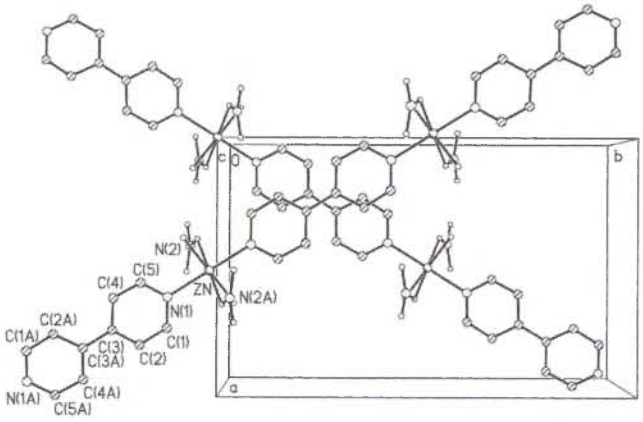
Crystal structure of diaqua-4,4′-bipyridinezinc nitrate $Zn(4,4'\text{-bipy})(H_2O)_2(NO_3)_2$: *a one-dimensional coordination polymer*

R.-G. Xiong, B. J. Lewandowski and S. D. Huang*

Kent State University, Department of Chemistry, P. O. Box 5190, Kent, OH 44242, USA

Received January 22, 1999, CCDC-No. 1267/122



Abstract

$C_{10}H_{12}N_4O_8Zn$, orthorhombic, *Pccn* (No. 56), $a = 11.9053(8)$ Å, $b = 19.348(1)$ Å, $c = 7.4578(5)$ Å, $V = 1717.9$ Å^3, $Z = 4$, $R_{gt}(F) = 0.051$, $wR(F) = 0.092$, $T = 296$ K.

Source of material

The title compound was prepared as single crystals from a hydrothermal reaction between zinc nitrate and 4,4′-bipyridine at 373 K.

Discussion

The asymmetric unit contains a Zn cation situated on the inversion center, a half molecule of 4,4′-bipyridine, a nitrate anion and a coordinated water molecule. The inversion operation gives rise to octahedral coordination to the Zn ion with two N atoms from the 4,4′-bipy ligand, two O atoms from the nitrate anions and two O atoms from the water molecules. The one-dimensional chain-like structure of the compound can be generated by a combination of inversion and lattice translation operations. The polymer chains are packed in a cross-hair fashion in [110] and [220] directions as shown in the figure.

Table 1. Data collection and handling.

Crystal:	pale rod, size 0.20 × 0.20 × 0.30 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	14.72 cm^{-1}
Diffractometer, scan mode:	Bruker CCD, ω, $\Delta\omega = 0.3°$
$2\theta_{max}$:	54.22°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	9066, 2056
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 3\ \sigma(I_{obs})$, 1155
$N(param)_{refined}$:	106
Programs:	SIR92 [1], teXsan [2]

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

Atom	Site	x	y	z	U_{iso}
H(1)	8*e*	0.2557	0.0503	0.4585	0.045
H(2)	8*e*	0.1522	0.1512	0.4578	0.046
H(3)	8*e*	0.4391	0.2581	0.5464	0.05
H(4)	8*e*	0.5338	0.1543	0.5418	0.049
H(5)	8*e*	0.3161	−0.0725	0.6033	0.042
H(6)	8*e*	0.3869	−0.0522	0.7853	0.042

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}
Zn	4*a*	1/2	0	1/2	0.0212(5)	0.0237(6)	0.0326(6)	0.0059(5)	−0.0008(6)	−0.0001(7)
O(1)	8*e*	0.3886(4)	−0.0348(3)	0.2857(7)	0.030(3)	0.051(4)	0.029(3)	0.005(3)	0.001(2)	−0.009(3)
O(2)	8*e*	0.3367(5)	−0.0686(4)	0.0254(7)	0.037(3)	0.075(4)	0.028(3)	−0.004(3)	−0.004(3)	−0.009(3)
O(3)	8*e*	0.5141(5)	−0.0671(4)	0.0940(9)	0.029(4)	0.095(6)	0.053(4)	0.018(4)	0.004(3)	−0.011(4)
O(4)	8*e*	0.3788(4)	−0.0509(3)	0.6586(7)	0.030(3)	0.048(4)	0.027(3)	−0.004(3)	−0.002(2)	0.001(3)
N(1)	8*e*	0.4048(5)	0.0930(3)	0.4983(9)	0.023(3)	0.023(3)	0.043(4)	0.006(2)	−0.002(4)	−0.003(4)
N(2)	8*e*	0.4152(5)	−0.0571(4)	0.1346(8)	0.030(3)	0.037(4)	0.027(3)	0.006(3)	0.000(3)	0.000(3)
C(1)	8*e*	0.2929(6)	0.0932(4)	0.476(1)	0.025(4)	0.021(3)	0.066(6)	0.001(3)	−0.008(4)	−0.006(4)
C(2)	8*e*	0.2312(6)	0.1533(4)	0.475(1)	0.017(3)	0.029(4)	0.067(6)	0.005(3)	−0.008(4)	−0.002(4)
C(3)	8*e*	0.2826(5)	0.2173(3)	0.502(1)	0.023(3)	0.022(3)	0.037(4)	0.004(3)	−0.001(4)	−0.001(4)
C(4)	8*e*	0.3990(6)	0.2163(4)	0.527(1)	0.024(4)	0.022(4)	0.079(7)	0.001(3)	−0.001(4)	−0.003(5)
C(5)	8*e*	0.4548(6)	0.1538(4)	0.524(1)	0.021(3)	0.029(4)	0.074(7)	0.003(3)	−0.008(4)	−0.002(5)

* Correspondence author (e-mail: shuang@kent.edu)

Acknowledgments. This work was supported by the U.S. National Science Foundation (Grant No. OSR-9452893) and the Department of Energy (DE-FC02-91ER75674).

References

1. Altomare, A.; Cascarano, M.; Giacovazzo, C.; Guagliardi, A.: Completion and refinement of crystal structures with SIR92. J. Appl. Crystallogr. **26** (1993) 343-350.
2. Molecular Structure Corporation. teXsan. Single Crystal Structure Analysis Software. Version 1.7. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA 1992-1997.