

Spin Transition in the Cu(hfac)₂ Complex with (4-Ethylpyridin-3-yl)-Substituted Nitronyl Nitroxide Caused by the “Asymmetric” Structural Rearrangement of Exchange Clusters in the Heterospin Molecule

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Table 1 SI. Crystallographic data and experiments details for [Cu(hfac)₂(L^{Et})₂].

T, K	295	240	200	50
Space group		<i>P</i> 2 ₁ / <i>c</i>		P-1
Z		2		2
<i>a</i> ,	13.1963(6)	13.0640(12)	13.0323(15)	13.012(5)
<i>b</i> ,	16.5504(8)	16.3791(14)	16.1955(19)	15.673(5)
<i>c</i> , Å	15.6804(7)	15.6909(14)	15.7062(17)	15.761(6)
α , °				89.670(17)
β , °	107.291(2)	107.388(6)	107.539(8)	89.813(15)
γ , °				71.729(17)
<i>V</i> , Å ³	3269.9(3)	3204.1(5)	3160.9(6)	3052(2)
<i>D</i> _{calc} g cm ⁻³	1.609	1.642	1.664	1.724
<i>I</i> _{hkl} total	29320	25827	25278	16895
uniq	8041	7672	7814	12096
<i>R</i> _{int}	0.1037	0.1306	0.1475	0.1670
$\theta_{\max}$, °	28.338	28.003	28.444	28.298
<i>I</i> >2 σ_I / N	3147 / 560	2866 / 560	2391 / 533	4416 /
Goof	0.826	0.796	0.958	0.788
<i>R</i> ₁ / w <i>R</i> ₂ (<i>I</i> >2 σ_I)	0.0497 / 0.1110	0.0550 / 0.1067	0.1024 / 0.2797	0.0847 / 0.1859
<i>R</i> ₁ / w <i>R</i> ₂ (all)	0.1511 / 0.1354	0.1608 / 0.1349	0.2835 / 0.3242	0.2282 / 0.2621

Table 2 SI. Crystallographic data and details of experiments for $[[\text{Cu}(\text{hfac})_2]_4(\text{L}^{\text{Et}})_2]$.

T, K	295	240	200	154	150	100	50	240*
Space group	$P2_1/c$							
Z	2	2	2	2	6	4	4	2
<i>a</i> , Å	15.933(4)	15.7740(14)	15.7701(14)	15.7115(16)	15.6154(6)	30.0780(18)	30.024(5)	15.7875(9)
<i>b</i> , Å	16.839(3)	16.7111(16)	16.7095(16)	16.6697(18)	49.9624(19)	17.4789(12)	17.399(3)	16.7372(10)
<i>c</i> , Å	18.876(4)	18.7239(17)	18.7214(17)	18.6560(20)	18.5882(7)	18.4869(10)	18.484(3)	18.7786(10)
β , °	105.222(15)	105.097(3)	105.086(3)	104.995(4)	104.731(2)	104.393(3)	104.292(4)	105.053(4)
<i>V</i> , Å ³	4887.0(18)	4765.3(8)	4763.3(8)	4719.8(9)	14025.5(9)	9414.1(10)	9357(2)	4791.8(5)
<i>V</i> / <i>Z</i> , Å ³	2443.5	2382.7	2381.6	2358.2	2337.6	2353.5	2339.2	2395.9
<i>D</i> _{calc} g cm ⁻³	1.726	1.770	1.771	1.787	1.804	1.792	1.803	1.760
<i>I</i> _{hkl} total	46296	46774	47325	33759	129178	53780	57734	43340
uniq	12184	8544	8548	7972	34443	22273	22802	11552
<i>R</i> _{int}	0.1720	0.0347	0.0649	0.0459	0.1086	0.1220	0.1268	0.0905
θ_{max} , °	28.487	67.746	67.738	67.203	28.283	28.041	28.340	28.078
<i>I</i> > 2 σ _I / N	3060 / 775	7775 / 813	7490 /	6159 / 814	12227 / 2170	9146 / 1387	10773 / 1387	3527 / 812
Goof	0.738	1.042	1.000	1.204	0.735	0.718	0.776	0.752
<i>R</i> ₁	0.0580	0.0458	0.0481	0.0619	0.0460	0.0547	0.0561	0.0449
<i>wR</i> ₂ (<i>I</i> > 2 σ _I)	0.1233	0.1327	0.1346	0.1862	0.0663	0.1020	0.1099	0.0793
<i>R</i> ₁	0.2402	0.0491	0.0522	0.0820	0.1714	0.1465	0.1279	0.1986
<i>wR</i> ₂ (all)	0.1706	0.1364	0.1385	0.2297	0.0832	0.1294	0.1311	0.1044

* – after the heating from 50 K.