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Bis(*N*-ethylpyridinium) bis(2-thioxo-1,3-dithiole-4,5-dithiolato)zincate(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.038
wR factor = 0.106
Data-to-parameter ratio = 16.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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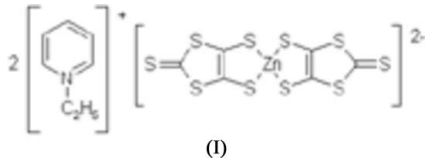
In the title compound, $(C_7H_{10}N)_2[Zn(C_3S_5)_2]$, the Zn^{II} ion is located on a twofold axis and coordinated by four 2-thioxo-1,3-dithiole-4,5-dithiolate S atoms with a distorted tetrahedral geometry. The asymmetric unit contains two independent *N*-ethylpyridinium cations, each having mirror symmetry.

Comment

$[Zn(dmit)_2]^{2-}$ salts (dmit is 2-thioxo-1,3-dithiole-4,5-dithiolate) have attracted much attention because of promising optical properties (Li *et al.*, 1996; Xia *et al.*, 1997; Dai *et al.*, 2000; Sun *et al.*, 2001). As part of an investigation of organic optical materials, the title compound, (I), was recently prepared in our laboratory.



(I)

The crystal structure of (I) consists of $[Zn(dmit)_2]^{2-}$ anions and ethylpyridinium cations (Fig. 1). The anion has C_2 symmetry. The Zn^{II} ion is located on a twofold axis and coordinated by four S atoms from two dmit ligands with a distorted tetrahedral geometry (Table 1). The dihedral angle between dmit planes is 69.44 (18)°. The Zn^{II} ion deviates from each dmit mean plane by 0.230 (1) Å. Both independent cations have mirror symmetry, with the ethyl C atoms, pyridine N atoms, and atoms C5 and C13 lying on the mirror planes.

In the crystal structure of (I), the S2···S2^{iii} separation of 3.6304 (13) Å [symmetry code: (iii) $\frac{1}{2} - x$,1/2 − y,1 − z] is much longer than 3.492 (2) Å found in a similar compound, bis(*N*-methylpyridinium)[Zn(dmit)$_2$] (Wang *et al.*, 2005), and indicates the normal van der Waals contact between S atoms.

Experimental

The title complex was prepared according to a literature procedure (Steimeck & Kirmse, 1979). The single crystals of (I) used for X-ray structure analysis were obtained by slow evaporation of an acetone solution of (I) at room temperature.

Crystal data

$(C_7H_{10}N)_2[Zn(C_3S_5)_2]$
M_r = 674.35
Monoclinic, $C2/m$
a = 19.948 (4) Å
b = 14.733 (3) Å
c = 10.001 (2) Å
β = 106.934 (2)°
V = 2811.7 (10) Å^3
Z = 4
D_x = 1.593 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3979 reflections
θ = 2.1–24.9°
μ = 1.63 mm^{-1}
T = 298 (2) K
Block, red
0.79 × 0.68 × 0.45 mm

Data collection

Bruker SMART CCD area-detector diffractometer	2593 independent reflections
φ and ω scans	2229 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)	$R_{int} = 0.030$
$T_{min} = 0.280$, $T_{max} = 0.476$	$\theta_{max} = 25.1^\circ$
7034 measured reflections	$h = -23 \rightarrow 23$
	$k = -17 \rightarrow 15$
	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0651P)^2 + 1.3911P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.106$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.97$ e Å^{-3}
2593 reflections	
162 parameters	
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

Zn1—S4	2.3323 (9)	S3—C1	1.721 (3)
Zn1—S5	2.3429 (8)	S3—C3	1.738 (3)
S1—C1	1.650 (3)	S4—C3	1.734 (3)
S2—C1	1.713 (3)	S5—C2	1.742 (3)
S2—C2	1.746 (3)		

H atoms were treated as riding, with C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXTL* (Bruker, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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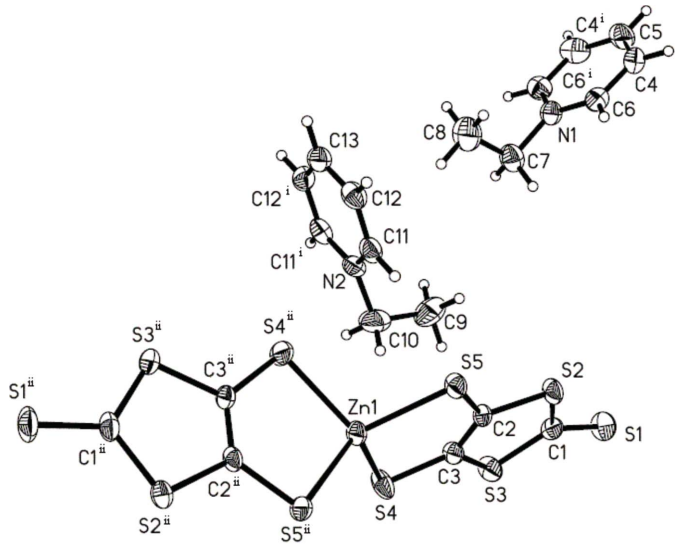

Figure 1
The structure of (I), with 50% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry codes: (i) $-x$, y, $1 - z$; (ii) x, $-y$, z].

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