

ELECTRONIC SUPPLEMENTARY INFORMATION

Spatial distribution of phases during gradual magnetostructural transitions in copper(II)-nitroxide based molecular magnets

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XRD study. The intensity data for single crystals of $\text{Cu}(\text{hfac})_2\text{L}^{\text{Pr}}$ were collected on a SMART APEX DUO CCD (Bruker AXS) automated diffractometer with a Cobra (Oxford Cryosystems) using the standard procedure (Cu K α radiation). The structures were solved by direct methods and refined by the full-matrix least-squares procedure anisotropically for non-hydrogen atoms. The H atoms were calculated geometrically and included in the refinement as riding groups. All calculations were fulfilled with the SHELXTL 6.14 program package. Experimental details, selected bond lengths and angles are summarized below in Tables S1 and S2. CIF structures (files) of the $\text{Cu}(\text{hfac})_2\text{L}^{\text{Pr}}$ at different temperatures (CCDC Nos. 1418246-1418252) are available.

Table S1. Crystal data and experimental details for Cu(hfac)₂L^{Pr}.

T, K	290	240	225	220		150	100
Space group, <i>Z</i>	<i>C2/c</i> , 8	<i>C2/c</i> , 8	<i>C2/c</i> , 8	<i>C2/c</i> , 8	<i>P2₁/n</i>	<i>P2₁/n</i>	<i>P2₁/n</i>
<i>a</i> ,	30.934(4)	30.6714(18)	30.5685(16)	30.4776(18)	30.4776(18)	30.086(3)	29.944(2)
<i>b</i> ,	9.5804(12)	9.5911(5)	9.6211(5)	9.6557(6)	9.6557(6)	9.6786(8)	9.6596(7)
<i>c</i> , Å	26.135(3)	25.970(2)	25.8714(13)	25.804(2)	25.804(2)	25.227(2)	25.0248(19)
β , °	125.328(4)	125.6211(17)	125.8858(17)	126.1147(19)	126.1147(19)	125.674(3)	125.423(2)
<i>V</i> , Å ³	6318.9(14)	6210.1(7)	6164.6(6)	6134.5(8)	6134.5(8)	5967.5(9)	5898.6(8)
<i>D_c</i> , g cm ⁻³	1.562	1.589	1.601	1.609	1.609	1.654	1.673
μ /cm ⁻¹	2.031	2.067	2.082	2.092	2.092	2.151	2.176
Mosaicity (xy / z), °	0.41/1.03	0.44/0.95	0.45/1.08	0.44/1.32	0.44/1.32	0.45/1.42	0.46/1.53
Exti	0.00043(3)	0.00008(2)	0.000003(13)	0.000008(13)	0.000000	0.000000	0.000000
<i>I</i> _{hkl} (read / reject)	32533 / 952	37321 / 1155	34281 / 1060	78646 / 40465	78646 / 2375	74459 / 2317	74459 / 2317
θ range, deg.	67.878	67.811	67.464	67.527	67.527	67.612	67.612
<i>I</i> _{hkl} (meas/uniq)	31581 / 5648	36166 / 5563	33221 / 5513	38181 / 5484	76271 / 10960	72142 / 10677	81561 / 10560
<i>R</i> _{int}	0.0316	0.019	0.0187	0.0310	0.0346	0.0311	0.0351
<i>I</i> _{hkl} (<i>I</i> > 2 σ _{<i>I</i>}) / N	5285 / 555	5269 / 554	5191 / 581	5156 / 581	8519 / 1077	9763 / 967	9820 / 940
<i>Goof</i>	1.030	1.021	1.051	1.080	1.021	1.051	1.072
<i>R</i> ₁	0.0378	0.0380	0.0342	0.0341	0.0450	0.0342	0.0312
<i>wR</i> ₂ (<i>I</i> > 2 σ _{<i>I</i>})	0.1103	0.1119	0.1013	0.0986	0.1334	0.0968	0.0876
<i>R</i> ₁	0.0396	0.0393	0.0359	0.0359	0.0551	0.0369	0.0333
<i>wR</i> ₂ (all data)	0.1125	0.1134	0.1034	0.1003	0.1449	0.0996	0.0895

Table S2. Selected bond lengths (Å) and angles (deg) in Cu(hfac)₂L^{Pr}.

T, K	290	240	225	220		150	100
Cu _O -O _{NO}	2.3155(14)	2.2632(15)	2.2248(14)	2.1930(15)	2.1938(18) 2.1962(18)	2.0591(13) 2.0626(12)	2.0207(11) 2.0224(11)
Cu _O -O _{hfac}	1.9848(15)	2.0223(16)	2.0522(15)	2.0802(16)	2.0796(19) 2.0821(19)	2.2183(14) 2.2226(14)	2.2659(12) 2.2682(12)
Cu _O -O _{NO} -N	127.93(12)	126.94(12)	126.41(11)	126.00(12)	126.75(14) 125.22(14)	124.28(10) 123.81(10)	124.62(9) 123.41(9)
Cu _N -N	2.4644(17)	2.4494(17)	2.4438(15)	2.4398(16)	2.4234(19)	2.3987(14)	2.3961(13) 2.4403(13)
N-O	1.294(2), 1.276(2)	1.296(2), 1.277(3)	1.299(2), 1.273(2)	1.301(2), 1.271(2)	1.303(3), 1.272(3) 1.302(3), 1.268(3)	1.3062(19), 1.273(2) 1.3049(19), 1.271(2)	1.3081(17), 1.2701(18) 1.3062(18), 1.2691(19)

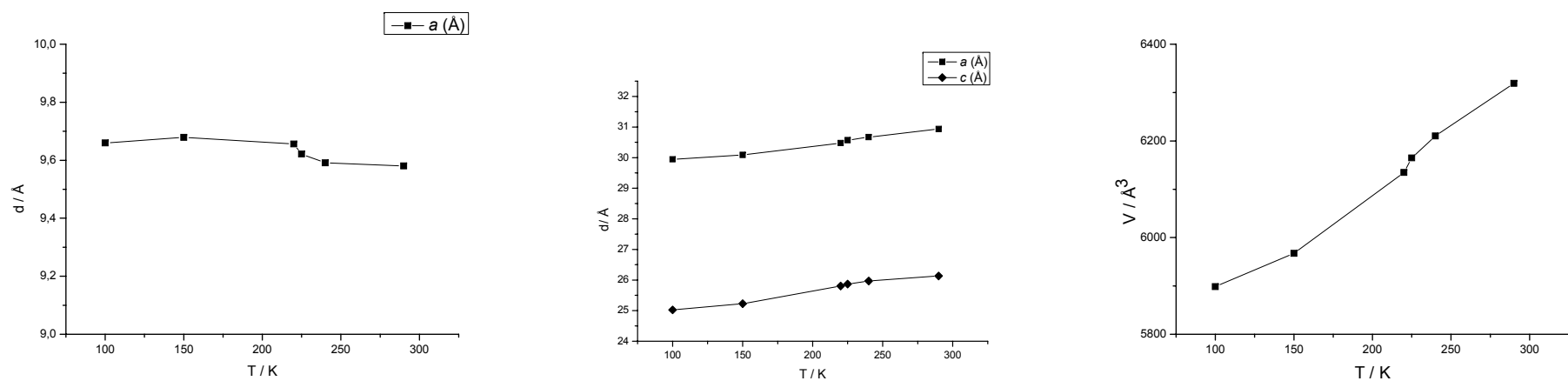


Figure S1. Temperature dynamics of unit cell parameters (a, b) and volume for Cu(hfac)₂L^{Pr}.