Crystal structure of dichloro-bis(3(5)-amino-5(3)-methylpyrazole)zinc(II), $ZnCl_2N_6C_8H_{14}$

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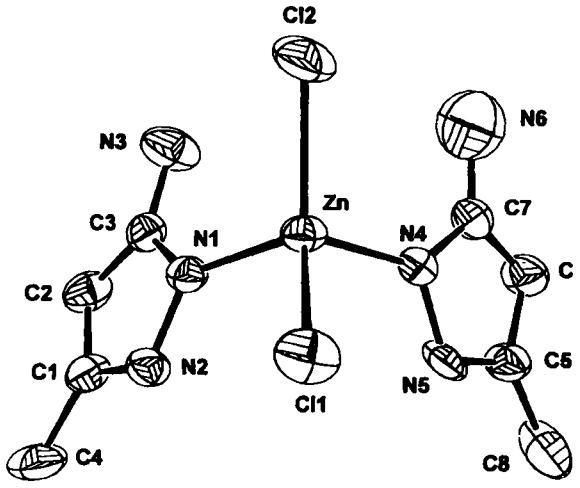

Source of material: Light yellow crystals are obtained by direct reaction of hot ethanolic solution of $ZnCl_2$ with the ligand 3(5)-amino-5(3)-methylpyrazole.

Obtained structure is deformed tetrahedrally where Zn(II) atom is coordinated with two chlorine atoms and two "pyridine" atoms of nitrogen from two pyrazole rings. The angle Cl1–Zn–Cl2 is 121.1(1)°. Distances: d(Zn–N) = 1.983(6) Å – 1.999(6) Å, d(Zn–Cl) = 2.237(2) Å. Similar deviation of Cl1-Zn-Cl2 from tetrahedron angle was found in complex with similar ligands (see ref. 1) in consequence of existence of inter and intramolecular bounds of N···H···Cl type.

$C_8H_{14}Cl_2N_6Zn$, monoclinic, $P12_1/n1$ (No. 14), a =8.564(1) Å, b =12.575(2) Å, c =13.140(3) Å, β =98.3(1)°, V =1400.1 Å^3, Z =4, ρ_m =1500.0 g·cm^{-3}, $R(F)$ =0.046, $R_w(F)$ =0.051.

Table 1. Parameters used for the X-ray data collection

Crystal:	light yellow prism, size 0.18 x 0.50 x 0.36 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	21.70 cm^{-1}
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	ω/2θ
$T_{measurement}$:	293 K
$2\theta_{max}$:	56°
N(hkl)$_{unique}$:	3098
Criterion for I_o:	$I_o > 4\,\sigma(I_o)$
N($param$)$_{refined}$:	155
Program:	SDP

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

Atom	Site	x	y	z	U_{iso}
HC(2)	4e	–0.269	–0.056	0.381	0.26
HN(2)	4e	0.188	–0.083	0.361	0.21
HN(5)	4e	0.283	0.001	0.125	0.26
HN(6)	4e	0.075	0.188	–0.098	0.29
H(1N3)	4e	–0.124	0.214	0.313	0.36
H(1C4)	4e	0.048	–0.238	0.458	0.38
H(1N6)	4e	0.009	0.349	0.026	0.64
H(1C8)	4e	0.158	–0.027	–0.139	0.41
H(2N3)	4e	–0.293	0.158	0.331	0.36
H(2C4)	4e	–0.011	–0.262	0.343	0.38
H(2N6)	4e	0.061	0.332	0.151	0.64
H(2C8)	4e	0.251	–0.085	–0.045	0.41
H(3C4)	4e	–0.131	–0.247	0.420	0.38
H(3C8)	4e	0.334	0.000	–0.104	0.41

Table 3. Final 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}
Zn	4e	0.2006(9)	0.1528(7)	0.2925(7)	0.0429(4)	0.0315(4)	0.0507(4)	0.0003(5)	0.0078(3)	0.0059(5)
Cl(1)	4e	0.4358(2)	0.0801(2)	0.3483(2)	0.0430(1)	0.0517(1)	0.0775(1)	–0.0010(1)	–0.0010(1)	–0.0020(1)
Cl(2)	4e	0.1440(4)	0.3191(2)	0.3356(2)	0.1093(1)	0.0325(1)	0.0890(2)	–0.013(1)	0.0120(2)	–0.007(1)
N(1)	4e	0.0491(7)	0.0518(5)	0.3404(5)	0.045(3)	0.032(3)	0.049(3)	0.001(3)	0.013(3)	–0.003(3)
N(2)	4e	0.0858(7)	–0.0532(5)	0.3599(5)	0.041(3)	0.036(3)	0.061(4)	0.001(3)	0.016(3)	0.006(3)
N(3)	4e	–0.1825(8)	0.1538(6)	0.3284(7)	0.049(4)	0.052(4)	0.139(7)	0.006(5)	0.027(4)	0.013(4)

Table 3. (Continued)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(4)	4*e*	0.1742(7)	0.1464(5)	0.1390(5)	0.057(3)	0.036(3)	0.046(3)	0.006(3)	0.013(3)	0.006(3)
N(5)	4*e*	0.2266(8)	0.0589(5)	0.0901(5)	0.075(4)	0.025(3)	0.054(4)	−0.002(3)	0.008(3)	0.011(3)
N(6)	4*e*	0.055(1)	0.3067(7)	0.0826(7)	0.239(9)	0.093(5)	0.071(6)	0.022(5)	0.035(6)	0.113(5)
C(1)	4*e*	−0.0410(9)	−0.1082(6)	0.3789(6)	0.048(4)	0.046(4)	0.056(5)	0.002(4)	0.017(4)	−0.008(4)
C(2)	4*e*	−0.1637(9)	−0.0401(7)	0.3710(7)	0.041(4)	0.058(5)	0.072(5)	0.000(5)	0.016(4)	−0.011(4)
C(3)	4*e*	−0.1046(9)	0.0592(6)	0.3478(6)	0.045(4)	0.042(4)	0.049(4)	−0.006(4)	0.014(3)	−0.004(4)
C(4)	4*e*	−0.033(1)	−0.2243(7)	0.4025(8)	0.093(6)	0.043(5)	0.096(7)	0.018(5)	0.031(5)	−0.014(5)
C(5)	4*e*	0.192(1)	0.0658(6)	−0.0108(6)	0.074(5)	0.040(4)	0.047(4)	0.004(4)	0.009(4)	−0.008(4)
C(6)	4*e*	0.116(1)	0.1605(7)	−0.0323(6)	0.075(5)	0.055(4)	0.049(4)	0.016(5)	0.004(4)	0.010(5)
C(7)	4*e*	0.110(1)	0.2074(7)	0.0626(6)	0.075(5)	0.050(5)	0.047(4)	0.017(4)	0.015(4)	0.018(4)
C(8)	4*e*	0.238(1)	−0.0192(8)	−0.0814(7)	0.15(1)	0.057(6)	1.062(6)	−0.019(5)	0.016(6)	0.005(7)

References

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