STRUCTURAL CHEMISTRY

Volume 71 (2015)

Supporting information for article:

(2-Aminopyrimidine-κN^1)aqua(pyridine-2,6-dicarboxylato-κ$^3O^2$,N,O^6)copper(II): X-ray and DFT calculated structure

Zakieh Yousefi, Hossein Eshtiagh-Hosseini, Alireza Salimi and Janet Soleimannejad

Table S1 A list of compounds with general formula [Cu(pydc)(*N*-coligand)] in the CSD associated with some structural features

No.	Refcode	Structure	Group	τ_5	Axial ligand	CN	Cu…plane	Cu-$O_{carboxylate}$	Cu-$N_{pyridine}$	Cu-O_{water}	Cu-$O_{bridged}$	Ref.
1	MAHKOW	Dimer	*i*	0.16	H_2O	5	0.190	2.069, 2.001	1.097	2.232	-	Song *et al.* 2004
		Dimer	*iii*	-	H_2O, $O_{carboxylate}$	6	-	2.017, 2.011	1.890	2.771	2.597	
2	MENLUN	Polymer	*ii*	0.08	$O_{carboxylate}$	5	0.216	2.011, 2.050	1.898	-	2.343	Xiang *et al.* 2006
3	NIBDIM	Dimer or Polymer	*ii* *or* *iii*	0.26 or -	$O_{carboxylate}$ or $O_{carboxylate}$,NH_2	5 or 6	-	1.995, 2.002	1.900	-	2.749 2.787($N_{bridged}$)	Uçar *et al.* 2007
4	NUNYEB	Monomer	*i*	0.17	H_2O	5	0.144	2.001, 2.052	1.898	2.242	-	Dong *et al.* 2010
5	OYEFEE	Monomer	*i*	0.12	H_2O	5	0.201	2.028, 2.042	1.898	2.275	-	van Albada *et al.* 2011
		Monomer	*i*	0.14	H_2O	5	0.198	2.032, 2.012	1.902	2.297	-	
6	OYEFII	Monomer	*i*	0.29	H_2O	5	0.126	2.042, 2.050	1.917	2.274	-	van Albada *et al.* 2011
7	OYEFOO	Polymer	*ii*	0.25	$O_{carboxylate}$	5	0.059	2.012, 2.025	1.898	-	2.509	van Albada *et al.* 2011
8	OYOZIM	Dimer	*ii*	0.24	NH_2	5	0.053	2.036, 1.991	1.909	-	2.689($N_{bridged}$)	Yenikaya *et al.* 2011
		Monomer	*i*	0.12	H_2O	5	0.190	2.032, 2.040	1.926	2.224	-	
9	PODXAI	Monomer	*i*	0.15	H_2O	5	0.198	2.002, 2.057	1.903	2.227	-	Mutambi, 2008
10	RALPUR	Monomer	*i*	0.24	H_2O	5	0.115	2.044, 2.001	1.868	2.307	-	Das & Baruah, 2012
11	TIMKUV	Dimer	*ii*	0.24	$O_{carboxylate}$	5	0.055	2.024, 1.998	1.899	-	2.589	Su & Chiu, 1996
12	TIMLAC	Polymer	*ii*	-	$O_{carboxylate}$	6	-	2.010, 2.001	1.897	-	2.659,2.865	Su & Chiu, 1996
		Monomer	*i*	0.11	H_2O	5	0.183	2.048, 2.040	1.840	2.270		
13	UGIXAK	Polymer	*ii*	-	$O_{carboxylate}$	6	-	2.018, 2.014, 2.021	1.861, 1.890		2.017,2.662	Seddiqi *et al.* 2009
14	WUKLEU	Monomer	*i*	0.26	H_2O	5	0.076	2.053,2.054	1.923	2.278	2.918($N_{bridged}$)	Yenikaya *et al.* 2009

		or Dimer	*or* *iii*	or -	or H_2O, NH_2	or 6	or -					
15	YADHUH	Polymer	*ii*	-	$O_{carboxylate}$	6	-	2.002, 2.003	1.888		2.795, 2.795	Gosh *et al.* 2004
16	KAYNEF	Monomer	*i*	0.15	H_2O	5	0.171	2.043, 2.022	1.899	2.244		Yang *et al.* 2012
17	AMAMIL	Monomer	*i*	0.11	H_2O	5	0.165	2.042, 2.050	1.911	2.318		Cui *et al.* 2011
18	AROSOP	Tetramer	*ii*	-	$O_{carboxylate}$	6	-	1.999, 2.001	1.889		2.541, 2.723	Chaigneau *et al.* 2004
19	AYOLOP	Dimer or polymer	*ii* *or* *iii*	0.30 or -	$O_{carboxylate}$ or $O_{carboxylate}$,NH_2	5 or 6	0.003	1.999, 2.020	1.898		2.742 2.783($N_{bridged}$)	Altin *etal.* 2004
20	CIHPAL	Polymer	*ii*	0.17	$O_{carboxylate}$	5	0.144	2.031, 2.039	1.897		2.225	Kirin *et al.* 2007
21	COMJOE	Monomer	*i*	0.12	H_2O	5	0.160	2.062, 1.998	1.91	2.255		Cui *et al.* 2008
22	COMJUK	Monomer	*i*	0.18	H_2O	5	0.132	2.025, 2.004	1.904	2.287		Cui *et al.* 2008
23	COMKAR	Monomer	*i*	0.09	H_2O	5	0.168	2.008, 2.049	1.911	2.286		Cui *et al.* 2008
24	ERIHAP	Monomer	*i*	0.18	H_2O	5	0.222	2.018, 2.039	1.9467	2.254		Kong & Yu, 2011
25	ERILEX	Monomer	*i*	0.06	H_2O	5	0.199	1.998, 2.017	1.906	2.231		Chen *et al.* 2011
26	FAZXEK	Monomer		-	-	4	-	1.987, 1.994	1.937			Perry *et al.* 2004
27	FONGAR	Monomer	*i*	0.14	CH_3OH	5	0.144	2.021, 2.036	1.906	2.269(CH_3OH)		Liu *et al.* 2005
28	FOQKUS	Polymer	*ii*	0.19	$O_{carboxylate}$	5	0.191	2.027, 2.034	1.904		2.192	Cui *et al.* 2009
29	IHOSOO	Polymer	*ii*	-	$O_{carboxylate}$	6	-	2.066, 2.053	1.901		2.434	Uçar *et al.*, 2009
30	JOFXEH	Monomer	*i*	0.18	H_2O	5	0.095	2.026, 2.015	1.895	2.390		Ang *et al.* 1991
31	JOFXIL	Monomer	*i*	0.17	H_2O	5	0.165	2.037, 2.046	1.918	2.295		Ang *et al.* 1991
32	JOFXOR	Monomer	*i*	0.15	H_2O	5	0.155	2.057, 2.019	1.903	2.287		Ang *et al.* 1991
33	FIKVAY	Polymer	*ii*	-	$O_{carboxylate}$	6	-	2.019, 2.019	1.881		2.860, 2.860	Mistri *et al.* 2013
34	XIPQAQ	Monomer	*i*	0.20	H_2O	5	0.144	2.052, 2.019	1.930	2.295		Wei *et al.* 2013
35	XIPQEU	Monomer	*i*	0.06	H_2O	5	0.195	2.027, 2.028	1.908	2.264		Wei *et al.* 2013

36	QANRII	Monomer	*i*	0.18	H_2O	5	0.132	2.034, 2.078	1.912	2.278		Patel *et al.* 2011
37	YEQDAA	Monomer	*i*	0.06	H_2O	5	0.018	2.009, 2.002	1.904	2.270		Ma *et al.* 2006
38	GIBQAL	Monomer	*i*	0.19	H_2O	5	0.132	2.016, 2.034	1.899	2.261		van Albada *et al.* 2013
39	GIBQEP	Monomer	*i*	0.13	H_2O	5	0.183	2.030, 2.010	1.913	2.208		van Albada *et al.* 2013
40	GIBQIT	Monomer	*i*	-	H_2O	6	-	2.038, 2.078	1.913	2.458, 2.463		van Albada *et al.* 2013
41	GILTOM	Monomer	*i*	0.11	H_2O	5	0.141	1.981, 2.044	1.910	2.310		Pilar Brandi-Blanco *et al.* 2013
42	QIJSAF	Monomer	*i*	0.20	H_2O	5	0.147	2.028, 2.063	1.938	2.301		Wang *et al.* 2014

References for Table S1 that are not in the main paper

Albada, G. A. van, Ghazzali, M., Al-Farhan, K., Bouwman, E. & Reedijk, J. (2013). *Polyhedron*, **52**, 1059–1064.
Ang, H. G., Kwik, W. L., Hanson, G. R., Crowther, J. A., McPartlin, M. & Choi, N. (1991). *J. Chem. Soc, Dalton Trans.* pp. 3193–3201.
Chaigneau, J., Marrot, J. & Riou, D. (2004). *Acta Cryst.* **C60**, m101–m103.
Cui, G.-H., Liu, T.-F. & Peng, X. (2011). *J. Chem. Crystallogr.* **41**, 322–327.
Cui, S., Zhao, Y., Zhang, J., Liu, Q. & Zhang, Y. (2008). *Cryst. Growth Des.* **8**, 3803–3809.
Cui, S.-X., Zhao, Y.-L., Zhang, J.-P., Liu, Q. & Zhang, Y. (2009). *Polyhedron*, **28**, 980–986.
Das, B. & Baruah, J. B. (2012). *Polyhedron*, **31**, 361–367.
Dong, G.-Y., Fan, L.-H., Yang, L.-X. & Khan, I. U. (2010). *Acta Cryst.* **E66**, m532.
Ghosh, S. K., Ribas, J. & Bharadwaj, P. K. (2004). *CrystEngComm*, **6**, 250–256.
Kirin, S. I., Ohr, K., Yennawar, H. P., Morgan, C. M., Levine, L. A. & Williams, M. E. (2007). *Inorg. Chem. Commun.* **10**, 652–656.
Kong, F. & Yu, Z. (2011). *Acta Cryst.* **E67**, m783.
Liu, S.-H., Li, Y.-Z. & Meng, Q.-J. (2005). *Acta Cryst.* **E61**, m1183.
Ma, Y., Gao, D.-Z., Zhang, W., Yoshimura, K., Liao, D.-Z., Jiang, Z.-H. & Yan, S.-P. (2006). *Inorg. Chim. Acta*, **359**, 4655-4659.
Mistri, S., Zangrando, E. & Manna, S.C. (2013). *Inorg. Chim. Acta*, **405**, 331**–**338.
Mutambi, E. M. (2008). *Acta Cryst.* **E64**, m979.
Patel, D. K., Choquesillo-Lazarte, D., Dominguez-Martín, A., Brandi-Blanco, M. P., Gonzalez-Perez, J. M., Castineiras, A. & Niclós-Gutiérrez, J. (2011). *Inorg. Chem.* **50**, 10549–10551.
Perry, J. J., McManus, G. J. & Zaworotko, M. J. (2004). *J. Chem. Crystallogr.* **34**, 877–881.
Pilar Brandi-Blanco, M. del, Choquesillo-Lazarte, D., Domínguez-Martín, A., Matilla-Hernandez, A., Gonzalez-Perez, J. M., Castineiras, A. & Niclós-Gutiérrez, J. (2013). *J. Inorg. Biochem.* **127**, 211–219.
Siddiqi, Z. A., Khalid, M., Kumar, S. & Shahid, M. (2009). *Anal. Sci.* **25**, 71–72.
Song, L.-H., Liang, F.-P., Hu, R.-X., Ma, Y.-S., Chen, M.-S. & Zhang, Z. (2004). *Chin. J. Struct. Chem.* **23**, 1069–1072.
Su, C.-C. & Chiu, S.-Y. (1996). *Polyhedron*, **15**, 2623–2631.
Uçar, I., Bulut, I., Bulut, A. & Karadağ, A. (2009). *Struct. Chem.* **20**, 825–838.
Wang, Y.-F., Li, Z., Sun, Y.-C. & Zhao, J.-S. (2014). *Synth. React. Inorg. Met-Org. Nano-Met Chem.* **44**, 277–281.
Wei, J., Zhang, D., Yang, Q., Chen, S. & Gao, S. (2013). *Inorg. Chem. Commun.* **30**, 13–16.
Xiang, J., Mei, P. & Li, Q. (2006). *Acta Cryst.* **E62**, m2380.
Yang, Q., Chen, S., Xie, G. & Gao, S. (2012). *J. Coord. Chem.* **65**, 2584–2592.
Yenikaya, C., Büyükkidan, N., Sari, M., Keşli, R., Ilkimen, H., Bülbül, M. & Büyükgüngor, O. (2011). *J. Coord. Chem.* **64**, 3353–3365.

Table S2. Optimized molecular specification of compounds (I) - (IV) at B3LYP/6-31g(d, p) level of theory

Compound I (dimer)			
	x	***y***	***z***
Cu	-2.35790100	-0.51810000	0.08649200
N	-1.41700700	-2.16296400	0.37065800
O	-3.69222400	-1.80334600	-0.68167100
O	-3.86267600	-3.95904300	-1.37152100
C	-3.28010000	-3.05053300	-0.80774100
C	-1.94793000	-3.28400600	-0.11260700
C	-1.28870000	-4.49846700	0.05864100
H	-1.73090000	-5.40510900	-0.33747700
C	-0.07129200	-4.49157700	0.74730000
H	0.46381900	-5.42332400	0.90466200
C	0.46620700	-3.29340400	1.23269500
H	1.41214700	-3.25510000	1.75978200
C	-0.25403900	-2.12159700	1.02015400
C	0.12755200	-0.69924000	1.39047700
O	-0.83035400	0.14728300	1.25648700
O	1.29905500	-0.44719200	1.72355700
N	-3.55655600	1.06014600	0.29130100
N	-5.02227200	0.49082200	-1.43447900
H	-5.83385000	0.74408700	-1.97428900
H	-4.66320700	-0.46498400	-1.44637000
C	-4.62234800	1.37113800	-0.50568800
N	-5.31356700	2.53228300	-0.42316700
C	-4.94412400	3.39027800	0.51733900
H	-5.51284300	4.31803200	0.56479700
C	-3.89397500	3.14792300	1.40924200
H	-3.61250400	3.85567800	2.17816200
C	-3.21594800	1.95380200	1.24066700
H	-2.36221600	1.67967600	1.85117500
O	-4.19521700	-1.74854200	2.12335500
H	-5.01669200	-1.41943200	2.50757600
H	-4.37899500	-1.83674700	1.17343900
Cu	2.35770300	0.51793800	-0.08616100
N	1.41682900	2.16280600	-0.37046100
O	3.69199900	1.80321400	0.68195100
O	3.86250200	3.95895900	1.37163400
C	3.27990500	3.05042100	0.80792200
C	1.94775200	3.28387000	0.11275100
C	1.28854100	4.49832800	-0.05858800
H	1.73074600	5.40499200	0.33747700
C	0.07114700	4.49141000	-0.74727100
H	-0.46395200	5.42315300	-0.90469900
C	-0.46635400	3.29321300	-1.23260800
H	-1.41228800	3.25488800	-1.75970500

C	0.25387800	2.12141300	-1.01998600
C	-0.12770600	0.69903600	-1.39024200
O	0.83022700	-0.14746200	-1.25623000
O	-1.29916600	0.44697200	-1.72343300
N	3.55663300	-1.06007600	-0.29142900
N	5.02251400	-0.49082300	1.43423200
H	5.83428900	-0.74400500	1.97378700
H	4.66327300	0.46491400	1.44636200
C	4.62265900	-1.37099900	0.50527200
N	5.31413700	-2.53195900	0.42234900
C	4.94470000	-3.38983600	-0.51826900
H	5.51364800	-4.31743200	-0.56607100
C	3.89432300	-3.14752000	-1.40991300
H	3.61287600	-3.85515900	-2.17894800
C	3.21604600	-1.95359900	-1.24092900
H	2.36214200	-1.67952400	-1.85121900
O	4.19558200	1.74923400	-2.12317700
H	5.01729400	1.42053500	-2.50724100
H	4.37897400	1.83697300	-1.17314400

Compound II (dimer)

	x	***y***	***z***
C	-4.93038500	-0.69251700	-0.77101200
C	-6.13075000	-0.17144200	-1.27832500
H	-6.72171000	-0.77067400	-1.96257200
C	-6.51781400	1.12465400	-0.87136100
H	-7.44358400	1.55350000	-1.24545500
C	-5.70863500	1.86855700	0.01601600
H	-5.96983600	2.86845900	0.34552900
C	-4.52412000	1.27934100	0.48538300
C	-4.31697700	-2.05013000	-1.09331300
C	-3.50825200	1.89889600	1.44036600
C	-0.06616100	-2.47514100	0.78511400
C	1.26861500	-2.76878600	1.21350100
H	1.75256800	-3.66426600	0.83533800
C	1.92058000	-1.90738800	2.08504100
H	2.93131900	-2.13549900	2.41485400
C	1.26591100	-0.73266400	2.53872300
H	1.75009100	-0.02885200	3.20621000
C	-0.02976200	-0.49338000	2.09711300
H	-0.58143200	0.39385200	2.38862900
N	-4.18907300	0.03834200	0.08287600
N	-0.69707800	-1.34186600	1.24611100
N	-0.72047500	-3.31041300	-0.06711200
O	-3.16440000	-2.25251200	-0.44873400
O	-4.87788100	-2.83319000	-1.89028500
O	-2.53256200	1.05431100	1.77772000

O	-3.64359000	3.08599000	1.82188400
O	-3.47153500	-1.29391800	2.84169100
Cu	-2.56675400	-0.77394500	0.80966300
H	-1.68534500	-3.11971700	-0.37264200
H	-0.22175800	-4.09539000	-0.46148200
H	-3.25085000	-0.47043500	3.32440200
H	-3.43478200	-2.08736500	3.40711500
C	4.93147200	0.69206600	0.76928900
C	6.13170100	0.17041500	1.27633200
H	6.72363900	0.76978900	1.95961000
C	6.51733600	-1.12643000	0.87040500
H	7.44296500	-1.55573500	1.24432000
C	5.70689400	-1.87049600	-0.01568500
H	5.96695700	-2.87097800	-0.34433500
C	4.52260700	-1.28067800	-0.48486100
C	4.31945300	2.05051200	1.09069600
C	3.50546500	-1.90032600	-1.43841400
C	0.06750200	2.47700800	-0.78467300
C	-1.26749800	2.77118600	-1.21198900
H	-1.75064400	3.66711700	-0.83385700
C	-1.92074200	1.90970600	-2.08249000
H	-2.93163800	2.13823700	-2.41152700
C	-1.26718200	0.73433200	-2.53609000
H	-1.75234300	0.03046000	-3.20280100
C	0.02868900	0.49444600	-2.09538900
H	0.57951100	-0.39334900	-2.38679100
N	4.18895600	-0.03896300	-0.08340100
N	0.69727000	1.34301000	-1.24546400
N	0.72318500	3.31246100	0.06633300
O	3.16659600	2.25323500	0.44672600
O	4.88161100	2.83390900	1.88644700
O	2.53045800	-1.05513900	-1.77618400
O	3.63923400	-3.08807900	-1.81847800
O	3.47079200	1.29154400	-2.84282100
Cu	2.56682600	0.77397700	-0.80992200
H	1.68822100	3.12132700	0.37111600
H	0.22555000	4.09836400	0.46020900
H	3.24944200	0.46793000	-3.32498900
H	3.43461200	2.08465800	-3.40875000

Compound III (dimer)			
	x	***y***	***z***
Cu	-2.33176400	0.61299300	-0.04720600
N	-1.39920000	2.23044000	-0.52920000
O	-0.80973700	-0.13833800	-1.21281600
N	-3.65298600	-0.87363700	-0.41086600
O	-3.58788800	1.93697200	0.68743900

O	-3.91445900	4.16683800	0.94014300
C	-1.94584000	3.38850900	-0.16459700
C	-0.23512600	2.13832200	-1.17351300
C	-3.27188100	3.20265100	0.56022100
C	-4.89038800	-1.03244700	0.15432000
C	-3.22935200	-1.85646000	-1.23282200
H	-2.24534000	-1.70931500	-1.66465100
C	0.47148100	3.29061200	-1.50460000
H	1.42082800	3.21133300	-2.02113400
N	-5.68347600	-2.11258700	-0.05098100
C	-1.30777000	4.58779200	-0.47195200
H	-1.76770700	5.52447300	-0.17912700
C	-5.22939500	-3.05408100	-0.86345600
H	-5.88421100	-3.91179200	-1.01224400
C	-0.08690400	4.52601800	-1.15184500
H	0.43522100	5.44347100	-1.40666100
C	-3.98866700	-2.97912000	-1.50598700
H	-3.63404300	-3.75385300	-2.17346800
O	1.33403800	0.40693500	-1.67601300
N	-5.36779500	-0.08407600	0.96956800
C	0.15337800	0.68901200	-1.39710400
H	-4.89903100	0.82105500	1.06259200
H	-6.30039600	-0.22707100	1.32189800
Cu	2.33176600	-0.61299000	0.04720300
N	1.39918000	-2.23042400	0.52920200
O	0.80975700	0.13836100	1.21283200
N	3.65301400	0.87362000	0.41086200
O	3.58786000	-1.93698700	-0.68745900
O	3.91439800	-4.16685900	-0.94016200
C	1.94579800	-3.38850000	0.16459100
C	0.23511100	-2.13829000	1.17352200
C	3.27183900	-3.20266200	-0.56023100
C	4.89042800	1.03240200	-0.15430600
C	3.22938400	1.85646100	1.23279900
H	2.24536500	1.70933700	1.66461800
C	-0.47151200	-3.29057000	1.50461000
H	-1.42085400	-3.21127700	2.02115100
N	5.68353200	2.11253000	0.05099600
C	1.30771100	-4.58777400	0.47194500
H	1.76763200	-5.52446200	0.17911500
C	5.22945500	3.05404200	0.86345200
H	5.88428800	3.91173900	1.01224800
C	0.08685000	-4.52598300	1.15184700
H	-0.43528800	-5.44342900	1.40666300
C	3.98871600	2.97910900	1.50596500
H	3.63409800	3.75385300	2.17343700
O	-1.33402400	-0.40688200	1.67603800

N	5.36782600	0.08402200	-0.96954900
C	-0.15337000	-0.68897500	1.39712200
H	4.89903200	-0.82109000	-1.06260200
H	6.30043000	0.22700200	-1.32187700

Compound III (Tetramer)

	x	***y***	***z***
Cu	-0.06584000	-8.48014700	0.31763400
N	-0.59121600	-7.60151600	1.95114700
O	-1.38173300	-7.06777800	-0.39810200
N	-0.33972500	-9.82053900	-1.17326900
O	0.82415500	-9.66061700	1.61628300
O	1.15408800	-9.97394300	3.83762800
C	-0.14178700	-8.10981800	3.09680600
C	-1.33868800	-6.49936600	1.88039500
C	0.69571900	-9.36342500	2.88683800
C	0.28902300	-11.02769400	-1.32782800
C	-1.17181300	-9.43802000	-2.16441800
H	-1.65492300	-8.47767900	-2.02068200
C	-1.69589600	-5.82283300	3.04279900
H	-2.29592200	-4.92264700	2.98004100
N	0.12767600	-11.83321300	-2.40665500
C	-0.46705100	-7.49904500	4.30549900
H	-0.10338000	-7.92752800	5.23220200
C	-0.69880700	-11.42059500	-3.35474000
H	-0.81178700	-12.08461300	-4.21087900
C	-1.25510100	-6.34405600	4.26603900
H	-1.52453900	-5.84336300	5.19116200
C	-1.39822800	-10.21052700	-3.28844600
H	-2.07550100	-9.88925500	-4.06921600
O	-2.03167900	-4.97991300	0.17040900
N	1.12305900	-11.46215100	-0.37590700
C	-1.63551300	-6.13027900	0.43976100
H	1.21523700	-10.97133800	0.51806400
H	1.53222000	-12.37091600	-0.52027100
Cu	-0.38751700	-3.80609700	-0.76887400
N	0.16401200	-4.60211700	-2.43720900
O	0.90191800	-5.26105900	-0.10293800
N	-0.06429800	-2.50222700	0.73107200
O	-1.26258500	-2.55758700	-2.02979800
O	-1.39933800	-2.04122900	-4.23254100
C	-0.22842300	-4.01050400	-3.56358000
C	0.90218000	-5.71219000	-2.40819200
C	-1.04417500	-2.75275200	-3.30027400
C	-0.79277300	-1.37968500	1.00518600
C	0.97792400	-2.76646000	1.54914800
H	1.52931600	-3.67235900	1.32094200

C	1.29812500	-6.31685100	-3.59771500
H	1.88806600	-7.22550100	-3.57085200
N	-0.53674800	-0.54153900	2.03425300
C	0.14471100	-4.54165300	-4.79579600
H	-0.16680900	-4.04393800	-5.70668400
C	0.50551500	-0.81917700	2.80874300
H	0.72206700	-0.10449800	3.60052000
C	0.91481700	-5.70967300	-4.80042100
H	1.21926000	-6.15037500	-5.74504900
C	1.31536300	-1.94513500	2.60704800
H	2.16294300	-2.16237400	3.24439800
O	1.52386300	-7.33110100	-0.76346400
N	-1.84514800	-1.07716800	0.22218300
C	1.15559400	-6.16206900	-0.98123100
H	-1.90901700	-1.47905900	-0.71344400
H	-2.28151600	-0.18845800	0.41073500
Cu	0.38751700	3.80609700	0.76887400
N	-0.16401200	4.60211700	2.43720900
O	-0.90191800	5.26105900	0.10293800
N	0.06429800	2.50222700	-0.73107200
O	1.26258500	2.55758700	2.02979800
O	1.39933800	2.04122900	4.23254100
C	0.22842300	4.01050400	3.56358000
C	-0.90218000	5.71219000	2.40819200
C	1.04417500	2.75275200	3.30027400
C	0.79277300	1.37968500	-1.00518600
C	-0.97792400	2.76646000	-1.54914800
H	-1.52931600	3.67235900	-1.32094200
C	-1.29812500	6.31685100	3.59771500
H	-1.88806600	7.22550100	3.57085200
N	0.53674800	0.54153900	-2.03425300
C	-0.14471100	4.54165300	4.79579600
H	0.16680900	4.04393800	5.70668400
C	-0.50551500	0.81917700	-2.80874300
H	-0.72206700	0.10449800	-3.60052000
C	-0.91481700	5.70967300	4.80042100
H	-1.21926000	6.15037500	5.74504900
C	-1.31536300	1.94513500	-2.60704800
H	-2.16294300	2.16237400	-3.24439800
O	-1.52386300	7.33110100	0.76346400
N	1.84514800	1.07716800	-0.22218300
C	-1.15559400	6.16206900	0.98123100
H	1.90901700	1.47905900	0.71344400
H	2.28151600	0.18845800	-0.41073500
Cu	0.06584000	8.48014700	-0.31763400
N	0.59121600	7.60151600	-1.95114700
O	1.38173300	7.06777800	0.39810200

N	0.33972500	9.82053900	1.17326900
O	-0.82415500	9.66061700	-1.61628300
O	-1.15408800	9.97394300	-3.83762800
C	0.14178700	8.10981800	-3.09680600
C	1.33868800	6.49936600	-1.88039500
C	-0.69571900	9.36342500	-2.88683800
C	-0.28902300	11.02769400	1.32782800
C	1.17181300	9.43802000	2.16441800
H	1.65492300	8.47767900	2.02068200
C	1.69589600	5.82283300	-3.04279900
H	2.29592200	4.92264700	-2.98004100
N	-0.12767600	11.83321300	2.40665500
C	0.46705100	7.49904500	-4.30549900
H	0.10338000	7.92752800	-5.23220200
C	0.69880700	11.42059500	3.35474000
H	0.81178700	12.08461300	4.21087900
C	1.25510100	6.34405600	-4.26603900
H	1.52453900	5.84336300	-5.19116200
C	1.39822800	10.21052700	3.28844600
H	2.07550100	9.88925500	4.06921600
O	2.03167900	4.97991300	-0.17040900
N	-1.12305900	11.46215100	0.37590700
C	1.63551300	6.13027900	-0.43976100
H	-1.21523700	10.97133800	-0.51806400
H	-1.53222000	12.37091600	0.52027100

Compound IV (dimer)			
	x	***y***	***z***
Cu	2.08548000	-1.13337200	-0.02993700
O	2.92796200	-2.75002600	-0.82059500
N	0.85603400	-2.47502300	0.59198900
O	0.86557900	-0.00871300	1.17077500
O	2.74100100	-5.00296000	-0.92341900
O	-1.30566700	-0.01329200	1.77814300
N	3.76631300	-0.03367200	0.27776700
N	5.19191700	-1.26840800	-1.10136400
C	-0.24975600	-0.58338900	1.44929100
N	6.03526100	0.63756800	-0.15069800
C	-1.15921400	-3.02531000	1.69598300
H	-2.03147100	-2.70144600	2.25205800
C	2.35439600	-3.89958100	-0.57313000
C	1.08108300	-3.73959900	0.24326900
C	0.19274300	-4.74015300	0.63070400
H	0.39521400	-5.76656000	0.34652600
C	4.99057400	-0.20638800	-0.30900500
C	4.65609700	1.95269400	1.28335100
H	4.51567700	2.81335500	1.92543100

C	3.63087900	1.05328300	1.06367200
H	2.65381100	1.18154900	1.51703600
C	5.87604500	1.69985100	0.63335900
C	-0.21877400	-2.08748100	1.28189000
C	-0.93469900	-4.36901300	1.36978500
H	-1.64631300	-5.12560000	1.68648200
C	7.07018200	2.59876300	0.80675400
H	7.75785800	2.16394600	1.54156000
H	7.61574800	2.68656700	-0.13548600
H	6.78185400	3.59172000	1.15979400
H	6.11952500	-1.37793200	-1.47700500
H	4.49618000	-2.01327000	-1.17920500
Cu	-2.08529000	1.13321400	0.03016900
O	-2.92880000	2.74947200	0.82047800
N	-0.85645400	2.47544200	-0.59166400
O	-0.86481500	0.00905600	-1.17026800
O	-2.74254400	5.00244000	0.92393800
O	1.30650100	0.01463400	-1.77738100
N	-3.76586200	0.03326400	-0.27809100
N	-5.19004000	1.26418200	1.10590400
C	0.25029600	0.58424900	-1.44869900
N	-6.03414800	-0.63951100	0.15121700
C	1.15872100	3.02660000	-1.69532400
H	2.03121900	2.70314400	-2.25125700
C	-2.35558000	3.89927300	0.57338600
C	-1.08211800	3.73990200	-0.24293100
C	-0.19414500	4.74084500	-0.63020400
H	-0.39708100	5.76715800	-0.34601700
C	-4.98953500	0.20425000	0.31046300
C	-4.65634200	-1.95068800	-1.28775800
H	-4.51645600	-2.80968300	-1.93217400
C	-3.63104300	-1.05157900	-1.06693600
H	-2.65439400	-1.17855100	-1.52157800
C	-5.87555100	-1.69980900	-0.63573000
C	0.21862100	2.08835400	-1.28139700
C	0.93356000	4.37020000	-1.36913500
H	1.64489400	5.12710200	-1.68571200
C	-7.06968000	-2.59865100	-0.80954100
H	-7.76328900	-2.15738500	-1.53481500
H	-7.60843600	-2.69645900	0.13568800
H	-6.78266700	-3.58775700	-1.17418900
H	-6.11759300	1.37315200	1.48187200
H	-4.49523500	2.01001200	1.18278800

Compound IV (Tetramer)

	x	***y***	***z***
Cu	-7.89018800	0.69166600	-0.58816200

O	-8.91384100	1.85649900	-1.80056100
N	-7.31613300	2.41102000	0.07023900
O	-6.80991000	0.13875800	1.07532600
O	-9.31214000	4.03214700	-2.30138400
O	-5.01267700	0.91308900	2.20610500
N	-9.13424800	-0.89643600	-0.59647200
N	-10.30657500	-0.34565600	-2.54236700
C	-6.04043700	1.06457700	1.52097100
N	-10.81351100	-2.33929100	-1.53449600
C	-5.98770600	3.68742800	1.54696900
H	-5.26960900	3.72227800	2.35769400
C	-8.76492800	3.15076300	-1.66019300
C	-7.79182700	3.49439400	-0.54054200
C	-7.39652700	4.76176700	-0.11927600
H	-7.79822100	5.63643700	-0.61750100
C	-10.08009200	-1.20236200	-1.53745200
C	-9.68158300	-2.97344600	0.46767900
H	-9.51994700	-3.67622400	1.27555200
C	-8.95904600	-1.80020900	0.39094600
H	-8.20150700	-1.54596800	1.12436900
C	-10.62270300	-3.21164000	-0.54986800
C	-6.44345500	2.45890700	1.07769300
C	-6.48548100	4.84702400	0.93862100
H	-6.15701000	5.82067800	1.28989800
C	-11.47901400	-4.44864500	-0.56237000
H	-12.42816100	-4.24758900	-0.05123800
H	-11.71328000	-4.73435100	-1.58967000
H	-10.99298900	-5.28117700	-0.04737000
H	-11.04823700	-0.59142900	-3.17767600
H	-9.90984300	0.59757000	-2.53271200
Cu	-3.38570500	-0.12472300	1.03472100
O	-2.43032100	-1.32629000	2.28214300
N	-4.02822800	-1.82634700	0.39012100
O	-4.43920200	0.44984700	-0.64784100
O	-2.10110300	-3.51138600	2.77576500
O	-6.25822600	-0.26677400	-1.78409800
N	-2.17848500	1.47509400	1.09800700
N	-0.62170300	0.67069000	2.64701300
C	-5.24256100	-0.44769200	-1.08540600
N	-0.41490300	2.85043500	1.97767600
C	-5.42679300	-3.06071900	-1.05947400
H	-6.14336600	-3.07149200	-1.87228500
C	-2.62459600	-2.60825300	2.13590400
C	-3.61534600	-2.92176400	1.02475400
C	-4.08578100	-4.17328900	0.63478900
H	-3.74191200	-5.05836700	1.15692900
C	-1.08706500	1.67978600	1.89343700

C	-1.93315700	3.74633700	0.37201000
H	-2.26458200	4.56579300	-0.25312300
C	-2.57576100	2.53000600	0.34853600
H	-3.43469600	2.35072100	-0.28736900
C	-0.82457400	3.87069300	1.23088000
C	-4.90464600	-1.84969700	-0.61501600
C	-4.99850900	-4.23211200	-0.42328000
H	-5.38309300	-5.19335500	-0.75112300
C	-0.04243100	5.14900000	1.31736000
H	0.51216700	5.19080900	2.25653800
H	-0.69464800	6.02298000	1.23198100
H	0.66886200	5.17100300	0.48382800
H	0.14129800	0.89150100	3.26544100
H	-1.11832900	-0.22000500	2.71100600
Cu	3.27719200	0.20322100	-0.12402100
O	1.94889500	1.46731800	-0.86402700
N	4.14818100	1.86995500	0.30738900
O	4.85813400	-0.45589200	1.02033800
O	1.53023800	3.67496900	-1.15345700
O	6.97979600	0.19473900	1.45074300
N	2.07827300	-1.37224600	0.20782100
N	0.27175900	-0.67156800	-1.09959800
C	5.78544300	0.41611800	1.17606000
N	0.18313000	-2.78645600	-0.22178600
C	6.00676300	3.02669400	1.19449300
H	6.97155900	2.99542400	1.68681900
C	2.22028900	2.73961200	-0.76904600
C	3.55455900	2.99616600	-0.08305400
C	4.16212100	4.22545100	0.16101100
H	3.67056100	5.13635100	-0.15973800
C	0.85674400	-1.62178000	-0.35426600
C	1.96215800	-3.56844000	1.16063300
H	2.40472100	-4.34062000	1.77717000
C	2.60051000	-2.36356000	0.96466200
H	3.56899100	-2.15272800	1.40397500
C	0.72291000	-3.75086700	0.51967000
C	5.33173400	1.84084600	0.92106200
C	5.40030100	4.22912600	0.81170200
H	5.89875700	5.17182100	1.01711800
C	-0.05698000	-5.02524100	0.66431100
H	-0.61461100	-5.23089200	-0.25235600
H	0.59521100	-5.87066900	0.89793300
H	-0.77751800	-4.90323500	1.48210900
H	-0.62329400	-0.89667400	-1.50155300
H	0.67265400	0.26348500	-1.18742600
Cu	8.02003100	-0.75661000	-0.29437600
O	9.35312100	-2.01037400	0.43032300

N	7.16015900	-2.42202100	-0.74539700
O	6.44414300	-0.09045000	-1.43765700
O	9.78849700	-4.21926500	0.70340800
O	4.32713600	-0.74500700	-1.88021100
N	9.25817400	0.78530000	-0.68900900
N	11.01138700	0.11890700	0.70562500
C	5.52090900	-0.96643200	-1.60585600
N	11.22595100	2.12963800	-0.37176200
C	5.32521300	-3.58135600	-1.67401800
H	4.36375700	-3.55382000	-2.17303800
C	9.09508100	-3.29057800	0.32357800
C	7.76741500	-3.54806400	-0.37637100
C	7.18145900	-4.77994200	-0.65765900
H	7.68976100	-5.69006100	-0.36108800
C	10.48749400	1.02090400	-0.13564800
C	9.49432600	2.87837800	-1.83261700
H	9.09305800	3.61620300	-2.51619600
C	8.79012000	1.73043000	-1.53179200
H	7.81194100	1.53137100	-1.95599200
C	10.74278600	3.04424600	-1.20657900
C	5.98217800	-2.39280800	-1.37001600
C	5.94739300	-4.78428200	-1.31608600
H	5.46426300	-5.72845900	-1.54935200
C	11.60584500	4.24805800	-1.47019100
H	12.29549100	4.03591800	-2.29601000
H	12.20815400	4.48024600	-0.58982600
H	11.00803400	5.11886100	-1.75118600
H	11.94136800	0.31149000	1.04058900
H	10.59629700	-0.81064400	0.80793600

Table S3 Wiberg and Mayer bond order indices of all of the computed coordination compounds at B3LYP/6–31g(d,p) level of theory.

Compound I (dimer)	**Wiberg indices**	**Mayer indices**
Cu1-O1	0.130	0.400
Cu1-O3	0.267	0.439
Cu1-N11	0.262	0.435
Cu1-N1	0.257	0.458
Cu1-O1W	0.130	0.238
Cu1a-O4a	0.108	0.191
Cu1a-O1a	0.244	0.400
Cu1a-O3a	0.267	0.439
Cu1a-N11a	0.262	0.435
Cu1a-O1Wa	0.130	0.238
Cu1a-O4a	0.108	0.191
Cu1a-N1a	0.257	0.458

Symmetry code: (a) 1-*x*, 1-*y*, 1-*z*

Compound II (dimer)	**Wiberg indices**	**Mayer indices**
Cu1-O3	0.269	0.435
Cu1-O1	0.277	0.464
Cu1-O5	0.150	0.270
Cu1-N2	0.289	0.476
Cu1-N1	0.000	0.001
Cu1-N3a	0.277	0.464
Cu1a-O1a	0.269	0.435
Cu1a-O3a	0.263	0.460
Cu1-N1a	0.289	0.476
Cu1a-N2a	0.150	0.270
Cu1a-O5a	0.000	0.001

Symmetry code: (a) 1-*x*, 1-*y*, 1-*z*

Compound III (dimer)	**Wiberg indices**	**Mayer indices**
Cu1-N2	0.284	0.474
Cu1-N1	0.280	0.443
Cu1-O1	0.252	0.385
Cu1-O2	0.303	0.483
Cu1-O4a	0.195	0.311
Cu1a-N2a	0.280	0.443
Cu29-N1a	0.285	0.474

Cu1a-O2a	0.303	0.483
Cu1a-O1a	0.252	0.385
Cu1a-O4	0.195	0.311

Symmetry code= (a) -*x*, 1-*y*, -*z*

Compound III (tetramer)	**Wiberg indices**	**Mayer indices**
Cu1-N1	0.286	0.476
Cu1-N2	0.281	0.443
Cu1-O1	0.253	0.385
Cu1-O2	0.303	0.483
Cu1-O4a	0.190	0.308
Cu1a-N1a	0.280	0.472
Cu1a-N2a	0.279	0.449
Cu1a-O1a	0.252	0.392
Cu1a-O2a	0.293	0.464
Cu1a-O4	0.193	0.317
Cu1a-N4b	0.000	0.002
Cu1b-N1b	0.280	0.472
Cu1b-N2b	0.279	0.449
Cu1b-O2b	0.291	0.464
Cu1b-O1b	0.252	0.392
Cu1b-N4a	0.000	0.002
Cu1b-O4c	0.193	0.317
Cu1c-N2c	0.281	0.443
Cu1c-N1c	0.286	0.476
Cu1c-O1c	0.253	0.385
Cu1c-O2c	0.303	0.483
Cu1c-O4b	0.190	0.308

Symmetry code= (a) -*x*, 1-*y*, -*z*; (b) *x*, 1+*y*, *z*; (c) –*x*, 2-*y*, -*z*

Compound IV (dimer)	**Wiberg indices**	**Mayer indices**
Cu1-N1	0.286	0.476
Cu1-N2	0.281	0.445
Cu1-O1	0.298	0.477
Cu1-O2	0.256	0.392
Cu1-O3a	0.192	0.314
Cu1a-N1a	0.286	0.476
Cu1a-N2a	0.281	0.445
Cu1a-O1a	0.298	0.477
Cu1a-O2a	0.256	0.392

Cu1-O3	0.192	0.314

Symmetry code= (a) 1-*x*, 1-*y*, -*z*

Compound IV (tetramer)	**Wiberg indices**	**Mayer indices**
Cu1-N1	0.284	0.473
Cu1-N2	0.283	0.447
Cu1-O1	0.302	0.482
Cu1-O2	0.252	0.384
Cu1-O3a	0.191	0.310
Cu1a-N1a	0.275	0.470
Cu1a-N2a	0.284	0.463
Cu1a-O2a	0.246	0.385
Cu1a-O1a	0.288	0.472
Cu1a-O3	0.183	0.298
Cu1a-N4b	0.004	0.027
Cu1b-N1b	0.279	0.471
Cu1b-N2b	0.285	0.460
Cu1b-O2b	0.250	0.385
Cu1b-O1b	0.292	0.467
Cu1b-N4a	0.003	0.018
Cu1b-3c	0.018	0.304
Cu1c-N1c	0.284	0.473
Cu1c-N2c	0.283	0.448
Cu1c-O2c	0.253	0.386
Cu1c-O1c	0.302	0.482
Cu1c-O3b	0.018	0.308

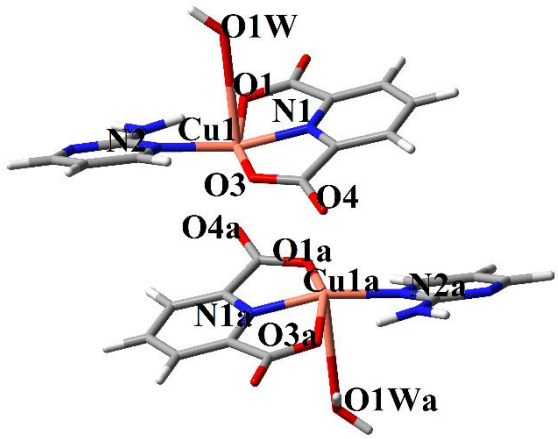
Symmetry code= (a) 1-*x*, 1-*y*, -*z*; (b) 1-*x*, 2-*y*, -*z*; (c) *x*, 1+*y*, *z*

Table S4. Optimized bond lengths (X-ray data), Mayer and Wiberg bond order indices of compound (I)

	Bond length (Exp.)	Wiberg bond order	Mayer bond order
Cu1-N1	1.916 (1.911)	0.257	0.458
Cu1-O1	2.051(2.027)	0.244	0.400
Cu1-O3	2.028 (2.017)	0.267	0.439
Cu1-N11	1.984 (1.988)	0.262	0.435
Cu1-O1W	2.406 (2.346)	0.130	0.238
Cu1-O4a	2.663 (2.968)	0.108	0.191
N1-C2	1.331 (1.331)	1.327	1.205
N1-C6	1.331 (1.330)	1.325	1.204
C2-C1	1.513 (1.519)	0.962	0.919
C1-O1	1.318 (1.275)	1.165	1.124
C1-O2	1.222 (1.218)	1.675	1.786
C2-C3	1.392 (1.372)	1.394	1.414
C3-C4	1.398 (1.382)	1.434	1.399
C4-C5	1.399 (1.388)	1.434	1.396
C5-C6	1.392 (1.379)	1.393	1.406
C6-C7	1.514 (1.517)	0.956	0.922
C7-O3	1.298 (1.284)	1.262	1.192
C7-O4	1.237 (1.222)	1.558	1.574
N11-C12	1.366 (1.365)	1.223	1.154
C12-N12	1.336 (1.321)	1.304	1.212
C12-N13	1.356 (1.353)	1.283	1.298
N13-C14	1.325 (1.318)	1.478	1.459
C14-C15	1.399 (1.372)	1.372	1.345
C15-C16	1.382 (1.364)	1.459	1.449
N11-C16	1.347 (1.340)	1.340	1.280
Cu1a-O1Wa	2.406	0.129	0.238
Cu1a-N1a	1.916	0.257	0.458
Cu1a-N11a	1.984	0.262	0.435
Cu1a-O1a	2.051	0.244	0.400
Cu1a-O3a	2.028	0.267	0.439
Cu1a-O4	2.661	0.108	0.191
N1a-C6a	1.331	1.325	1.204
C6a-C5a	1.392	1.393	1.406
C5a-C4a	1.399	1.434	1.396
C4a-C3a	1.398	1.434	1.399
C3a-C2a	1.392	1.394	1.414
C2a-C1a	1.513	0.962	0.919
C1a-O1a	1.318	1.165	1.124
C1a-O2a	1.222	1.675	1.786
C7a-O3a	1.298	1.262	1.192
C7a-O4a	1.237	1.558	1.574
N11a-C12a	1.366	1.223	1.154
N12a-C12a	1.336	1.304	1.212
C12a-N13a	1.356	1.283	1.298
N13a-C14a	1.325	1.478	1.459
C14a-C15a	1.399	1.372	1.346
C15a-C16a	1.382	1.459	1.449
C16a-N11a	1.347	1.340	1.280

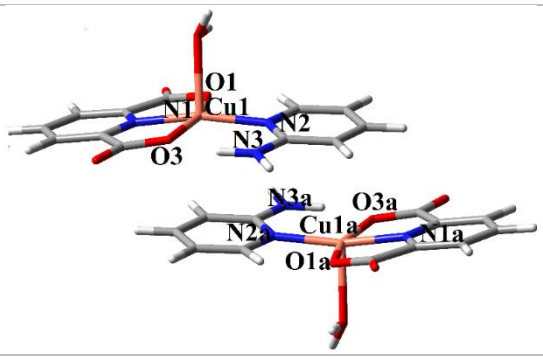
Compound (I), optimized dimer fragment

Symmetry code: a) 1-x,



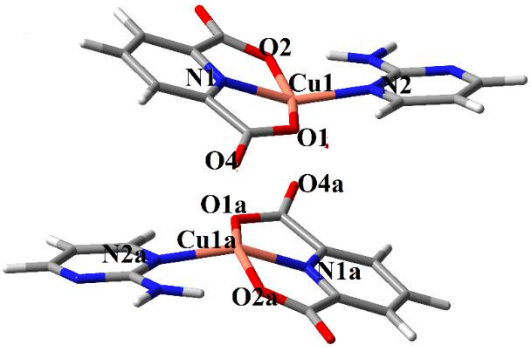
Symmetry code: (a) 1-*x*, 1-*y*, 1-*z*

Compound (II), optimized dimer fragment



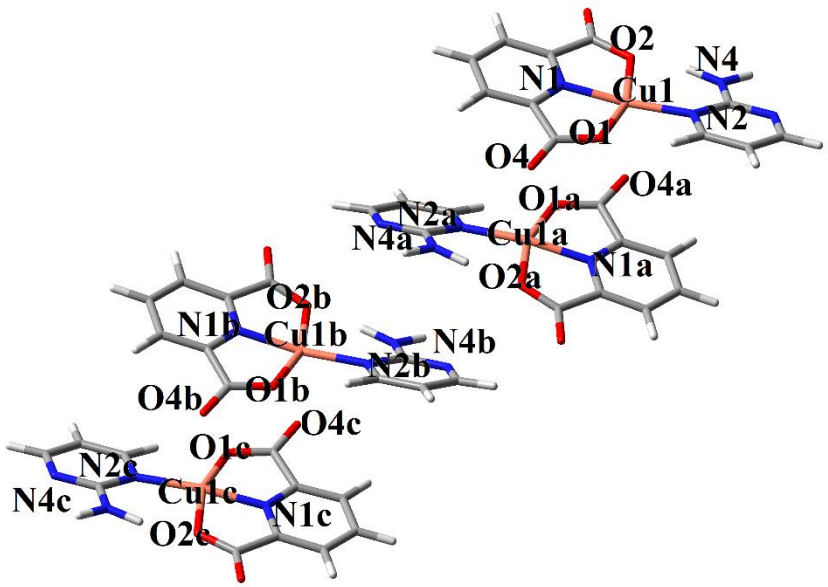
Symmetry code: (a) 1-*x*, 1-*y*, 1-*z*

Compound (III), optimized dimer fragment



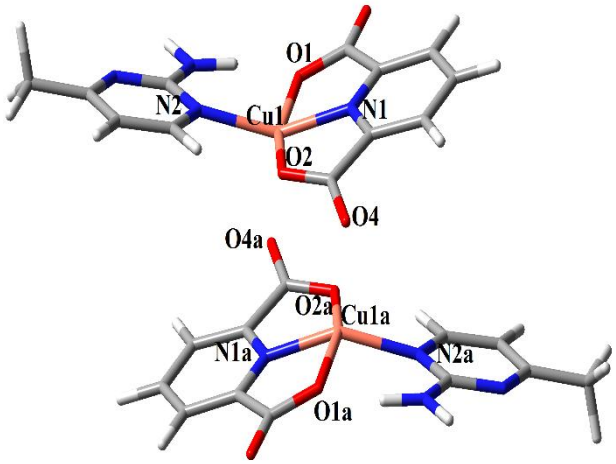
Symmetry code= (a) -*x*, 1-*y*, -*z*

Compound (III), optimized tetramer fragment



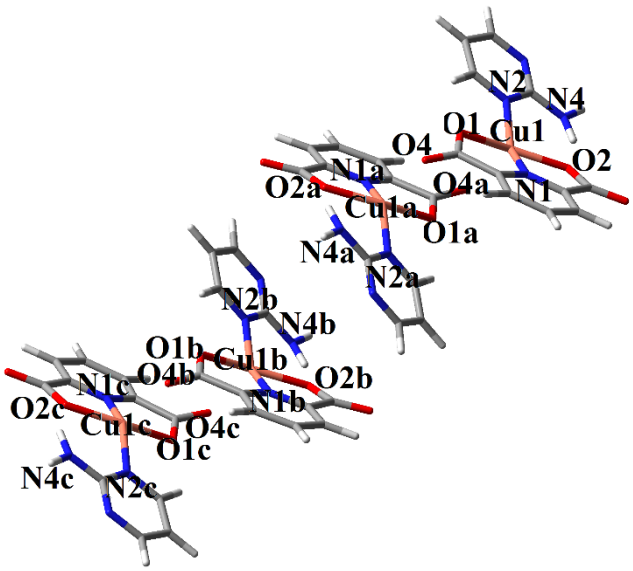
Symmetry code= (a) -*x*, 1-*y*, -*z*; (b) *x*, 1+*y*, *z*; (c) –*x*, 2-*y*, -*z*

Compound (IV), optimized dimer fragment



Symmetry code= (a) 1-*x*, 1-*y*, -*z*

Compound (IV), optimized tetramer fragment



Symmetry code= (a) 1-*x*, 1-*y*, -*z*; (b) 1-*x*, 2-*y*, -*z*; (c) *x*, 1+*y*, *z*

Figure S1: Optimized structures for all fragments of compounds I, II, III and IV at B3lYP/6–31g(d,p)