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Poly[tetra-*n*-butylammonium [(dimethyl sulfoxide-κO)sesqui(μ_2-terephthalato-$\kappa^2 O:O'$)zincate(II)] 0.67-dimethyl sulfoxide 0.25-pyrazine solvate]

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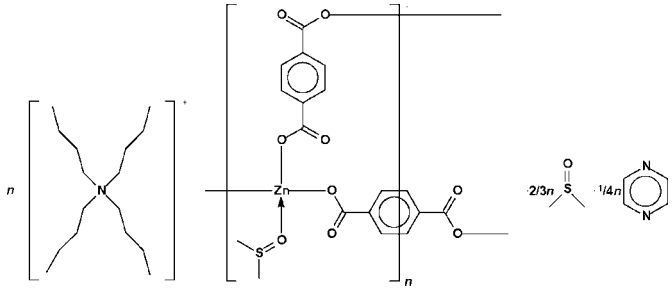
Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.060; wR factor = 0.181; data-to-parameter ratio = 20.5.

The anion of the title compound, $\{(C_{16}H_{36}N)[Zn(C_8H_4O_4)_{1.5}\text{-}(C_2H_6OS)]\cdot 0.67C_2H_6OS\cdot 0.25C_4H_4N_2\}_n$, exists as a polyanionic layer in which the dimethyl sulfoxide-coordinated Zn atom is bridged by two terephthalate anions (one of which lies on a general position and the other about a center of inversion). The honeycomb layers are wavy, and the sterically bulky cation as well as the dimethyl sulfoxide and pyrazine solvent molecules occupy the space between adjacent layers. These do not interact with the layers. The geometry of the Zn atom is tetrahedral.

Related literature

For other zinc terephthalate adducts of DMSO, see Wang *et al.* (2001) and Yang *et al.* (2005). For a report of the intercalation of DMSO in organic compounds, see Nangia & Desiraju (1999).



Experimental

Crystal data

$(C_{16}H_{36}N)[Zn(C_8H_4O_4)_{1.5}\text{-}(C_2H_6OS)]\cdot 0.67C_2H_6OS\cdot\text{-}0.25C_4H_4N_2$
M_r = 704.26
Monoclinic, $P2_1/n$
a = 11.1722 (5) Å
b = 24.8188 (11) Å
c = 13.9443 (6) Å
β = 97.968 (1)°
V = 3829.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 223 (2) K
0.48 × 0.47 × 0.38 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.626, T_{max} = 0.752
43211 measured reflections
8752 independent reflections
7451 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.181
S = 1.05
8752 reflections
427 parameters
105 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1	1.959 (2)	Zn1—O3^{i}	1.993 (2)
Zn1—O5	1.972 (2)	Zn1—O7	2.047 (2)

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2568).

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supplementary materials

Acta Cryst. (2007). E**63**, m2788 [**doi:10.1107/S1600536807050672**]

Poly[tetra-*n*-butylammonium [(dimethyl sulfoxide-κO)sesqui(μ_2-terephthalato-$\kappa^2 O:O'$)zincate(II)] 0.67-dimethyl sulfoxide 0.25-pyrazine solvate]

S.-Y. Yang, C. Du, R.-B. Huang and S. W. Ng

Comment

Dimethyl sulfoxide (DMSO) occassionally gets trapped in organic molecular crystals through multi-point recognition between the solvent and molecule (Nangia & Desiraju, 1999). Similarly, coordination polymers synthesized using DMSO as solvent sometimes intercalate DMSO as solvated molecule (Wang *et al.*, 2001, Yang *et al.*, 2005). Our attempt to synthesize porous coordination polymers with the zinc ion, terephthalate dianion and pyrazine in DMSO resulted in the formation of the title compound, (I).

The zinc atom exists in a tetrahedral geometry (Table 1), being coordinated to one oxygen atom from a DMSO moleucle and three oxygen atoms from three different terephthalate anions (Fig. 1). The manner of bridging generates a wavy, honeycomb polyanionic layer (Figure 2). The space between adjacent layers is occupied by the bulky cation as well as the DMSO and pyrazine solvent molecules. The guest cations and molecules take up more than 60% of the unit cell volume. These guests interact with the layers through weak van der Waals interactions.

Experimental

Pyrazine (0.4 mmol), tetra-*n*-butylammonium terephthalate (0.4 mmol), zinc nitrate hexahydrate (0.4 mmol) and dimethylsulfoxide (2 ml) was placed in a thin glass tube. The contents were set aside for a month for the formation of colourless blocks of (I).

Refinement

There is some disorder in the terminal carbon atom of one of the four butyl chains of the cation. For the cation, the four N–C bonds were restrained to within 0.01 Å of each other as were the C–C distances. The C32 atom is disordered over two sites; the U^{ij} values for C28 were set to those of C28'.

As one of the geometrically generated H atoms of the uncoordinated DMSO (S2/O8/C15/C16) molecule is too close to one of the geometrically generated H of the C28' atom, the occupancy of this DMSO molecule is not unity, and refining gave a value close to 0.667. Furthermore, the refinement of the occupancy of the C28/C28' pair of atoms gave a ratio of nearly 0.67/0.33. Consequently, the occupany of the DMSO was fixed as 2/3; the occupancy of C32 would then also be 2/3.

The pyrazine molecule lies on an inversion centre; its C—C and C—N bond distances were restrained to 1.35 (1) Å; the U^{ij} values were restrained to be nearly isotropic. The carbon-bound H atoms were placed at calculated positions (C–H 0.93 to 0.98 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2 to 1.5U_{eq}(C). The final difference Fourier map had a large peak in the vicinity of S1, but was otherwise essentially featureless.

Figures

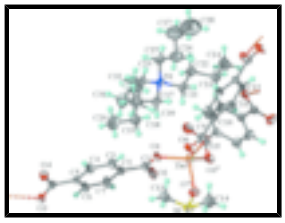

Fig. 1. **Figure 1**. View of a portion of the layer structure of (I); displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius. Symmetry code: $i = 1/2 + x, 3/2 - y, 1/2 - z$.] The solvent DMSO and pyrazine molecules, and the minor disorder component are not shown.

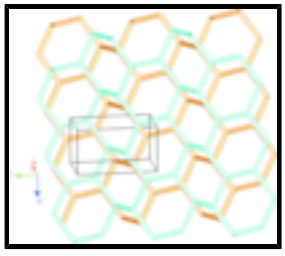

Fig. 2. **Figure 2**. Extended layer structure of (I).

Poly[tetra-*n*-butylammonium [(dimethyl sulfoxide-κ*O*) sesqui(μ$_2$-terephthalato-κ^2*O*:*O*$^{\prime}$)zincate(II)] 0.67-dimethyl sulfoxide 0.25-pyrazine solvate]

Crystal data

$(C_{16}H_{36}N)[Zn(C_8H_4O_4)_{1.5}(C_2H_6OS)]\cdot 0.67C_2H_6OS\cdot 0.25C_4H_4N_2$	$F_{000} = 1558$
$M_r = 704.26$	$D_x = 1.267$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 6737 reflections
$a = 11.1722$ (5) Å	$\theta = 2.2$–27.6º
$b = 24.8188$ (11) Å	$\mu = 0.80$ mm^{-1}
$c = 13.9443$ (6) Å	$T = 223$ (2) K
$\beta = 97.968$ (1)º	Irregular block, colorless
$V = 3829.2$ (3) Å^3	0.48 × 0.47 × 0.38 mm
$Z = 4$	

Data collection

Bruker APEX area-detector diffractometer	8752 independent reflections
Radiation source: fine-focus sealed tube	7451 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.038$
$T = 223(2)$ K	$\theta_{max} = 27.5$º
φ and ω scans	$\theta_{min} = 1.6$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -14 \rightarrow 14$
$T_{min} = 0.626$, $T_{max} = 0.752$	$k = -32 \rightarrow 32$
43211 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.060$	H-atom parameters constrained
$wR(F^2) = 0.181$	$w = 1/[\sigma^2(F_o^2) + (0.1092P)^2 + 3.742P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
8752 reflections	$\Delta\rho_{max} = 1.44$ e Å^{-3}
427 parameters	$\Delta\rho_{min} = -0.61$ e Å^{-3}
105 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.64399 (3)	0.642867 (13)	0.33508 (2)	0.02661 (13)	
S1	0.38991 (8)	0.57300 (4)	0.32477 (7)	0.0474 (2)	
S2	0.5688 (3)	0.98156 (14)	0.66626 (17)	0.1035 (8)	0.67
O1	0.59927 (19)	0.67880 (9)	0.45005 (15)	0.0349 (5)	
O2	0.5151 (2)	0.74012 (12)	0.34659 (16)	0.0518 (7)	
O3	0.1890 (2)	0.83652 (10)	0.70662 (17)	0.0425 (5)	
O4	0.3049 (2)	0.78816 (13)	0.81478 (17)	0.0531 (7)	
O5	0.7673 (2)	0.58738 (9)	0.37480 (16)	0.0396 (5)	
O6	0.6877 (2)	0.54688 (10)	0.49407 (19)	0.0460 (6)	
O7	0.4824 (2)	0.60747 (10)	0.28330 (17)	0.0445 (6)	
O8	0.5191 (8)	1.0295 (4)	0.6328 (7)	0.150 (4)	0.67
N1	0.9806 (2)	0.68523 (11)	0.59716 (18)	0.0379 (6)	
C1	0.5326 (3)	0.72000 (13)	0.4272 (2)	0.0333 (6)	
C2	0.4686 (3)	0.74255 (13)	0.5077 (2)	0.0326 (6)	
C3	0.4834 (3)	0.71959 (14)	0.5987 (2)	0.0406 (7)	
H3	0.5360	0.6901	0.6122	0.049*	
C4	0.4214 (3)	0.73963 (15)	0.6704 (2)	0.0414 (7)	
H4	0.4339	0.7242	0.7326	0.050*	
C5	0.3412 (3)	0.78209 (13)	0.6515 (2)	0.0330 (6)	
C6	0.3251 (3)	0.80457 (15)	0.5598 (2)	0.0422 (8)	
H6	0.2704	0.8332	0.5457	0.051*	
C7	0.3888 (3)	0.78525 (15)	0.4887 (2)	0.0444 (8)	
H7	0.3779	0.8012	0.4270	0.053*	
C8	0.2740 (3)	0.80337 (14)	0.7308 (2)	0.0380 (7)	
C9	0.7701 (2)	0.55514 (11)	0.4462 (2)	0.0302 (6)	
C10	0.8894 (2)	0.52593 (11)	0.4732 (2)	0.0284 (6)	
C11	0.9800 (3)	0.52863 (12)	0.4141 (2)	0.0319 (6)	
H11	0.9665	0.5480	0.3556	0.038*	
C12	1.0895 (3)	0.50312 (12)	0.4406 (2)	0.0330 (6)	

H12	1.1501	0.5054	0.4003	0.040*	
C13	0.4011 (3)	0.58585 (16)	0.4505 (3)	0.0484 (8)	
H13A	0.3699	0.6216	0.4607	0.073*	
H13B	0.4850	0.5838	0.4794	0.073*	
H13C	0.3543	0.5593	0.4803	0.073*	
C14	0.4521 (4)	0.50670 (17)	0.3325 (3)	0.0630 (11)	
H14A	0.4536	0.4926	0.2678	0.095*	
H14B	0.4028	0.4835	0.3671	0.095*	
H14C	0.5338	0.5079	0.3668	0.095*	
C15	0.4521 (17)	0.9380 (6)	0.6315 (9)	0.180 (8)	0.67
H15A	0.3880	0.9442	0.6705	0.270*	0.67
H15B	0.4807	0.9012	0.6404	0.270*	0.67
H15C	0.4213	0.9439	0.5637	0.270*	0.67
C16	0.6612 (17)	0.9648 (10)	0.5953 (10)	0.226 (11)	0.67
H16A	0.7320	0.9877	0.6065	0.339*	0.67
H16B	0.6231	0.9688	0.5288	0.339*	0.67
H16C	0.6850	0.9275	0.6070	0.339*	0.67
C17	0.8735 (3)	0.65174 (13)	0.6193 (2)	0.0385 (7)	
H17A	0.8038	0.6605	0.5711	0.046*	
H17B	0.8927	0.6137	0.6109	0.046*	
C18	0.8364 (4)	0.65861 (16)	0.7188 (3)	0.0487 (9)	
H18A	0.8068	0.6953	0.7263	0.058*	
H18B	0.9058	0.6524	0.7687	0.058*	
C19	0.7367 (3)	0.61794 (15)	0.7296 (3)	0.0486 (8)	
H19A	0.6725	0.6218	0.6745	0.058*	
H19B	0.7699	0.5815	0.7272	0.058*	
C20	0.6817 (5)	0.6240 (2)	0.8225 (4)	0.0817 (16)	
H20A	0.6194	0.5970	0.8246	0.123*	
H20B	0.6465	0.6596	0.8249	0.123*	
H20C	0.7441	0.6193	0.8776	0.123*	
C21	0.9985 (3)	0.66980 (14)	0.4949 (2)	0.0410 (7)	
H21A	1.0147	0.6310	0.4942	0.049*	
H21B	0.9219	0.6759	0.4528	0.049*	
C22	1.0968 (3)	0.69794 (15)	0.4500 (2)	0.0471 (8)	
H22A	1.1731	0.6963	0.4940	0.056*	
H22B	1.0755	0.7359	0.4382	0.056*	
C23	1.1112 (3)	0.67031 (16)	0.3550 (2)	0.0466 (8)	
H23A	1.0320	0.6682	0.3150	0.056*	
H23B	1.1399	0.6334	0.3686	0.056*	
C24	1.1989 (4)	0.6992 (2)	0.2981 (3)	0.0621 (11)	
H24A	1.2036	0.6800	0.2381	0.093*	
H24B	1.2783	0.7004	0.3363	0.093*	
H24C	1.1706	0.7357	0.2835	0.093*	
C25	1.0928 (3)	0.67370 (15)	0.6683 (3)	0.0476 (8)	
H25A	1.0782	0.6854	0.7328	0.057*	
H25B	1.1594	0.6955	0.6503	0.057*	
C26	1.1329 (4)	0.61516 (19)	0.6747 (4)	0.0784 (15)	
H26A	1.0694	0.5929	0.6963	0.094*	
H26B	1.1470	0.6024	0.6107	0.094*	

C27	1.2475 (5)	0.6102 (3)	0.7453 (5)	0.111 (2)	
H27A	1.3083	0.6344	0.7244	0.133*	
H27B	1.2311	0.6227	0.8089	0.133*	
C28	1.2987 (10)	0.5555 (4)	0.7559 (10)	0.224 (7)	
H28A	1.3708	0.5559	0.8035	0.337*	
H28B	1.3193	0.5434	0.6941	0.337*	
H28C	1.2397	0.5312	0.7772	0.337*	
C29	0.9563 (3)	0.74534 (13)	0.6051 (2)	0.0433 (8)	
H29A	0.9532	0.7541	0.6732	0.052*	
H29B	1.0244	0.7652	0.5848	0.052*	
C30	0.8404 (3)	0.76503 (14)	0.5455 (3)	0.0507 (9)	
H30A	0.7707	0.7515	0.5737	0.061*	
H30B	0.8353	0.7509	0.4794	0.061*	
C31	0.8365 (5)	0.82621 (16)	0.5425 (4)	0.0676 (12)	
H31A	0.8426	0.8399	0.6088	0.081*	0.33
H31B	0.7583	0.8377	0.5078	0.081*	0.33
H31C	0.8578	0.8406	0.6080	0.081*	0.67
H31D	0.8956	0.8396	0.5025	0.081*	0.67
C32	0.9368 (9)	0.8511 (4)	0.4936 (10)	0.124 (4)	0.67
H32A	0.9296	0.8900	0.4941	0.186*	0.67
H32B	0.9302	0.8385	0.4272	0.186*	0.67
H32C	1.0146	0.8406	0.5282	0.186*	0.67
C32'	0.7109 (11)	0.8452 (9)	0.501 (2)	0.124 (4)	0.33
H32D	0.7092	0.8843	0.4991	0.186*	0.33
H32E	0.6527	0.8322	0.5409	0.186*	0.33
H32F	0.6905	0.8313	0.4355	0.186*	0.33
N2	0.4355 (13)	0.5001 (6)	0.0732 (9)	0.121 (4)	0.50
C33	0.5243 (17)	0.5325 (8)	0.0698 (14)	0.143 (6)	0.50
H33	0.5428	0.5581	0.1193	0.171*	0.50
C34	0.415 (2)	0.4692 (8)	−0.0040 (14)	0.160 (7)	0.50
H34	0.3468	0.4465	−0.0087	0.192*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02605 (19)	0.0307 (2)	0.02437 (19)	0.00432 (12)	0.00790 (13)	0.00481 (11)
S1	0.0347 (4)	0.0568 (5)	0.0500 (5)	−0.0105 (4)	0.0032 (4)	0.0037 (4)
S2	0.122 (2)	0.121 (2)	0.0642 (13)	−0.0155 (17)	0.0000 (13)	−0.0061 (13)
O1	0.0355 (11)	0.0379 (11)	0.0336 (11)	0.0072 (9)	0.0129 (9)	−0.0017 (9)
O2	0.0593 (15)	0.0694 (17)	0.0298 (12)	0.0266 (13)	0.0177 (11)	0.0070 (11)
O3	0.0408 (12)	0.0531 (14)	0.0364 (12)	−0.0006 (11)	0.0155 (10)	−0.0137 (10)
O4	0.0504 (14)	0.0816 (19)	0.0298 (12)	−0.0007 (13)	0.0150 (10)	−0.0096 (12)
O5	0.0367 (11)	0.0418 (12)	0.0417 (12)	0.0163 (9)	0.0103 (9)	0.0117 (10)
O6	0.0299 (11)	0.0521 (14)	0.0580 (15)	0.0089 (10)	0.0130 (10)	0.0165 (12)
O7	0.0396 (12)	0.0562 (15)	0.0369 (12)	−0.0133 (11)	0.0029 (10)	0.0057 (10)
O8	0.117 (6)	0.156 (8)	0.166 (8)	0.031 (6)	−0.015 (6)	−0.084 (7)
N1	0.0393 (14)	0.0420 (15)	0.0326 (13)	−0.0105 (11)	0.0052 (11)	−0.0086 (11)
C1	0.0305 (14)	0.0401 (16)	0.0309 (15)	0.0048 (12)	0.0099 (11)	−0.0010 (12)

C2	0.0324 (14)	0.0384 (16)	0.0280 (14)	0.0042 (12)	0.0079 (11)	−0.0014 (11)
C3	0.0427 (17)	0.0472 (18)	0.0334 (16)	0.0118 (14)	0.0104 (13)	0.0022 (13)
C4	0.0436 (18)	0.056 (2)	0.0264 (14)	0.0049 (15)	0.0098 (13)	0.0029 (13)
C5	0.0288 (14)	0.0431 (17)	0.0286 (14)	−0.0046 (12)	0.0092 (11)	−0.0096 (12)
C6	0.0461 (18)	0.0479 (19)	0.0347 (16)	0.0172 (15)	0.0126 (14)	0.0006 (14)
C7	0.055 (2)	0.052 (2)	0.0281 (15)	0.0188 (16)	0.0132 (14)	0.0054 (13)
C8	0.0319 (15)	0.0488 (18)	0.0354 (16)	−0.0121 (13)	0.0119 (12)	−0.0157 (13)
C9	0.0274 (13)	0.0252 (13)	0.0378 (15)	0.0023 (10)	0.0037 (11)	−0.0016 (11)
C10	0.0258 (12)	0.0233 (12)	0.0365 (15)	0.0015 (10)	0.0055 (11)	0.0000 (10)
C11	0.0339 (14)	0.0291 (14)	0.0335 (14)	0.0056 (11)	0.0080 (12)	0.0066 (11)
C12	0.0309 (14)	0.0314 (14)	0.0387 (15)	0.0043 (11)	0.0125 (12)	0.0046 (12)
C13	0.0408 (18)	0.054 (2)	0.054 (2)	−0.0038 (15)	0.0181 (16)	0.0072 (17)
C14	0.069 (3)	0.049 (2)	0.074 (3)	−0.012 (2)	0.019 (2)	−0.006 (2)
C15	0.26 (2)	0.166 (13)	0.096 (9)	−0.097 (14)	−0.041 (11)	0.013 (8)
C16	0.23 (2)	0.34 (3)	0.098 (10)	0.12 (2)	0.002 (11)	0.045 (14)
C17	0.0384 (16)	0.0379 (16)	0.0398 (17)	−0.0107 (13)	0.0070 (13)	−0.0077 (13)
C18	0.055 (2)	0.049 (2)	0.0441 (19)	−0.0156 (17)	0.0165 (16)	−0.0104 (15)
C19	0.050 (2)	0.0446 (19)	0.053 (2)	−0.0083 (16)	0.0139 (16)	−0.0013 (16)
C20	0.095 (4)	0.082 (3)	0.078 (3)	−0.040 (3)	0.047 (3)	−0.017 (3)
C21	0.0430 (17)	0.0466 (19)	0.0340 (16)	−0.0096 (14)	0.0078 (13)	−0.0116 (13)
C22	0.0471 (19)	0.052 (2)	0.0436 (19)	−0.0092 (16)	0.0125 (15)	−0.0061 (15)
C23	0.0387 (17)	0.058 (2)	0.0449 (19)	0.0006 (15)	0.0111 (15)	−0.0018 (16)
C24	0.055 (2)	0.077 (3)	0.058 (2)	0.001 (2)	0.0230 (19)	0.005 (2)
C25	0.0404 (18)	0.059 (2)	0.0416 (18)	−0.0096 (16)	−0.0001 (14)	−0.0061 (16)
C26	0.060 (3)	0.073 (3)	0.094 (4)	0.012 (2)	−0.017 (3)	−0.007 (3)
C27	0.089 (5)	0.098 (5)	0.133 (6)	0.014 (4)	−0.029 (4)	0.010 (4)
C28	0.152 (9)	0.199 (12)	0.287 (16)	0.094 (9)	−0.093 (10)	−0.078 (11)
C29	0.0515 (19)	0.0412 (18)	0.0379 (17)	−0.0113 (15)	0.0091 (14)	−0.0084 (14)
C30	0.060 (2)	0.046 (2)	0.046 (2)	−0.0014 (17)	0.0043 (17)	−0.0071 (15)
C31	0.089 (3)	0.045 (2)	0.070 (3)	0.001 (2)	0.015 (2)	0.004 (2)
C32	0.123 (8)	0.094 (7)	0.154 (10)	0.011 (6)	0.018 (7)	0.054 (6)
C32'	0.123 (8)	0.094 (7)	0.154 (10)	0.011 (6)	0.018 (7)	0.054 (6)
N2	0.147 (8)	0.129 (8)	0.090 (6)	−0.034 (7)	0.027 (6)	−0.004 (6)
C33	0.163 (10)	0.151 (10)	0.117 (9)	−0.015 (8)	0.031 (8)	0.029 (8)
C34	0.172 (11)	0.167 (11)	0.142 (10)	−0.029 (9)	0.029 (9)	0.017 (9)

Geometric parameters (Å, °)

Zn1—O1	1.959 (2)	C18—H18A	0.9800
Zn1—O5	1.972 (2)	C18—H18B	0.9800
Zn1—O3^{i}	1.993 (2)	C19—C20	1.516 (5)
Zn1—O7	2.047 (2)	C19—H19A	0.9800
S1—O7	1.516 (2)	C19—H19B	0.9800
S1—C13	1.769 (4)	C20—H20A	0.9700
S1—C14	1.784 (5)	C20—H20B	0.9700
S2—O8	1.368 (10)	C20—H20C	0.9700
S2—C16	1.581 (17)	C21—C22	1.509 (4)
S2—C15	1.712 (13)	C21—H21A	0.9800
O1—C1	1.279 (4)	C21—H21B	0.9800

O2—C1	1.220 (4)	C22—C23	1.519 (4)
O3—C8	1.266 (4)	C22—H22A	0.9800
O3—Zn1^{ii}	1.993 (2)	C22—H22B	0.9800
O4—C8	1.234 (4)	C23—C24	1.524 (4)
O5—C9	1.274 (4)	C23—H23A	0.9800
O6—C9	1.228 (4)	C23—H23B	0.9800
N1—C25	1.515 (4)	C24—H24A	0.9700
N1—C21	1.517 (4)	C24—H24B	0.9700
N1—C17	1.523 (4)	C24—H24C	0.9700
N1—C29	1.523 (4)	C25—C26	1.519 (5)
C1—C2	1.519 (4)	C25—H25A	0.9800
C2—C3	1.380 (4)	C25—H25B	0.9800
C2—C7	1.387 (4)	C26—C27	1.508 (5)
C3—C4	1.385 (4)	C26—H26A	0.9800
C3—H3	0.9400	C26—H26B	0.9800
C4—C5	1.385 (5)	C27—C28	1.473 (7)
C4—H4	0.9400	C27—H27A	0.9800
C5—C6	1.383 (4)	C27—H27B	0.9800
C5—C8	1.516 (4)	C28—H28A	0.9700
C6—C7	1.384 (4)	C28—H28B	0.9700
C6—H6	0.9400	C28—H28C	0.9700
C7—H7	0.9400	C29—C30	1.519 (4)
C8—Zn1^{ii}	2.567 (3)	C29—H29A	0.9800
C9—C10	1.518 (4)	C29—H29B	0.9800
C10—C11	1.392 (4)	C30—C31	1.519 (5)
C10—C12^{iii}	1.393 (4)	C30—H30A	0.9800
C11—C12	1.382 (4)	C30—H30B	0.9800
C11—H11	0.9400	C31—C32'	1.518 (8)
C12—C10^{iii}	1.393 (4)	C31—C32	1.520 (7)
C12—H12	0.9400	C31—H31A	0.9800
C13—H13A	0.9700	C31—H31B	0.9800
C13—H13B	0.9700	C31—H31C	0.9800
C13—H13C	0.9700	C31—H31D	0.9800
C14—H14A	0.9700	C32—H32A	0.9700
C14—H14B	0.9700	C32—H32B	0.9700
C14—H14C	0.9700	C32—H32C	0.9700
C15—H15A	0.9700	C32'—H32D	0.9700
C15—H15B	0.9700	C32'—H32E	0.9700
C15—H15C	0.9700	C32'—H32F	0.9700
C16—H16A	0.9700	N2—C33	1.283 (15)
C16—H16B	0.9700	N2—C34	1.316 (15)
C16—H16C	0.9700	C33—C34^{iv}	1.218 (16)
C17—C18	1.511 (4)	C33—H33	0.9400
C17—H17A	0.9800	C34—C33^{iv}	1.218 (16)
C17—H17B	0.9800	C34—H34	0.9400
C18—C19	1.526 (4)		
O1—Zn1—O5	109.61 (9)	C18—C19—H19B	108.8

O1—Zn1—O3^{i}	138.01 (10)	H19A—C19—H19B	107.6
O5—Zn1—O3^{i}	100.27 (10)	C19—C20—H20A	109.5
O1—Zn1—O7	99.87 (10)	C19—C20—H20B	109.5
O5—Zn1—O7	110.29 (10)	H20A—C20—H20B	109.5
O3^{i}—Zn1—O7	96.49 (10)	C19—C20—H20C	109.5
O7—S1—C13	108.55 (16)	H20A—C20—H20C	109.5
O7—S1—C14	105.26 (19)	H20B—C20—H20C	109.5
C13—S1—C14	97.7 (2)	C22—C21—N1	118.2 (3)
O8—S2—C16	106.6 (9)	C22—C21—H21A	107.8
O8—S2—C15	101.3 (7)	N1—C21—H21A	107.8
C16—S2—C15	101.2 (11)	C22—C21—H21B	107.8
C1—O1—Zn1	111.44 (18)	N1—C21—H21B	107.8
C8—O3—Zn1^{ii}	101.6 (2)	H21A—C21—H21B	107.1
C9—O5—Zn1	126.77 (19)	C21—C22—C23	108.9 (3)
S1—O7—Zn1	136.20 (14)	C21—C22—H22A	109.9
C25—N1—C21	111.3 (3)	C23—C22—H22A	109.9
C25—N1—C17	111.5 (3)	C21—C22—H22B	109.9
C21—N1—C17	105.2 (2)	C23—C22—H22B	109.9
C25—N1—C29	106.1 (2)	H22A—C22—H22B	108.3
C21—N1—C29	111.3 (3)	C22—C23—C24	113.3 (3)
C17—N1—C29	111.5 (2)	C22—C23—H23A	108.9
O2—C1—O1	124.8 (3)	C24—C23—H23A	108.9
O2—C1—C2	119.9 (3)	C22—C23—H23B	108.9
O1—C1—C2	115.3 (3)	C24—C23—H23B	108.9
C3—C2—C7	118.9 (3)	H23A—C23—H23B	107.7
C3—C2—C1	121.3 (3)	C23—C24—H24A	109.5
C7—C2—C1	119.7 (3)	C23—C24—H24B	109.5
C2—C3—C4	120.5 (3)	H24A—C24—H24B	109.5
C2—C3—H3	119.8	C23—C24—H24C	109.5
C4—C3—H3	119.8	H24A—C24—H24C	109.5
C5—C4—C3	120.7 (3)	H24B—C24—H24C	109.5
C5—C4—H4	119.7	N1—C25—C26	115.4 (3)
C3—C4—H4	119.7	N1—C25—H25A	108.4
C6—C5—C4	118.8 (3)	C26—C25—H25A	108.4
C6—C5—C8	121.3 (3)	N1—C25—H25B	108.4
C4—C5—C8	119.9 (3)	C26—C25—H25B	108.4
C5—C6—C7	120.5 (3)	H25A—C25—H25B	107.5
C5—C6—H6	119.7	C27—C26—C25	109.4 (4)
C7—C6—H6	119.7	C27—C26—H26A	109.8
C6—C7—C2	120.6 (3)	C25—C26—H26A	109.8
C6—C7—H7	119.7	C27—C26—H26B	109.8
C2—C7—H7	119.7	C25—C26—H26B	109.8
O4—C8—O3	123.5 (3)	H26A—C26—H26B	108.2
O4—C8—C5	119.0 (3)	C28—C27—C26	115.0 (6)
O3—C8—C5	117.5 (3)	C28—C27—H27A	108.5
O4—C8—Zn1^{ii}	74.17 (18)	C26—C27—H27A	108.5
O3—C8—Zn1^{ii}	49.51 (14)	C28—C27—H27B	108.5

C5—C8—Zn1^{ii}	166.2 (3)	C26—C27—H27B	108.5
O6—C9—O5	126.2 (3)	H27A—C27—H27B	107.5
O6—C9—C10	119.0 (3)	C27—C28—H28A	109.5
O5—C9—C10	114.8 (2)	C27—C28—H28B	109.5
C11—C10—C12^{iii}	119.1 (3)	H28A—C28—H28B	109.5
C11—C10—C9	121.0 (3)	C27—C28—H28C	109.5
C12^{iii}—C10—C9	119.9 (3)	H28A—C28—H28C	109.5
C12—C11—C10	120.5 (3)	H28B—C28—H28C	109.5
C12—C11—H11	119.7	C30—C29—N1	115.0 (3)
C10—C11—H11	119.7	C30—C29—H29A	108.5
C11—C12—C10^{iii}	120.4 (3)	N1—C29—H29A	108.5
C11—C12—H12	119.8	C30—C29—H29B	108.5
C10^{iii}—C12—H12	119.8	N1—C29—H29B	108.5
S1—C13—H13A	109.5	H29A—C29—H29B	107.5
S1—C13—H13B	109.5	C29—C30—C31	110.8 (3)
H13A—C13—H13B	109.5	C29—C30—H30A	109.5
S1—C13—H13C	109.5	C31—C30—H30A	109.5
H13A—C13—H13C	109.5	C29—C30—H30B	109.5
H13B—C13—H13C	109.5	C31—C30—H30B	109.5
S1—C14—H14A	109.5	H30A—C30—H30B	108.1
S1—C14—H14B	109.5	C32'—C31—C30	110.0 (10)
H14A—C14—H14B	109.5	C32'—C31—C32	113.7 (10)
S1—C14—H14C	109.5	C30—C31—C32	113.4 (6)
H14A—C14—H14C	109.5	C30—C31—H31A	108.9
H14B—C14—H14C	109.5	C32—C31—H31A	108.9
S2—C15—H15A	109.5	C30—C31—H31B	108.9
S2—C15—H15B	109.5	C32—C31—H31B	108.9
H15A—C15—H15B	109.5	H31A—C31—H31B	107.7
S2—C15—H15C	109.5	C32'—C31—H31C	109.7
H15A—C15—H15C	109.5	C30—C31—H31C	109.7
H15B—C15—H15C	109.5	C32'—C31—H31D	109.7
S2—C16—H16A	109.5	C30—C31—H31D	109.7
S2—C16—H16B	109.5	H31C—C31—H31D	108.2
H16A—C16—H16B	109.5	C31—C32—H32A	109.5
S2—C16—H16C	109.5	C31—C32—H32B	109.5
H16A—C16—H16C	109.5	H32A—C32—H32B	109.5
H16B—C16—H16C	109.5	C31—C32—H32C	109.5
C18—C17—N1	116.6 (3)	H32A—C32—H32C	109.5
C18—C17—H17A	108.1	H32B—C32—H32C	109.5
N1—C17—H17A	108.1	C31—C32'—H32D	109.5
C18—C17—H17B	108.1	C31—C32'—H32E	109.5
N1—C17—H17B	108.1	H32D—C32'—H32E	109.5
H17A—C17—H17B	107.3	C31—C32'—H32F	109.5
C17—C18—C19	108.3 (3)	H32D—C32'—H32F	109.5
C17—C18—H18A	110.0	H32E—C32'—H32F	109.5
C19—C18—H18A	110.0	C33—N2—C34	112.6 (14)
C17—C18—H18B	110.0	C34^{iv}—C33—N2	121 (2)

C19—C18—H18B	110.0	C34^{iv}—C33—H33	119.3
H18A—C18—H18B	108.4	N2—C33—H33	119.3
C20—C19—C18	114.0 (3)	C33^{iv}—C34—N2	126 (2)
C20—C19—H19A	108.8	C33^{iv}—C34—H34	117.1
C18—C19—H19A	108.8	N2—C34—H34	117.1
C20—C19—H19B	108.8		
O5—Zn1—O1—C1	170.8 (2)	C6—C5—C8—Zn1^{ii}	−7.4 (11)
O3^{i}—Zn1—O1—C1	38.0 (3)	C4—C5—C8—Zn1^{ii}	172.1 (7)
O7—Zn1—O1—C1	−73.4 (2)	Zn1—O5—C9—O6	12.2 (5)
C8^{i}—Zn1—O1—C1	63.7 (2)	Zn1—O5—C9—C10	−166.51 (19)
O1—Zn1—O5—C9	40.6 (3)	O6—C9—C10—C11	171.8 (3)
O3^{i}—Zn1—O5—C9	−169.3 (3)	O5—C9—C10—C11	−9.4 (4)
O7—Zn1—O5—C9	−68.4 (3)	O6—C9—C10—C12^{iii}	−9.7 (4)
C13—S1—O7—Zn1	25.2 (3)	O5—C9—C10—C12^{iii}	169.1 (3)
C14—S1—O7—Zn1	−78.6 (3)	C12^{iii}—C10—C11—C12	−0.4 (5)
O1—Zn1—O7—S1	−49.4 (3)	C9—C10—C11—C12	178.2 (3)
O5—Zn1—O7—S1	65.9 (3)	C10—C11—C12—C10^{iii}	0.4 (5)
O3^{i}—Zn1—O7—S1	169.4 (2)	C25—N1—C17—C18	58.4 (4)
Zn1—O1—C1—O2	−11.5 (4)	C21—N1—C17—C18	179.2 (3)
Zn1—O1—C1—C2	165.9 (2)	C29—N1—C17—C18	−60.0 (4)
O2—C1—C2—C3	177.8 (3)	N1—C17—C18—C19	−174.6 (3)
O1—C1—C2—C3	0.3 (5)	C17—C18—C19—C20	−174.2 (4)
O2—C1—C2—C7	1.2 (5)	C25—N1—C21—C22	−61.2 (4)
O1—C1—C2—C7	−176.3 (3)	C17—N1—C21—C22	178.0 (3)
C7—C2—C3—C4	−1.3 (5)	C29—N1—C21—C22	57.0 (4)
C1—C2—C3—C4	−177.9 (3)	N1—C21—C22—C23	171.3 (3)
C2—C3—C4—C5	1.7 (5)	C21—C22—C23—C24	173.8 (3)
C3—C4—C5—C6	−0.7 (5)	C21—N1—C25—C26	−60.2 (4)
C3—C4—C5—C8	179.8 (3)	C17—N1—C25—C26	57.0 (4)
C4—C5—C6—C7	−0.6 (5)	C29—N1—C25—C26	178.6 (4)
C8—C5—C6—C7	178.9 (3)	N1—C25—C26—C27	178.0 (5)
C5—C6—C7—C2	0.9 (6)	C25—C26—C27—C28	−178.0 (9)
C3—C2—C7—C6	0.0 (6)	C25—N1—C29—C30	−175.0 (3)
C1—C2—C7—C6	176.7 (3)	C21—N1—C29—C30	63.8 (4)
Zn1^{ii}—O3—C8—O4	4.9 (4)	C17—N1—C29—C30	−53.5 (4)
Zn1^{ii}—O3—C8—C5	−174.4 (2)	N1—C29—C30—C31	−168.9 (3)
C6—C5—C8—O4	−168.5 (3)	C29—C30—C31—C32'	−168.5 (12)
C4—C5—C8—O4	10.9 (5)	C29—C30—C31—C32	62.9 (8)
C6—C5—C8—O3	10.8 (5)	C34—N2—C33—C34^{iv}	−5(4)
C4—C5—C8—O3	−169.7 (3)	C33—N2—C34—C33^{iv}	5(4)

Symmetry codes: (i) *x*+1/2, −*y*+3/2, *z*−1/2; (ii) *x*−1/2, −*y*+3/2, *z*+1/2; (iii) −*x*+2, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*.

Fig. 1

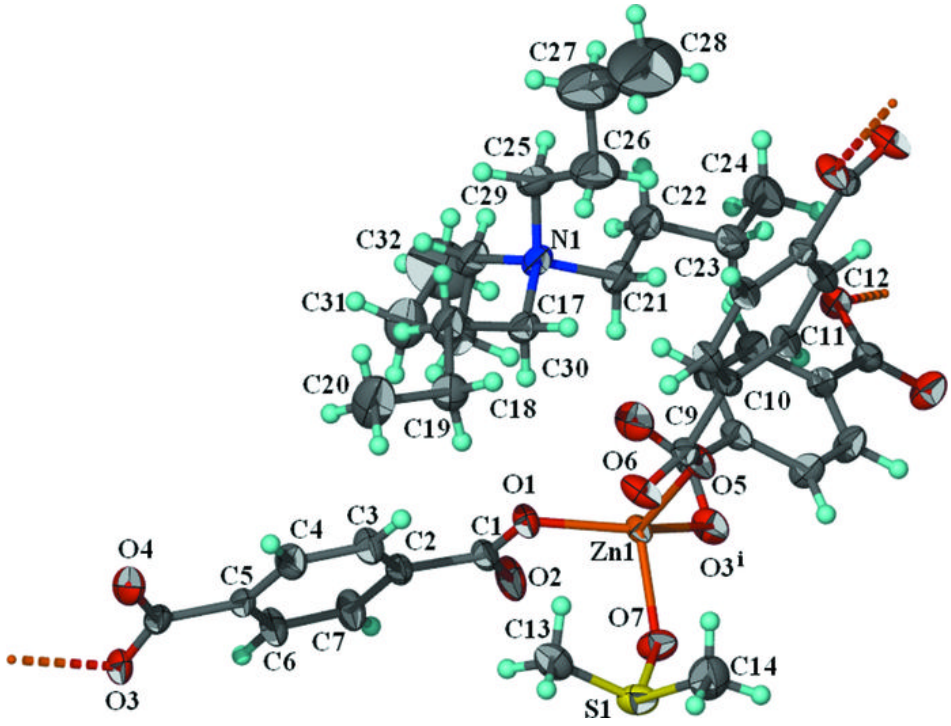
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Fig. 2