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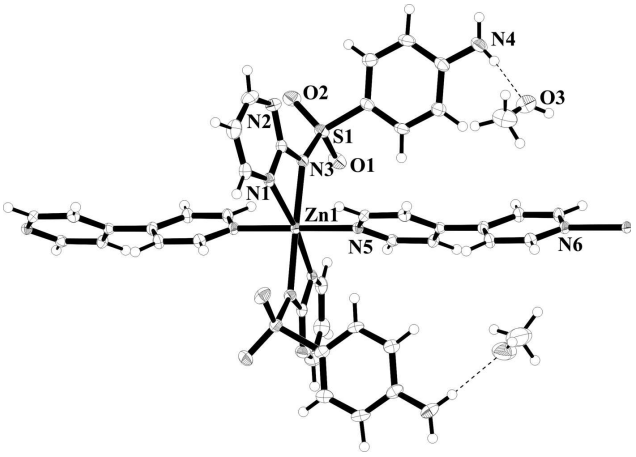
The crystal structure of *catena*-poly[bis((4-aminophenyl)sulfonyl)(pyrimidin-2-yl)amido-κ²*N*,*N*′)-bis(μ₂-4,4′-bipyridine-*N*,*N*′-κ²*N*:*N*′)zinc(II) – methanol (1/2), $C_{32}H_{34}N_{10}O_6S_2Zn$



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Abstract

$C_{32}H_{34}N_{10}O_6S_2Zn$, monoclinic, $C2/c$ (no. 15), $a = 24.243(4)$ Å, $b = 11.2766(17)$ Å, $c = 15.799(5)$ Å, $\beta = 127.986(2)°$, $V = 3404.0(13)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0432$, $wR_{ref}(F^2) = 0.1146$, $T = 100(2)$ K.

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A part of the title 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.

Source of material

The title structure was synthesized by adding methanol solution containing 4,4′-bipyridine (bipy; 0.234 g, 1.5 mmol) to the mixture of $Zn(NO_3)_2{\cdot}6(H_2O)$ (0.297 g, 1.0 mmol) and sodium sulfadiazine (0.545 g, 2 mmol) in methanol. The resulted precipitate was filtered off after stirring for half an hour. The remaining solution was kept undisturbed at room temperature for slow evaporation. Colorless plate-shaped crystals of $[Zn(4,4'\text{-bipy})_2(\text{sulfa})_2\text{MeOH}]_n$ were yielded after 4 days.

Table 1: Data collection and handling.

Crystal:	Plate, clear light colorless
Size:	0.22 × 0.18 × 0.08 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.91 mm^{-1}
Diffractometer, scan mode:	Bruker CCD, φ and ω-scans
θ_{max}, completeness:	27.8°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	16708, 4046, 0.056
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3237
$N(param)_{refined}$:	290
Programs:	Bruker programs [1], SHELX [2, 3]

Experimental details

All hydrogen atoms were added using the standard riding model implemented in the software [3].

Discussion

The two-fold rotation axis runs through the Zn(II) centers and the 4,4′-bipyridine molecules leaving the asymmetric unit consisting of a sulfadiazine ligand, a 4,4′-bipyridine, 1/2 Zn(II) and a methanol molecule (*cf.* the figure). The central Zn(II) cation is coordinated by six nitrogen atoms as a distorted octahedron with the average Zn—N distance of 2.17 Å. Two of the six are from two bipy ligands, and the other four are from two bidentate sulfadiazine ligands in chelating modes. This kind of coordination mode with both sulfadiazine ligands chelating to the metal center was reported for Cd(II) [4–6], Mn(II) [7], Ni(II) [8, 9], Cu(II) [10] and Co(II) [11–13] complexes. In Zn(II) complexes containing the sulfadiazine ligand [14–16], two ligands interact with the central Zn(II) by one of the N atoms. Englert's group reported that a second N atom in the sulfadiazine switching from non-bonding to bonding to the Zn(II) center with the temperature increasing from 100 K to 200 K in the structure of $Zn(\text{sulfadiazine})_2(NH_3)_2$ [17].

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.0000	0.14239(3)	0.2500	0.01386(12)
S1	0.07699(3)	0.15190(6)	0.52500(5)	0.01826(15)
O1	0.00421(10)	0.15525(17)	0.48048(15)	0.0260(4)
O2	0.12024(11)	0.06124(17)	0.60341(14)	0.0287(4)
O3	0.13995(14)	0.8055(2)	0.5657(2)	0.0542(7)
N1	0.11400(11)	0.12746(17)	0.32621(16)	0.0161(4)
N2	0.19885(11)	0.1198(2)	0.51812(17)	0.0213(5)
N3	0.07539(11)	0.14472(17)	0.42251(16)	0.0153(4)
N4	0.18757(13)	0.6219(2)	0.7334(2)	0.0270(5)
N5	0.0000	0.3305(2)	0.2500	0.0140(6)
N6	0.0000	0.9548(2)	0.2500	0.0145(6)
C1	0.13298(13)	0.1307(2)	0.42715(19)	0.0160(5)
C2	0.16388(14)	0.1053(2)	0.3165(2)	0.0214(5)
C3	0.23282(15)	0.0890(3)	0.4057(2)	0.0282(6)
C4	0.24687(15)	0.0995(3)	0.5039(2)	0.0270(6)
C5	0.11329(13)	0.2907(2)	0.58771(19)	0.0185(5)
C6	0.07968(14)	0.3939(2)	0.5301(2)	0.0208(5)
C7	0.10454(14)	0.5033(3)	0.5773(2)	0.0226(5)
C8	0.16421(13)	0.5132(2)	0.6847(2)	0.0218(5)
C9	0.19770(14)	0.4087(3)	0.7418(2)	0.0246(6)
C10	0.17227(14)	0.2985(3)	0.6943(2)	0.0229(6)
C11	0.04883(13)	0.3922(2)	0.25339(19)	0.0156(5)
C12	0.05063(12)	0.5146(2)	0.25382(19)	0.0159(5)
C13	0.0000	0.5779(3)	0.2500	0.0136(6)
C14	0.0000	0.7090(3)	0.2500	0.0157(7)
C15	0.01618(13)	0.7722(2)	0.19207(19)	0.0169(5)
C16	0.01553(13)	0.8944(2)	0.19388(19)	0.0166(5)
C17	0.1623(2)	0.7956(4)	0.4988(3)	0.0608(11)
H2	0.1497(16)	0.101(3)	0.248(2)	0.030(8)*
H3	0.2712(17)	0.070(3)	0.399(2)	0.035(9)*
H3A	0.1108(19)	0.852(3)	0.557(4)	0.064(15)*
H4	0.2885(19)	0.098(3)	0.566(3)	0.041(10)*
H4A	0.2277(12)	0.626(3)	0.7967(18)	0.040(10)*
H4B	0.1744(19)	0.678(3)	0.688(2)	0.049(11)*
H6	0.0398(16)	0.391(3)	0.462(2)	0.024(8)*
H7	0.0796(13)	0.573(2)	0.538(2)	0.013(7)*
H9	0.2406(16)	0.418(3)	0.815(2)	0.028(8)*
H10	0.1934(15)	0.234(3)	0.731(2)	0.024(8)*
H11	0.0841(15)	0.347(2)	0.257(2)	0.017(7)*
H12	0.0863(14)	0.553(2)	0.255(2)	0.016(7)*
H15	0.0254(13)	0.732(2)	0.149(2)	0.014(6)*
H16	0.0256(13)	0.936(2)	0.1536(19)	0.008(6)*
H17A	0.1329	0.8465	0.4354	0.091*
H17B	0.1578	0.7131	0.4759	0.091*
H17C	0.2113	0.8206	0.5400	0.091*

Nevertheless, both bidentate sulfadiazine in the same zinc compound has not been reported.

The 4,4′-bipyridine ligands bridge the Zn(II) centers connecting the structure to a one dimensional polymer along crystallographic *b* direction. The terminal amine $-NH_2$ group of sulfadiazine does not participate in the coordination but it captures the methanol *via* N—H···O hydrogen bond on one side and connects with the uncoordinated pyrimidine–N atom in the adjacent polymer chain on another, thus extending the 1D polymer to a hydrogen bonded 2D network. The hydroxyl group of the methanol forms weak hydrogen bonds to the sulfoxyl O from the same polymer chain as the hydroxyl-O bound with the ammine. The O—H···O bond is weak (A···D) = 3.042 Å and A···H···D angle = 130.3°.

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