

Preparation and Characterization of Cr^{III}, Mn^{II}, Fe^{II}, Co^{II} and Ni^{II} complexes of a hexaaza-dithiophenolate macrocycle

SUPPORTING INFORMATION

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CONTENT:

1. Magnetic susceptibility data of [(L^{Me})Mn^{II}₂(μ-OAc)]BPh₄ (**2**·BPh₄) as a function of the temperature.
2. Magnetic susceptibility data of [(L^{Me})Fe^{II}₂(μ-OAc)]BPh₄ (**3**·BPh₄) as a function of the temperature.
3. Magnetic susceptibility data of [(L^{Me})Co^{II}₂(μ-OAc)]BPh₄ (**4**·BPh₄) as a function of the temperature.
4. Magnetic susceptibility data of [(L^{Me})Ni^{II}₂(μ-OAc)]BPh₄ (**5**·BPh₄) as a function of the

temperature.

1) Magnetic susceptibility data of $[(L^{M_c})Mn^{II}_2(\mu-OAc)]BPh_4$ (**2**· BPh_4) as a function of the temperature. Sample = 0.02306 [g]; $M_r = 1157.23$ [g mol⁻¹], diamagnetic correction = -0.005491 [cm³/mol], $H = 0.1$ Tesla

T / K	$\chi_{M,exp} / cm^3 mol^{-1}$	$\chi_{M,calcd} / cm^3 mol^{-1}$	$(\chi_{M,exp} - \chi_{M,calcd.})$
299.990	0.02348	0.02379	-3.080E-4
295.200	0.02415	0.02411	3.400E-5
289.340	0.02449	0.02452	-3.000E-5
284.420	0.02489	0.02487	1.900E-5
279.430	0.02526	0.02524	2.700E-5
274.410	0.02566	0.02561	3.900E-5
269.420	0.02604	0.02600	3.400E-5
264.440	0.02646	0.02640	6.100E-5
259.430	0.02687	0.02682	5.100E-5
254.440	0.02729	0.02724	4.900E-5
249.440	0.02786	0.02768	1.800E-4
244.450	0.02837	0.02813	2.390E-4
239.450	0.02884	0.02859	2.480E-4
234.490	0.02934	0.02907	2.720E-4
229.470	0.02988	0.02957	3.120E-4
224.480	0.03032	0.03008	2.370E-4
219.480	0.03078	0.03061	1.760E-4
214.490	0.03125	0.03115	1.020E-4
209.500	0.03190	0.03172	1.810E-4
204.510	0.03252	0.03230	2.190E-4
199.510	0.03312	0.03290	2.200E-4
194.510	0.03378	0.03353	2.490E-4
189.540	0.03447	0.03417	2.980E-4
184.530	0.03507	0.03484	2.280E-4
179.560	0.03583	0.03553	2.960E-4
174.570	0.03656	0.03625	3.140E-4
169.560	0.03728	0.03700	2.870E-4
164.580	0.03810	0.03776	3.390E-4
159.580	0.03885	0.03856	2.890E-4
154.600	0.03967	0.03939	2.790E-4
149.600	0.04057	0.04025	3.250E-4
144.620	0.04137	0.04113	2.430E-4
139.620	0.04237	0.04205	3.220E-4
134.640	0.04336	0.04300	3.590E-4
129.650	0.04427	0.04398	2.880E-4
124.660	0.04527	0.04499	2.770E-4
119.670	0.04623	0.04604	1.870E-4
114.700	0.04741	0.04711	2.950E-4

109.750	0.04836	0.04821	1.530E-4
104.790	0.04948	0.04933	1.420E-4
99.860	0.05071	0.05047	2.360E-4
97.820	0.05099	0.05095	4.100E-5
95.740	0.05134	0.05144	-1.010E-4
93.740	0.05199	0.05191	7.600E-5
91.750	0.05233	0.05238	-4.800E-5
89.770	0.05289	0.05285	4.100E-5
87.800	0.05332	0.05332	2.000E-6
85.800	0.05358	0.05379	-2.060E-4
83.820	0.05416	0.05425	-9.000E-5
81.850	0.05464	0.05472	-7.700E-5
79.870	0.05506	0.05518	-1.180E-4
78.070	0.05526	0.05559	-3.250E-4
76.070	0.05581	0.05604	-2.330E-4
74.070	0.05626	0.05649	-2.300E-4
72.070	0.05655	0.05693	-3.780E-4
70.070	0.05724	0.05735	-1.130E-4
68.090	0.05738	0.05776	-3.800E-4
66.090	0.05797	0.05816	-1.880E-4
64.060	0.05809	0.05855	-4.650E-4
62.100	0.05870	0.05891	-2.120E-4
60.090	0.05889	0.05926	-3.640E-4
58.100	0.05926	0.05958	-3.220E-4
56.090	0.05957	0.05987	-3.090E-4
54.090	0.05975	0.06014	-3.870E-4
52.080	0.06008	0.06038	-2.980E-4
50.070	0.06018	0.06058	-4.000E-4
48.040	0.06068	0.06075	-6.700E-5
46.030	0.06085	0.06088	-2.300E-5
44.020	0.06103	0.06096	6.700E-5
42.020	0.06131	0.06100	3.080E-4
40.010	0.06105	0.06100	4.800E-5
38.010	0.06085	0.06095	-1.020E-4
36.000	0.06068	0.06084	-1.600E-4
34.000	0.06044	0.06069	-2.540E-4
32.000	0.06011	0.06048	-3.720E-4
30.000	0.05985	0.06022	-3.700E-4
27.990	0.05945	0.05989	-4.380E-4
25.990	0.05901	0.05949	-4.770E-4
23.990	0.05862	0.05901	-3.990E-4
22.000	0.05797	0.05844	-4.770E-4
20.000	0.05708	0.05775	-6.740E-4
19.000	0.05679	0.05734	-5.530E-4
18.000	0.05639	0.05689	-5.000E-4
17.000	0.05567	0.05638	-7.120E-4
16.000	0.05531	0.05580	-4.970E-4
15.000	0.05454	0.05514	-5.980E-4

14.010	0.05370	0.05439	-6.870E-4
13.000	0.05308	0.05349	-4.140E-4
12.010	0.05189	0.05246	-5.680E-4
10.970	0.05049	0.05114	-6.520E-4
10.030	0.04920	0.04967	-4.780E-4
9.020	0.04719	0.04770	-5.070E-4
8.010	0.04467	0.04510	-4.320E-4
7.000	0.04149	0.04157	-7.600E-5
6.000	0.03682	0.03666	1.600E-4
5.000	0.03024	0.02977	4.680E-4
4.000	0.02125	0.02083	4.150E-4
3.000	0.01252	0.01180	7.180E-4
2.010	0.00758	0.00777	-1.900E-4

2) Magnetic susceptibility data of $[(L^{Me})Fe_2(\mu-OAc)]BPh_4$ (**3**· BPh_4) as a function of the temperature. Sample = 0.02273 [g]; M_r = 1159.05 [g/mol], diamagnetic correction = - 0.0055000 [cm³/mol], H = 0.2 Tesla

T / K	$\chi_{M,exp} / \text{cm}^3 \text{mol}^{-1}$	$\chi_{M,calcd.} / \text{cm}^3 \text{mol}^{-1}$	$(\chi_{M,exp} - \chi_{M,calcd.})$
299.990	0.01725	0.01741	-1.600E-4
295.200	0.01769	0.01762	7.500E-5
289.340	0.01795	0.01789	6.200E-5
284.410	0.01817	0.01811	5.600E-5
279.400	0.01843	0.01835	8.000E-5
274.380	0.01868	0.01860	8.000E-5
269.410	0.01907	0.01885	2.200E-4
264.420	0.01932	0.01910	2.210E-4
259.430	0.01962	0.01937	2.550E-4
254.420	0.01990	0.01964	2.610E-4
249.410	0.02015	0.01991	2.420E-4
244.420	0.02041	0.02019	2.170E-4
239.460	0.02071	0.02048	2.290E-4
234.470	0.02097	0.02078	1.880E-4
229.470	0.02125	0.02108	1.740E-4
224.470	0.02155	0.02139	1.590E-4
219.460	0.02187	0.02171	1.630E-4
214.480	0.02217	0.02204	1.350E-4
209.480	0.02248	0.02237	1.120E-4
204.490	0.02281	0.02271	9.600E-5
199.510	0.02316	0.02306	9.900E-5
194.500	0.02349	0.02342	7.000E-5
189.510	0.02386	0.02379	7.500E-5
184.520	0.02418	0.02416	2.100E-5
179.520	0.02456	0.02455	1.300E-5
174.550	0.02494	0.02493	2.000E-6
169.550	0.02534	0.02533	2.000E-6

164.570	0.02573	0.02574	-1.300E-5
159.580	0.02612	0.02615	-2.800E-5
154.580	0.02655	0.02657	-2.300E-5
149.600	0.02698	0.02700	-1.900E-5
144.610	0.02737	0.02743	-6.000E-5
139.600	0.02780	0.02786	-6.500E-5
134.610	0.02823	0.02830	-7.100E-5
129.640	0.02866	0.02873	-7.500E-5
124.660	0.02904	0.02917	-1.320E-4
119.680	0.02949	0.02960	-1.100E-4
114.690	0.02989	0.03002	-1.310E-4
109.750	0.03031	0.03044	-1.280E-4
104.820	0.03071	0.03083	-1.220E-4
99.890	0.03108	0.03121	-1.360E-4
97.800	0.03118	0.03137	-1.880E-4
95.730	0.03130	0.03151	-2.090E-4
93.740	0.03147	0.03165	-1.820E-4
91.750	0.03162	0.03179	-1.660E-4
89.760	0.03172	0.03191	-1.900E-4
87.780	0.03183	0.03204	-2.080E-4
85.790	0.03195	0.03215	-1.960E-4
83.800	0.03211	0.03226	-1.520E-4
81.820	0.03221	0.03236	-1.540E-4
79.860	0.03223	0.03246	-2.250E-4
78.060	0.03228	0.03254	-2.510E-4
76.060	0.03240	0.03261	-2.160E-4
74.070	0.03245	0.03269	-2.380E-4
72.070	0.03252	0.03275	-2.230E-4
70.090	0.03259	0.03280	-2.090E-4
68.070	0.03261	0.03284	-2.310E-4
66.100	0.03265	0.03287	-2.250E-4
64.080	0.03267	0.03289	-2.190E-4
62.090	0.03270	0.03290	-2.030E-4
60.090	0.03266	0.03290	-2.340E-4
58.090	0.03266	0.03288	-2.260E-4
56.100	0.03265	0.03285	-2.050E-4
54.090	0.03259	0.03281	-2.240E-4
52.080	0.03261	0.03275	-1.430E-4
50.070	0.03250	0.03268	-1.820E-4
48.030	0.03246	0.03260	-1.400E-4
46.030	0.03232	0.03250	-1.810E-4
44.030	0.03221	0.03238	-1.690E-4
42.020	0.03209	0.03225	-1.560E-4
40.010	0.03194	0.03210	-1.560E-4
38.010	0.03177	0.03193	-1.560E-4
36.000	0.03155	0.03173	-1.840E-4
34.000	0.03133	0.03151	-1.770E-4
32.000	0.03106	0.03126	-2.000E-4

30.000	0.03077	0.03097	-2.020E-4
27.990	0.03045	0.03063	-1.750E-4
25.990	0.03011	0.03023	-1.250E-4
23.990	0.02964	0.02976	-1.260E-4
21.990	0.02912	0.02919	-7.100E-5
20.000	0.02851	0.02848	3.100E-5
19.000	0.02806	0.02806	9.000E-6
18.000	0.02765	0.02757	7.900E-5
17.000	0.02717	0.02701	1.560E-4
16.000	0.02658	0.02636	2.220E-4
15.000	0.02591	0.02559	3.180E-4
14.010	0.02513	0.02470	4.250E-4
13.010	0.02417	0.02364	5.370E-4
12.010	0.02305	0.02238	6.670E-4
10.980	0.02144	0.02086	5.800E-4
10.030	0.01982	0.01927	5.530E-4
9.020	0.01784	0.01741	4.300E-4
8.010	0.01556	0.01552	4.000E-5
7.000	0.01312	0.01385	-7.280E-4
6.000	0.01072		
5.010	0.00866		
4.000	0.00745		
3.000	0.00753		
2.000	0.00850		

3) Magnetic susceptibility data of $[(L^{Me})Co_2(\mu-OAc)]BPh_4$ ($4 \cdot BPh_4$) as a function of the temperature. Sample = 0.03051 [g]; $M_r = 1165.22$ [g/mol], diamagnetic correction = -0.0055309 [cm^3/mol], $H = 0.2$ Tesla

T / K	$\chi_{M,exp.} / cm^3 mol^{-1}$	$\chi_{M,calcd.} / cm^3 mol^{-1}$	$(\chi_{M,exp.} - \chi_{M,calcd.})$
2.000	0.30715	0.30347	3.680E-3
3.000	0.26316	0.21402	4.914E-2
4.000	0.22882	0.17925	4.957E-2
5.000	0.20912	0.16827	4.085E-2
6.000	0.19711	0.16724	2.987E-2
7.000	0.18749	0.16928	1.821E-2
8.010	0.18131	0.17135	9.960E-3
9.020	0.17773	0.17231	5.420E-3
10.030	0.17372	0.17199	1.730E-3
10.970	0.17035	0.17069	-3.400E-4
12.000	0.16623	0.16840	-2.170E-3
13.000	0.16327	0.16557	-2.300E-3
14.010	0.15995	0.16230	-2.350E-3
15.000	0.15659	0.15887	-2.280E-3
16.000	0.15286	0.15528	-2.420E-3
17.000	0.14929	0.15165	-2.360E-3

18.000	0.14447	0.14804	-3.570E-3
19.000	0.14213	0.14449	-2.360E-3
20.000	0.13966	0.14104	-1.380E-3
22.000	0.13263	0.13446	-1.830E-3
23.990	0.12594	0.12839	-2.450E-3
25.990	0.12178	0.12279	-1.010E-3
27.990	0.11745	0.11765	-2.000E-4
29.990	0.11276	0.11295	-1.900E-4
32.000	0.10838	0.10862	-2.400E-4
34.000	0.10455	0.10467	-1.200E-4
36.000	0.10087	0.10103	-1.600E-4
38.010	0.09733	0.09765	-3.200E-4
40.010	0.09426	0.09454	-2.800E-4
42.020	0.09154	0.09163	-9.000E-5
44.020	0.08897	0.08894	3.000E-5
46.030	0.08635	0.08641	-6.000E-5
48.040	0.08395	0.08404	-9.000E-5
50.060	0.08151	0.08181	-3.000E-4
52.080	0.07941	0.07970	-2.900E-4
54.090	0.07741	0.07772	-3.100E-4
56.080	0.07560	0.07587	-2.700E-4
58.090	0.07396	0.07409	-1.300E-4
60.080	0.07217	0.07241	-2.400E-4
62.080	0.07046	0.07081	-3.500E-4
64.100	0.06877	0.06927	-5.000E-4
66.060	0.06712	0.06783	-7.100E-4
68.080	0.06614	0.06642	-2.800E-4
70.070	0.06471	0.06508	-3.700E-4
72.070	0.06354	0.06379	-2.500E-4
74.060	0.06195	0.06256	-6.100E-4
76.060	0.06046	0.06137	-9.100E-4
78.070	0.05972	0.06022	-5.000E-4
79.880	0.05918	0.05922	-4.000E-5
81.820	0.05821	0.05818	3.000E-5
83.800	0.05723	0.05716	7.000E-5
85.780	0.05598	0.05617	-1.900E-4
87.780	0.05527	0.05520	7.000E-5
89.750	0.05435	0.05428	7.000E-5
91.750	0.05347	0.05338	9.000E-5
93.740	0.05239	0.05251	-1.200E-4
95.730	0.05175	0.05166	9.000E-5
97.810	0.05067	0.05081	-1.400E-4
99.840	0.05035	0.05000	3.500E-4
104.800	0.04848	0.04812	3.600E-4
109.740	0.04645	0.04638	7.000E-5
114.700	0.04518	0.04475	4.300E-4
119.660	0.04337	0.04322	1.500E-4
124.640	0.04220	0.04179	4.100E-4

129.620	0.04088	0.04044	4.400E-4
134.600	0.03960	0.03918	4.200E-4
139.600	0.03838	0.03798	4.000E-4
144.580	0.03724	0.03685	3.900E-4
149.550	0.03593	0.03579	1.400E-4
154.610	0.03463	0.03477	-1.400E-4
159.560	0.03432	0.03382	5.000E-4
164.550	0.03307	0.03292	1.500E-4
169.530	0.03225	0.03206	1.900E-4
174.530	0.03131	0.03124	7.000E-5
179.510	0.03065	0.03047	1.800E-4
184.520	0.03014	0.02972	4.200E-4
189.510	0.02925	0.02901	2.400E-4
194.480	0.02837	0.02834	3.000E-5
199.490	0.02763	0.02769	-6.000E-5
204.470	0.02721	0.02708	1.300E-4
209.440	0.02683	0.02649	3.400E-4
214.460	0.02608	0.02592	1.600E-4
219.440	0.02541	0.02538	3.000E-5
224.450	0.02489	0.02485	4.000E-5
229.430	0.02441	0.02435	6.000E-5
234.430	0.02387	0.02387	0
239.380	0.02329	0.02341	-1.200E-4
244.410	0.02284	0.02296	-1.200E-4
249.380	0.02241	0.02254	-1.300E-4
254.400	0.02200	0.02212	-1.200E-4
259.360	0.02162	0.02172	-1.000E-4
264.370	0.02123	0.02134	-1.100E-4
269.380	0.02085	0.02096	-1.100E-4
274.390	0.02049	0.02060	-1.100E-4
279.370	0.02015	0.02025	-1.000E-4
284.380	0.01980	0.01992	-1.200E-4
289.600	0.01951	0.01958	-7.000E-5
294.100	0.01922	0.01929	-7.000E-5

4) Magnetic susceptibility data of $[(L^{Me})Ni_2(\mu-OAc)]BPh_4$ (**5**·BPh₄) as a function of the temperature. Sample = 0.02396 [g]; $M_r = 1164.74$ [g/mol], diamagnetic correction = -0.0055285 [cm³/mol], $H = 0.2$ Tesla

T / K	$\chi_M T_{exp} / cm^3 K mol^{-1}$	$\chi_M T_{calcd} / cm^3 K mol^{-1}$	$\chi_M T_{exp} - \chi_M T_{calcd}$
299.990	4.50336	4.53468	3.132E-2
294.160	4.50851	4.53735	2.884E-2
289.450	4.51772	4.53955	2.183E-2
284.420	4.51640	4.54194	2.554E-2
279.410	4.51826	4.54438	2.612E-2

274.410	4.51861	4.54686	2.825E-2
269.380	4.53724	4.54940	1.216E-2
264.400	4.55264	4.55196	-6.757E-4
259.390	4.55685	4.55458	-2.267E-3
254.410	4.55852	4.55729	-1.234E-3
249.440	4.56361	4.56001	-3.597E-3
244.420	4.56343	4.56286	-5.693E-4
239.440	4.56440	4.56572	1.319E-3
234.440	4.56623	4.56870	2.465E-3
229.430	4.56895	4.57175	2.803E-3
224.450	4.56194	4.57487	1.293E-2
219.450	4.56369	4.57810	1.441E-2
214.470	4.56799	4.58139	1.340E-2
209.470	4.56895	4.58478	1.583E-2
204.480	4.57420	4.58830	1.410E-2
199.490	4.57743	4.59193	1.450E-2
194.490	4.58459	4.59568	1.109E-2
189.500	4.59417	4.59954	5.366E-3
184.520	4.60044	4.60354	3.104E-3
179.530	4.60695	4.60770	7.539E-4
174.540	4.61120	4.61201	8.149E-4
169.530	4.61233	4.61650	4.166E-3
164.550	4.61701	4.62113	4.124E-3
159.570	4.61961	4.62599	6.385E-3
154.590	4.62194	4.63104	9.099E-3
149.570	4.62860	4.63636	7.757E-3
144.590	4.63663	4.64188	5.251E-3
139.600	4.64171	4.64768	5.971E-3
134.620	4.65359	4.65376	1.669E-4
129.640	4.64645	4.66014	1.369E-2
124.660	4.65462	4.66686	1.224E-2
119.690	4.66629	4.67395	7.664E-3
114.880	4.65977	4.68118	2.141E-2
109.850	4.69192	4.68920	-2.718E-3
104.850	4.70018	4.69765	-2.533E-3
99.880	4.71123	4.70659	-4.644E-3
97.820	4.69618	4.71045	1.427E-2
95.730	4.70911	4.71450	5.386E-3
93.740	4.71344	4.71843	4.992E-3
91.760	4.72081	4.72247	1.657E-3
89.760	4.72657	4.72664	6.720E-5
87.780	4.73553	4.73089	-4.641E-3
85.800	4.74523	4.73525	-9.980E-3
83.820	4.75684	4.73973	-1.711E-2
81.840	4.76021	4.74434	-1.587E-2
79.860	4.76365	4.74907	-1.458E-2
77.900	4.77379	4.75390	-1.990E-2
75.920	4.78057	4.75891	-2.166E-2

74.060	4.76491	4.76373	-1.178E-3
72.060	4.76910	4.76908	-1.670E-5
70.080	4.78501	4.77452	-1.049E-2
68.060	4.78425	4.78022	-4.026E-3
66.080	4.80286	4.78599	-1.688E-2
64.080	4.80868	4.79196	-1.672E-2
62.080	4.81533	4.79810	-1.723E-2
60.080	4.82072	4.80442	-1.630E-2
58.090	4.82155	4.81086	-1.069E-2
56.080	4.82744	4.81755	-9.894E-3
54.080	4.83150	4.82436	-7.143E-3
52.080	4.83695	4.83133	-5.617E-3
50.070	4.84389	4.83849	-5.400E-3
48.040	4.84860	4.84585	-2.747E-3
46.040	4.85676	4.85322	-3.536E-3
44.030	4.86268	4.86072	-1.956E-3
42.020	4.86884	4.86827	-5.674E-4
40.010	4.87926	4.87583	-3.427E-3
38.010	4.88262	4.88330	6.771E-4
36.010	4.88639	4.89062	4.230E-3
34.000	4.89309	4.89774	4.647E-3
32.000	4.89767	4.90445	6.783E-3
30.000	4.89946	4.91061	1.115E-2
28.000	4.90550	4.91601	1.051E-2
25.990	4.90892	4.92038	1.147E-2
23.990	4.91145	4.92332	1.187E-2
21.990	4.91194	4.92437	1.243E-2
20.000	4.90770	4.92295	1.525E-2
19.000	4.90281	4.92106	1.825E-2
18.000	4.89824	4.91823	1.999E-2
17.000	4.89636	4.91432	1.796E-2
16.000	4.89350	4.90917	1.567E-2
15.000	4.88786	4.90260	1.474E-2
14.010	4.88393	4.89446	1.053E-2
13.010	4.87639	4.88436	7.965E-3
12.010	4.86753	4.87207	4.538E-3
10.980	4.88057	4.85678	-2.379E-2
10.030	4.87861	4.83997	-3.864E-2
9.020	4.86556	4.81885	-4.671E-2
8.000	4.84769	4.79366	-5.403E-2
7.000	4.82412	4.76477	-5.935E-2
5.990	4.79119	4.73097	-6.023E-2
5.010	4.76768	4.69334	-7.434E-2
4.000	4.72834	4.64880	-7.954E-2
3.000	4.62471	4.59589	-2.882E-2
2.010	4.38404	4.51989	1.358E-1