

Supplementary Material: Two-Dimensional Nitronyl Nitroxide–Cu Networks Based on Multi-Dentate Nitronyl Nitroxides: Structures and Magnetic Properties

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Table S1. Selected bond lengths [Å] and angles [°] for complex 1.

1			
Cu(1)–O(1)	1.947(3)	Cu(1)–O(2)	1.956(3)
Cu(1)–O(3)	2.166(3)	Cu(1)–O(4)	1.947(3)
Cu(1)–N(1)	1.991(3)	Cu(2)–O(9)	1.935(2)
Cu(2)–O(9)#3	1.935(2)	Cu(2)–O(10)	1.951(2)
Cu(2)–O(10)#3	1.951(2)	Cu(2)–O(15)	2.553(2)
Cu(2)–O(15)#3	2.553(2)	Cu(3)–O(5)	1.913(3)
Cu(3)–O(6)	2.146(3)	Cu(3)–O(7)	1.963(3)
Cu(3)–O(8)	1.904(3)	Cu(3)–O(16)	1.989(3)
Cu(4)–O(13)	1.930(3)	Cu(4)–O(13)#1	1.930(3)
Cu(4)–O(14)	1.943(3)	Cu(4)–O(14)#1	1.943(3)
Cu(4)–O(17)	2.428(3)	Cu(4)–O(17)#1	2.428(3)
Cu(5)–O(11)	1.950(3)	Cu(5)–O(11)#2	1.950(3)
Cu(5)–O(12)	1.941(3)	Cu(5)–O(12)#2	1.941(3)
O(15)–N(2)	1.281(4)	O(16)–N(3)	1.294(4)
O(18)–N(4)	1.296(4)	O(17)–N(5)	1.281(4)
N(1)–Cu(1)–O(3)	101.18(1)	O(15)–Cu(2)–O(15)#3	180.00(1)
N(2)–O(15)–Cu(2)	149.51(2)	N(3)–O(16)–Cu(3)	122.8(2)
N(5)–O(17)–Cu(4)	147.12(2)	O(17)–Cu(4)–O(17)#3	180.00(1)
O(18)–Cu(5)–O(18)#2	180.00(1)	N(4)–O(18)–Cu(5)	133.65(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y,-z; #2 -x+2,-y+1,-z; #3 -x+2,-y+1,-z+1

Table S2. Selected bond lengths [Å] and angles [°] for complex 2.

2			
Cu(1)-O(9)	2.039(5)	Cu(1)-O(9)#1	2.039(5)
Cu(1)-O(10)	2.229(5)	Cu(1)-O(10)#1	2.229(5)
Cu(1)-N(1)	2.018(5)	Cu(1)-N(1)#1	2.018(5)
Cu(2)-O(1)	2.326(5)	Cu(2)-O(5)	2.002(6)
Cu(2)-O(6)	1.952(6)	Cu(2)-O(7)	2.237(7)
Cu(2)-O(8)	1.945(6)	Cu(2)-N(2)	2.061(6)
Cu(3)-O(2)	2.362(5)	Cu(3)-O(2)#1	2.362(5)
Cu(3)-O(3)	1.947(5)	Cu(3)-O(3)#1	1.947(5)
Cu(3)-O(4)	1.942(5)	Cu(3)-O(4)#1	1.942(5)
O(1)-N(3)	1.278(7)	O(2)-N(4)	1.270(7)
N(1)-Cu(1)-N(1)#1	180.00(1)	N(2)-Cu(2)-O(1)	87.4(2)
N(3)-O(1)-Cu(2)	126.0(4)	N(4)-O(2)-Cu(3)	150.7(5)
O(2)#1-Cu(3)-O(2)	180.00(1)		

Symmetry transformations used to generate equivalent atoms: #1 -x,-y+2,-z-1

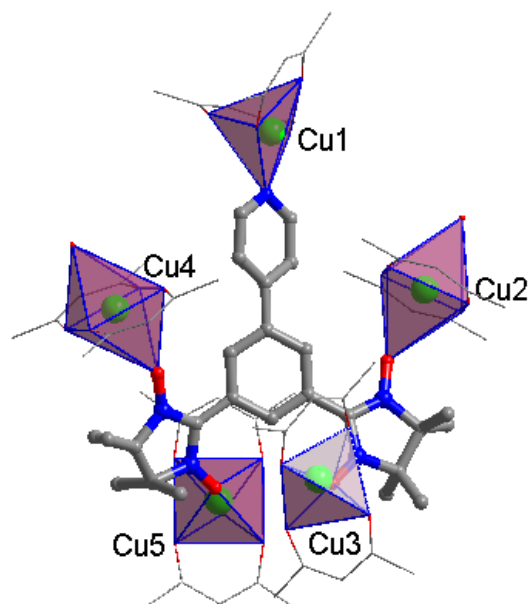


Figure S1. The coordination polyhedron of five Cu(II) ions in complex 1. All of the fluorine and hydrogen atoms are omitted for clarity.

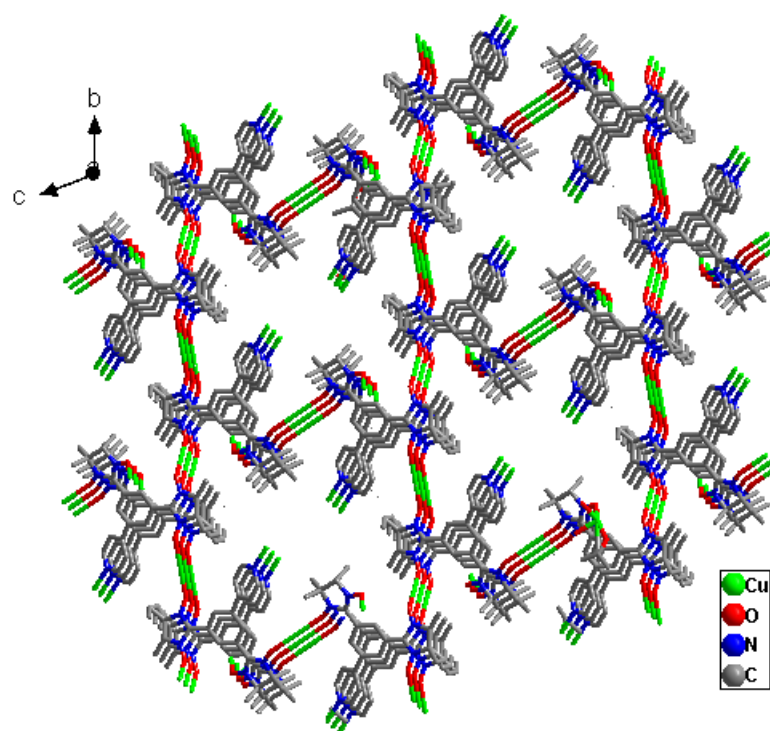


Figure S2. Crystal packing arrangement for complex 1. All of the hydrogen and hfac coligands are omitted for clarity.

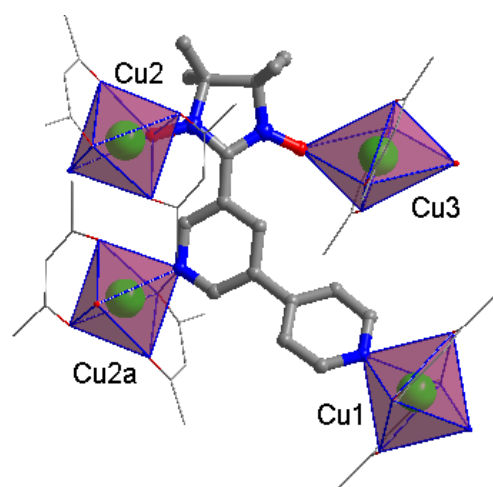


Figure S3. The coordination polyhedron of four Cu(II) ions in complex 2. All of the fluorine and hydrogen atoms are omitted for clarity.

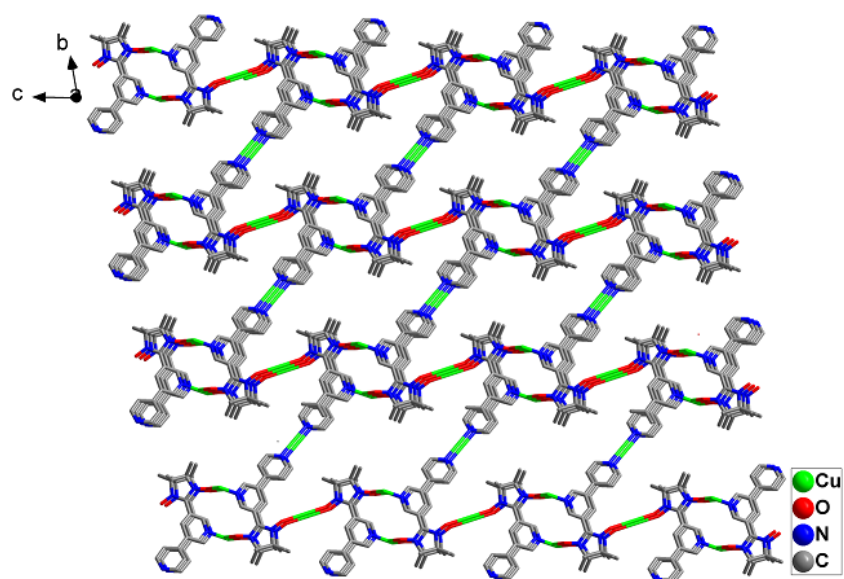
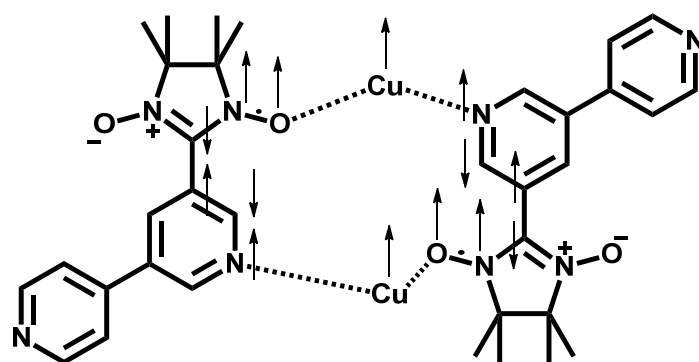


Figure S4. Crystal packing arrangement for complex 2. All of the hydrogen and hfac coligands are omitted for clarity.



Scheme S1. Spin polarization mechanism for the magnetic coupling mediated by NIT-3Py-5-4Py ligand.