Electronic Supplementary Information for Dalton Transactions

Supplementary Information

Steric, geometrical and solvent effects on redox potentials in salen-type copper(II) complexes

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Experimental

Cyclic voltammetric measurements. Cyclic voltammetric measurements were performed using an ALS/CHI600A volammetric analyzer (Bioanalytical Systems Inc.). Cyclic voltammograms were recorded at room temperature. A glassy carbon disk electrode with a diameter of 3 mm was used as a working electrode. A platinum wire auxiliary electrode and an Ag/Ag^+ (Ag/0.01 M $AgNO_3$, 1 M = 1 mol dm^{-3}) reference electrode were used in a three electrode system. Sample solutions containing 0.1 M Bu_4NBF_4 as a supporting electrolyte were prepared in the concentration of 0.5—2.4 mM and deoxygenated with pure argon before measurements. The electrode potentials reported here were corrected using the redox potential of ferrocenium/ferrocene $E^{o'}(Fc^{+/0})$ as an external standard redox couple.

Cyclic voltammetry was performed at various scan rates. No significant change of $E_{1/2}$ for the $Cu^{II/I}$ couple was observed when the scan rate was varied from 50 to 1000 mVs^{-1}. The data at 100 mVs^{-1} were presented in the text (Fig. 3 and Table 3). Figs. S1, S2, and S3 show the cyclic voltammograms of ***rac*-1**, ***meso*-1**, and **2** in acetonitrile, respectively, at scan rates at 50, 100, 300, 500, and 1000 mVs^{-1}.

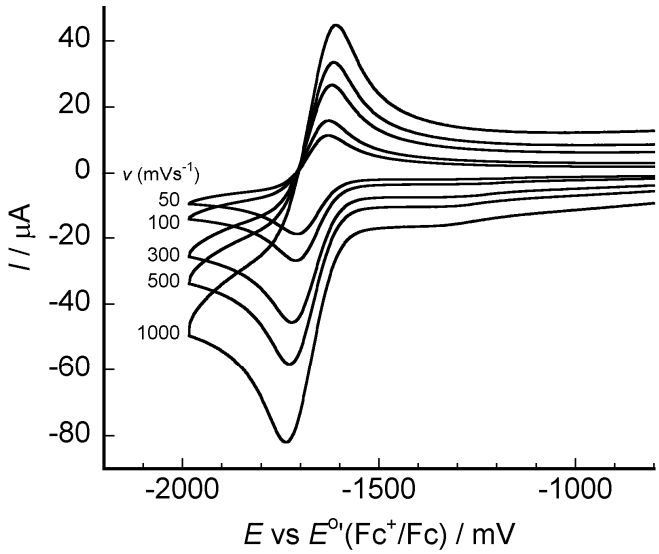

Fig. S1. Cyclic voltammograms of ***rac*-1** (1.1 mM) in acetonitrile containing 0.1 M Bu_4NBF_4; scan rate (v), 50, 100, 300, 500, 1000 mVs^{-1}; working electrode, glassy carbon; auxiliary electrode, platinum wire; reference electrode, Ag/Ag^+.

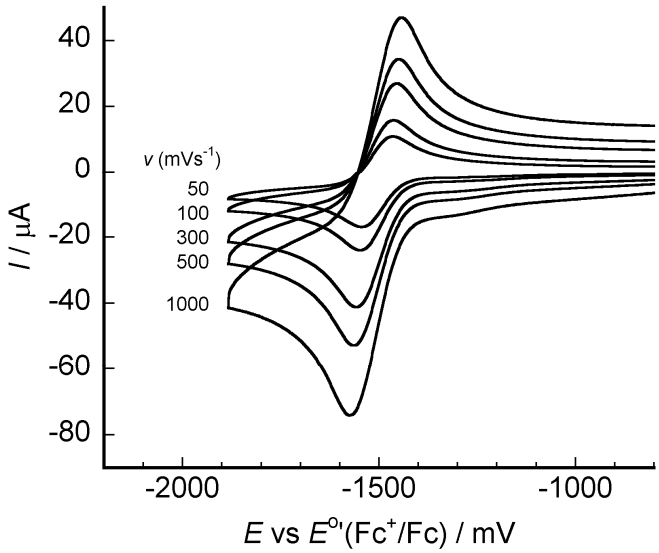

Fig. S2. Cyclic voltammograms of ***meso*-1** (1.1 mM) in acetonitrile containing 0.1 M Bu_4NBF_4; scan rate (v), 50, 100, 300, 500, 1000 mVs^{-1}; working electrode, glassy carbon; auxiliary electrode, platinum wire; reference electrode, Ag/Ag^+.

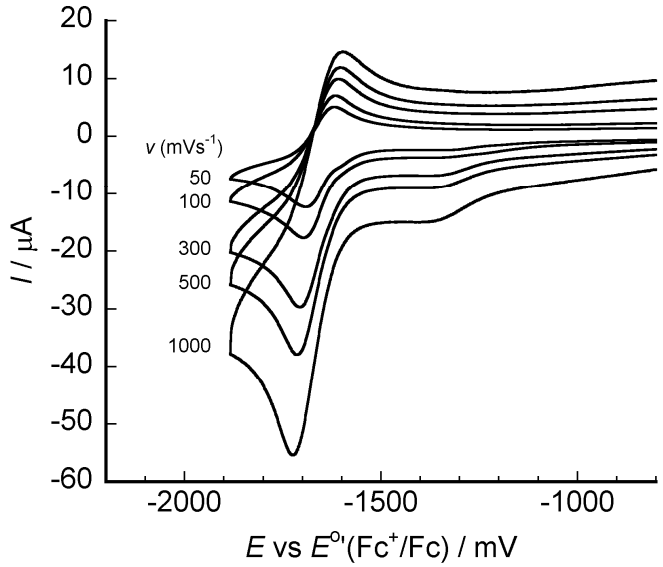

Fig. S3. Cyclic voltammograms of **2** (0.49 mM) in acetonitrile containing 0.1 M Bu_4NBF_4; scan rate (v), 50, 100, 300, 500, 1000 mVs^{-1}; working electrode, glassy carbon; auxiliary electrode, platinum wire; reference electrode, Ag/Ag^+.

Computational details. Structure optimization of the complexes was performed using the Gaussian 03 program package.[1] The B3LYP density functional method and the LANL2DZ basis set were used for complexes ***rac*-1**, ***meso*-1**, and **2**. The initial models for ***rac*-1** and ***meso*-1** were obtained from the crystal structures analyzed in this work. The initial model for **2** was obtained the crystal structure in reference 2. The calculations of copper(I) complexes [***rac*-1**]$^-$, [***meso*-1**]$^-$, and [**2**]$^-$ were performed using the optimized structures of the corresponding copper(II) complexes as the initial model. The optimized structures of ***rac*-1**, ***meso*-1**, **2**, [***rac*-1**]$^-$, [***meso*-1**]$^-$, and [**2**]$^-$ were shown in Figs. S4, S5, S6, S7, S8, and S9, and their molecular coordinates are listed in Tables S1, S2, S3, S4, S5, and S6, respectively.

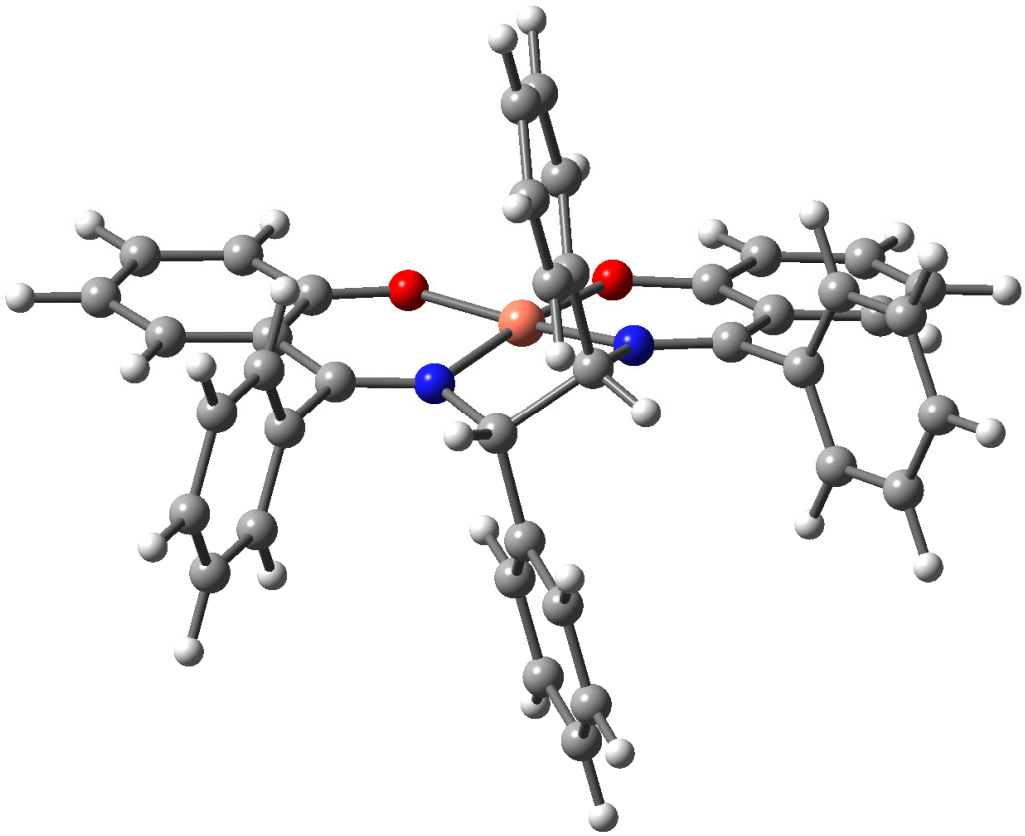

Fig. S4. Molecular structure of ***rac*-1** optimized by the DFT calculation.

Table S4. Molecular coordinates of ***rac*-1** optimized by the density functional calculation

	Atomic number	*x*/Å	*y*/Å	*z*/Å
1	29	-0.000062	1.652242	0.000143
2	8	-1.374634	2.987441	0.035001
3	8	1.374480	2.987517	-0.034390
4	7	-1.346167	0.203342	-0.169360
5	7	1.346159	0.203439	0.169512
6	6	-2.687863	2.827814	0.136797
7	6	-3.478348	4.015807	0.285599
8	6	-4.860868	3.960705	0.405782
9	6	-5.538749	2.709171	0.380458
10	6	-4.801934	1.541524	0.230452

11	6	-3.372965	1.549495	0.103618
12	6	-2.667878	0.289132	-0.076363
13	6	-3.496623	-0.974804	-0.163347
14	6	-3.816695	-1.693002	1.008725
15	6	-4.588523	-2.867489	0.932047
16	6	-5.049716	-3.331476	-0.315635
17	6	-4.733972	-2.614701	-1.486225
18	6	-3.961247	-1.440744	-1.410791
19	6	-0.659651	-1.084921	-0.424541
20	6	-0.361340	-1.309704	-1.913889
21	6	-0.011021	-2.610925	-2.338397
22	6	0.294917	-2.873817	-3.684614
23	6	0.254154	-1.832607	-4.633597
24	6	-0.100356	-0.535139	-4.220761
25	6	-0.407898	-0.275804	-2.871295
26	6	2.687655	2.827929	-0.137002
27	6	3.478032	4.015940	-0.286213
28	6	4.860487	3.960867	-0.407173
29	6	5.538412	2.709350	-0.382243
30	6	4.801707	1.541684	-0.231830
31	6	3.372810	1.549628	-0.104220
32	6	2.667838	0.289258	0.076154
33	6	3.496663	-0.974619	0.163195
34	6	3.961626	-1.440220	1.410640
35	6	4.734399	-2.614138	1.486178
36	6	5.049864	-3.331202	0.315689
37	6	4.588338	-2.867548	-0.931993
38	6	3.816449	-1.693108	-1.008775
39	6	0.659715	-1.084767	0.425103
40	6	0.361465	-1.309107	1.914534
41	6	0.407946	-0.274906	2.871619
42	6	0.100520	-0.533871	4.221185
43	6	-0.253789	-1.831257	4.634442
44	6	-0.294479	-2.872763	3.685779
45	6	0.011337	-2.610243	2.339464
46	1	-2.938138	4.957832	0.302607
47	1	-5.429049	4.881877	0.520130

48	1	-6.620288	2.668429	0.474620
49	1	-5.323498	0.590230	0.206884
50	1	-3.465619	-1.334407	1.973417
51	1	-4.831163	-3.412317	1.841125
52	1	-5.649507	-4.236570	-0.374381
53	1	-5.088184	-2.964412	-2.452765
54	1	-3.723651	-0.887871	-2.316038
55	1	-1.265959	-1.926780	-0.072841
56	1	0.010803	-3.426569	-1.616511
57	1	0.556157	-3.883338	-3.993843
58	1	0.488643	-2.032100	-5.676504
59	1	-0.138727	0.275574	-4.944405
60	1	-0.693456	0.729345	-2.574222
61	1	2.937796	4.957956	-0.302896
62	1	5.428583	4.882053	-0.521829
63	1	6.619898	2.668634	-0.477018
64	1	5.323299	0.590397	-0.208562
65	1	3.724242	-0.887119	2.315804
66	1	5.088863	-2.963596	2.452717
67	1	5.649695	-4.236265	0.374514
68	1	4.830755	-3.412606	-1.840993
69	1	3.465090	-1.334787	-1.973466
70	1	1.266041	-1.926715	0.073644
71	1	0.693342	0.730196	2.574229
72	1	0.138823	0.277072	4.944574
73	1	-0.488187	-2.030461	5.677425
74	1	-0.555571	-3.882223	3.995332
75	1	-0.010445	-3.426112	1.617830

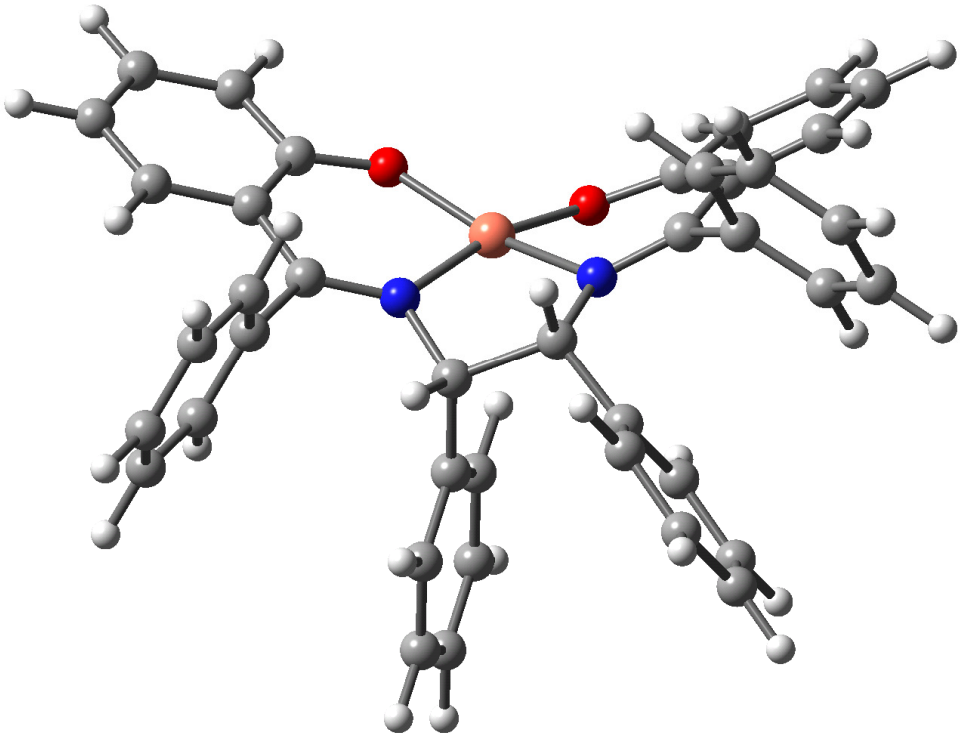

Fig. S5. Molecular structure of ***meso*-1** optimized by the DFT calculation.

Table S2. Molecular coordinates of ***meso*-1** optimized by the density functional calculation

	Atomic number	*x*/Å	*y*/Å	*z*/Å
1	29	0.263601	1.664103	0.430954
2	8	-0.994406	2.808068	1.316856
3	8	1.670790	2.965146	0.411739
4	7	-1.199753	0.403670	-0.057193
5	7	1.484184	0.225074	-0.113281
6	6	-2.263399	2.968092	0.961025
7	6	-2.951008	4.114228	1.478820
8	6	-4.250960	4.417632	1.093873
9	6	-4.940283	3.586398	0.167377
10	6	-4.312404	2.447928	-0.323372
11	6	-2.983792	2.075778	0.069677
12	6	-2.421503	0.811472	-0.396211

13	6	-3.261135	-0.028224	-1.334410
14	6	-4.393383	-0.745784	-0.896964
15	6	-5.152732	-1.499759	-1.808024
16	6	-4.797807	-1.533749	-3.170853
17	6	-3.677457	-0.806875	-3.616700
18	6	-2.911759	-0.060116	-2.702086
19	6	-0.673858	-0.947741	-0.419721
20	6	-1.521921	-2.128604	0.053125
21	6	-2.168272	-2.130339	1.307103
22	6	-2.888521	-3.257380	1.735453
23	6	-2.968632	-4.403759	0.919645
24	6	-2.324342	-4.410084	-0.331572
25	6	-1.607867	-3.276831	-0.758975
26	6	2.882650	2.837573	-0.117041
27	6	3.690170	4.021245	-0.185240
28	6	4.964417	4.004178	-0.737885
29	6	5.513129	2.795193	-1.250808
30	6	4.762474	1.628340	-1.184983
31	6	3.442741	1.597936	-0.624019
32	6	2.732338	0.328279	-0.550275
33	6	3.466695	-0.919599	-0.991020
34	6	4.268439	-1.640291	-0.081881
35	6	4.948825	-2.798787	-0.501051
36	6	4.835542	-3.245826	-1.832014
37	6	4.038868	-2.526182	-2.744109
38	6	3.358765	-1.367118	-2.325393
39	6	0.808499	-1.080018	0.109369
40	6	0.960909	-1.522582	1.572663
41	6	0.704397	-0.664399	2.664944
42	6	0.862932	-1.117999	3.985816
43	6	1.281421	-2.438555	4.240056
44	6	1.542707	-3.300512	3.158684
45	6	1.386669	-2.841244	1.838305
46	1	-2.392570	4.747437	2.161965
47	1	-4.738058	5.305800	1.491733
48	1	-5.947603	3.837995	-0.152480
49	1	-4.847144	1.818768	-1.026542

50	1	-4.672173	-0.722156	0.152581
51	1	-6.016941	-2.056931	-1.455329
52	1	-5.389232	-2.113503	-3.875514
53	1	-3.405153	-0.813553	-4.669422
54	1	-2.058954	0.516602	-3.054892
55	1	-0.595520	-1.007191	-1.515403
56	1	-2.112122	-1.252688	1.944575
57	1	-3.380865	-3.244990	2.705082
58	1	-3.525633	-5.276186	1.253574
59	1	-2.385888	-5.286453	-0.972735
60	1	-1.128094	-3.281948	-1.736665
61	1	3.249468	4.931418	0.210839
62	1	5.546266	4.922972	-0.778798
63	1	6.509330	2.784469	-1.684040
64	1	5.187797	0.706867	-1.569614
65	1	4.360651	-1.296283	0.944939
66	1	5.565427	-3.346173	0.207532
67	1	5.364387	-4.139183	-2.155255
68	1	3.953125	-2.859884	-3.775382
69	1	2.755751	-0.804293	-3.034770
70	1	1.263222	-1.863018	-0.507280
71	1	0.375961	0.358945	2.505547
72	1	0.661495	-0.440645	4.812223
73	1	1.404619	-2.787235	5.262730
74	1	1.867782	-4.322217	3.340951
75	1	1.594828	-3.514131	1.008779

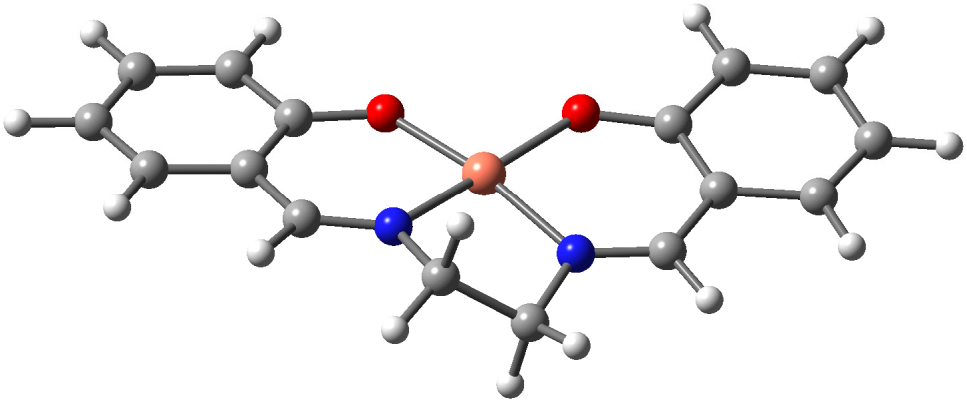

Fig. S6. Molecular structure of **2** optimized by the DFT calculation.

Table S3. Molecular coordinates of **2** optimized by the density functional calculation

	Atomic number	*x*/Å	*y*/Å	*z*/Å
1	29	0.000019	0.124268	-0.000078
2	8	1.399739	-1.203840	-0.053575
3	8	-1.399770	-1.203828	0.053339
4	7	1.314963	1.592724	0.204635
5	7	-1.314932	1.592706	-0.204316
6	6	2.715003	-1.033150	-0.044076
7	6	3.555185	-2.190202	-0.156870
8	6	4.941652	-2.080274	-0.155275
9	6	5.581559	-0.811324	-0.039426
10	6	4.795602	0.328297	0.073538
11	6	3.366465	0.255546	0.074099
12	6	2.625772	1.478573	0.203691
13	6	0.656154	2.901738	0.404809
14	6	-0.656147	2.901779	-0.404336
15	6	-2.625751	1.478529	-0.203887
16	6	-3.366482	0.255523	-0.074374
17	6	-4.795608	0.328287	-0.073957
18	6	-5.581578	-0.811312	0.039289
19	6	-4.941681	-2.080205	0.155595

20	6	-3.555214	-2.190167	0.157263
21	6	-2.715005	-1.033166	0.044072
22	1	3.059078	-3.152332	-0.243530
23	1	5.548882	-2.979146	-0.243268
24	1	6.665561	-0.742430	-0.038395
25	1	5.265858	1.307368	0.165796
26	1	3.224354	2.392309	0.314245
27	1	1.302211	3.737684	0.098191
28	1	0.423078	3.020783	1.473058
29	1	-1.302229	3.737654	-0.097583
30	1	-0.423094	3.021002	-1.472573
31	1	-3.224292	2.392260	-0.314693
32	1	-5.265860	1.307332	-0.166496
33	1	-6.665579	-0.742407	0.038112
34	1	-5.548910	-2.979047	0.243922
35	1	-3.059142	-3.152288	0.244218

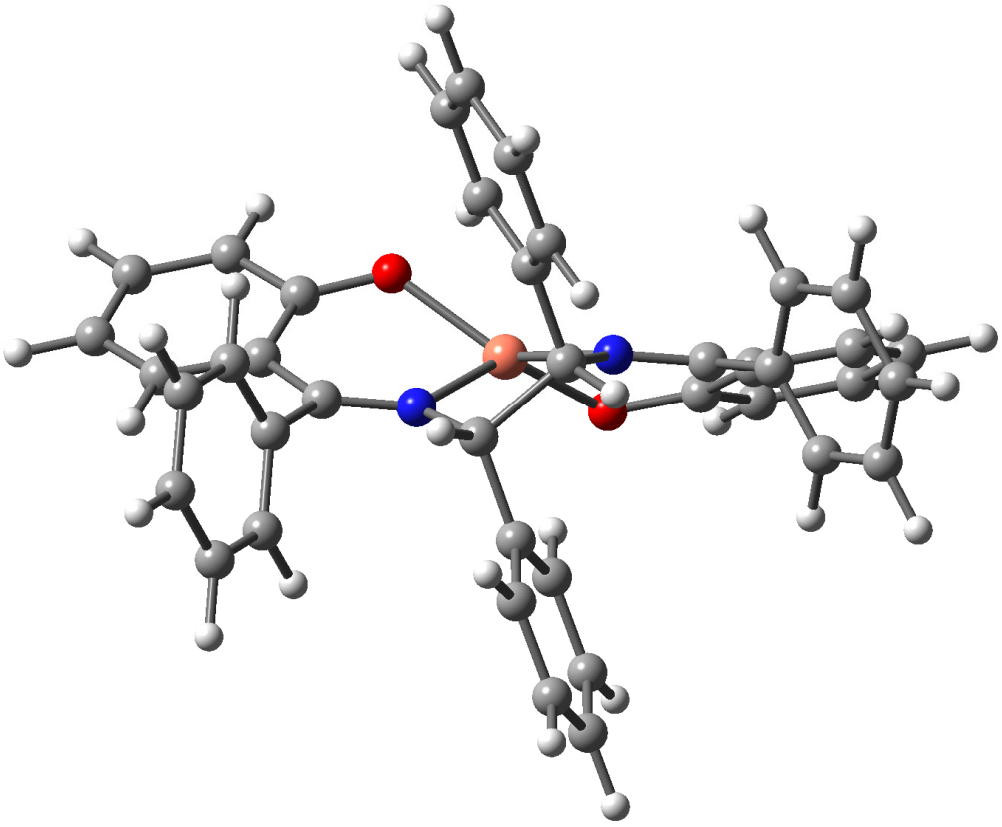

Fig. S7. Molecular structure of [***rac*-1**]$^-$ optimized by the DFT calculation.

Table S4. Molecular coordinates of [***rac*-1**]$^-$ optimized by the density functional calculation

	Atomic number	*x*/Å	*y*/Å	*z*/Å
1	29	-0.000323	1.851088	-0.000913
2	8	1.552364	2.785849	-0.915060
3	8	-1.553204	2.784654	0.915793
4	7	1.342241	0.247454	0.427316
5	7	-1.342296	0.246986	-0.426822
6	6	2.818387	2.663990	-0.581574
7	6	3.709912	3.759704	-0.891066
8	6	5.059313	3.748364	-0.559250
9	6	5.629034	2.621046	0.094203
10	6	4.809649	1.528764	0.380745
11	6	3.416788	1.494636	0.064999

12	6	2.658635	0.269661	0.373486
13	6	3.466483	-0.998245	0.591174
14	6	4.138996	-1.606231	-0.492409
15	6	4.874153	-2.791341	-0.306459
16	6	4.963469	-3.376772	0.972639
17	6	4.302415	-2.772068	2.059757
18	6	3.553341	-1.595513	1.867302
19	6	0.577521	-1.009626	0.549793
20	6	-0.003054	-1.210910	1.951281
21	6	0.063545	-2.493405	2.540416
22	6	-0.485849	-2.738505	3.813122
23	6	-1.110390	-1.693632	4.521348
24	6	-1.178250	-0.410606	3.942037
25	6	-0.633527	-0.166716	2.667889
26	6	-2.818960	2.663342	0.581099
27	6	-3.710483	3.759357	0.889518
28	6	-5.059611	3.748207	0.556553
29	6	-5.629047	2.620851	-0.097091
30	6	-4.809656	1.528334	-0.382744
31	6	-3.417076	1.494058	-0.065851
32	6	-2.658727	0.269048	-0.373599
33	6	-3.466375	-0.998975	-0.591222
34	6	-3.552356	-1.596919	-1.867092
35	6	-4.301320	-2.773562	-2.059437
36	6	-4.963138	-3.377677	-0.972459
37	6	-4.874707	-2.791565	0.306390
38	6	-4.139665	-1.606366	0.492216
39	6	-0.577394	-1.010085	-0.548369
40	6	0.003287	-1.212446	-1.949661
41	6	0.633219	-0.168662	-2.667329
42	6	1.178140	-0.413530	-3.941202
43	6	1.111031	-1.697188	-4.519190
44	6	0.487034	-2.741676	-3.809915
45	6	-0.062559	-2.495580	-2.537491
46	1	3.252946	4.614830	-1.384517
47	1	5.682465	4.610581	-0.798647
48	1	6.682165	2.608321	0.366206

49	1	5.248905	0.666932	0.877514
50	1	4.079298	-1.147467	-1.476114
51	1	5.377205	-3.252474	-1.154110
52	1	5.539185	-4.288804	1.118997
53	1	4.365729	-3.213541	3.052334
54	1	3.036883	-1.136637	2.706670
55	1	1.191963	-1.890471	0.313661
56	1	0.558649	-3.301092	2.002744
57	1	-0.422446	-3.734076	4.249381
58	1	-1.534607	-1.875132	5.507461
59	1	-1.660054	0.405023	4.477320
60	1	-0.702411	0.825936	2.231598
61	1	-3.253772	4.614509	1.383164
62	1	-5.682784	4.610616	0.795205
63	1	-6.681965	2.608290	-0.369929
64	1	-5.248654	0.666467	-0.879692
65	1	-3.035322	-1.138502	-2.706356
66	1	-4.363955	-3.215560	-3.051824
67	1	-5.538767	-4.289777	-1.118730
68	1	-5.378362	-3.252235	1.153934
69	1	-4.080651	-1.147056	1.475707
70	1	-1.191786	-1.890787	-0.311582
71	1	0.701462	0.824472	-2.232039
72	1	1.659510	0.401817	-4.477303
73	1	1.535407	-1.879472	-5.505088
74	1	0.424217	-3.737733	-4.245147
75	1	-0.557232	-3.302994	-1.999014

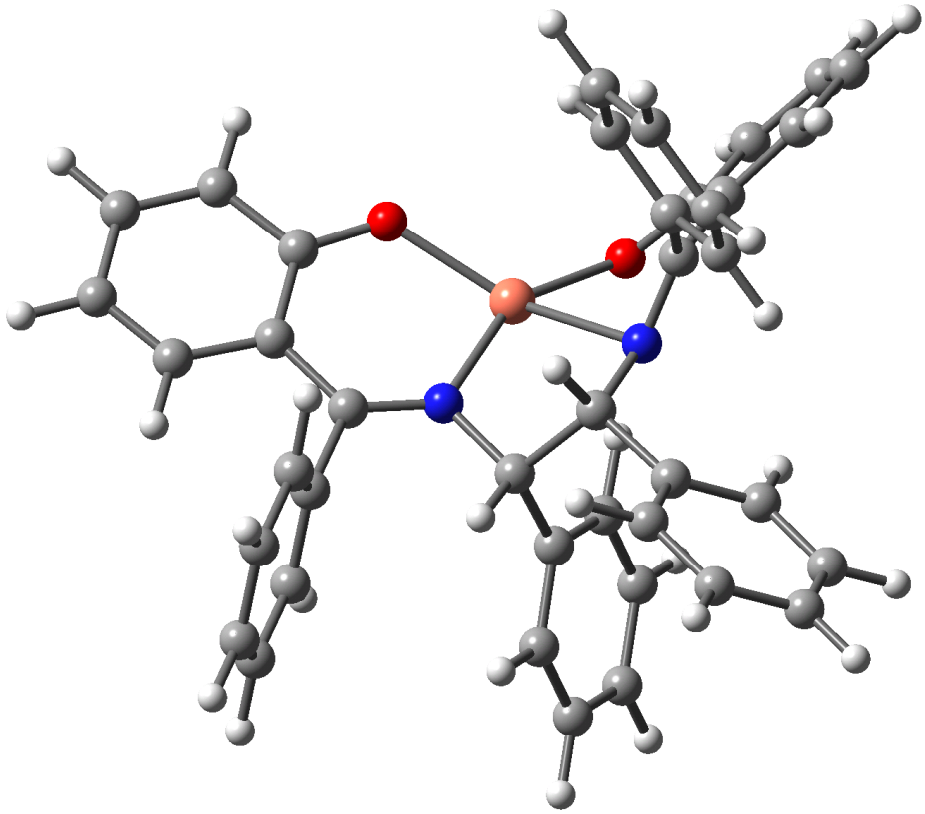

Fig. S8. Molecular structure of [***meso*-1**]$^{-}$ optimized by the DFT calculation.

Table S5. Molecular coordinates of [***meso*-1**]$^{-}$ optimized by the density functional calculation

	Atomic number	*x*/Å	*y*/Å	*z*/Å
1	29	-0.195601	-1.528507	-1.081780
2	8	-1.821297	-1.731641	-2.189949
3	8	0.752635	-3.249030	-0.555311
4	7	-1.452051	0.310216	-0.271127
5	7	1.301811	-0.402456	-0.343675
6	6	-3.048015	-1.715871	-1.695729
7	6	-4.086646	-2.421204	-2.401398
8	6	-5.393806	-2.499867	-1.925281
9	6	-5.748467	-1.893578	-0.690686
10	6	-4.765102	-1.203874	0.025081

11	6	-3.428717	-1.066052	-0.445595
12	6	-2.470308	-0.268377	0.341199
13	6	-2.667201	-0.239728	1.844941
14	6	-3.002235	0.938484	2.547555
15	6	-3.180618	0.916480	3.944591
16	6	-3.014674	-0.283392	4.662282
17	6	-2.676143	-1.464194	3.970154
18	6	-2.513419	-1.443085	2.573671
19	6	-0.464566	1.141230	0.435353
20	6	-0.891413	2.609538	0.529070
21	6	-1.800742	3.176676	-0.388894
22	6	-2.152822	4.535693	-0.298567
23	6	-1.600447	5.351180	0.709042
24	6	-0.691336	4.792458	1.628956
25	6	-0.342395	3.432383	1.536266
26	6	1.989688	-3.357493	-0.137009
27	6	2.535573	-4.690515	0.010626
28	6	3.838303	-4.926592	0.424346
29	6	4.698860	-3.835453	0.734155
30	6	4.207430	-2.537657	0.621432
31	6	2.870821	-2.236415	0.198699
32	6	2.463031	-0.826286	0.137860
33	6	3.456330	0.183626	0.692278
34	6	4.326012	0.888957	-0.165894
35	6	5.244656	1.821544	0.352556
36	6	5.301408	2.065683	1.738939
37	6	4.434891	1.365881	2.602314
38	6	3.523850	0.427659	2.081354
39	6	0.923829	1.038881	-0.310699
40	6	0.945361	1.651287	-1.715497
41	6	0.147428	1.160633	-2.777049
42	6	0.222268	1.755685	-4.049775
43	6	1.082414	2.845984	-4.288817
44	6	1.874180	3.342913	-3.236220
45	6	1.803875	2.744768	-1.963755
46	1	-3.793533	-2.901450	-3.332638
47	1	-6.145886	-3.040367	-2.500946

48	1	-6.765535	-1.959947	-0.309911
49	1	-5.033360	-0.728964	0.967305
50	1	-3.132690	1.868588	2.001862
51	1	-3.446556	1.833430	4.467138
52	1	-3.148285	-0.300034	5.742472
53	1	-2.543013	-2.397256	4.514020
54	1	-2.265057	-2.355502	2.036932
55	1	-0.270043	0.780480	1.461459
56	1	-2.225532	2.543678	-1.162022
57	1	-2.855263	4.957569	-1.014842
58	1	-1.874974	6.402265	0.778040
59	1	-0.261390	5.410364	2.415444
60	1	0.349973	3.002415	2.259050
61	1	1.858402	-5.504644	-0.237344
62	1	4.204264	-5.949975	0.509662
63	1	5.724103	-4.009959	1.052804
64	1	4.875182	-1.715465	0.860615
65	1	4.280579	0.705536	-1.236410
66	1	5.910164	2.354581	-0.323373
67	1	6.009302	2.788123	2.140368
68	1	4.471872	1.544690	3.675088
69	1	2.866876	-0.124447	2.749609
70	1	1.622633	1.621853	0.301736
71	1	-0.538269	0.336545	-2.603893
72	1	-0.398249	1.364295	-4.853477
73	1	1.133184	3.300700	-5.276932
74	1	2.539750	4.188434	-3.402313
75	1	2.417933	3.134275	-1.153336

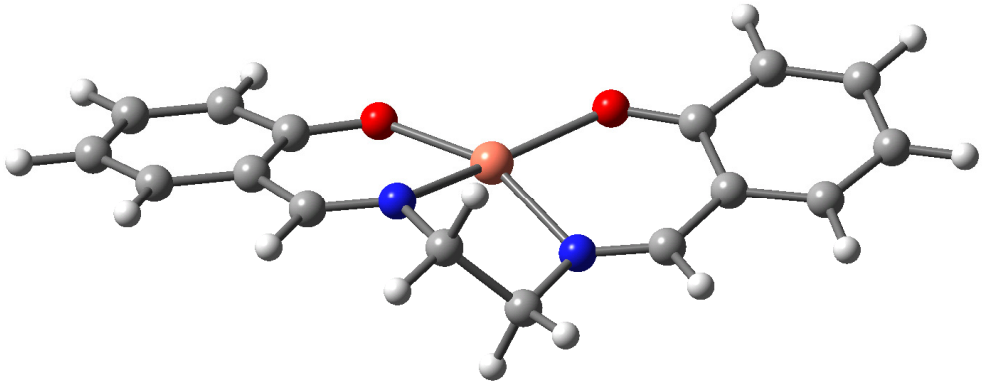

Fig. S9. Molecular structure of [**2**]$^{-}$ optimized by the DFT calculation.

Table S6. Molecular coordinates of [**2**]$^{-}$ optimized by the density functional calculation

	Atomic number	*x*/Å	*y*/Å	*z*/Å
1	29	-0.000001	-0.161756	0.000051
2	8	1.690368	-1.359798	-0.100728
3	8	-1.690418	-1.359810	0.101013
4	7	1.294858	1.453284	0.477637
5	7	-1.294774	1.453245	-0.477475
6	6	2.957447	-1.030346	-0.072770
7	6	3.961190	-2.048956	-0.307095
8	6	5.325392	-1.778498	-0.273968
9	6	5.804621	-0.459415	-0.028641
10	6	4.869753	0.555597	0.179330
11	6	3.463664	0.319605	0.174367
12	6	2.600553	1.470198	0.358648
13	6	0.555556	2.723392	0.542804
14	6	-0.555470	2.723350	-0.542725
15	6	-2.600488	1.470169	-0.358693
16	6	-3.463641	0.319608	-0.174424
17	6	-4.869725	0.555632	-0.179587
18	6	-5.804642	-0.459343	0.028332

19	6	-5.325474	-1.778424	0.273803
20	6	-3.961284	-2.048914	0.307118
21	6	-2.957485	-1.030339	0.072864
22	1	3.587351	-3.052520	-0.499366
23	1	6.037911	-2.587211	-0.441748
24	1	6.872225	-0.250615	-0.009605
25	1	5.215090	1.576626	0.358460
26	1	3.125958	2.444593	0.367381
27	1	1.208413	3.608388	0.402126
28	1	0.075119	2.801792	1.530003
29	1	-1.208337	3.608350	-0.402122
30	1	-0.075027	2.801681	-1.529927
31	1	-3.125884	2.444565	-0.367633
32	1	-5.215015	1.576657	-0.358830
33	1	-6.872238	-0.250520	0.009148
34	1	-6.038035	-2.587107	0.441545
35	1	-3.587493	-3.052475	0.499497

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