Crystal structure of aqua-*bis*[*N*-(5-*p*-tolyl-1,3,4-oxadiazol-2-yl) benzamide-$\kappa^2 N,O$]zinc(II), $Zn(C_{16}H_{12}N_3O_2)_2(H_2O)$, $C_{32}H_{26}N_6O_5Zn$

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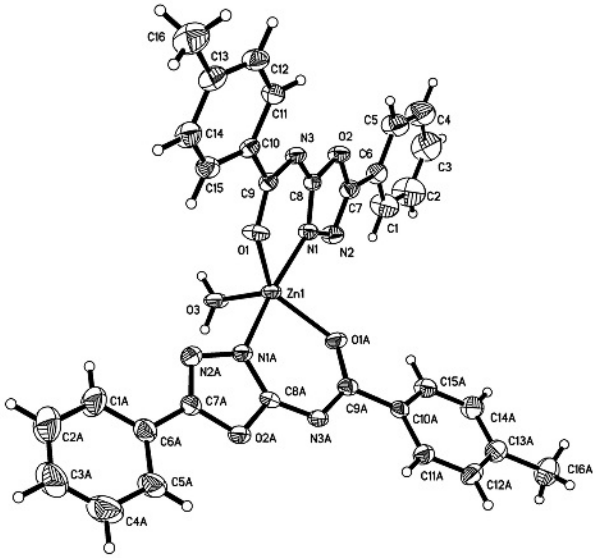

Abstract

$C_{32}H_{26}N_6O_5Zn$, orthorhombic, *Pbcn* (no. 60), $a = 31.793(1)$ Å, $b = 8.0862(4)$ Å, $c = 11.6099(4)$ Å, $V = 2984.8$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0583$, $wR_{ref}(F^2) = 0.1205$, $T = 293$ K.

Table 1. Data collection and handling.

Crystal:	colourless prisms, size 0.15×0.2×0.2 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.74 cm^{-1}
Diffractometer, scan mode:	Oxford Diffraction Xcalibur Eos Gemini, φ and ω
$2\theta_{max}$:	52.74°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8925, 3045
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2110
$N(param)_{refined}$:	204
Programs:	SHELXS-97 [8]

Source of material

A methanol solution of $Zn(NO_3)_2$ (0.1 mol/L, 10 mL) was added to a ethanol solution of *N*-(5-*p*-tolyl-1,3,4-oxadiazol-2-yl)-benzamide (279 mg, 1 mmol). The mixture was stirred and neutralized with NaOH aqueous solution. The solution was then evaporated to a small volume. The product was obtained by filtration. The colourless crystals were obtained by recrystallization from methanol/hexane solution.

Discussion

Oxadiazole derivatives have received considerable attentions in electro-active and opto-active materials due to their high electron affinities, which make them good candidates for electron injection and transportation [1-4]. By introducing different metal ions and ligands, oxadiazole metal complexes can easily tailor the emission color, thermal stability, film formation properties as well as other required properties, and thus have been employed in light-emitting diodes [5-7].

The crystal structure analysis of the title compound revealed that the Zn^{2+} ion is coordinated by two O atoms and two N atoms from two ligands and one water O atom in a trigonal-bipyramidal geometry (Fig.). The two ligand molecules are deprotoned to make the complex neutral. The ligand behaves as a chelating unit that binds through the N atom an O atom, giving a six-membered chelate ring. In the crystal of the title compound there exist intermoleculer O–H···N hydrogen bonds (H3···N3 1.95 Å, 160.4°), which link the molecules into a 1D chain structure.

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

Atom	Site	*x*	*y*	*z*	U_{iso}
H(1)	8*d*	0.3349	–0.0144	0.3779	0.100
H(2)	8*d*	0.2671	–0.0462	0.4383	0.137
H(3A)	8*d*	0.2463	0.0549	0.6146	0.128
H(4)	8*d*	0.2939	0.1890	0.7280	0.122
H(5)	8*d*	0.3633	0.2182	0.6707	0.090
H(11)	8*d*	0.5372	0.4567	0.6587	0.056
H(12)	8*d*	0.5936	0.5762	0.7481	0.067
H(14)	8*d*	0.6707	0.3850	0.5131	0.072
H(15)	8*d*	0.6145	0.2642	0.4237	0.062
H(16A)	8*d*	0.6667	0.6803	0.7298	0.134
H(16B)	8*d*	0.6973	0.5895	0.6450	0.134
H(16C)	8*d*	0.6846	0.5055	0.7617	0.134
H(3)	8*d*	0.499(1)	–0.195(1)	0.3098(5)	0.134

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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*c*	½	0.11010(5)	¼	0.0443(2)	0.0461(2)	0.0223(2)	0	0.0026(2)	0
O(1)	8*d*	0.53897(5)	0.2202(2)	0.3682(1)	0.054(1)	0.075(1)	0.0281(8)	–0.012(1)	0.0075(8)	–0.0106(8)
O(2)	8*d*	0.42805(5)	0.1972(2)	0.5447(1)	0.0443(9)	0.062(1)	0.0310(8)	–0.0041(9)	0.0039(8)	0.0004(8)
O(3)	4*c*	½	–0.1355(3)	¼	0.094(2)	0.042(1)	0.025(1)	0	0.006(1)	0
N(1)	8*d*	0.45596(6)	0.1315(3)	0.3781(1)	0.038(1)	0.049(1)	0.0295(9)	–0.002(1)	0.0029(9)	–0.0013(9)
N(2)	8*d*	0.41393(6)	0.0845(3)	0.3755(2)	0.045(1)	0.064(2)	0.039(1)	–0.008(1)	–0.001(1)	–0.004(1)
N(3)	8*d*	0.49760(6)	0.2626(3)	0.5293(2)	0.040(1)	0.051(1)	0.0267(9)	–0.001(1)	0.0017(9)	0.0028(9)
C(1)	8*d*	0.32698(9)	0.0270(5)	0.4493(3)	0.048(2)	0.123(3)	0.080(2)	–0.018(2)	0.001(2)	–0.022(2)
C(2)	8*d*	0.2864(1)	0.0079(6)	0.4852(3)	0.056(2)	0.171(4)	0.116(3)	–0.031(3)	0.001(2)	–0.018(3)
C(3)	8*d*	0.2739(1)	0.0679(6)	0.5899(3)	0.051(2)	0.163(4)	0.107(3)	–0.010(2)	0.022(2)	0.014(3)
C(4)	8*d*	0.3024(1)	0.1467(6)	0.6572(3)	0.073(2)	0.161(4)	0.070(2)	0.005(3)	0.024(2)	0.007(2)
C(5)	8*d*	0.34390(9)	0.1659(5)	0.6230(2)	0.052(2)	0.118(3)	0.057(2)	–0.006(2)	0.016(2)	0.001(2)
C(6)	8*d*	0.35602(8)	0.1052(4)	0.5158(2)	0.042(1)	0.062(2)	0.052(2)	–0.002(1)	0.005(1)	0.006(1)
C(7)	8*d*	0.39868(7)	0.1250(3)	0.4752(2)	0.041(1)	0.047(2)	0.040(1)	–0.002(1)	0.000(1)	0.004(1)
C(8)	8*d*	0.46348(7)	0.1981(3)	0.4804(2)	0.039(1)	0.038(1)	0.029(1)	0.003(1)	0.007(1)	0.006(1)
C(9)	8*d*	0.53313(8)	0.2699(3)	0.4699(2)	0.047(1)	0.037(1)	0.032(1)	0.003(1)	0.000(1)	0.006(1)
C(10)	8*d*	0.56959(7)	0.3462(3)	0.5295(2)	0.040(1)	0.039(1)	0.033(1)	–0.002(1)	–0.002(1)	0.008(1)
C(11)	8*d*	0.56406(8)	0.4416(3)	0.6287(2)	0.047(1)	0.051(2)	0.041(1)	–0.002(1)	0.002(1)	–0.006(1)
C(12)	8*d*	0.59798(8)	0.5131(4)	0.6822(2)	0.057(2)	0.065(2)	0.045(1)	–0.007(2)	–0.009(1)	–0.010(1)
C(13)	8*d*	0.63805(8)	0.4941(4)	0.6415(2)	0.056(2)	0.070(2)	0.053(2)	–0.008(2)	–0.010(1)	0.004(2)
C(14)	8*d*	0.64380(8)	0.3996(4)	0.5430(2)	0.038(1)	0.084(2)	0.058(2)	–0.004(2)	–0.003(1)	0.003(2)
C(15)	8*d*	0.60992(8)	0.3276(4)	0.4894(2)	0.052(2)	0.063(2)	0.041(1)	0.002(2)	0.005(1)	0.003(1)
C(16)	8*d*	0.6750(1)	0.5746(5)	0.6998(3)	0.068(2)	0.113(3)	0.087(2)	–0.025(2)	–0.021(2)	–0.004(2)

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References

1. Peng, Z.; Bao, Z.; Galvin M. E.: Polymers with bipolar carrier transport abilities for light emitting diodes. Chem. Mater. **10** (1998) 2086-2090.
2. Wang, J. F.; Jabbour, G. E.; Mash, E. A.; Anderson, J.; Zhang, Y. D.; Lee, P. A.; Armstrong, N. R.; Peghambarian, N.; Kippelen, B.: Oxadiazole Metal Complex for Organic Light-Emitting Diodes. Adv. Mater. **11** (1999) 1266-1269.
3. Hughes, G.; Bryce, M. R.: Electron-transporting materials for organic electroluminescent and electrophosphorescent devices. J. Mater. Chem. **15** (2005) 94-107.
4. Yang, X. H.; Wu, F. I.; Neher, D.; Chein, C. H.; Shu, C. F.: Efficient red-emitting electrophosphorescent polymers. Chem. Mater. **20** (2008) 1629-1635.
5. Wang, Y. T.; Tong, M. L.; Fan. H. H.; Wang, H. Z.; Chen, X. M.: Homochiral crystallization of helical coordination chains bridged by achiral ligands:can it be controlled by the ligand structure? Dalton Trans. (2005) 424-426.
6. Chen, L. Q.; Yang, C. L.; Qin, J. G.; Gao, J.; You, H.; Ma, D. G.: Synthesis, structure, electrochemistry, photophysica and electroluminescence of 1,3,4-oxadiazole-based ortho-metalated iridium(III) complexes. J. Organomet. Chem. **691** (2006) 3519-3530.
7. Zhang, F. L.; Hou, Y. H.; Du, C. X.; Wu, Y.J: Synthesis, structure, photo- and electro-luminescent properties of novel oxadiazole-functionlized europium(III) benzamide complexes. Dalton Trans. (2009) 7359-7367.
8. Sheldrick, G. M.: A short history of SHELX. Acta Crystallogr. **A64** (2008) 112-122.