Supplementary Material

Asymmetric Transformation of a Double-Stranded, Dicopper(I) Helicate Containing Achiral Bis(Bidentate) Schiff-Bases

Nicolle C. Habermehl[a], Patricia M. Angus[b], Nathan L. Kilah[a], Lasse Norén[a], A. David Rae[a], Anthony C. Willis[a], and S. Bruce Wild[a*]

[a] *Research School of Chemistry, Institute of Advanced Studies, Australian National University, Canberra, ACT 0200, Australia*

[b] *Department of Chemistry, Faculty of Science, Australian National University, Canberra, ACT 0200, Australia*

[*] Author to whom correspondence should be addressed. E-mail: sbw@rsc.anu.edu.au

Kinetic Analysis

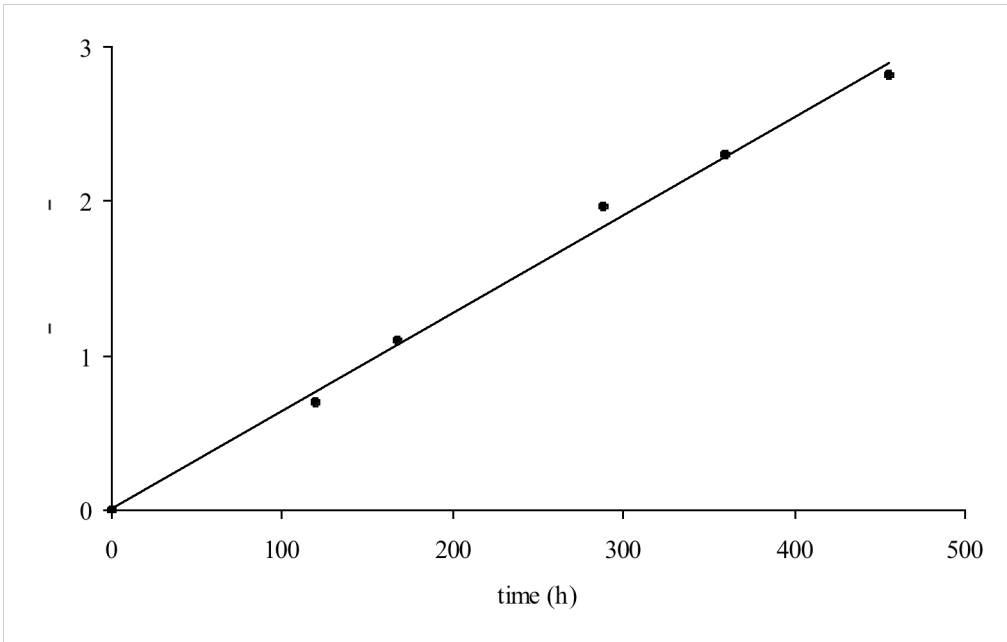

Figure 1 Plot of $\ln\{([A]_0-[A]_e)/([A]_t-[A]_e)\}$ (where A = **A** + **B**) versus time for ligand exchange between (*R**,*R**)-(±)-$[Cu_2(\mathbf{1a})_2](PF_6)_2$ (**A**) and (*R**,*R**)-(±)-$[Cu_2(\mathbf{1b})_2](PF_6)_2$ (**B**) (acetone-d_6, 23 °C).

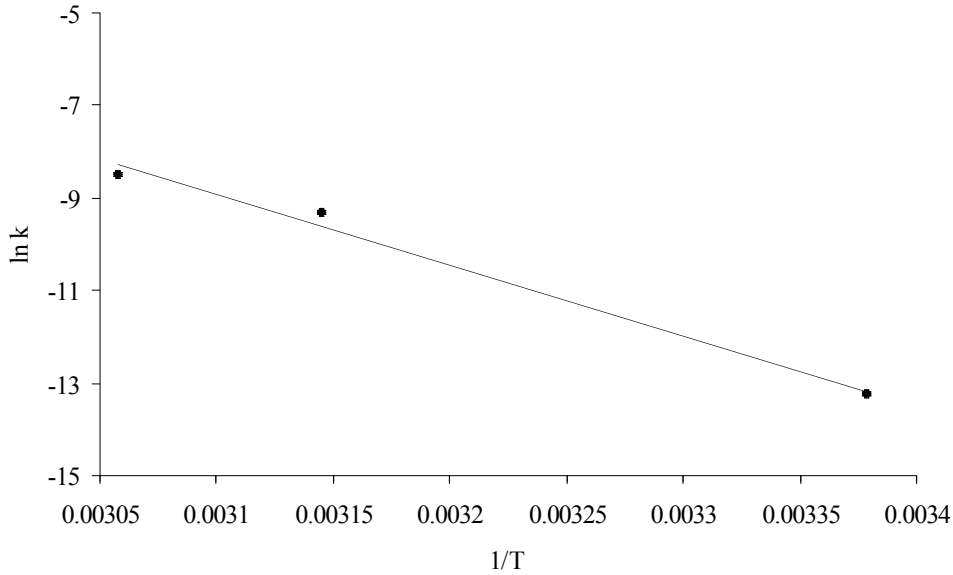

Figure 2 Plot of ln k versus 1/T for the ligand exchange between (*R**,*R**)-(±)-$[Cu_2(\mathbf{1a})_2](PF_6)_2$ and (*R**,*R**)-(±)-$[Cu_2(\mathbf{1b})_2](PF_6)_2$ in acetone-d_6.

NMR Spectra

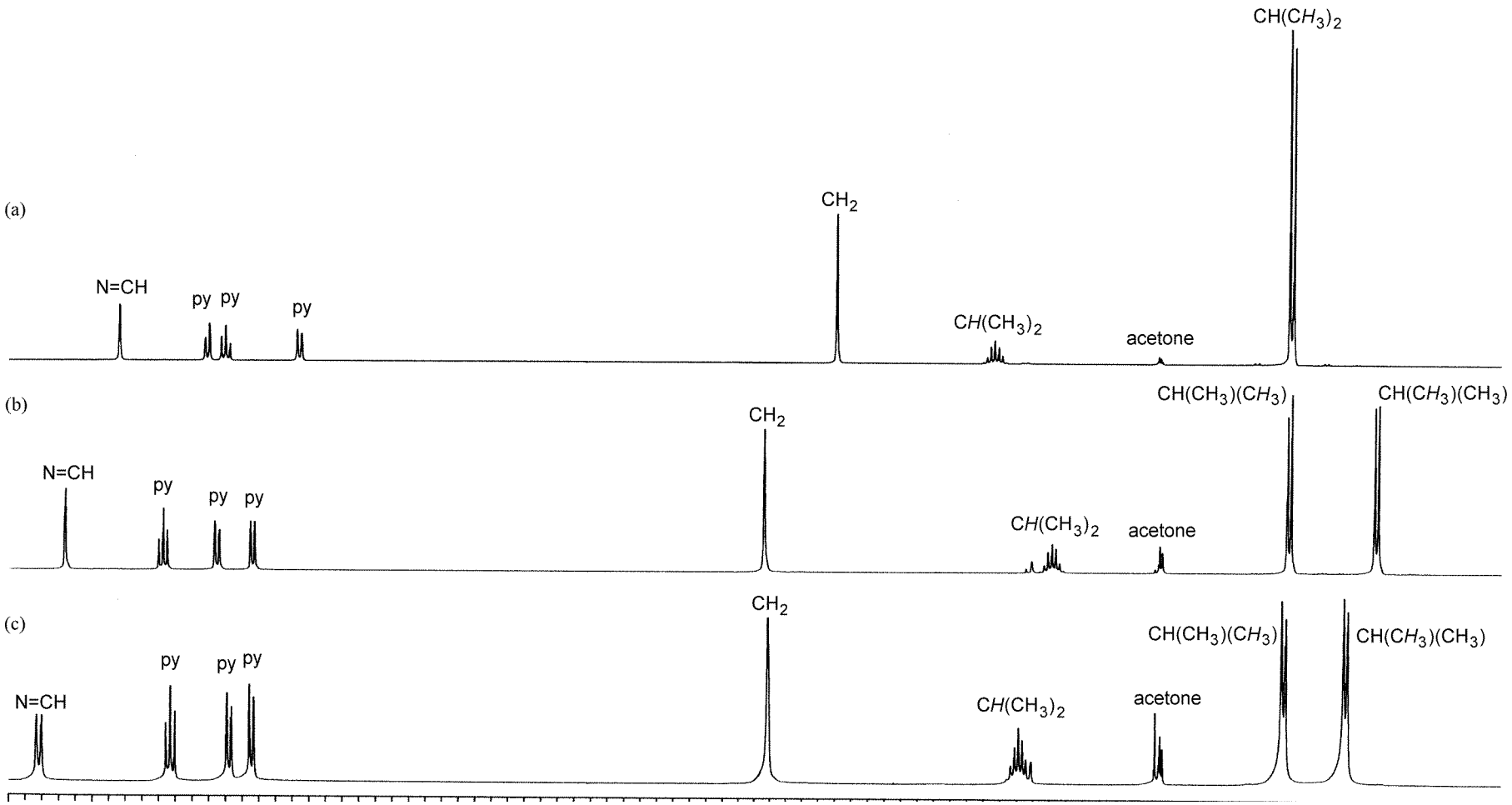

Figure 3 ^{1}H NMR spectra (acetone-d_6, 20 °C, 300 MHz) of (a) **1c**, (b) (R*,R*)-(±)-[Cu_2(**1c**)$_2$](PF_6)$_2$, and (c) (R*,R*)-(±)-[Ag_2(**1c**)$_2$](PF_6)$_2$.

X-ray Powder Diffraction Data

The following list is the observed and calculated powder pattern (*d*-spacings) of the compound $C_{40}H_{52}Cu_2N_8 \cdot 2(C_{18}H_{12}AsO_6) \cdot CH_2Cl_2$. The calculated pattern is based on the single crystal data obtained at 200 K and omitting the hydrogen atoms. The unit cell parameters of the observed powder pattern are those obtained from a refinement based on 40 lines at 300 K (a = 12.359(1) Å, b = 26.211(3) Å, c = 12.541(1) Å, β = 111.51 (1)°). The observed intensities are estimated by eye; b = broad and diffuse line, s = unusually sharp line. The cell based on 105 reflections is a = 12.357(1) Å, b = 26.223(3) Å, c = 12.544(1) Å, β = 111.54(1)°.

	Observed			**Calculated**	
Index	**d-value**	**Int.**	**Int.**	**d-value**	**Index**
$10\bar{1}$	10.302	70	100	10.290	$10\bar{1}$
021	8.731	40	51	8.715	021
120	8.649	1	12	8.643	120
$12\bar{1}$	8.114	2	16	8.093	$12\bar{1}$
130	6.985	90	35	6.994	031
			61	6.956	130
111	6.773	50	86	6.768	111
$13\bar{1}$	6.661	<1	7	6.660	$13\bar{1}$
040	6.558	2	10	6.553	040
121	6.186	5	20	6.178	121
$21\bar{1}$	5.964	<1	7	5.963	$21\bar{1}$
002	5.832	2	3	5.832	002
140	5.702	10	3	5.695	012
			18	5.693	140
210	5.618	30	27	5.615	210
			18	5.604	$12\bar{2}$
$14\bar{1}$	5.545	20_b	16	5.548	$22\bar{1}$
			22	5.527	$14\bar{1}$
$02\bar{2}$	5.332	10	14	5.330	$02\bar{2}$

220	5.271	15	17	5.265	220
$13\bar{2}$	5.061	5	10	5.056	$13\bar{2}$
$23\bar{1}$	5.015	2	13	5.014	$23\bar{1}$
$03\bar{2}$	4.855	1	5	4.852	$03\bar{2}$
150	4.782	30_b	4	4.785	141
			7	4.782	051
			15	4.770	150
$15\bar{1}$	4.670	<1	6	4.671	$15\bar{1}$
112	4.502	40_s	5	4.504	$14\bar{2}$
			30	4.502	112
$24\bar{1}$	4.475	1	5	4.474	$24\bar{1}$
			2	4.473	211
042	4.354	<1	4	4.357	042
240	4.321	5	7	4.322	240
			7	4.315	122
151	4.196	5_s	8	4.197	151
$11\bar{3}$	4.125	1	3	4.126	$11\bar{3}$
160	4.096	3	2	4.091	061
			3	4.084	160
132	4.049	6_s	7	4.050	132
			5	4.047	$24\bar{2}$
$15\bar{2}$	4.010	2	4	4.003	$15\bar{2}$
$12\bar{3}$	3.981	5_s	18	3.981	$12\bar{3}$
052	3.908	2	4	3.899	052
013	3.848	1_b	7	3.847	013
$22\bar{3}$	3.796	35_s	28	3.796	$22\bar{3}$
			11	3.792	310
$32\bar{2}$	3.766	1	4	3.767	$32\bar{2}$
$33\bar{1}$	3.725	10_b	2	3.729	023
			14	3.724	$33\bar{1}$
			8	3.707	161
$25\bar{2}$	3.676	5_s	2	3.679	320
			9	3.672	$25\bar{2}$
not observed			5	3.611	$23\bar{3}$
not observed			3	3.586	$33\bar{2}$

071	3.566	100	3	3.571	$16\bar{2}$
			34	3.565	071
			6	3.560	170
			3	3.553	$26\bar{1}$
$17\bar{1}$	3.516	1	4	3.519	$17\bar{1}$
062	3.500	5	9	3.497	062
152	3.448	8	6	3.445	152
$31\bar{3}$	3.399	1_s	4	3.401	$31\bar{3}$
			1	3.393	$24\bar{3}$
043	3.348	$<1_s$	1	3.345	043
301	3.300	5_s	1	3.302	171
			3	3.300	301
321	3.199	15_s	4	3.205	$17\bar{2}$
			10	3.200	321
			3	3.194	$27\bar{1}$
			1	3.193	$33\bar{3}$
162	3.156	2	3	3.158	162
			1	3.154	081
			2	3.151	072
			2	3.151	180
350	3.092	1	4	3.094	350
			2	3.091	$11\bar{4}$
$40\bar{1}$	3.063	<1	2	3.064	$40\bar{1}$
$12\bar{4}$	3.027	1	4	3.028	$12\bar{4}$
			2	3.028	$27\bar{2}$
181	2.966	1	1	2.970	143
			5	2.968	181
not observed			2	2.936	$26\bar{3}$
not observed			2	2.932	$13\bar{4}$
$23\bar{4}$	2.921	1_b	?	2.923	$36\bar{2}$
			1	2.922	$23\bar{4}$
172	2.896	1	1	2.899	014
			1	2.897	$18\bar{2}$
			1	2.896	172
$43\bar{1}$	2.887	1	2	2.891	$43\bar{1}$
			1	2.889	$43\bar{2}$
			1	2.889	$28\bar{1}$

091	2.829	<1	1	2.826	091
			1	2.823	190
420	2.807	3	3	2.808	420
034	2.768	<1	?	2.767	213
			1	2.767	034
223	2.720	1	1	2.723	$27\overline{3}$
			2	2.722	223
191	2.688	2	4	2.689	191
$25\overline{4}$	2.667	1	3	2.668	$25\overline{4}$
			1	2.665	044
$45\overline{1}$	2.644	3	3	2.645	$45\overline{1}$
			1	2.644	$45\overline{2}$
			1	2.642	$33\overline{4}$
			1	2.641	332
092	2.605	2_b	1	2.609	104
			3	2.606	092
			1	2.598	290
272	2.557	2	1	2.558	272
			1	2.557	$0\cdot10\cdot1$
$1\cdot10\cdot\overline{1}$	2.539	1	2	2.540	$1\cdot10\cdot\overline{1}$
$46\overline{2}$	2.506	<1	2	2.507	$46\overline{2}$
			1	2.506	$20\overline{5}$
173	2.489	2	1	2.490	380
			1	2.489	173
$50\overline{2}$	2.471	1	1	2.471	$50\overline{2}$
$1\cdot10\cdot1$	2.454	3_b	3	2.455	$1\cdot10\cdot1$
			2	2.450	352
064	2.425	1	1	2.427	$30\overline{5}$
			2	2.426	064
$23\overline{5}$	2.410	<1	2	2.409	$23\overline{5}$
			?	2.408	$50\overline{3}$
$52\overline{1}$	2.391	4_b	1	2.393	282
			2	2.391	$0\cdot10\cdot2$
			2	2.391	$52\overline{1}$
			1	2.389	$19\overline{3}$
			1	2.388	$27\overline{4}$
$13\overline{5}$	2.377	<1	2	2.377	$13\overline{5}$

093	2.333	5	1	2.334	005
			1	2.333	$1\cdot 11\cdot 0$
			2	2.331	093
313	2.324	<1	1	3.326	313
			1	2.325	381
451	2.315	1	2	2.317	$53\overline{3}$
			2	2.315	451
not observed			2	2.301	074
not observed			2	2.291	510
292	2.240	1	2	2.239	292
not observed			2	2.206	$55\overline{1}$
193	2.193	1	3	2.193	193
442	2.145	1	1	2.145	442
$47\overline{4}$	2.122	<1	1	2.120	$47\overline{4}$
550	2.105	<1	1	2.107	511
			2	2.106	550
			1	2.105	$56\overline{3}$
$21\overline{6}$	2.083	1	1	2.083	$27\overline{5}$
			3	2.083	$21\overline{6}$
$1\cdot 10\cdot 3$	2.061	1	1	2.062	$3\cdot 11\cdot\overline{1}$
			1	2.062	$17\overline{5}$
			1	2.060	$1\cdot 10\cdot 3$
$3\cdot 11\cdot\overline{2}$	2.038	$<1_b$	1	2.039	$57\overline{1}$
			1	2.038	$3\cdot 11\cdot\overline{2}$
			1	2.037	$37\overline{5}$
not observed			2	2.022	$57\overline{3}$
$33\overline{6}$	2.011	1_b	1	2.012	541
			2	2.011	$33\overline{6}$
			1	2.009	$46\overline{5}$
$62\overline{1}$	1.989	1_b	1	1.992	$4\cdot 10\cdot\overline{1}$
			2	1.991	$13\overline{6}$
			2	1.989	$62\overline{1}$
$1\cdot 12\cdot 2$	1.971	10	1	1.972	324
			1	1.971	$34\overline{6}$
			2	1.971	$1\cdot 12\cdot 2$

$1\cdot13\cdot1$	1.938	2	1	1.940	433
			2	1.938	$1\cdot13\cdot1$
			1	1.936	$47\overline{5}$
$15\overline{6}$	1.904	1	1	1.908	$2\cdot10\cdot3$
			1	1.906	$0\cdot13\cdot2$
			2	1.905	$15\overline{6}$
			1	1.904	$0\cdot12\cdot3$
$65\overline{1}$	1.881	<1	1	1.881	$4\cdot11\cdot\overline{1}$
			2	1.879	$65\overline{1}$
630	1.871	<1	1	1.872	$0\cdot14\cdot0$
			1	1.872	630
			1	1.869	532
$1\cdot10\cdot4$	1.848	<1	1	1.849	$1\cdot10\cdot4$
$1\cdot14\cdot\overline{1}$	1.842	<1	1	1.845	$1\cdot13\cdot2$
			1	1.843	$2\cdot13\cdot1$
			1	1.842	$1\cdot14\cdot\overline{1}$
$53\overline{6}$	1.818	<1	1	1.818	$53\overline{6}$
			1	1.816	$1\cdot13\cdot\overline{3}$
116	1.808	<1	1	1.809	$37\overline{6}$
			1	1.807	116
$5\cdot10\cdot\overline{2}$	1.797	<1	1	1.798	$5\cdot10\cdot\overline{2}$
$0\cdot13\cdot3$	1.789	2_b	1	1.792	$1\cdot14\cdot\overline{2}$
			1	1.792	$67\overline{3}$
			1	1.791	185
			1	1.790	$0\cdot13\cdot3$
$12\overline{7}$	1.727	1	2	1.728	$12\overline{7}$
156	1.712	1	1	1.712	$71\overline{1}$
			1	1.712	156
			1	1.711	591
$25\overline{7}$	1.691	2	1	1.690	$3\cdot14\cdot\overline{2}$
			2	1.690	$25\overline{7}$
$6\cdot10\cdot\overline{3}$	1.611	<1	1	1.612	$1\cdot15\cdot\overline{3}$
			1	1.610	$6\cdot10\cdot\overline{3}$
057	1.588	<1	1	1.588	057
$1\cdot16\cdot2$	1.542	$<1_b$	1	1.542	$1\cdot16\cdot2$