Fu-Jie Liu* and Guo-Xi Wang

Crystal Structure of tris(tetrakis{1-vinyl-1*H*-imidazole- κ N}copper(II)) bis [tri- μ_2 -bromido-tetrabromido-bis(1-vinyl-1*H*-imidazole- κ N)tetracopper(I)], $C_{80}H_{96}N_{32}Cu_{11}Br_{14}$

$\gamma = 74.464(2)^\circ$, $V = 2750.9(8) \text{ \AA}^3$, $Z = 1$, $R_{gt}(F) = 0.0432$, $wR_{ref}(F^2) = 0.0859$, $T = 296(2) \text{ K}$.

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The crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	$0.18 \times 0.17 \times 0.16 \text{ mm}$
Wavelength:	Mo $K\alpha$ radiation ($0.71073 \text{ \AA}$)
μ :	7.22 mm^{-1}
Diffraction, scan mode:	Bruker SMART, φ and ω -scans
$\theta_{\max}$, completeness:	25° , $>99\%$
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	41708, 9671, 0.083
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 5665
$N(\text{param})_{\text{refined}}$:	629
Programs:	Bruker programs [1], SHELX [2, 3], OLEX2 [4]

Source of material

1-Vinyl-1*H*-imidazole (1 mmol), copper(I) bromide (1 mmol), and methanol (2 mL) were added to deionized water (0.2 mL) in the heat-resistant glass tube. The mixtures were carefully stirred, and then frozen the tube, finally sealed with a gas burner. The tube was placed in the oven at 60°C under the hydro-thermal reaction conditions for 3 days to get good quality yellow block crystal appeared in the tube wall.

Experimental details

Hydrogen atoms were added using geometric restraints.

Discussion

Imidazole is of considerable interest as a versatile organic ligand in metal-organic systems in which it offers potential coordinate sites to synthesis coordination polymers [5–8]. The rational design of crystal structures based on the imidazole derivatives is an exciting research topic in metal-organic chemistry [9–11]. The transition metal (Cu)

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Abstract

$C_{80}H_{96}N_{32}Cu_{11}Br_{14}$, triclinic, $P\bar{1}$ (no. 2), $a = 11.370(2) \text{ \AA}$, $b = 14.287(3) \text{ \AA}$, $c = 17.621(3) \text{ \AA}$, $\alpha = 85.929(2)^\circ$, $\beta = 88.392(2)^\circ$,

***Corresponding author:** Fu-Jie Liu, Zhenjiang Key Laboratory of Functional Chemistry and Institute of Medicine and Chemical Engineering, Zhenjiang College, Zhenjiang, Jiangsu 212028, P.R. China; and Department of Chemical and Materials Engineering, Zhenjiang College, Zhenjiang, Jiangsu 212028, P.R. China, e-mail: liufj2019@126.com

Guo-Xi Wang: Zhenjiang Key Laboratory of Functional Chemistry and Institute of Medicine and Chemical Engineering, Zhenjiang College, Zhenjiang, Jiangsu 212028, P.R. China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
Br1	0.69435(6)	0.33237(5)	0.14653(4)	0.0563(2)
Br2	0.73557(8)	0.54387(6)	0.28770(4)	0.0710(2)
Br3	1.02242(6)	0.39541(5)	0.16195(4)	0.04680(19)
Br4	1.06701(6)	0.11054(5)	0.16952(4)	0.0587(2)
Br5	1.33063(6)	0.13219(5)	0.32275(4)	0.04979(19)
Br6	1.40609(6)	−0.07729(5)	0.16794(4)	0.0526(2)
Br7	1.16922(7)	−0.16903(7)	0.31610(5)	0.0850(3)
Cu1	0.52157(7)	0.24233(5)	0.24128(4)	0.0411(2)
Cu2	0.80650(8)	0.42127(6)	0.20410(5)	0.0552(2)
Cu3 ^a	1.0033(8)	0.2556(4)	0.2380(2)	0.0593(8)
Cu3A ^b	0.963(5)	0.2623(15)	0.228(2)	0.057(6)
Cu4	1.0000	0.5000	0.0000	0.0361(3)
Cu5	1.26290(8)	0.05462(6)	0.22447(5)	0.0585(3)
Cu6	1.35474(8)	−0.12991(7)	0.29517(5)	0.0685(3)
N1	0.3915(5)	0.3709(4)	0.2412(3)	0.0414(14)
N2	0.2281(5)	0.4756(4)	0.2814(3)	0.0464(14)
N3	0.8180(4)	0.5491(3)	0.0094(3)	0.0347(12)
N4	0.6311(4)	0.6099(4)	0.0525(3)	0.0399(13)
N5	0.4691(4)	0.2061(3)	0.1430(3)	0.0349(12)
N6	0.3621(4)	0.1742(3)	0.0507(3)	0.0356(12)
N7	0.9764(4)	0.3811(4)	−0.0451(3)	0.0355(12)
N8	0.9183(4)	0.2471(4)	−0.0497(3)	0.0455(14)
N9	0.5732(4)	0.2693(4)	0.3436(3)	0.0412(13)
N10	0.6227(4)	0.3411(4)	0.4394(3)	0.0435(14)
N11	0.9759(5)	0.2322(4)	0.3456(3)	0.0532(15)
N12	1.0208(6)	0.1570(6)	0.4580(4)	0.0656(18)
N13	0.6493(4)	0.1151(4)	0.2503(3)	0.0394(13)
N14	0.7352(5)	−0.0413(4)	0.2562(3)	0.0421(14)
N15	1.4873(5)	−0.1576(4)	0.3703(3)	0.0507(15)
N16	1.6396(5)	−0.2385(5)	0.4419(4)	0.0612(17)
C1	0.4036(6)	0.4629(5)	0.2245(4)	0.0468(18)
H1	0.4700	0.4781	0.1995	0.056*
C2	0.3034(7)	0.5283(5)	0.2500(4)	0.0510(19)
H2	0.2888	0.5956	0.2468	0.061*
C3	0.2838(6)	0.3830(5)	0.2745(4)	0.0460(18)
H3	0.2509	0.3321	0.2912	0.055*
C4	0.1078(8)	0.5075(6)	0.3176(4)	0.069(2)
H4	0.0613	0.4631	0.3254	0.083*
C5	0.0663(8)	0.5887(7)	0.3378(5)	0.091(3)
H5A	0.1111	0.6344	0.3306	0.109*
H5B	−0.0106	0.6058	0.3606	0.109*
C6	0.7340(6)	0.5394(5)	−0.0432(4)	0.0481(18)
H6	0.7536	0.5109	−0.0894	0.058*
C7	0.6209(6)	0.5772(5)	−0.0175(4)	0.0459(17)
H7	0.5487	0.5807	−0.0425	0.055*
C8	0.7511(6)	0.5911(4)	0.0661(4)	0.0403(16)
H8	0.7831	0.6060	0.1103	0.048*
C9	0.5379(7)	0.6546(5)	0.1031(4)	0.058(2)
H9	0.5614	0.6716	0.1492	0.069*
C10	0.4219(7)	0.6737(5)	0.0899(5)	0.073(2)
H10A	0.3951	0.6577	0.0444	0.087*
H10B	0.3655	0.7034	0.1260	0.087*
C11	0.5470(6)	0.1602(4)	0.0880(4)	0.0437(17)
H11	0.6317	0.1450	0.0900	0.052*

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
C12	0.4835(6)	0.1404(4)	0.0312(3)	0.0441(17)
H12	0.5152	0.1099	−0.0127	0.053*
C13	0.3586(5)	0.2133(4)	0.1181(3)	0.0344(15)
H13	0.2870	0.2419	0.1440	0.041*
C14	0.2607(6)	0.1683(5)	0.0097(4)	0.0529(19)
H14	0.1839	0.1940	0.0308	0.063*
C15	0.2653(7)	0.1306(5)	−0.0542(4)	0.072(2)
H15A	0.3404	0.1041	−0.0772	0.086*
H15B	0.1936	0.1295	−0.0778	0.086*
C16	0.9755(6)	0.3587(5)	−0.1195(4)	0.0478(18)
H16	0.9965	0.3949	−0.1612	0.057*
C17	0.9398(6)	0.2764(5)	−0.1231(4)	0.0533(19)
H17	0.9315	0.2457	−0.1667	0.064*
C18	0.9403(5)	0.3115(5)	−0.0056(4)	0.0426(17)
H18	0.9314	0.3082	0.0471	0.051*
C19	0.8814(7)	0.1617(6)	−0.0201(5)	0.075(3)
H19	0.8762	0.1506	0.0324	0.090*
C20	0.8570(7)	0.1043(6)	−0.0602(6)	0.102(3)
H20A	0.8615	0.1137	−0.1129	0.122*
H20B	0.8338	0.0507	−0.0384	0.122*
C21	0.6000(6)	0.2045(5)	0.4066(4)	0.0513(19)
H21	0.5970	0.1400	0.4080	0.062*
C22	0.6307(6)	0.2467(5)	0.4650(4)	0.0506(18)
H22	0.6531	0.2180	0.5133	0.061*
C23	0.5885(5)	0.3509(5)	0.3666(4)	0.0445(17)
H23	0.5770	0.4083	0.3359	0.053*
C24	0.6427(6)	0.4183(5)	0.4799(4)	0.059(2)
H24	0.6381	0.4774	0.4528	0.071*
C25	0.6670(6)	0.4117(6)	0.5524(4)	0.081(3)
H25A	0.6723	0.3536	0.5812	0.098*
H25B	0.6791	0.4651	0.5752	0.098*
C26	0.9248(6)	0.2930(6)	0.3998(5)	0.067(2)
H26	0.8772	0.3565	0.3902	0.081*
C27	0.9522(7)	0.2487(7)	0.4699(5)	0.079(3)
H27	0.9290	0.2753	0.5165	0.095*
C28	1.0335(6)	0.1500(6)	0.3820(5)	0.061(2)
H28	1.0771	0.0946	0.3586	0.073*
C29	1.0756(9)	0.0891(8)	0.5186(6)	0.099(3)
H29	1.0478	0.1027	0.5678	0.118*
C30	1.1548(9)	0.0161(7)	0.5107(6)	0.110(4)
H30A	1.1848	0.0002	0.4623	0.132*
H30B	1.1863	−0.0249	0.5529	0.132*
C31	0.7736(6)	0.0991(5)	0.2558(4)	0.052(2)
H31	0.8147	0.1473	0.2562	0.063*
C32	0.8257(6)	0.0042(5)	0.2604(4)	0.057(2)
H32	0.9087	−0.0258	0.2656	0.069*
C33	0.6313(6)	0.0290(5)	0.2506(3)	0.0425(17)
H33	0.5547	0.0179	0.2474	0.051*
C34	0.7427(6)	−0.1427(5)	0.2585(4)	0.0546(19)
H34	0.6725	−0.1608	0.2480	0.065*
C35	0.8367(7)	−0.2084(6)	0.2737(4)	0.078(3)
H35A	0.9086	−0.1929	0.2845	0.093*
H35B	0.8354	−0.2733	0.2742	0.093*
C36	1.5169(7)	−0.0959(5)	0.4179(4)	0.0559(19)
H36	1.4783	−0.0299	0.4192	0.067*

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C37	1.6101(7)	−0.1452(6)	0.4628(4)	0.063(2)
H37	1.6468	−0.1205	0.5004	0.076*
C38	1.5636(7)	−0.2422(6)	0.3872(4)	0.061(2)
H38	1.5646	−0.2986	0.3636	0.073*
C39	1.7327(8)	−0.3250(8)	0.4672(6)	0.099(3)
H39	1.7478	−0.3788	0.4381	0.119*
C40	1.7908(10)	−0.3307(9)	0.5233(6)	0.142(5)
H40A	1.7774	−0.2778	0.5533	0.170*
H40B	1.8497	−0.3880	0.5370	0.170*

Occupancies: ^a = 0.86(3), ^b = 0.14(3).

together with organic ligands, leads to synthesis of a functional complex. Which have the potential applications, such as catalytic organic reaction [12]. Here, we report the 1-vinyl-1H-imidazole react with copper(I) bromide to obtain the title complex.

Single crystal X-ray diffraction reveals that the copper atoms have four different coordination environments in its crystal structure, presenting a mixed-valence Cu (I/II) complex. The $Cu_1(II)$ and $Cu_4(II)$ atoms are in twisted tetrahedron coordination environments, respectively, resulting from four coordination of the N atoms of four ligands. The $Cu_2(I)$ and $Cu_5(I)$ atoms are in distorted trigonal planar geometry, which is defined by a terminal Br atom and two μ -bridging Br atoms. The center of $Cu_6(I)$ coordinates a N atom of the ligand, a terminal Br atom and a μ_2 -Br atom, and completes its coordination environment to a twisted triangle geometry. The central $Cu_3(I)$ coordinated with a N atom of the ligand and two μ_2 -Br atoms to form a distorted triangle geometry. Weak secondary interactions may be present, which gives $Cu_1(II)$ —Br₁ and $Cu_4(II)$ —Br₃ bond lengths with 3.0276(11) Å and 3.1102(8) Å. The Cu—Br bond lengths range from 2.3220(11) Å and 2.4196(12) Å in the complex, respectively. The Cu—N bonds lengths range from 1.993(5) Å and 2.2026(5) Å, which are all within a reasonable range [13].

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