

**Na<sup>I</sup>/Cu<sup>I-II</sup> Heterometallic Cages Interconnected by an Unusual Linear  
2-Coordinate OCN-Cu(I)-NCO Links: Synthesis, Structural,  
Magnetostructural Correlation and Computational Studies**

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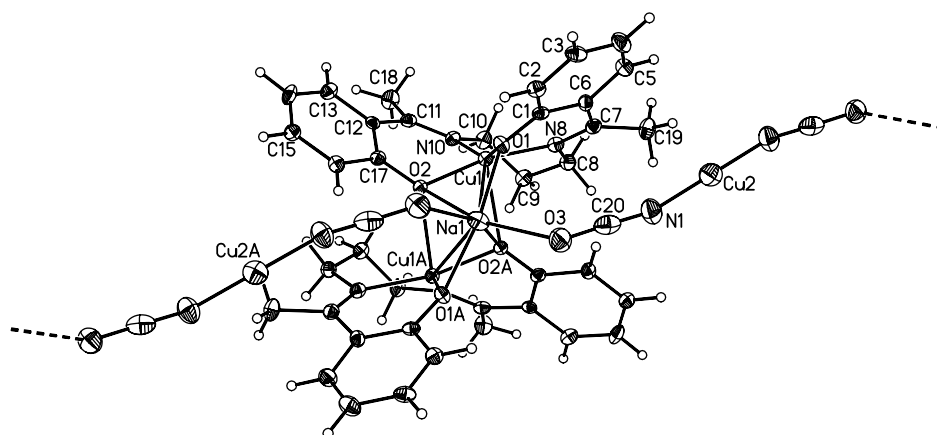
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**Fig. S1:** Probability ellipsoids of **1** drawn at the 40% probability level.

The suffix A denotes symmetry code:  $-x, y, 0.5-z$

**Table S1:** The delocalization of the electrons from copper to the ligands in OCN-Cu-NCO linkage. The NBO second-order perturbative stabilization energies are obtained at the NBO/B3LYP//B3LYP/6-31G\*,LANL2DZ level of theory.

Acceptor orbitals	Delocalization energies (kcal/mol)
$\pi^*$ 2px (N(1)-C20)	3.07
$\pi^*$ 2py (N(1)-C20)	3.07
$\pi^*$ 2px (N(1)#2-C20)	3.07
$\pi^*$ 2py (N(1)#2-C20)	3.07

Total electronic energies (in a.u) and Cartesian coordinates of geometries optimized at the B3LYP/6-31G\*,LANL2DZ level of theory

2			
Et = -1192.2015312			
6	-2.995608	-0.280066	0.429196
6	-2.425466	-1.158897	-0.562031
6	-3.052141	-2.426140	-0.766580
6	-4.123574	-2.836607	-0.004604
6	-4.650937	-2.000341	1.001812
6	-4.098217	-0.750981	1.193305
8	-1.397224	-0.866915	-1.295604
29	0.006841	0.283716	-0.680921
7	1.571078	1.471998	-0.161001
6	1.408955	2.916313	-0.348215
6	0.045532	3.288727	-0.924053
6	-1.136214	2.972289	-0.006669
7	-1.434281	1.534514	0.028764
6	-2.552403	1.099502	0.559129
6	-3.474236	2.042353	1.320787
8	1.284570	-1.060535	-1.186554
6	2.300042	-1.355433	-0.436014
6	3.004122	-0.406635	0.392185
6	4.056166	-0.883871	1.220678
6	4.448573	-2.206457	1.228299
6	3.809141	-3.115733	0.359842
6	2.776470	-2.701827	-0.452653
6	2.708949	1.014435	0.308054
6	3.782726	2.008131	0.720475
1	-2.622986	-3.060061	-1.536252
1	-4.559348	-3.818679	-0.174473
1	-5.482948	-2.331912	1.615572
1	-4.521342	-0.116525	1.964827
1	-4.497489	1.975726	0.940760
1	-3.500221	1.754868	2.378332
1	-3.158023	3.082471	1.277015
1	-2.009090	3.526035	-0.374172
1	-0.914285	3.350568	1.003203

1	0.050494	4.370004	-1.111431
1	-0.103149	2.802863	-1.898308
1	1.542053	3.445555	0.608189
1	2.187333	3.295902	-1.025873
1	3.994527	2.696174	-0.105822
1	3.452432	2.621864	1.567993
1	4.719573	1.523752	0.983848
1	2.259989	-3.390601	-1.113940
1	4.124496	-4.156576	0.339911
1	5.241134	-2.539633	1.891323
1	4.550829	-0.198104	1.901274
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<b>3</b>				1	-5.165323	2.694881	-1.543585
Et = -2384.374014				1	-4.453773	5.021569	-1.788434
6	-1.868258	-0.500125	-2.907183	1	-2.485744	5.859766	-0.486572
6	-0.884080	-1.203638	-2.170572	1	-1.235897	4.312836	1.000975
6	-0.351005	-2.419308	-2.720369	1	0.383352	-0.405431	5.744252
6	-0.812078	-2.838466	-3.984509	1	2.042064	1.378612	6.013794
6	-1.765207	-2.122095	-4.697583	1	2.994300	2.506644	3.997942
6	-2.301173	-0.950405	-4.144041	1	2.225911	1.829656	1.726373
8	-0.493898	-0.742938	-0.999581	1	-0.602766	-3.512089	4.121060
29	1.451666	-0.538835	-0.701548	1	0.161637	-2.408686	5.264523
7	3.382536	-0.393351	-0.176801	1	-1.608097	-2.463259	5.115649
6	4.001440	-1.585411	0.415508	1	-5.809647	-0.076379	-1.069517
6	3.006388	-2.687885	0.793148	1	-6.041770	-0.012183	0.675721
6	2.403793	-3.477145	-0.376241	1	-6.176702	1.467659	-0.269372
7	1.454397	-2.675812	-1.140159	1	-4.499332	-1.858205	-0.364037
6	0.647751	-3.226889	-1.989404	1	-4.720522	-1.529893	1.353612
6	0.693382	-4.725618	-2.250809	1	-2.152044	-2.672796	0.136216
29	-1.431042	-0.036211	0.833472	1	-3.490407	-3.626627	0.776220
7	-3.369492	-0.237573	0.358782	1	-3.155417	-2.558697	3.036250

6	-3.966170	-1.565357	0.551327	1	-1.848817	-3.597025	2.470679
6	-2.957639	-2.671665	0.879693	1	1.642836	-5.014030	-2.719482
6	-2.349181	-2.633945	2.287830	1	0.628274	-5.274958	-1.304360
7	-1.419779	-1.522268	2.445802	1	-0.126098	-5.063949	-2.883323
6	-0.624328	-1.453893	3.463821	1	-2.252146	0.416218	-2.470507
6	-0.662806	-2.509440	4.559762	1	-3.046134	-0.380522	-4.694304
8	-1.753267	1.857579	1.383280	1	-2.082453	-2.465235	-5.677917
6	-2.456822	2.595120	0.591963	1	-0.389614	-3.730126	-4.438231
6	-3.626420	2.131167	-0.126474	1	5.111234	3.136430	-0.224152
6	-4.315202	3.044590	-0.964693	1	4.375692	5.188918	-1.328686
6	-3.916816	4.359505	-1.115810	1	2.419705	5.123611	-2.891409
6	-2.802444	4.823611	-0.387554	1	1.203989	2.990213	-3.263298
6	-2.100862	3.973625	0.439235	1	1.923923	-4.380661	0.028557
6	-4.134898	0.770680	0.032167	1	3.213441	-3.827106	-1.038021
6	-5.624274	0.534939	-0.176637	1	2.198626	-2.265050	1.402074
8	0.508995	-0.008121	1.206793	1	3.546927	-3.401754	1.429155
6	0.882600	0.315956	2.427472	1	4.749233	-2.008050	-0.275028
6	0.355853	-0.354002	3.584482	1	4.545992	-1.298201	1.325689
6	0.802175	0.058196	4.855957	1	5.787873	0.597472	0.944476
6	1.735477	1.074774	5.017208	1	6.056081	-0.326972	-0.531414
6	2.265194	1.707978	3.883598	1	6.155790	1.430618	-0.581009
6	1.845881	1.337524	2.615954				
8	1.744830	0.752807	-2.198336				
6	2.434481	1.814902	-1.954449				
6	2.064966	3.037009	-2.603536				
6	2.747092	4.214777	-2.390835				
6	3.854768	4.255480	-1.519555				
6	4.267426	3.087727	-0.906327				
6	3.600499	1.849820	-1.094481				
6	4.127308	0.643184	-0.461153				
6	5.614993	0.595979	-0.139737				

NImag=0

4

Et = -532.4774127

6	-3.031964	0.008730	0.000022
7	-1.838509	-0.001884	0.000020
29	0.000021	-0.014834	-0.000003
7	1.838465	-0.004872	-0.000010
6	3.031842	0.008218	-0.000005
8	4.239930	0.024190	0.000007
8	-4.239875	0.022782	-0.000019

NImag=0