819
6	7	0	-1.438678	0.375048	-0.305211
7	9	0	-5.097531	-0.166520	-2.575398
8	9	0	-7.571753	-2.706894	1.615879
9	9	0	-7.803160	-0.429935	-2.558035
10	9	0	-9.053431	-1.707357	-0.472749
11	9	0	4.995350	-0.262797	-2.659117
12	9	0	9.016306	-1.821812	-0.698392
13	9	0	-0.748054	4.183945	-2.235539
14	9	0	7.696868	-0.552060	-2.745588
15	9	0	-0.717800	6.891866	-1.978366
16	9	0	7.609202	-2.789197	1.454936
17	9	0	0.094125	8.043719	0.379850
18	9	0	0.817809	3.752841	2.254716
19	9	0	4.909376	-2.480384	1.571380
20	6	0	2.575097	2.338351	-0.215558
21	1	0	2.764817	3.410724	-0.185860
22	6	0	-2.632479	-2.359010	-0.573098
23	9	0	0.866103	6.462933	2.489896
24	6	0	4.856561	-1.360946	-0.540596
25	6	0	-3.007724	-3.726138	-0.828180
26	1	0	-4.026851	-4.085542	-0.971625
27	6	0	-4.885614	-1.287913	-0.476335
28	6	0	0.074467	6.704803	0.257824
29	6	0	-5.563844	-1.936895	0.575239
30	6	0	-1.250370	1.746590	-0.189757
31	6	0	5.610673	-0.877351	-1.629270
32	6	0	-2.812892	0.118423	-0.344128
33	6	0	-3.401029	-1.166701	-0.465827
34	6	0	0.031763	3.873711	0.000853
35	6	0	-5.677702	-0.785372	-1.528943
36	6	0	7.005317	-1.021876	-1.690259
37	6	0	6.960152	-2.172496	0.448793
38	6	0	-0.744797	-3.595146	-0.679868
39	6	0	5.567901	-2.008559	0.490033

40	6	0	0.014673	2.384940	-0.127855
41	6	0	-1.836565	-4.488023	-0.896527
42	1	0	-1.763869	-5.557188	-1.095821
43	6	0	-2.547837	2.376240	-0.145772
44	1	0	-2.723133	3.447517	-0.054411
45	6	0	0.681121	-3.606698	-0.669064
46	6	0	-7.075259	-0.916325	-1.535752
47	6	0	-6.957412	-2.088151	0.588957
48	6	0	-3.500448	1.381402	-0.237013
49	1	0	-4.582650	1.507340	-0.236348
50	6	0	7.680950	-1.674832	-0.647810
51	6	0	-7.715986	-1.573282	-0.473891
52	6	0	0.471988	5.895553	1.333290
53	6	0	3.374180	-1.222119	-0.475368
54	6	0	-0.355873	4.715572	-1.060945
55	6	0	-0.343623	6.114284	-0.944590
56	6	0	1.759224	-4.517496	-0.883972
57	1	0	1.669490	-5.584943	-1.085265
58	6	0	3.512311	1.327542	-0.307151
59	1	0	4.594996	1.439469	-0.351533
60	6	0	2.807253	0.072191	-0.354049
61	6	0	0.443164	4.499785	1.194490
62	6	0	2.586474	-2.401574	-0.555911
63	6	0	2.940787	-3.774251	-0.813364
64	1	0	3.954635	-4.148847	-0.954334
65	6	0	1.269912	1.725558	-0.192772
66	6	0	-1.379557	-1.495284	2.696500
67	6	0	0.635206	-0.834599	3.259324
68	6	0	-0.044629	-1.105147	4.433113
69	7	0	-1.314900	-1.519893	4.056583
70	1	0	-2.067898	-1.796625	4.681394
71	7	0	-0.216975	-1.085568	2.183468
72	1	0	0.258266	-1.040060	5.475062
73	1	0	-2.268014	-1.769410	2.130112
74	6	0	2.040570	-0.347035	3.089005
75	1	0	2.644802	-1.052450	2.494424
76	1	0	2.063733	0.626541	2.570880
77	1	0	2.524210	-0.225350	4.071119

(TPFC)Mn^{III}(Py)

1	25	0	0.005952	-0.923904	-0.165725
2	7	0	1.251158	-2.352760	-0.451996
3	7	0	-1.436253	0.340166	-0.347457
4	7	0	-1.227188	-2.358972	-0.474306

5	9	0	5.038766	-2.110685	-2.571157
6	7	0	1.442448	0.347596	-0.343661
7	9	0	4.910004	-0.586419	1.953868
8	9	0	7.743170	-2.349447	-2.404957
9	9	0	7.618665	-0.800914	2.094594
10	9	0	9.046545	-1.688069	-0.079095
11	9	0	-4.953449	-0.566323	1.840485
12	9	0	-9.033729	-1.724436	-0.273161
13	9	0	-0.840226	3.956048	1.873705
14	9	0	-7.663919	-0.788419	1.917610
15	9	0	-0.872040	6.675954	1.863243
16	9	0	-7.670063	-2.426278	-2.551944
17	9	0	-0.041953	8.055857	-0.363249
18	9	0	0.820600	3.970585	-2.602634
19	9	0	-4.963608	-2.179417	-2.655739
20	6	0	-2.562959	2.332630	-0.464831
21	1	0	-2.747775	3.404296	-0.529582
22	6	0	2.624514	-2.406497	-0.462441
23	9	0	0.809352	6.690476	-2.590262
24	6	0	-4.865370	-1.356024	-0.415256
25	6	0	2.995701	-3.794016	-0.572015
26	1	0	4.016062	-4.175526	-0.607160
27	6	0	4.881700	-1.331954	-0.318478
28	6	0	-0.031590	6.711380	-0.363830
29	6	0	5.644856	-1.789051	-1.411399
30	6	0	1.261241	1.725799	-0.350737
31	6	0	-5.598475	-1.009811	0.737840
32	6	0	2.816024	0.078694	-0.352144
33	6	0	3.396987	-1.215830	-0.383905
34	6	0	-0.008805	3.868320	-0.364642
35	6	0	5.584198	-1.006667	0.859204
36	6	0	-6.994769	-1.123715	0.797979
37	6	0	-6.996382	-1.968873	-1.480045
38	6	0	0.729478	-3.634565	-0.563474
39	6	0	-5.599358	-1.838177	-1.517502
40	6	0	-0.001512	2.373817	-0.362012
41	6	0	1.821056	-4.550462	-0.639595
42	1	0	1.747207	-5.633412	-0.738515
43	6	0	2.562953	2.347199	-0.350826
44	1	0	2.745619	3.421114	-0.352886
45	6	0	-0.696984	-3.638359	-0.573390
46	6	0	6.979005	-1.116547	0.952169
47	6	0	7.041113	-1.915523	-1.341600
48	6	0	3.510038	1.341898	-0.351287

49	1	0	4.593086	1.459755	-0.372153
50	6	0	-7.695484	-1.607038	-0.318201
51	6	0	7.709390	-1.574690	-0.155547
52	6	0	0.406504	6.012100	-1.499024
53	6	0	-3.380409	-1.233928	-0.445224
54	6	0	-0.438451	4.601874	0.759416
55	6	0	-0.458519	6.004740	0.771072
56	6	0	-1.782328	-4.560798	-0.659428
57	1	0	-1.701065	-5.643737	-0.752530
58	6	0	-3.505411	1.322844	-0.473695
59	1	0	-4.586704	1.433842	-0.549973
60	6	0	-2.806804	0.063963	-0.409660
61	6	0	0.408445	4.608721	-1.489024
62	6	0	-2.600112	-2.420781	-0.501571
63	6	0	-2.961947	-3.810947	-0.609517
64	1	0	-3.979552	-4.198625	-0.654930
65	6	0	-1.260488	1.718462	-0.383654
66	6	0	-1.175492	-1.001402	2.818489
67	6	0	-1.229758	-1.047783	4.217608
68	6	0	-0.027696	-1.075150	4.939894
69	6	0	1.184706	-1.054906	4.234848
70	6	0	1.150596	-1.008631	2.835044
71	7	0	-0.007441	-0.982631	2.135745
72	1	0	-0.035659	-1.109956	6.034063
73	1	0	-2.089291	-0.973345	2.215398
74	1	0	-2.199140	-1.059617	4.723801
75	1	0	2.146718	-1.072693	4.754757
76	1	0	2.073153	-0.986829	2.245185

(TPFC)Mn^{III}(2-MI)

1	25	0	-0.023115	-0.926418	-0.062837
2	7	0	-1.273383	-2.343423	-0.411455
3	7	0	1.425899	0.334658	-0.274242
4	7	0	1.206579	-2.361699	-0.415740
5	9	0	-4.907663	-2.454979	1.644026
6	7	0	-1.451228	0.358344	-0.289672
7	9	0	-5.081629	-0.177129	-2.553511
8	9	0	-7.611380	-2.731349	1.595624
9	9	0	-7.787438	-0.433680	-2.569326
10	9	0	-9.065449	-1.717510	-0.504636
11	9	0	4.956198	-0.350283	-2.715770
12	9	0	9.002305	-1.830650	-0.745096
13	9	0	-0.821845	4.162702	-2.237828
14	9	0	7.657918	-0.637497	-2.821693

15	9	0	-0.787088	6.870698	-1.991659
16	9	0	7.621056	-2.721988	1.457622
17	9	0	0.090563	8.032929	0.337907
18	9	0	0.869322	3.750451	2.209847
19	9	0	4.921092	-2.413195	1.592468
20	6	0	2.560540	2.327339	-0.267769
21	1	0	2.749339	3.400289	-0.258557
22	6	0	-2.643155	-2.379324	-0.514981
23	9	0	0.923358	6.460408	2.431596
24	6	0	4.843440	-1.373746	-0.559268
25	6	0	-3.017951	-3.749374	-0.755548
26	1	0	-4.036985	-4.110202	-0.895408
27	6	0	-4.897179	-1.306873	-0.455372
28	6	0	0.068006	6.693553	0.221840
29	6	0	-5.588435	-1.960701	0.585253
30	6	0	-1.264160	1.730896	-0.188037
31	6	0	5.584325	-0.927200	-1.672399
32	6	0	-2.825317	0.099645	-0.320719
33	6	0	-3.412805	-1.186786	-0.428917
34	6	0	0.019280	3.860472	-0.022514
35	6	0	-5.675519	-0.798354	-1.515552
36	6	0	6.978720	-1.071111	-1.743242
37	6	0	6.959635	-2.144296	0.436274
38	6	0	-0.755987	-3.616424	-0.604486
39	6	0	5.567674	-1.981618	0.485953
40	6	0	0.000985	2.371490	-0.142984
41	6	0	-1.847444	-4.512175	-0.812051
42	1	0	-1.774324	-5.583708	-0.997828
43	6	0	-2.562215	2.359305	-0.142483
44	1	0	-2.738945	3.430891	-0.058148
45	6	0	0.669850	-3.626942	-0.604000
46	6	0	-7.072935	-0.926077	-1.540017
47	6	0	-6.982874	-2.108262	0.580198
48	6	0	-3.513727	1.362644	-0.222539
49	1	0	-4.596032	1.486909	-0.216445
50	6	0	7.667193	-1.685027	-0.685523
51	6	0	-7.727577	-1.586398	-0.488867
52	6	0	0.496492	5.888599	1.288615
53	6	0	3.361392	-1.236308	-0.482023
54	6	0	-0.398183	4.698444	-1.076275
55	6	0	-0.383792	6.097648	-0.965603
56	6	0	1.746783	-4.540371	-0.813811
57	1	0	1.656034	-5.611200	-0.995786
58	6	0	3.498112	1.316272	-0.360896

59	1	0	4.579757	1.429278	-0.426031
60	6	0	2.794222	0.059626	-0.378869
61	6	0	0.464088	4.492567	1.155931
62	6	0	2.574765	-2.418322	-0.531251
63	6	0	2.928312	-3.795045	-0.767688
64	1	0	3.941118	-4.171129	-0.912609
65	6	0	1.256709	1.713297	-0.216893
66	6	0	0.695212	-0.713096	3.176232
67	6	0	-1.350965	-1.425884	2.832113
68	6	0	-1.196120	-1.359356	4.198526
69	7	0	0.101709	-0.908008	4.395581
70	1	0	0.547823	-0.743807	5.294849
71	1	0	-2.224292	-1.731364	2.259539
72	7	0	-0.176772	-1.025113	2.207056
73	1	0	-1.865151	-1.585362	5.024362
74	6	0	2.097210	-0.218185	3.016997
75	1	0	2.576178	-0.084803	4.000421
76	1	0	2.705534	-0.926455	2.431650
77	1	0	2.114682	0.750195	2.489956

(TPFC)Mn^{III}(5-MI)

1	25	0	0.001196	-0.901076	-0.108290
2	7	0	-1.244719	-2.325883	-0.434643
3	7	0	1.444010	0.369788	-0.296658
4	7	0	1.235566	-2.330745	-0.460474
5	9	0	-4.971520	-2.497398	1.498967
6	7	0	-1.431878	0.380364	-0.313981
7	9	0	-4.967345	-0.108389	-2.639624
8	9	0	-7.670303	-2.761239	1.333321
9	9	0	-7.669209	-0.352101	-2.771730
10	9	0	-9.035102	-1.684436	-0.795190
11	9	0	4.927971	-0.173956	-2.723464
12	9	0	9.022916	-1.746787	-0.936827
13	9	0	-0.727220	4.253452	-2.197708
14	9	0	7.625369	-0.438401	-2.907205
15	9	0	-0.706401	6.953020	-1.863360
16	9	0	7.695567	-2.778455	1.237039
17	9	0	0.067351	8.039580	0.537506
18	9	0	0.773148	3.700850	2.305089
19	9	0	5.001535	-2.494130	1.452792
20	6	0	2.574621	2.363324	-0.222265
21	1	0	2.760823	3.436074	-0.180829
22	6	0	-2.613252	-2.361768	-0.558849
23	9	0	0.810286	6.400389	2.614785

24	6	0	4.866514	-1.320235	-0.625770
25	6	0	-2.981909	-3.727434	-0.828646
26	1	0	-3.998486	-4.087739	-0.986212
27	6	0	-4.869881	-1.290033	-0.562889
28	6	0	0.052890	6.704938	0.377213
29	6	0	-5.604967	-1.970801	0.430061
30	6	0	-1.252071	1.752010	-0.193280
31	6	0	5.581153	-0.806023	-1.727825
32	6	0	-2.805061	0.114903	-0.355091
33	6	0	-3.387159	-1.171999	-0.480440
34	6	0	0.021889	3.880826	0.038645
35	6	0	-5.603835	-0.752360	-1.641089
36	6	0	6.973628	-0.938134	-1.839953
37	6	0	7.008399	-2.140974	0.269336
38	6	0	-0.721967	-3.593637	-0.653560
39	6	0	5.616989	-1.988944	0.363518
40	6	0	0.011535	2.395823	-0.126025
41	6	0	-1.809409	-4.487717	-0.886560
42	1	0	-1.732330	-5.555004	-1.094232
43	6	0	-2.552897	2.374222	-0.146852
44	1	0	-2.735411	3.444010	-0.051031
45	6	0	0.704960	-3.596638	-0.662706
46	6	0	-6.999198	-0.873660	-1.726516
47	6	0	-6.998895	-2.112178	0.362161
48	6	0	-3.499110	1.373752	-0.247241
49	1	0	-4.582018	1.492905	-0.245134
50	6	0	7.688838	-1.611016	-0.837529
51	6	0	-7.698377	-1.558927	-0.721172
52	6	0	0.435867	5.866563	1.435650
53	6	0	3.385772	-1.192542	-0.516370
54	6	0	-0.352850	4.751948	-1.004019
55	6	0	-0.345603	6.147167	-0.847350
56	6	0	1.785659	-4.499882	-0.894152
57	1	0	1.700769	-5.568573	-1.091192
58	6	0	3.514678	1.356662	-0.327313
59	1	0	4.597036	1.472563	-0.370354
60	6	0	2.814328	0.098513	-0.383096
61	6	0	0.411540	4.476546	1.253811
62	6	0	2.603500	-2.376812	-0.584982
63	6	0	2.962793	-3.747099	-0.846588
64	1	0	3.976702	-4.115295	-1.002907
65	6	0	1.271689	1.744837	-0.205717
66	6	0	0.221469	0.115471	2.944160
67	6	0	-0.229380	-2.015087	2.979353

68	6	0	-0.154518	-1.628625	4.304859
69	7	0	0.133043	-0.265791	4.253229
70	1	0	0.258942	0.346328	5.056315
71	7	0	0.004719	-0.930628	2.148112
72	1	0	0.433140	1.133580	2.621995
73	1	0	-0.438079	-3.002288	2.571671
74	6	0	-0.320056	-2.383754	5.585617
75	1	0	0.596869	-2.363413	6.201973
76	1	0	-1.147198	-1.984008	6.199596
77	1	0	-0.549135	-3.437312	5.365741

(TPFC)Mn^{III}(2-IPI)

1	25	0	-0.099547	-0.901874	-0.126534
2	7	0	-1.338986	-2.323624	-0.498565
3	7	0	1.334495	0.379721	-0.341258
4	7	0	1.144775	-2.316424	-0.517232
5	9	0	-4.994587	-2.424266	1.582301
6	7	0	-1.543515	0.371070	-0.326350
7	9	0	-5.143139	-0.227113	-2.656514
8	9	0	-7.698582	-2.719431	1.515058
9	9	0	-7.848569	-0.501314	-2.694000
10	9	0	-9.137884	-1.754653	-0.618054
11	9	0	4.723722	-0.143348	-2.921230
12	9	0	8.903697	-1.664018	-1.293705
13	9	0	-0.890255	4.179242	-2.286244
14	9	0	7.413570	-0.384696	-3.214039
15	9	0	-0.885360	6.888696	-2.042872
16	9	0	7.676570	-2.690009	0.941894
17	9	0	-0.088095	8.059781	0.310829
18	9	0	0.669379	3.786551	2.210966
19	9	0	4.991115	-2.431096	1.265731
20	6	0	2.442452	2.388463	-0.345805
21	1	0	2.616254	3.463803	-0.326028
22	6	0	-2.708378	-2.372448	-0.600088
23	9	0	0.694055	6.496539	2.430388
24	6	0	4.759326	-1.273077	-0.814584
25	6	0	-3.069862	-3.742224	-0.862507
26	1	0	-4.085691	-4.110944	-1.005201
27	6	0	-4.973785	-1.319717	-0.538250
28	6	0	-0.095245	6.720208	0.195412
29	6	0	-5.670238	-1.957110	0.508464
30	6	0	-1.370435	1.744604	-0.213327
31	6	0	5.423220	-0.761244	-1.949163
32	6	0	-2.915007	0.100842	-0.371628

33	6	0	-3.489820	-1.189427	-0.500436
34	6	0	-0.111132	3.887477	-0.047459
35	6	0	-5.744103	-0.834397	-1.614550
36	6	0	6.811273	-0.881652	-2.117433
37	6	0	6.944992	-2.066827	-0.002063
38	6	0	-0.809086	-3.586815	-0.716541
39	6	0	5.557570	-1.926209	0.146378
40	6	0	-0.112323	2.397838	-0.170082
41	6	0	-1.891788	-4.491065	-0.936193
42	1	0	-1.807469	-5.558260	-1.141222
43	6	0	-2.674163	2.360676	-0.169514
44	1	0	-2.860446	3.430087	-0.077960
45	6	0	0.616373	-3.582004	-0.732589
46	6	0	-7.140548	-0.971069	-1.649761
47	6	0	-7.063793	-2.112689	0.493684
48	6	0	-3.616054	1.356084	-0.266111
49	1	0	-4.699628	1.469524	-0.267927
50	6	0	7.573986	-1.539842	-1.140463
51	6	0	-7.800968	-1.615641	-0.592372
52	6	0	0.307559	5.920061	1.275695
53	6	0	3.282817	-1.160314	-0.646026
54	6	0	-0.504872	4.720416	-1.114057
55	6	0	-0.505811	6.119805	-1.004718
56	6	0	1.695995	-4.474885	-1.005383
57	1	0	1.611248	-5.540312	-1.219242
58	6	0	3.390038	1.392366	-0.478398
59	1	0	4.467705	1.520965	-0.572655
60	6	0	2.702785	0.125827	-0.492419
61	6	0	0.291972	4.523547	1.143153
62	6	0	2.508613	-2.351582	-0.689053
63	6	0	2.869363	-3.716025	-0.978503
64	1	0	3.880419	-4.074294	-1.172142
65	6	0	1.149128	1.755455	-0.266745
66	6	0	0.617664	-1.011926	3.139397
67	6	0	-1.527259	-1.245090	2.732520
68	6	0	-1.389715	-1.312532	4.100370
69	7	0	-0.030768	-1.161755	4.338361
70	1	0	0.420644	-1.172770	5.249560
71	1	0	-2.431521	-1.334127	2.134232
72	1	0	-2.108124	-1.457741	4.902792
73	7	0	-0.281547	-1.057766	2.145275
74	6	0	2.103133	-0.798467	3.017410
75	6	0	2.490640	0.663151	3.348934
76	6	0	2.901590	-1.801527	3.878656

77	1	0	2.279003	0.901150	4.407182
78	1	0	3.569876	0.814957	3.180344
79	1	0	1.941016	1.379954	2.719343
80	1	0	2.756549	-1.621802	4.960606
81	1	0	2.614868	-2.843058	3.660102
82	1	0	3.978528	-1.695889	3.673815
83	1	0	2.346931	-0.986807	1.958466

(TPFC)Mn^{III}(4-IPi)

1	25	0	0.087679	-0.876937	-0.165594
2	7	0	-1.152867	-2.283424	-0.588005
3	7	0	1.530777	0.402308	-0.333092
4	7	0	1.329677	-2.285316	-0.586992
5	9	0	-4.970233	-2.432862	1.254781
6	7	0	-1.346054	0.406728	-0.340377
7	9	0	-4.768293	-0.080816	-2.899062
8	9	0	-7.661244	-2.690962	0.967227
9	9	0	-7.462614	-0.322446	-3.156551
10	9	0	-8.921985	-1.632892	-1.233569
11	9	0	5.165513	-0.176251	-2.667257
12	9	0	9.128118	-1.723993	-0.581256
13	9	0	0.863717	4.234147	-2.235550
14	9	0	7.871035	-0.456424	-2.667945
15	9	0	0.861359	6.940434	-1.954909
16	9	0	7.656279	-2.696540	1.526944
17	9	0	0.078358	8.078874	0.419368
18	9	0	-0.673093	3.779635	2.262577
19	9	0	4.952605	-2.395583	1.557938
20	6	0	2.658828	2.390258	-0.137476
21	1	0	2.843308	3.458174	-0.026828
22	6	0	-2.518521	-2.317498	-0.743588
23	9	0	-0.692985	6.487377	2.521212
24	6	0	4.963974	-1.281713	-0.559479
25	6	0	-2.879556	-3.674791	-1.064377
26	1	0	-3.892127	-4.030317	-1.254938
27	6	0	-4.772784	-1.243064	-0.810029
28	6	0	0.083581	6.741033	0.285338
29	6	0	-5.554590	-1.912131	0.153587
30	6	0	-1.162931	1.781299	-0.243503
31	6	0	5.750439	-0.791499	-1.621571
32	6	0	-2.715063	0.152642	-0.482112
33	6	0	-3.294155	-1.130023	-0.660115
34	6	0	0.095842	3.912551	0.003170
35	6	0	-5.453292	-0.714930	-1.926750

36	6	0	7.147256	-0.930783	-1.637202
37	6	0	7.038029	-2.083635	0.498922
38	6	0	-0.624249	-3.541689	-0.840965
39	6	0	5.645238	-1.924808	0.492989
40	6	0	0.097504	2.424590	-0.140582
41	6	0	-1.705041	-4.429852	-1.124505
42	1	0	-1.620648	-5.489283	-1.366354
43	6	0	-2.458044	2.412851	-0.300877
44	1	0	-2.633550	3.487219	-0.259006
45	6	0	0.801317	-3.544314	-0.833377
46	6	0	-6.843406	-0.835002	-2.076528
47	6	0	-6.944087	-2.052119	0.022996
48	6	0	-3.404605	1.417235	-0.440125
49	1	0	-4.483505	1.544550	-0.520308
50	6	0	7.791512	-1.582499	-0.574138
51	6	0	-7.590316	-1.508844	-1.098018
52	6	0	-0.313663	5.926368	1.356780
53	6	0	3.479441	-1.151440	-0.539958
54	6	0	0.484381	4.759637	-1.054057
55	6	0	0.486726	6.157333	-0.925510
56	6	0	1.885353	-4.442588	-1.068822
57	1	0	1.802537	-5.504759	-1.299111
58	6	0	3.602387	1.388783	-0.250102
59	1	0	4.685844	1.504012	-0.249941
60	6	0	2.902947	0.135060	-0.382608
61	6	0	-0.300237	4.531572	1.205256
62	6	0	2.699787	-2.332144	-0.680433
63	6	0	3.063332	-3.695374	-0.971706
64	1	0	4.079892	-4.060495	-1.118957
65	6	0	1.355892	1.773756	-0.194860
66	6	0	1.524540	-1.426143	2.582208
67	6	0	-0.579298	-1.261885	3.186478
68	6	0	0.141831	-1.612666	4.315479
69	7	0	1.466350	-1.708331	3.912809
70	1	0	2.256611	-1.964867	4.499262
71	7	0	0.305453	-1.150182	2.111929
72	1	0	-0.161299	-1.800933	5.341736
73	1	0	2.445064	-1.454161	2.001883
74	6	0	-2.056244	-0.981480	3.056654
75	6	0	-2.354517	0.523003	3.260311
76	6	0	-2.892117	-1.845174	4.021749
77	1	0	-2.343404	-1.249246	2.023786
78	1	0	-1.766878	1.151778	2.573251
79	1	0	-3.423617	0.730632	3.083332

80	1	0	-2.113133	0.828818	4.294105
81	1	0	-2.684264	-2.919634	3.886918
82	1	0	-2.688311	-1.584801	5.076430
83	1	0	-3.967231	-1.680328	3.843910

(TPFC)Mn^{III}(5-IPi)

1	25	0	0.006560	-1.023249	-0.219466
2	7	0	-1.240672	-2.475713	-0.385602
3	7	0	1.451445	0.218094	-0.535942
4	7	0	1.239197	-2.485311	-0.411185
5	9	0	-4.954575	-2.454563	1.558682
6	7	0	-1.424813	0.229745	-0.565727
7	9	0	-4.975844	-0.480707	-2.793952
8	9	0	-7.653604	-2.729662	1.436702
9	9	0	-7.678255	-0.731400	-2.883448
10	9	0	-9.032369	-1.863311	-0.777769
11	9	0	4.953408	-0.596051	-2.870780
12	9	0	9.031244	-1.959129	-0.883381
13	9	0	-0.795544	3.900280	-2.797089
14	9	0	7.652384	-0.878081	-2.999627
15	9	0	-0.779836	6.618200	-2.725506
16	9	0	7.683121	-2.744207	1.379183
17	9	0	0.072941	7.934770	-0.470037
18	9	0	0.867113	3.789173	1.682157
19	9	0	4.987689	-2.438701	1.537369
20	6	0	2.584421	2.206125	-0.675722
21	1	0	2.772988	3.276529	-0.751441
22	6	0	-2.609632	-2.522966	-0.504195
23	9	0	0.899686	6.505102	1.727350
24	6	0	4.872650	-1.501728	-0.659393
25	6	0	-2.979857	-3.909234	-0.622134
26	1	0	-3.996867	-4.283842	-0.738636
27	6	0	-4.864796	-1.453768	-0.612304
28	6	0	0.060281	6.590687	-0.499813
29	6	0	-5.594316	-2.033746	0.446434
30	6	0	-1.243172	1.606311	-0.581602
31	6	0	5.597385	-1.113113	-1.805246
32	6	0	-2.797942	-0.037407	-0.566936
33	6	0	-3.381816	-1.329707	-0.551346
34	6	0	0.032887	3.746152	-0.562428
35	6	0	-5.605848	-1.022737	-1.732943
36	6	0	6.990757	-1.256430	-1.889370
37	6	0	7.005439	-2.218090	0.340435
38	6	0	-0.718948	-3.760851	-0.464126

39	6	0	5.613315	-2.056997	0.404519
40	6	0	0.021071	2.252619	-0.582508
41	6	0	-1.807784	-4.673182	-0.596630
42	1	0	-1.732628	-5.756978	-0.686221
43	6	0	-2.543738	2.231167	-0.587085
44	1	0	-2.725693	3.305251	-0.594045
45	6	0	0.708367	-3.765505	-0.471695
46	6	0	-7.001888	-1.149844	-1.796900
47	6	0	-6.988571	-2.179545	0.401942
48	6	0	-3.490881	1.226938	-0.580038
49	1	0	-4.573642	1.347347	-0.579214
50	6	0	7.696367	-1.813708	-0.811992
51	6	0	-7.695084	-1.733162	-0.725277
52	6	0	0.485794	5.859096	0.619856
53	6	0	3.391255	-1.361401	-0.577130
54	6	0	-0.382866	4.512285	-1.670217
55	6	0	-0.378581	5.915906	-1.649355
56	6	0	1.789372	-4.689485	-0.594715
57	1	0	1.704640	-5.773576	-0.670770
58	6	0	3.523314	1.193178	-0.667570
59	1	0	4.605927	1.303088	-0.717979
60	6	0	2.821371	-0.062875	-0.588036
61	6	0	0.462631	4.457843	0.575189
62	6	0	2.607837	-2.545577	-0.521118
63	6	0	2.967188	-3.936610	-0.625560
64	1	0	3.981662	-4.320668	-0.732556
65	6	0	1.280396	1.594961	-0.594231
66	6	0	-0.427678	-1.738382	2.891010
67	6	0	0.261095	0.324868	2.760995
68	6	0	0.045899	0.087555	4.107531
69	7	0	-0.392439	-1.235984	4.160276
70	1	0	-0.638102	-1.746039	5.005844
71	1	0	0.599126	1.237671	2.275446
72	7	0	-0.035256	-0.810916	2.020554
73	1	0	-0.735103	-2.752288	2.643620
74	6	0	0.167630	0.955026	5.335496
75	6	0	-1.223664	1.304620	5.919529
76	6	0	0.977340	2.229526	5.031170
77	1	0	0.721473	0.376784	6.104303
78	1	0	-1.811329	0.401587	6.158697
79	1	0	-1.116233	1.892412	6.846947
80	1	0	-1.805822	1.901727	5.197331
81	1	0	1.987809	1.986180	4.664408
82	1	0	0.476634	2.845500	4.265126

83	1	0	1.078891	2.842829	5.941550
(TPFC)Mn ^{III}					
1	25	0	-0.002426	-1.010443	-0.009901
2	7	0	-1.242154	-2.449513	-0.064778
3	7	0	1.433951	0.242849	0.016752
4	7	0	1.232539	-2.454606	-0.039132
5	9	0	-4.940560	-2.508696	2.014730
6	7	0	-1.434793	0.247380	0.018143
7	9	0	-5.008120	-0.386630	-2.264036
8	9	0	-7.644909	-2.769166	1.918750
9	9	0	-7.714321	-0.629324	-2.331909
10	9	0	-9.045707	-1.826323	-0.248499
11	9	0	5.056057	-0.366633	-2.153118
12	9	0	9.041194	-1.854195	-0.069667
13	9	0	0.803776	3.968355	-2.052443
14	9	0	7.762064	-0.616629	-2.162051
15	9	0	0.819889	6.685835	-1.912875
16	9	0	7.587681	-2.829764	2.047813
17	9	0	0.016745	7.951739	0.389122
18	9	0	-0.791758	3.758316	2.441310
19	9	0	4.883152	-2.561652	2.086195
20	6	0	2.562487	2.231418	0.180723
21	1	0	2.748969	3.300795	0.270847
22	6	0	-2.616741	-2.502511	-0.105370
23	9	0	-0.792863	6.477248	2.560561
24	6	0	4.873462	-1.453076	-0.031435
25	6	0	-2.983729	-3.890353	-0.194225
26	1	0	-4.003444	-4.270892	-0.248204
27	6	0	-4.879068	-1.435609	-0.119799
28	6	0	0.013438	6.609479	0.325127
29	6	0	-5.595196	-2.047073	0.929915
30	6	0	-1.256730	1.628893	0.074518
31	6	0	5.651507	-0.965195	-1.101989
32	6	0	-2.814543	-0.022604	-0.012268
33	6	0	-3.394163	-1.313127	-0.075664
34	6	0	0.005854	3.771178	0.189997
35	6	0	-5.630125	-0.965246	-1.216829
36	6	0	7.048819	-1.089792	-1.123426
37	6	0	6.959149	-2.228078	1.020929
38	6	0	-0.719014	-3.740588	-0.127260
39	6	0	5.563595	-2.084732	1.024011
40	6	0	0.002581	2.278040	0.118677
41	6	0	-1.809111	-4.652419	-0.205474

42	1	0	-1.736937	-5.738050	-0.267032
43	6	0	-2.558381	2.244525	0.080307
44	1	0	-2.742493	3.317649	0.111565
45	6	0	0.705400	-3.743304	-0.116435
46	6	0	-7.026953	-1.086258	-1.268798
47	6	0	-6.990807	-2.186706	0.896816
48	6	0	-3.504350	1.238655	0.033423
49	1	0	-4.587014	1.357655	0.035180
50	6	0	7.703786	-1.726180	-0.057656
51	6	0	-7.708530	-1.701814	-0.207489
52	6	0	-0.403187	5.854498	1.432602
53	6	0	3.388761	-1.326151	-0.020246
54	6	0	0.414297	4.558840	-0.904965
55	6	0	0.426412	5.960967	-0.849146
56	6	0	1.792918	-4.658756	-0.187653
57	1	0	1.717433	-5.743710	-0.256743
58	6	0	3.505425	1.222313	0.140948
59	1	0	4.587532	1.334780	0.193962
60	6	0	2.812511	-0.033646	0.036414
61	6	0	-0.398533	4.453407	1.354843
62	6	0	2.607297	-2.512449	-0.067419
63	6	0	2.970102	-3.901120	-0.160010
64	1	0	3.988887	-4.285050	-0.207009
65	6	0	1.259704	1.623366	0.101495