

Synthesis, Characterization, and Crystal Structure of a Dinuclear Ni(II) Complex with an Edge Sharing Bis(Square-pyramidal) $\text{N}_3\text{Ni}(\mu\text{-S}_2)\text{NiN}_3$ Core

Ulrike Lehmann, Jochen Lach and Berthold Kersting*

Leipzig, Institut für Anorganische Chemie der Universität

Received

Ulrike Lehmann, Jochen Lach and Berthold Kersting*

Institut für Anorganische Chemie, Universität Leipzig, D-04103 Leipzig, Germany. Fax: 49
341 973 6199; Tel: +49 341 973 6143; E-mail: b.kersting@uni-leipzig.de

Supporting Information

Content:

1) Figure S1. Structure of the $[\text{Ni}_2\text{L}_2]^{2+}$ cation in crystals of **5**·MeOH. Thermal ellipsoids are drawn at the 30% probability level. Hydrogen atoms are omitted for reasons of clarity.

Symmetry code used to generate equivalent atoms: $x, 1.5-y, z$ (')

2) Table S1. Experimental and calculated $\chi_{\text{M}}T$ [$\text{cm}^3\text{Kmol}^{-1}$] and μ_{eff} [μ_{B}] for **5**.

3) Table S2. Experimental and calculated $\chi_{\text{M}}T$ [$\text{cm}^3\text{Kmol}^{-1}$] and μ_{eff} [μ_{B}] for **7**.

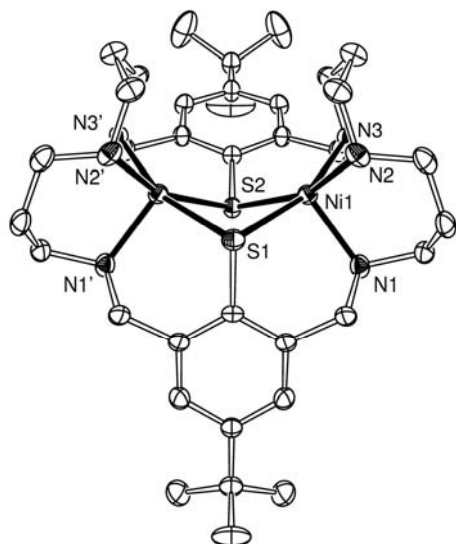


Figure S1. Structure of the $[\text{Ni}_2\text{L}_2]^{2+}$ cation in crystals of **5**·MeOH. Thermal ellipsoids are drawn at the 30 % probability level. Hydrogen atoms are omitted for reasons of clarity. Symmetry code used to generate equivalent atoms: : $x, 1.5-y, z$ (').

Table S1. Experimental and calculated $\chi_{\text{M}}T$ [$\text{cm}^3\text{Kmol}^{-1}$] and μ_{eff} [μ_{B}] for **5**.

T [K]	$\chi_{\text{M}}T_{(\text{exp})}$	$\chi_{\text{M}}T_{(\text{calc})}$	$\mu_{\text{eff}(\text{exp})}$	$\mu_{\text{eff}(\text{calc})}$
2.000	0.011	--	0.300	--
3.002	0.010	--	0.288	--
4.003	0.011	--	0.292	--
5.016	0.012	--	0.306	--
6.014	0.013	--	0.321	--
7.004	0.014	--	0.336	--
8.004	0.015	--	0.348	--
9.005	0.016	--	0.358	--
10.004	0.017	--	0.365	--
11.021	0.017	--	0.370	--
12.003	0.017	--	0.373	--
13.019	0.018	--	0.375	--
14.037	0.018	--	0.376	--
15.003	0.018	--	0.377	--

16.004	0.018	--	0.377	--
17.004	0.018	--	0.378	--
18.005	0.018	--	0.378	--
19.003	0.018	--	0.378	--
20.003	0.018	--	0.378	--
29.999	0.018	--	0.377	--
40.009	0.017	--	0.374	--
50.045	0.017	--	0.367	--
60.073	0.016	--	0.359	--
70.070	0.015	--	0.351	--
80.039	0.015	--	0.343	--
90.017	0.014	--	0.335	--
100.008	0.013	0.013	0.327	0.325
109.992	0.013	0.013	0.320	0.319
119.985	0.012	0.012	0.313	0.313
129.988	0.012	0.012	0.306	0.307
139.979	0.011	0.011	0.300	0.301
149.987	0.011	0.011	0.294	0.295
159.981	0.010	0.010	0.288	0.290
169.986	0.010	0.010	0.283	0.284
179.973	0.010	0.010	0.278	0.279
189.944	0.009	0.009	0.273	0.274
199.955	0.009	0.009	0.268	0.269
209.897	0.009	0.009	0.264	0.264
219.918	0.008	0.008	0.260	0.260
229.892	0.008	0.008	0.256	0.256
239.868	0.008	0.008	0.252	0.252
249.837	0.008	0.008	0.248	0.248
259.828	0.007	0.007	0.245	0.244

269.834	0.007	0.007	0.241	0.240
279.751	0.007	0.007	0.238	0.237
289.744	0.007	0.007	0.235	0.234
299.711	0.007	0.007	0.232	0.230
309.720	0.007	0.006	0.229	0.227
319.892	0.006	0.006	0.226	0.224
330.012	0.006	0.006	0.223	0.221

Table S2. Experimental and calculated $\chi_{\text{M}}T$ [$\text{cm}^3\text{Kmol}^{-1}$] and μ_{eff} [μ_{B}] for **7**.

T [K]	$\chi_{\text{M}}T_{(\text{exp})}$	$\chi_{\text{M}}T_{(\text{calc})}$	$\mu_{\text{eff}(\text{exp})}$	$\mu_{\text{eff}(\text{calc})}$
1.993	0.597	0.148	2.185	1.088
3.000	0.724	0.364	2.407	1.707
4.001	0.843	0.571	2.597	2.136
5.033	0.954	0.767	2.762	2.477
6.013	1.054	0.936	2.904	2.736
7.004	1.149	1.086	3.032	2.948
8.003	1.238	1.217	3.147	3.120
9.004	1.320	1.329	3.250	3.261
10.003	1.395	1.426	3.341	3.377
11.020	1.466	1.510	3.425	3.476
12.001	1.529	1.580	3.497	3.556
13.018	1.589	1.644	3.565	3.626
14.039	1.643	1.699	3.626	3.687
15.002	1.689	1.745	3.676	3.736
16.005	1.733	1.788	3.723	3.782
17.006	1.772	1.825	3.766	3.822
18.007	1.808	1.859	3.804	3.857

19.011	1.841	1.890	3.838	3.888
20.002	1.871	1.917	3.869	3.916
30.028	2.073	2.093	4.073	4.092
40.011	2.177	2.181	4.173	4.177
50.043	2.239	2.233	4.232	4.227
60.075	2.279	2.268	4.270	4.260
70.055	2.305	2.293	4.295	4.283
80.021	2.325	2.311	4.313	4.300
89.989	2.338	2.325	4.325	4.313
99.958	2.348	2.337	4.334	4.324
109.937	2.356	2.346	4.341	4.332
119.907	2.362	2.354	4.347	4.340
129.909	2.368	2.361	4.352	4.346
139.893	2.372	2.366	4.356	4.351
149.880	2.376	2.371	4.360	4.355
159.876	2.380	2.375	4.363	4.359
169.850	2.383	2.379	4.366	4.363
179.851	2.387	2.382	4.369	4.366
189.800	2.389	2.385	4.372	4.368
199.780	2.392	2.388	4.374	4.371
209.775	2.395	2.390	4.377	4.373
219.723	2.396	2.393	4.378	4.375
229.707	2.400	2.395	4.382	4.377
239.706	2.402	2.396	4.383	4.378
249.677	2.404	2.398	4.386	4.380

259.649	2.407	2.400	4.388	4.381
269.585	2.408	2.401	4.389	4.383
279.533	2.413	2.402	4.393	4.384
289.488	2.417	2.404	4.397	4.385
299.480	2.421	2.405	4.401	4.386
309.418	2.426	2.406	4.405	4.387
319.741	2.435	2.407	4.413	4.388
330.019	2.434	2.408	4.413	4.389
