Crystal structure of bis(1-phenylimidazolium) tetrachlorocuprate(II), $(C_9H_9N_2)_2(CuCl_4)$

U. Casellato[I], R. Ettorre[II] and R. Graziani*,[II]

[I] CNR, Istituto di Chimica e Tecnologie Inorganiche e dei Materiali Avanzati, Area della Ricerca, Corso Stati Uniti 4, I-35127 Padua, Italy
[II] Universita' di Padova, Dipartimento di Chimica Inorganica, Metallorganica e Analitica, Via Marzolo 1, I-35131 Padua, Italy

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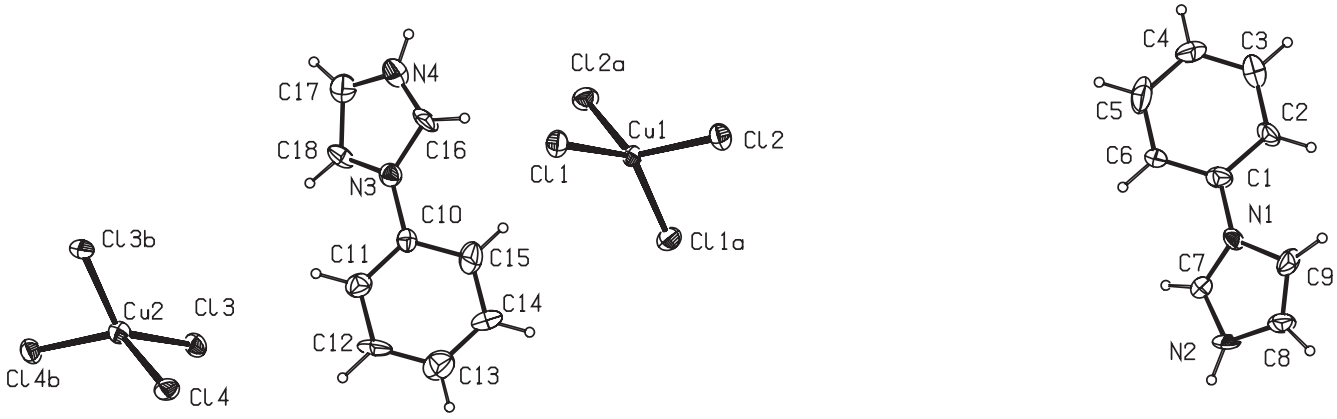

Abstract

$C_{18}H_{18}Cl_4CuN_4$, monoclinic, *C*121 (No. 5), a = 14.109(3) Å, b = 10.263(2) Å, c = 15.290(3) Å, β = 102.61(3)°, V = 2160.6 Å^3, Z = 4, $R_{gt}(F)$ = 0.040, $wR_{all}(F^2)$ = 0.124, T = 293 K.

Source of material

Crystals of the compound were obtained by slow evaporation of a mixture of $C_9H_8N_2$ and $CuCl_2$ (molar ratio 2 : 1) in concentrated HCl.

Discussion

The $(C_9H_9N_2)_2(CuCl_4)$ compound crystallizes in the monoclinic system and the unit cell of the *C*2 space group contains 4 $CuCl_4^{2-}$ anions and 8 organic cations. The copper atoms lie in special positions on different 2-fold symmetry axes. The structure consists of discrete anions and organic cations involved in a network of N–H···Cl bonds. The metal ions are in a distorted tetrahedral configuration with an average Cl–Cu–Cl *trans* angle of 133° which can be compared with values ranging from 125° and 145° [1] for the bulk of compounds containing isolated $CuCl_4^{2-}$ anions. All Cu—Cl bonds are comprised between 2.235(4) Å and 2.258(3) Å. The torsional angle between the imidazole and the phenyl rings is 31.5° which is significantly smaller than that of 46.5° corresponding to the torsional potential energy minimum calculated for unprotonated 1-phenylimidazole [2].

Table 1. Data collection and handling.

Crystal:	yellow block, size 0.222 × 0.289 × 0.578 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	15.16 cm^{-1}
Diffractometer, scan mode:	Bruker, $\theta/2\theta$
$2\theta_{max}$:	52°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1925, 1842
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 4\,\sigma(I_{obs})$, 1746
$N(param)_{refined}$:	222
Programs:	SHELXS-86 [3], SHELXL-93 [4]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2N)	4*c*	0.0937(8)	0.272(1)	0.8596(8)	0.092
H(4N)	4*c*	–0.1022(9)	0.171(1)	–0.368(1)	0.104
H(2)	4*c*	0.1413(6)	0.7837(8)	0.8372(5)	0.077
H(3)	4*c*	0.129(1)	0.9569(7)	0.7379(9)	0.101
H(4)	4*c*	0.109(1)	0.918(1)	0.5855(8)	0.115
H(5)	4*c*	0.102(1)	0.705(1)	0.5326(4)	0.145
H(6)	4*c*	0.115(1)	0.5321(8)	0.6319(7)	0.082
H(7)	4*c*	0.045(1)	0.415(1)	0.7333(8)	0.085

* Correspondence author (e-mail: rodolfo.graziani@unipd.it)

Table 2. Continued.

Atom	Site	*x*	*y*	*z*	U_{iso}
H(8)	4*c*	0.202(1)	0.390(1)	0.981(1)	0.082
H(9)	4*c*	0.2270(9)	0.602(2)	0.9269(8)	0.085
H(11)	4*c*	–0.1446(5)	–0.3476(8)	–0.3321(5)	0.082
H(12)	4*c*	–0.132(1)	–0.5168(6)	–0.230(1)	0.103
H(13)	4*c*	–0.109(1)	–0.472(1)	–0.0778(8)	0.120
H(14)	4*c*	–0.0994(9)	–0.257(1)	–0.0285(4)	0.111
H(15)	4*c*	–0.112(1)	–0.0881(8)	–0.1310(7)	0.111
H(16)	4*c*	–0.057(1)	0.059(1)	–0.237(1)	0.084
H(17)	4*c*	–0.204(1)	0.058(2)	–0.484(1)	0.104
H(18)	4*c*	–0.2253(9)	–0.163(1)	–0.415(1)	0.082

Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	2*a*	0	0.1377	0	0.0459(8)	0.047(1)	0.038(1)	0	0.0052(7)	0
Cl(1)	4*c*	0.1043(2)	0.0537(5)	–0.0770(2)	0.075(2)	0.071(2)	0.052(2)	0.007(2)	0.013(2)	–0.008(2)
Cl(2)	4*c*	0.1049(3)	0.2285(4)	0.1146(3)	0.068(2)	0.062(2)	0.059(2)	0.000(2)	0.004(2)	–0.013(2)
Cu(2)	2*b*	0	–0.6952(1)	1/2	0.082(1)	0.050(1)	0.053(2)	0	0.011(1)	0
Cl(3)	4*c*	–0.1042(2)	–0.6112(4)	–0.4219(2)	0.078(2)	0.044(2)	0.062(2)	0.013(2)	0.015(2)	–0.006(2)
Cl(4)	4*c*	0.1060(2)	–0.7851(4)	–0.3846(3)	0.068(2)	0.054(2)	0.057(2)	0.006(2)	0.005(1)	0.013(2)
N(1)	4*c*	0.1381(7)	0.539(1)	0.8034(8)	0.051(5)	0.045(6)	0.057(6)	–0.020(5)	0.013(4)	–0.014(5)
N(2)	4*c*	0.1131(8)	0.351(1)	0.8567(8)	0.106(8)	0.052(6)	0.074(8)	–0.041(6)	0.026(7)	0.017(5)
N(3)	4*c*	–0.1343(8)	–0.096(1)	–0.3048(9)	0.057(5)	0.053(6)	0.059(7)	0.002(5)	0.018(5)	–0.004(6)
N(4)	4*c*	–0.1206(9)	0.093(1)	–0.363(1)	0.107(9)	0.064(7)	0.09(1)	–0.001(6)	0.027(8)	–0.019(7)
C(2)	4*c*	0.1335(6)	0.7680(8)	0.7762(5)	0.085(8)	0.034(5)	0.068(8)	0.010(6)	0.009(7)	–0.008(6)
C(3)	4*c*	0.1261(6)	0.8718(6)	0.7166(6)	0.081(8)	0.09(1)	0.080(9)	0.003(8)	0.007(7)	–0.032(7)
C(4)	4*c*	0.1143(7)	0.8482(8)	0.6254(6)	0.15(2)	0.07(1)	0.08(1)	0.00(1)	0.03(1)	0.032(9)
C(5)	4*c*	0.1100(7)	0.7210(9)	0.5936(4)	0.18(2)	0.13(2)	0.057(9)	0.01(1)	0.04(1)	–0.03(1)
C(6)	4*c*	0.1174(7)	0.6172(7)	0.6532(5)	0.109(9)	0.043(6)	0.053(7)	–0.025(7)	0.020(7)	0.000(6)
C(1)	4*c*	0.1291(6)	0.6407(7)	0.7444(5)	0.069(7)	0.044(6)	0.077(9)	0.009(7)	0.023(6)	0.009(7)
C(7)	4*c*	0.090(1)	0.433(1)	0.7864(8)	0.107(9)	0.062(7)	0.043(6)	–0.019(7)	0.020(6)	0.002(5)
C(8)	4*c*	0.175(1)	0.421(1)	0.924(1)	0.086(9)	0.049(7)	0.066(9)	–0.001(6)	0.007(7)	0.022(6)
C(9)	4*c*	0.1901(9)	0.535(2)	0.8948(8)	0.072(7)	0.10(1)	0.034(5)	–0.009(7)	–0.006(5)	0.006(6)
C(11)	4*c*	–0.1356(5)	–0.3295(8)	–0.2713(5)	0.066(7)	0.076(9)	0.066(8)	–0.011(7)	0.021(6)	0.006(7)
C(12)	4*c*	–0.1278(7)	–0.4309(6)	–0.2098(7)	0.11(1)	0.034(5)	0.12(1)	0.004(6)	0.036(9)	0.034(6)
C(13)	4*c*	–0.1143(7)	–0.4038(9)	–0.1189(6)	0.11(1)	0.11(2)	0.10(1)	0.01(1)	0.04(1)	0.01(1)
C(14)	4*c*	–0.1085(6)	–0.275(1)	–0.0894(4)	0.13(1)	0.076(9)	0.076(9)	–0.014(9)	0.036(9)	0.032(8)
C(15)	4*c*	–0.1162(6)	–0.1740(8)	–0.1508(5)	0.11(1)	0.10(1)	0.07(1)	0.01(1)	0.046(9)	–0.02(1)
C(10)	4*c*	–0.1298(5)	–0.2011(7)	–0.2417(5)	0.037(4)	0.055(6)	0.045(6)	–0.003(5)	0.008(4)	–0.008(5)
C(16)	4*c*	–0.095(1)	0.028(1)	–0.291(1)	0.075(7)	0.041(6)	0.09(1)	–0.031(5)	0.015(7)	–0.021(6)
C(17)	4*c*	–0.177(1)	0.029(2)	–0.427(1)	0.10(1)	0.09(1)	0.07(1)	–0.014(9)	0.022(9)	–0.009(9)
C(18)	4*c*	–0.1872(9)	–0.094(1)	–0.387(1)	0.065(7)	0.044(6)	0.09(1)	–0.019(6)	0.006(7)	–0.011(6)

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