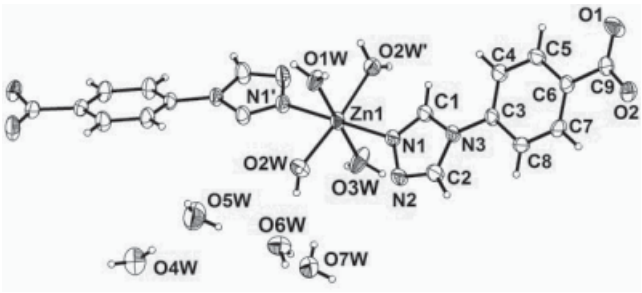
Crystal structure of tetraaqua-bis(4-(1,2,4-triazol-4-yl)benzoato-κ*N*)-zinc(II) decahydrate, $C_{18}H_{40}N_6O_{18}Zn$

Songbai Han* and Hongli Wang

China Institute of Atomic Energy, Department of Nuclear Physics, P.O.BOX 275(30), Beijing, P. R. China

Received November 22, 2012, accepted June 06, 2013, available online June 14, 2013, CCDC no. 1267/3988



Abstract

$C_{18}H_{40}N_6O_{18}Zn$, monoclinic, *C*2/*c* (no. 15), $a = 25.84(2)$ Å, $b = 7.910(5)$ Å, $c = 16.856(1)$ Å, $\beta = 112.734(9)°$, $V = 3177$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0319$, $wR_{ref}(F^2) = 0.0757$, $T = 293$ K.

Table 1. Data collection and handling.

Crystal:	colourless block, size 0.18×0.20×0.22 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.55 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	52.8°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8856, 3248
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2574
$N(param)_{refined}$:	252
Programs:	SAINT [3], SHELX[4]

Source of material

The title complex was prepared by reaction of an aqueous solution of $Zn(NO_3)_2{\cdot}6H_2O$ (0.297 g, 1 mmol) with 4-(*p*-benzoxy)-1,2,4-triazole (*HL*) (0.378 g, 2 mmol) in 18 mL water. This suspending solution was rigidly stirred at room temperature for 5 h and then was filtrated. The clear solution was sealed in a 25 mL acid digestion bomb at 140 °C for 4 days. Colourless block crystals were obtained by filtration and dried in air.

Discussion

Metal-organic supermolecular compounds with various network structures have received wide attention because of their attractive structures and potential application in many research areas [1]. Herein, we employed 4-(*p*-benzoxy)-1,2,4-triazole (*L*) ligand to construct a new zinc complex [2]. The title structure consists of mononuclear $[Zn(L)_2(H_2O)_4]$ units and lattice water molecules in the ratio 1:10 as shown in the figure. The $[Zn(L)_2(H_2O)_4]$ unit has a crystallographically imposed C_2 symmetry. The ligand adopts the unique Zn–N coordination fashion, in which the uncoordinated carboxylate groups exhibits strong intermolecular hdyrogen bonding interaction with water molecules. It is noteworth that the title compound self-assembles into a three-dimensional (3D) supramolecular architecture through intermolecular O-H···O hydrogen-bonding interactions.

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1A)	8*f*	0.6337	0.9797	0.8217	0.039
H(2A)	8*f*	0.6472	0.8713	1.0549	0.049
H(4A)	8*f*	0.7186	1.1037	0.8756	0.043
H(5A)	8*f*	0.8124	1.1723	0.9270	0.044
H(7A)	8*f*	0.8361	0.9438	1.1494	0.042
H(8A)	8*f*	0.7422	0.8690	1.0974	0.042
H(5WB)	8*f*	0.3231(9)	0.788(3)	0.789(2)	0.08(1)
H(4WB)	8*f*	0.170(1)	0.737(4)	0.711(2)	0.10(1)
H(4WA)	8*f*	0.2250(7)	0.730(3)	0.728(2)	0.08(1)
H(1WA)	8*f*	0.5216(8)	1.236(2)	0.784(1)	0.054(7)
H(6WB)	8*f*	0.398(1)	0.579(2)	0.850(2)	0.063(9)
H(6WA)	8*f*	0.402(1)	0.678(3)	0.9137(7)	0.069(9)
H(2WB)	8*f*	0.458(1)	0.996(2)	0.859(1)	0.051(7)
H(3WA)	8*f*	0.5237(8)	0.578(2)	0.782(1)	0.070(9)
H(7WB)	8*f*	0.405(1)	0.367(4)	0.759(1)	0.08(1)
H(8WB)	8*f*	0.472(1)	0.184(3)	0.980(1)	0.066(9)
H(2WA)	8*f*	0.437(1)	0.844(2)	0.838(2)	0.059(8)
H(8WA)	8*f*	0.5097(6)	0.237(3)	0.949(2)	0.078(9)
H(7WA)	8*f*	0.4242(8)	0.310(3)	0.838(1)	0.072(9)
H(5WA)	8*f*	0.299(2)	0.940(2)	0.765(2)	0.11(2)

* Correspondence author (e-mail: hansb@ciae.ac.cn)

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)	4*e*	$\frac{1}{2}$	0.90451(4)	$\frac{3}{4}$	0.0177(2)	0.0340(2)	0.0251(2)	0	0.0040(1)	0
C(1)	8*f*	0.62539(7)	0.9472(2)	0.8685(1)	0.0227(9)	0.049(1)	0.0231(9)	–0.0027(8)	0.0051(7)	0.0023(8)
C(2)	8*f*	0.63261(8)	0.8877(3)	0.9957(1)	0.027(1)	0.066(2)	0.027(1)	–0.006(1)	0.0068(8)	0.006(1)
C(3)	8*f*	0.72162(7)	0.9814(2)	0.9819(1)	0.0183(9)	0.036(1)	0.0262(9)	–0.0024(8)	0.0035(7)	–0.0017(8)
C(4)	8*f*	0.74231(8)	1.0713(3)	0.9307(1)	0.0238(9)	0.056(1)	0.0208(9)	–0.0038(9)	0.0013(7)	0.0038(9)
C(5)	8*f*	0.79836(8)	1.1126(3)	0.9619(1)	0.028(1)	0.054(1)	0.026(1)	–0.007(1)	0.0098(8)	0.004(1)
C(6)	8*f*	0.83421(7)	1.0671(2)	1.0441(1)	0.0225(9)	0.035(1)	0.0256(9)	–0.0018(8)	0.0049(7)	–0.0027(8)
C(7)	8*f*	0.81252(8)	0.9759(3)	1.0941(1)	0.025(1)	0.043(1)	0.026(1)	–0.0018(9)	–0.0018(8)	0.0069(9)
C(8)	8*f*	0.75631(8)	0.9315(2)	1.0635(1)	0.027(1)	0.044(1)	0.029(1)	–0.0064(9)	0.0057(8)	0.0087(9)
C(9)	8*f*	0.89464(8)	1.1214(2)	1.0789(1)	0.0244(9)	0.036(1)	0.032(1)	–0.0015(8)	0.0063(8)	–0.0045(9)
N(1)	8*f*	0.57595(6)	0.9025(2)	0.86387(9)	0.0223(8)	0.0393(9)	0.0267(8)	–0.0022(7)	0.0057(6)	0.0013(7)
N(2)	8*f*	0.58051(6)	0.8635(2)	0.9459(1)	0.0233(8)	0.064(1)	0.0289(9)	–0.0067(8)	0.0068(7)	0.0083(8)
N(3)	8*f*	0.66307(6)	0.9401(2)	0.9504(1)	0.0191(7)	0.042(1)	0.0240(8)	–0.0032(7)	0.0042(6)	0.0009(7)
O(1W)	4*e*	$\frac{1}{2}$	1.1701(3)	$\frac{3}{4}$	0.030(1)	0.031(1)	0.039(1)	0	–0.0019(9)	0
O(1)	1*e*	0.91369(6)	1.1889(2)	1.02955(9)	0.0300(8)	0.085(1)	0.0365(8)	–0.0200(8)	0.0081(7)	0.0004(8)
O(2)	1*e*	0.92267(5)	1.0987(2)	1.15823(8)	0.0254(7)	0.0476(8)	0.0305(7)	–0.0045(6)	–0.0016(6)	–0.0011(7)
O(2W)	1*e*	0.45031(6)	0.9245(2)	0.82168(9)	0.0350(8)	0.048(1)	0.0344(8)	–0.0083(7)	0.0171(7)	–0.0052(8)
O(3W)	4*e*	$\frac{1}{2}$	0.6423(3)	$\frac{3}{4}$	0.043(1)	0.030(1)	0.054(2)	0	–0.016(1)	0
O(4W)	1*e*	0.19535(9)	0.6784(3)	0.7071(1)	0.052(1)	0.065(1)	0.065(1)	0.003(1)	0.017(1)	–0.011(1)
O(5W)	1*e*	0.29604(9)	0.8385(3)	0.7551(2)	0.056(1)	0.069(2)	0.087(2)	0.004(1)	0.010(1)	0.007(1)
O(6W)	1*e*	0.39372(7)	0.6781(2)	0.8614(1)	0.058(1)	0.053(1)	0.045(1)	–0.0041(9)	0.0246(9)	0.0030(9)
O(7W)	1*e*	0.39768(7)	0.3598(2)	0.8021(1)	0.045(1)	0.064(1)	0.054(1)	0.0097(8)	0.0219(9)	0.0105(9)
O(8W)	1*e*	0.47906(6)	0.1918(2)	0.9367(1)	0.0344(9)	0.069(1)	0.0323(9)	–0.0114(8)	0.0123(7)	–0.0057(8)

Acknowledgments. This work was supported by State Key Development Program of Basic Research of China (grant No. 2010CB833101).

References

1. Yaghi, O. M.; O'Keeffe, M.; Ockwig, N. W.; Chae, H. K.; Eddaoudi, M.; Kim, J.: Reticular Synthesis and the Design of New Materials. Nature **423** (2003) 705-714.
2. Zou, R. Q.; Cai, L. Z.; Guo, G. C.: A hydrogen-bonded 3D coordination network of Co^{II} with 4-(*p*-benzoxy)-1,2,4-triazole: hydrothermal synthesis, characterization, crystal structure and emission property. J. Mole. Stuct. **737** (2005) 125-129.
3. Bruker (1998). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
4. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.