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Di-μ-sulfito-$\kappa^6O,O':O',O''$-bis[(2,2′-bipyridine-κ^2N,N')zinc(II)]

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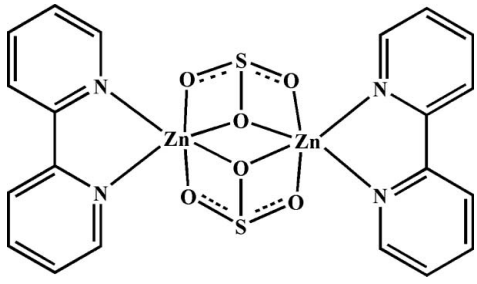
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.025; wR factor = 0.054; data-to-parameter ratio = 11.4.

In the title compound, $[Zn_2(SO_3)_2(C_{10}H_8N_2)_2]$, Zn^{2+} and SO_3^{2-} form a dinuclear unit, with an inversion center at the mid-point of the Zn···Zn vector. Each Zn atom has distorted octahedral geometry and is coordinated by four O atoms from two SO_3^{2-} anions and two N atoms of the 2,2′-bipyridine ligand.

Related literature

For related literature, see: Nguyen *et al.* (2006).



Experimental

Crystal data

$[Zn_2(SO_3)_2(C_{10}H_8N_2)_2]$
M_r = 603.23
Monoclinic, $P2_1/n$
a = 8.1444 (1) Å
b = 13.2118 (2) Å
c = 10.3020 (1) Å
β = 109.970 (1)°
V = 1041.86 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.55 mm^{-1}
T = 273 (2) K
0.21 × 0.13 × 0.10 mm

Data collection

Siemens SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.700, T_{max} = 0.800
8021 measured reflections
1756 independent reflections
1413 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.054
S = 0.94
1756 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O3^i	2.0651 (19)	Zn1—N2	2.105 (2)
Zn1—O1	2.0963 (17)	Zn1—O2	2.2016 (16)
Zn1—N1	2.102 (2)	Zn1—O2^i	2.2932 (19)
O3^i—Zn1—O1	156.65 (7)	N1—Zn1—O2	99.90 (7)
O3^i—Zn1—N1	103.97 (7)	N2—Zn1—O2	167.47 (8)
O1—Zn1—N1	96.46 (7)	O3^i—Zn1—O2^i	66.11 (6)
O3^i—Zn1—N2	94.52 (8)	O1—Zn1—O2^i	94.10 (7)
O1—Zn1—N2	100.69 (7)	N1—Zn1—O2^i	169.26 (7)
N1—Zn1—N2	78.21 (8)	N2—Zn1—O2^i	97.96 (7)
O3^i—Zn1—O2	97.94 (7)	O2—Zn1—O2^i	85.98 (7)
O1—Zn1—O2	67.07 (6)		

Symmetry code: (i) $-x, -y, -z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2163).

References

Nguyen, D.-T., Chew, E., Zhang, Q., Choi, A. & Bu, X. (2006). *Inorg. Chem.* **45**, 10722–10727.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
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supplementary materials

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Di-μ-sulfito-$\kappa^6O,O':O',O''$-bis[(2,2'-bipyridine-κ^2N,N')zinc(II)]

E Yang, X.-C. Song, S.-Z. Shen and Y.-D. Lin

Comment

Metal organic frameworks based on the SO_3^{2-} unit are of current interest (Nguyen *et al.*, 2006). We report here a new zinc sulfite structure, $Zn_2(SO_3)_2$(2,2'-bipyridine)$_2$.

In the title compound, Zn^{2+} and SO_3^{2-} form an dinuclear unit, with an inversion center at the mid-point of the Zn···Zn vector (Fig.1). Each Zn atom has distorted octahedral geometry and is coordinated by four O atoms from two different SO_3^{2-} anions and two N atoms from the 2,2'-bipyridine ligand. It is worth noting that Zn1 and Zn1a share two common oxygen sites from two SO_3^{2-} anions. In the SO_3^{2-} group, one oxygen site is linked to two Zn^{2+} and one S^{4+} sites; the other two oxygen sites are each linked to one Zn^{2+} and one S^{4+} sites. The 2,2'-bipyridine ligands chelate the Zn sites.

Experimental

A mixture of $ZnSO_3$ (0.145 g, 1 mmol), 2,2'-bipyridine (0.168 g, 1 mmol) and H_2O (18 ml) was sealed in a 25 ml Teflon-lined stainless steel reactor and was heated at 373 K for 3 d. On completion of the reaction, the reactor was cooled slowly to room temperature and the mixture was filtered, giving colorless single crystals suitable for X-ray analysis.

Refinement

All H atoms were placed at calculated positions, and refined using a riding model [C—H = 0.93Å and U_{iso}(H) = 1.2U_{eq}(C)].

Figures

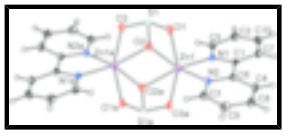


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids [symmetry code: (*a*) −*x*,-*y*,-*z*].

Di-μ-sulfito-κ^6*O*,*O*':*O*',*O*''-bis[(2,2'-bipyridine-κ^2*N*,*N*')zinc(II)]

Crystal data

$[Zn_2(SO_3)_2(C_{10}H_8N_2)_2]$	$Z = 2$
$M_r = 603.23$	$F_{000} = 608$
Monoclinic, $P2_1/n$	$D_x = 1.923$ Mg m^{-3}
Hall symbol: -P2yn	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å

a = 8.1444 (1) Å	θ = 2.6–25.0º
b = 13.2118 (2) Å	μ = 2.55 mm^{-1}
c = 10.3020 (1) Å	T = 273 (2) K
β = 109.970 (1)º	Prism, colorless
V = 1041.86 (2) Å^3	0.21 × 0.13 × 0.10 mm

Data collection

Siemens SMART 1K CCD area-detector diffractometer	1756 independent reflections
Radiation source: fine-focus sealed tube	1413 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 273(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −9→9
T_{min} = 0.700, T_{max} = 0.800	k = −15→15
8021 measured reflections	l = −12→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.025	H-atom parameters constrained
$wR(F^2)$ = 0.054	$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.94	$(\Delta/\sigma)_{max} < 0.001$
1756 reflections	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
154 parameters	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}

Zn1	0.07078 (4)	0.00807 (2)	0.16944 (3)	0.01426 (11)
S1	0.27778 (9)	−0.00925 (5)	0.00581 (7)	0.01588 (17)
O2	0.1343 (2)	−0.08446 (12)	0.01526 (18)	0.0166 (4)
N2	0.0632 (3)	0.11128 (15)	0.3230 (2)	0.0141 (5)
N1	0.2190 (3)	−0.06780 (14)	0.3510 (2)	0.0135 (5)
O1	0.2832 (2)	0.06485 (13)	0.12097 (18)	0.0188 (4)
C6	0.1471 (3)	0.08117 (18)	0.4537 (3)	0.0127 (6)
C5	0.3016 (4)	−0.15614 (19)	0.3572 (3)	0.0177 (6)
H5A	0.2819	−0.1922	0.2758	0.021*
C4	0.1365 (4)	0.13747 (19)	0.5649 (3)	0.0179 (6)
H4A	0.1936	0.1159	0.6550	0.021*
C3	−0.0344 (4)	0.19588 (18)	0.3002 (3)	0.0172 (6)
H3A	−0.0953	0.2149	0.2096	0.021*
C2	0.4143 (4)	−0.1964 (2)	0.4782 (3)	0.0202 (7)
H2A	0.4680	−0.2587	0.4793	0.024*
C1	0.2462 (3)	−0.01508 (18)	0.4696 (3)	0.0131 (6)
O3	0.1804 (3)	0.04415 (13)	−0.13110 (18)	0.0186 (4)
C10	0.4447 (4)	−0.14091 (19)	0.5983 (3)	0.0201 (7)
H10A	0.5227	−0.1647	0.6815	0.024*
C9	−0.0478 (4)	0.25539 (19)	0.4057 (3)	0.0199 (7)
H9A	−0.1145	0.3142	0.3870	0.024*
C8	0.0400 (4)	0.22563 (19)	0.5396 (3)	0.0203 (7)
H8A	0.0343	0.2649	0.6128	0.024*
C7	0.3591 (4)	−0.05038 (19)	0.5940 (3)	0.0177 (6)
H7A	0.3772	−0.0133	0.6744	0.021*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01481 (19)	0.01848 (17)	0.00850 (19)	−0.00008 (14)	0.00271 (16)	−0.00131 (13)
S1	0.0132 (4)	0.0205 (3)	0.0136 (4)	−0.0016 (3)	0.0043 (3)	0.0005 (3)
O2	0.0164 (11)	0.0184 (9)	0.0146 (11)	−0.0031 (8)	0.0046 (10)	0.0002 (8)
N2	0.0130 (14)	0.0178 (11)	0.0102 (13)	−0.0021 (9)	0.0024 (12)	−0.0007 (9)
N1	0.0133 (13)	0.0173 (11)	0.0102 (13)	−0.0029 (9)	0.0044 (11)	−0.0037 (9)
O1	0.0209 (12)	0.0238 (10)	0.0104 (11)	−0.0070 (8)	0.0036 (10)	−0.0026 (8)
C6	0.0116 (15)	0.0152 (13)	0.0112 (16)	−0.0032 (11)	0.0039 (14)	−0.0008 (10)
C5	0.0193 (17)	0.0200 (14)	0.0144 (17)	0.0009 (12)	0.0067 (15)	−0.0026 (11)
C4	0.0215 (17)	0.0213 (14)	0.0107 (16)	−0.0026 (12)	0.0054 (15)	−0.0022 (11)
C3	0.0165 (17)	0.0182 (13)	0.0156 (17)	0.0027 (11)	0.0038 (15)	0.0038 (11)
C2	0.0211 (18)	0.0197 (14)	0.0212 (18)	0.0046 (12)	0.0091 (16)	0.0031 (12)
C1	0.0117 (15)	0.0175 (13)	0.0108 (15)	−0.0040 (11)	0.0047 (14)	0.0007 (11)
O3	0.0195 (12)	0.0257 (10)	0.0094 (11)	−0.0042 (8)	0.0034 (10)	0.0020 (8)
C10	0.0175 (18)	0.0249 (15)	0.0146 (17)	−0.0003 (12)	0.0013 (15)	0.0069 (12)
C9	0.0212 (18)	0.0154 (13)	0.0254 (18)	0.0011 (12)	0.0108 (16)	−0.0019 (12)
C8	0.0231 (19)	0.0210 (14)	0.0192 (18)	−0.0045 (12)	0.0101 (16)	−0.0083 (12)
C7	0.0200 (18)	0.0226 (14)	0.0096 (16)	−0.0034 (12)	0.0040 (15)	−0.0007 (11)

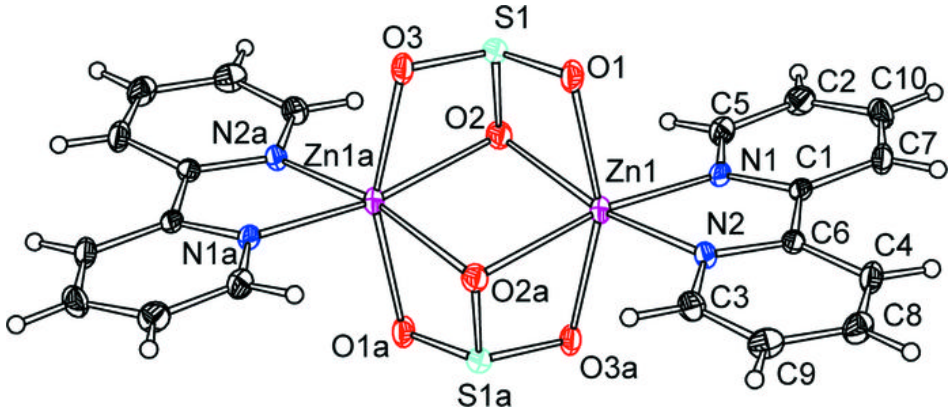
Geometric parameters (Å, °)

Zn1—O3^{i}	2.0651 (19)	C6—C1	1.485 (3)
Zn1—O1	2.0963 (17)	C5—C2	1.378 (4)
Zn1—N1	2.102 (2)	C5—H5A	0.9300
Zn1—N2	2.105 (2)	C4—C8	1.379 (4)
Zn1—O2	2.2016 (16)	C4—H4A	0.9300
Zn1—O2^{i}	2.2932 (19)	C3—C9	1.375 (3)
Zn1—S1	2.7708 (6)	C3—H3A	0.9300
Zn1—S1^{i}	2.7961 (8)	C2—C10	1.386 (4)
S1—O1	1.5271 (17)	C2—H2A	0.9300
S1—O3	1.5337 (19)	C1—C7	1.378 (4)
S1—O2	1.5618 (18)	O3—Zn1^{i}	2.0651 (19)
S1—Zn1^{i}	2.7961 (8)	C10—C7	1.378 (4)
O2—Zn1^{i}	2.2932 (19)	C10—H10A	0.9300
N2—C6	1.345 (3)	C9—C8	1.377 (4)
N2—C3	1.345 (3)	C9—H9A	0.9300
N1—C5	1.337 (3)	C8—H8A	0.9300
N1—C1	1.357 (3)	C7—H7A	0.9300
C6—C4	1.393 (3)		
O3^{i}—Zn1—O1	156.65 (7)	Zn1—O2—Zn1^{i}	94.02 (7)
O3^{i}—Zn1—N1	103.97 (7)	C6—N2—C3	119.2 (2)
O1—Zn1—N1	96.46 (7)	C6—N2—Zn1	115.17 (16)
O3^{i}—Zn1—N2	94.52 (8)	C3—N2—Zn1	125.06 (19)
O1—Zn1—N2	100.69 (7)	C5—N1—C1	118.7 (2)
N1—Zn1—N2	78.21 (8)	C5—N1—Zn1	125.85 (18)
O3^{i}—Zn1—O2	97.94 (7)	C1—N1—Zn1	115.07 (16)
O1—Zn1—O2	67.07 (6)	S1—O1—Zn1	98.54 (9)
N1—Zn1—O2	99.90 (7)	N2—C6—C4	120.8 (2)
N2—Zn1—O2	167.47 (8)	N2—C6—C1	115.8 (2)
O3^{i}—Zn1—O2^{i}	66.11 (6)	C4—C6—C1	123.4 (2)
O1—Zn1—O2^{i}	94.10 (7)	N1—C5—C2	123.3 (2)
N1—Zn1—O2^{i}	169.26 (7)	N1—C5—H5A	118.3
N2—Zn1—O2^{i}	97.96 (7)	C2—C5—H5A	118.3
O2—Zn1—O2^{i}	85.98 (7)	C8—C4—C6	119.1 (3)
O3^{i}—Zn1—S1	128.67 (5)	C8—C4—H4A	120.4
O1—Zn1—S1	33.03 (5)	C6—C4—H4A	120.4
N1—Zn1—S1	102.59 (6)	N2—C3—C9	122.6 (3)
N2—Zn1—S1	133.68 (6)	N2—C3—H3A	118.7
O2—Zn1—S1	34.25 (5)	C9—C3—H3A	118.7
O2^{i}—Zn1—S1	87.35 (4)	C5—C2—C10	117.7 (2)
O3^{i}—Zn1—S1^{i}	32.58 (5)	C5—C2—H2A	121.2
O1—Zn1—S1^{i}	125.64 (5)	C10—C2—H2A	121.2
N1—Zn1—S1^{i}	136.49 (6)	N1—C1—C7	121.0 (2)

N2—Zn1—S1^{i}	101.41 (6)	N1—C1—C6	115.1 (2)
O2—Zn1—S1^{i}	88.53 (5)	C7—C1—C6	123.8 (2)
O2^{i}—Zn1—S1^{i}	33.95 (4)	S1—O3—Zn1^{i}	100.93 (8)
S1—Zn1—S1^{i}	107.589 (18)	C7—C10—C2	119.7 (3)
O1—S1—O3	106.75 (10)	C7—C10—H10A	120.1
O1—S1—O2	100.56 (9)	C2—C10—H10A	120.1
O3—S1—O2	100.78 (10)	C3—C9—C8	118.3 (2)
O1—S1—Zn1	48.44 (7)	C3—C9—H9A	120.9
O3—S1—Zn1	106.88 (7)	C8—C9—H9A	120.9
O2—S1—Zn1	52.49 (6)	C9—C8—C4	119.9 (2)
O1—S1—Zn1^{i}	104.57 (8)	C9—C8—H8A	120.1
O3—S1—Zn1^{i}	46.48 (7)	C4—C8—H8A	120.1
O2—S1—Zn1^{i}	55.09 (7)	C10—C7—C1	119.6 (2)
Zn1—S1—Zn1^{i}	72.411 (18)	C10—C7—H7A	120.2
S1—O2—Zn1	93.26 (8)	C1—C7—H7A	120.2
S1—O2—Zn1^{i}	90.96 (8)		

Symmetry codes: (i) −*x*, −*y*, −*z*.

Fig. 1


S1
O3
O1
C2
C10
C5
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N2a
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Zn1
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C1
C7
N2
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C4
N1a
O2a
C3
C8
O1a
O3a
C9
S1a