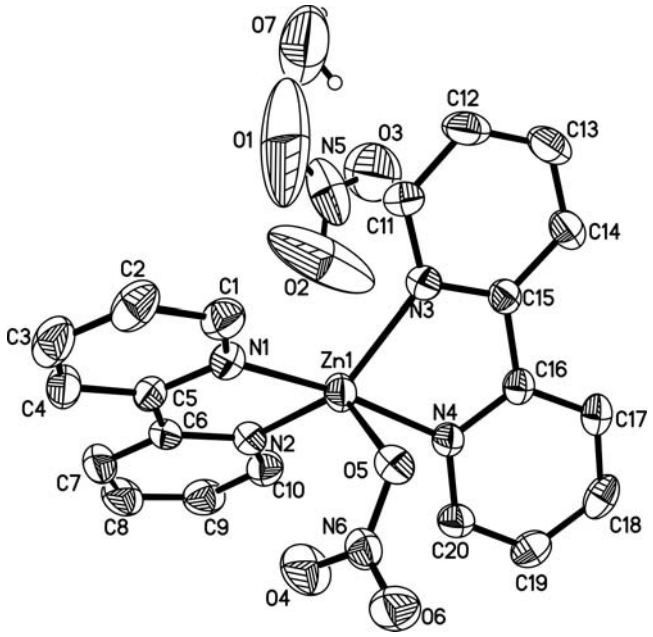
Crystal structure of bis(2,2′-bipyridine-*N*,*N*′)-(nitrato-*O*)zinc(II) nitrate monohydrate, $[Zn(C_{10}H_8N_2)(NO_3)][NO_3] \cdot H_2O$

Lianwen Zhou*

Dezhou University, Department of Chemistry, Dezhou 253023, Shandong, P. R. China

Received December 14, 2010, accepted and available on-line January 24, 2011; CCDC no. 1267/3334



Abstract

$C_{20}H_{18}N_6O_7Zn$, triclinic, $P\bar{1}$ (no. 2), a = 7.472(5) Å, b = 9.992(8) Å, c = 15.01(2) Å, α = 73.97(1)°, β = 88.43(1)°, γ = 90.023(9)°, V = 1076.8 Å^3, Z = 2, $R_{gt}(F)$ = 0.052, $wR_{ref}(F^2)$ = 0.156, T = 293 K.

Source of material

A mixture of 2,2′-bipyridine, $Zn(NO_3)_2 \cdot 6H_2O$ (molar ratio 2:1) and H_2O (20 ml) was sealed in a Teflon-lined autoclave (25 ml) and heated at about 400 K for sevral hours. Upon cooling slowly and opening the bomb, colorless crystals suitable for X-ray diffraction were obtained with a yield about 50 % (based on 2,2′-bipyridine).

Discussion

As already has been known, bidentate chelating ligands, such as 2,2′-bipyridine, 1,10-phenanthroline and their derivatives, have been widely employed to construct transition metal complexes [1-3].

The coordination sphere of the Zn(II) ion in the title crystal structure should be described as a distorted square-pyramidal, in which four positions are occupied by four N atoms from the two chelating bipyridine ligands, and the fifth site is occupied by the O atom of the coordinated nitrate. The average Zn—N bond length 2.01 Å is in agreement with the corresponding distances found in other zinc bipyridine complexes [4,5]. The bond length d(Zn—$O_{nitrate}$) = 2.297(4) Å is slightly longer than the Zn—O bond length in the above complexes.

Table 1. Data collection and handling.

Crystal:	colorless block, size 0.19 × 0.25 × 0.34 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	11.97 cm^{-1}
Diffractometer, scan mode:	Bruker SMART APEX II CCD, φ/ω
$2\theta_{max}$:	50°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5428, 3731
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2974
$N(param)_{refined}$:	307
Programs:	SHELXS-97, SHELXL-97 [6]

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

Atom	Site	x	y	z	U_{iso}
H(1O7)	2*i*	0.2001	0.4985	0.4204	0.309
H(207)	2*i*	0.1309	0.5545	0.4848	0.309
H(20)	2*i*	0.7304	0.1075	0.0437	0.069
H(19)	2*i*	0.6274	0.2174	–0.0993	0.076
H(18)	2*i*	0.6199	0.4568	–0.1472	0.074
H(17)	2*i*	0.7187	0.5819	–0.0487	0.064
H(14)	2*i*	0.7847	0.6814	0.0598	0.070
H(13)	2*i*	0.8977	0.7735	0.1722	0.086
H(12)	2*i*	1.0114	0.6255	0.3047	0.085
H(11)	2*i*	1.0147	0.3900	0.3214	0.070
H(1)	2*i*	1.2259	0.2180	0.3066	0.075
H(2)	2*i*	1.3832	0.0822	0.4281	0.090
H(3)	2*i*	1.2748	–0.1353	0.5061	0.095
H(4)	2*i*	1.0080	–0.2109	0.4616	0.079
H(7)	2*i*	0.7364	–0.2559	0.4194	0.081
H(8)	2*i*	0.4669	–0.2946	0.3567	0.092
H(9)	2*i*	0.3521	–0.1243	0.2348	0.084
H(10)	2*i*	0.5150	0.0745	0.1738	0.071

* e-mail: lwzhoudz@126.com

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(1)	2*i*	0.88529(7)	0.19043(4)	0.20548(3)	0.0729(4)	0.0435(3)	0.0481(3)	–0.0052(2)	–0.0159(2)	–0.0053(2)
O(1)	2*i*	0.595(2)	0.363(2)	0.412(1)	0.21(1)	0.36(2)	0.31(1)	–0.02(1)	–0.12(1)	0.20(1)
O(2)	2*i*	0.571(1)	0.290(1)	0.306(1)	0.26(1)	0.176(7)	0.58(2)	–0.139(7)	0.30(1)	–0.23(1)
O(3)	2*i*	0.429(1)	0.4484(7)	0.3188(5)	0.255(9)	0.139(5)	0.167(6)	0.058(6)	–0.098(6)	–0.038(4)
O(4)	2*i*	1.0587(5)	–0.0078(4)	0.1312(3)	0.093(3)	0.067(2)	0.110(3)	–0.032(2)	0.014(2)	–0.023(2)
O(5)	2*i*	1.1500(5)	0.1957(3)	0.1230(2)	0.091(2)	0.045(2)	0.062(2)	–0.003(1)	0.006(2)	–0.015(1)
O(6)	2*i*	1.2885(5)	0.0750(4)	0.0463(2)	0.074(2)	0.078(2)	0.081(2)	0.010(2)	0.010(2)	–0.029(2)
O(7)	2*i*	0.200(2)	0.4966(9)	0.4753(6)	0.36(1)	0.219(9)	0.148(6)	0.126(9)	0.044(7)	0.023(6)
N(1)	2*i*	1.0214(5)	0.0911(3)	0.3159(2)	0.060(2)	0.052(2)	0.044(2)	0.004(2)	–0.008(2)	–0.011(2)
N(2)	2*i*	0.7201(4)	0.0262(3)	0.2544(2)	0.058(2)	0.042(2)	0.047(2)	–0.002(1)	0.000(2)	–0.012(1)
N(3)	2*i*	0.9099(4)	0.3956(3)	0.2016(2)	0.054(2)	0.046(2)	0.048(2)	–0.002(1)	0.001(1)	–0.014(1)
N(4)	2*i*	0.7780(4)	0.2746(3)	0.0843(2)	0.055(2)	0.042(2)	0.043(2)	–0.001(1)	–0.006(1)	–0.010(1)
N(5)	2*i*	0.5306(9)	0.3684(7)	0.3440(7)	0.101(4)	0.074(4)	0.176(7)	0.001(3)	–0.024(5)	0.021(4)
N(6)	2*i*	1.1671(5)	0.0852(3)	0.0998(2)	0.056(2)	0.046(2)	0.055(2)	0.003(2)	–0.008(2)	–0.009(2)
C(20)	2*i*	0.7255(6)	0.2042(4)	0.0254(3)	0.072(3)	0.050(2)	0.054(2)	0.001(2)	–0.010(2)	–0.019(2)
C(19)	2*i*	0.6653(6)	0.2693(5)	–0.0604(3)	0.066(3)	0.077(3)	0.051(2)	–0.001(2)	–0.011(2)	–0.024(2)
C(18)	2*i*	0.6610(5)	0.4108(5)	–0.0889(3)	0.049(2)	0.089(3)	0.040(2)	0.008(2)	–0.008(2)	–0.005(2)
C(17)	2*i*	0.7185(5)	0.4851(4)	–0.0301(3)	0.050(2)	0.053(2)	0.048(2)	0.004(2)	0.000(2)	0.001(2)
C(16)	2*i*	0.7756(5)	0.4144(4)	0.0567(2)	0.039(2)	0.046(2)	0.043(2)	0.002(2)	0.002(2)	–0.007(2)
C(15)	2*i*	0.8422(5)	0.4825(4)	0.1251(2)	0.044(2)	0.042(2)	0.046(2)	–0.001(2)	0.005(2)	–0.011(2)
C(14)	2*i*	0.8339(6)	0.6236(4)	0.1128(3)	0.062(3)	0.042(2)	0.068(3)	0.001(2)	0.005(2)	–0.011(2)
C(13)	2*i*	0.8994(7)	0.6780(5)	0.1798(4)	0.083(3)	0.046(2)	0.089(3)	–0.008(2)	0.010(3)	–0.028(2)
C(12)	2*i*	0.9674(7)	0.5902(5)	0.2583(4)	0.083(3)	0.064(3)	0.078(3)	–0.012(2)	0.002(3)	–0.041(3)
C(11)	2*i*	0.9700(6)	0.4495(4)	0.2677(3)	0.071(3)	0.058(2)	0.052(2)	–0.003(2)	–0.003(2)	–0.024(2)
C(1)	2*i*	1.1794(6)	0.1316(5)	0.3397(3)	0.064(3)	0.070(3)	0.056(2)	0.003(2)	–0.008(2)	–0.022(2)
C(2)	2*i*	1.2758(7)	0.0499(6)	0.4115(3)	0.061(3)	0.107(4)	0.056(3)	0.016(3)	–0.016(2)	–0.022(3)
C(3)	2*i*	1.2118(8)	–0.0783(6)	0.4577(3)	0.081(4)	0.097(4)	0.055(3)	0.036(3)	–0.015(2)	–0.013(3)
C(4)	2*i*	1.0525(7)	–0.1226(5)	0.4317(3)	0.086(3)	0.058(3)	0.047(2)	0.019(2)	0.003(2)	–0.003(2)
C(5)	2*i*	0.9584(6)	–0.0355(4)	0.3610(3)	0.064(3)	0.048(2)	0.038(2)	0.010(2)	0.000(2)	–0.010(2)
C(6)	2*i*	0.7849(6)	–0.0697(4)	0.3281(3)	0.073(3)	0.038(2)	0.043(2)	0.005(2)	0.005(2)	–0.014(2)
C(7)	2*i*	0.6918(7)	–0.1901(4)	0.3685(3)	0.090(4)	0.045(2)	0.059(3)	0.002(2)	0.012(2)	–0.005(2)
C(8)	2*i*	0.5300(8)	–0.2119(5)	0.3318(4)	0.096(4)	0.051(3)	0.083(3)	–0.022(2)	0.020(3)	–0.021(2)
C(9)	2*i*	0.4624(7)	–0.1119(5)	0.2589(3)	0.075(3)	0.069(3)	0.072(3)	–0.019(2)	0.012(2)	–0.030(3)
C(10)	2*i*	0.5608(6)	0.0056(5)	0.2227(3)	0.066(3)	0.058(2)	0.054(2)	–0.006(2)	–0.006(2)	–0.016(2)

References

1. van Albada, G. A.; Mohamadou, A.; Mutikainen, I.; Turpeinen, U.; Reedijk, J.: Synthesis, characterisation, croperties and X-ray structures of Cu(II) coordination compounds with 5,5′-dimethylbipyridine and various anions: control of stoichiometry and structure by the sounterions. Eur. J. Inorg. Chem. (2004) 3733-3742.
2. Zhang, D. P.; Tian, N. C.; Zhang, X. M.: Bis(1,10-phenanthroline)bis-(isocyanato)cobalt(II). Acta Crystallogr. **E66** (2010) m614.
3. Dell'Amico, D. B.; Calderazzo, F.; Curiardi, M.; Labella, L.; Marchetti, F.: Bis-qtpy (qtpy = 2,2′: 6′, 2″: 6″, 2‴-quaterpyridine) metal complexes, $[M(qtpy)_2]^{2+}$. Inorg. Chem. **43** (2004) 5459-5465.
4. Liu, M.; Arora, S. K.: Structure of aquabis(2,2′-bipyridyl)zinc(II) diperchlorate. Acta Crystallogr. **C49** (1993) 372-374.
5. Chen, X. M.; Xu, Z. T.; Yu, X. L.; Mak, T. C. W.: Preparation and crystal structures of bis(*o*-phenanthroline)(acetato)zinc(II) perchlorate and bis(2,2′-bipyridine)(pyridinioacetato)zinc(II) diperchlorate. Polyhedron **13** (1993) 2079-2083.
6. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.