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Crystal structure of bis(acetato- κO)bis{2-((1*H*-tetrazol-1-yl)methyl)-1*H*-benzo[*d*]imidazole- κN } zinc(II), C₂₂H₂₂N₁₂O₄Zn

Table 1: Data collection and handling.

Crystal:	Prism, colorless
Size:	0.21 × 0.20 × 0.17 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.03 mm ⁻¹
Diffractometer, scan mode:	Rigaku Saturn, ω -scans
$\theta_{\max}$, completeness:	26°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	17553, 4940, 0.085
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3966
$N(\text{param})_{\text{refined}}$:	352
Programs:	Rigaku programs [1], SHELX [2]

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Abstract

C₂₂H₂₂N₁₂O₄Zn, monoclinic, $P2_1/c$ (no. 14), $a = 9.864(2)$ Å, $b = 8.6657(17)$ Å, $c = 30.803(8)$ Å, $\beta = 106.67(3)^\circ$, $V = 2522.3(10)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0630$, $wR_{\text{ref}}(F^2) = 0.1625$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

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Source of material

All reagents and solvents were commercially available except for 1-[(1*H*-benzimidazol-2-yl) methyl]-1*H*-tetrazole (Hbimt), which was synthesized according to the literature [3]. A methanol solution (3 mL) of Hbimt (0.05 mmol) was added dropwise to a methanol solution (2 mL) of Zn(Ac)₂·2H₂O (0.05 mmol). Colourless block-shaped crystals (55% yield, based on Zn) were obtained after five weeks through slow crystallization in a closed container at room temperature.

Experimental details

All hydrogen atoms were positioned geometrically and refined using a riding model, with $d(\text{C}-\text{H}) = 0.93$ (aromatic), 0.96 (CH₃), 0.97 (CH₂) Å and $d(\text{N}-\text{H}) = 0.86$ Å. H atoms were refined with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C}, \text{N})$ otherwise.

Discussion

It is well known that benzimidazole, tetrazole and their derivatives are widely used as ligands due to their strong coordination ability to metal ions and variety of coordination modes [4–6]. Up to now, numerous complexes with intriguing architectures and interesting properties have been constructed from these kinds of ligands [7–9]. But it is still a challenge to predict the structures and compositions of the products since many factors can influence the formation [10]. For example, the reaction of CdCl₂ with 2-[(1*H*-imidazol-1-yl)methyl]-1*H*-benzimidazole (imb)

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
Zn1	0.78277(5)	0.13054(5)	0.12736(2)	0.03259(17)
O1	0.6507(3)	0.0068(3)	0.14921(9)	0.0401(7)
O2	0.4851(3)	0.0328(4)	0.08375(9)	0.0487(8)
O3	0.7494(3)	0.3512(3)	0.11472(10)	0.0450(7)
O4	0.7603(4)	0.3824(4)	0.18653(10)	0.0503(8)
N1	0.9735(3)	0.1073(4)	0.17470(10)	0.0310(7)
N2	1.1460(3)	0.0518(4)	0.23676(10)	0.0336(7)
H2C	1.1887	0.0126	0.2627	0.040*
N3	0.8410(3)	0.0544(4)	0.25874(10)	0.0328(7)
N4	0.9144(4)	0.1276(5)	0.29681(14)	0.0566(11)
N5	0.8244(5)	0.2140(5)	0.30870(14)	0.0586(11)
N6	0.6936(4)	0.1975(5)	0.28007(13)	0.0598(11)
N7	0.7995(3)	0.0542(4)	0.06654(10)	0.0327(7)
N8	0.7356(3)	0.0020(4)	−0.00705(10)	0.0359(8)
H8B	0.6890	0.0062	−0.0353	0.043*
N9	0.6203(3)	0.3397(4)	−0.00565(10)	0.0345(7)
N10	0.5760(5)	0.3479(5)	−0.05128(13)	0.0560(11)
N11	0.6080(5)	0.4864(6)	−0.06059(17)	0.0692(13)
N12	0.6714(5)	0.5672(5)	−0.0233(2)	0.0721(14)
C1	0.7083(5)	0.1006(6)	0.24951(16)	0.0528(13)
H1A	0.6355	0.0684	0.2246	0.063*
C2	0.9095(4)	−0.0510(5)	0.23433(13)	0.0349(9)
H2A	0.8381	−0.1022	0.2103	0.042*
H2B	0.9614	−0.1294	0.2550	0.042*
C3	1.0087(4)	0.0352(4)	0.21443(12)	0.0287(8)
C4	1.0986(4)	0.1778(5)	0.17147(12)	0.0322(8)
C5	1.1247(5)	0.2701(5)	0.13828(14)	0.0466(11)
H5A	1.0527	0.2952	0.1123	0.056*
C6	1.2607(5)	0.3240(6)	0.14468(18)	0.0579(13)
H6A	1.2817	0.3836	0.1223	0.069*
C7	1.3681(5)	0.2897(6)	0.18479(18)	0.0571(13)
H7A	1.4581	0.3304	0.1888	0.069*
C8	1.3440(4)	0.1988(6)	0.21789(16)	0.0475(11)
H8A	1.4158	0.1752	0.2441	0.057*
C9	1.2069(4)	0.1427(4)	0.21071(13)	0.0328(8)
C10	0.6782(5)	0.4729(6)	0.01044(19)	0.0565(12)
H10A	0.7176	0.4961	0.0409	0.068*
C11	0.5925(4)	0.2016(5)	0.01762(14)	0.0381(9)
H11A	0.5058	0.1537	−0.0005	0.046*
H11B	0.5786	0.2313	0.0464	0.046*
C12	0.7104(4)	0.0866(5)	0.02596(12)	0.0318(8)
C13	0.8488(4)	−0.0928(5)	0.01181(13)	0.0344(9)
C14	0.9177(5)	−0.2036(5)	−0.00674(16)	0.0475(11)
H14A	0.8925	−0.2224	−0.0378	0.057*
C15	1.0252(5)	−0.2843(6)	0.02319(19)	0.0559(13)
H15A	1.0725	−0.3608	0.0121	0.067*
C16	1.0647(5)	−0.2540(5)	0.06952(17)	0.0519(12)
H16A	1.1377	−0.3109	0.0886	0.062*
C17	0.9988(5)	−0.1424(5)	0.08783(14)	0.0420(10)
H17A	1.0270	−0.1220	0.1188	0.050*
C18	0.8880(4)	−0.0606(4)	0.05833(13)	0.0331(8)
C19	0.5249(4)	−0.0157(5)	0.12271(13)	0.0364(9)
C20	0.4272(5)	−0.1074(6)	0.14227(16)	0.0528(12)
H20A	0.4757	−0.1358	0.1729	0.079*
H20B	0.3457	−0.0462	0.1419	0.079*
H20C	0.3976	−0.1989	0.1245	0.079*

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
C21	0.7493(4)	0.4364(5)	0.14831(15)	0.0436(10)
C22	0.7357(7)	0.6067(5)	0.13931(18)	0.0711(17)
H22A	0.7284	0.6260	0.1080	0.107*
H22B	0.6524	0.6445	0.1460	0.107*
H22C	0.8175	0.6585	0.1582	0.107*

and 1,4-benzenedicarboxylic acid (H₂bdc) can give complex [CdCl(bdic)_{1/2}(imb)₂]_n in water solution and complex {[Cd(bdic)(imb)(H₂O)]·DMF·2H₂O]_n in DMF-water solution [10]. In the reported complexes, the two-dimensional complex [Zn₂(bimt)₂(Ac)(OH)]_n was obtained by the reaction of Zn(Ac)₂·2H₂O with 1-[(1*H*-benzimidazol-2-yl) methyl]-1*H*-tetrazole (Hbimt) in DMF-water solution [11]. In order to explore the influence of solvent on the formation of complexes, we change the solvent of the above reaction system from DMF-water to methanol and get a new complex [Zn(Ac)₂(Hbimt)₂].

The asymmetrical unit of the title structure contains one Zn(II) ion, two Hbimt ligands and two acetate anions. The central Zn(II) ion is four-coordinated by two N atoms (N1, N7) from two Hbimt ligands and two O atoms (O1, O3) from two acetate anions leading to distorted tetrahedral coordination environment. The distances of Zn–N are 2.033(3) and 2.038(3) Å and the Zn–O bond length are 1.950(3) and 1.961(3) Å, all of which are close to those in a literature known Zn(II) complex [12]. In addition, there are some non-classical C–H···O hydrogen bonds. Molecules are linked by N2–H···O4' (' = 2 – *x*, *y* – 1/2, –*z* + 1/2) and N8–H···O2'' ('' = 1 – *x*, –*y*, –*z*) hydrogen bonds forming two-dimensional layered structure. Adjacent layers are further linked by non-classical hydrogen bonds resulting in a three-dimensional supramolecular architecture in the solid state.

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