

Prof. Dr. Jorge A. R. Navarro, Prof. Dr. Juan Manuel Salas, Prof. Dr. Miguel Quirós and Dr. Elisa Barea

Departamento de Química Inorgánica, Universidad de Granada,

Av. Fuentenueva S/N, E-18071 Granada (Spain)

Fax: (+34)958248526

E-mail: jarn@ugr.es; jsalas@ugr.es; mquiros@ugr.es; ebaream@ugr.es

Heteroleptic Pyrimidine-2-olate and 4,4'-bipyridine Copper(II) Layered Metal-organic Frameworks with Swelling Properties

Elisa Barea,^a Miguel Quirós,^a Jorge A. R. Navarro^{a*} and Juan M. Salas^{a*}

^aDepartamento de Química Inorgánica, Universidad de Granada, Av. Fuentenueva S/N, E-18071 Granada, Spain

Table S.1. Selected bond distances [Å] and angles [°] for **1a**.

Bond distances		Angles	
Cu1-O3	1.941(7)	O3-Cu1-O2	178.7(3)
Cu1-O2	1.968(8)	O3-Cu1-N21	90.0(3)
Cu1-N21	2.029(9)	O2-Cu1-N21	90.3(3)
Cu1-N11	2.058(9)	O3-Cu1-N11	88.9(3)
Cu1-Cl3	2.773(3)	O2-C1-N11	90.8(3)
Cu1-Cl2	2.873(3)	N21-Cu1-N11	178.5(4)
Cu2-O2	1.929(7)	O3-Cu1-Cl3	96.2(2)
Cu2-N3P	2.014(9)	O2-Cu1-Cl3	85.0(2)
Cu2-N41	2.032(9)	N21-Cu1-Cl3	89.8(3)
Cu2-N31	2.051(8)	N11-Cu1-Cl3	91.3(2)
Cu2-Cl3	2.607(3)	O3-Cu1-Cl2	81.9(2)
Cu3-O3	1.908(7)	O2-Cu1-Cl2	96.9(2)
Cu3-N1P	1.977(9)	N21-Cu1-Cl2	87.1(3)
Cu3-N51	2.041(8)	N11-Cu1-Cl2	91.8(2)
Cu3-N61	2.064(9)	Cl3-Cu1-Cl2	176.35(9)
Cu3-Cl2	2.650(3)	O2-Cu2-N3P	175.7(3)
N3P-Cu2	2.014(9)	O2-Cu2-N41	91.4(3)
		N3P-Cu2-N41	89.6(3)
		O2-Cu2-N31	90.7(3)
		N3P-Cu2-N31	87.1(3)
		N41-Cu2-N31	162.2(3)

O2-Cu2-Cl3	90.6(2)
N3P-Cu2-Cl3	93.4(3)
N41-Cu2-Cl3	98.6(3)
N31-Cu2-Cl3	99.1(3)
O3-Cu3-N1P	177.3(4)
O3-Cu3-N51	91.7(3)
N1P-Cu3-N51	88.3(3)
O3-Cu3-N61	91.0(3)
N1P-Cu3-N61	88.2(3)
N51-Cu3-N61	162.5(3)
O3-Cu3-Cl2	88.8(2)
N1P-Cu3-Cl2	93.9(3)
N51-Cu3-Cl2	99.0(3)
N61-Cu3-Cl2	98.4(3)
Cu3-Cl2-Cu1	72.62(9)
Cu2-Cl3-Cu1	73.29(8)
Cu2-O2-Cu1	111.1(4)
Cu3-O3-Cu1	116.7(4)

Table S.2. Selected H-bond distances [Å] for **1a**.

H-Bond distances	
O2P...O3W	2.719
Cl2...O2W	3.136
Cl2...O7W	3.002
Cl3...O1W	3.134
O2...O9W	3.075
O3...O6W	2.829
O3N...O4W	2.772