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Hexaaquazinc(II) D-camphor-10-sulfonate

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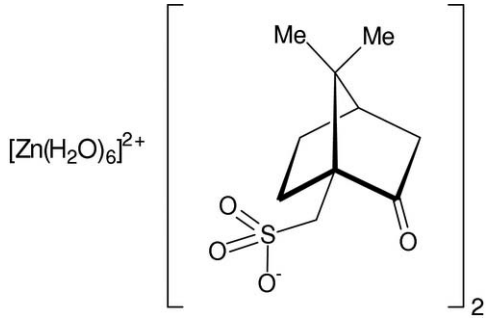
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.087; data-to-parameter ratio = 22.0.

The structure of the title compound, $[Zn(H_2O)_6](C_{10}H_{15}O_4S)_2$, consists of two D-camphor-10-sulfonate anions, together with essentially regular octahedral $[Zn(H_2O)_6]^{2+}$ cations. The coordinated water molecules around the zinc ion are engaged in an extensive network of hydrogen bonds with the O atoms of the sulfonate groups. Distances between hydrogen-bonded O atoms are in the range 2.704 (4)–2.845 (4) Å. The title compound and its nickel and copper analogues are isomorphous.

Related literature

For related literature, see: Couldwell *et al.* (1978); Henderson & Nicholson (1995); Sheldrick (1990).



Experimental

Crystal data

$[Zn(H_2O)_6](C_{10}H_{15}O_4S)_2$
M_r = 636.03
Monoclinic, $P2_1$
a = 11.7293 (14) Å
b = 7.0854 (8) Å
c = 17.169 (2) Å
β = 93.841 (10)°
V = 1423.7 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.07 mm^{-1}
T = 173 (2) K
0.60 × 0.60 × 0.20 mm

Data collection

Siemens $P4$ diffractometer
Absorption correction: multi-scan (*XEMP*; Siemens, 1994)
T_{min} = 0.565, T_{max} = 0.814
7590 measured reflections
7364 independent reflections
5903 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
3 standard reflections
every 247 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.087
S = 0.97
7364 reflections
334 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}
Absolute structure: Flack (1983), with 3392 Friedel pairs
Flack parameter: −0.005 (10)

Data collection: *XSCANS* (Fait, 1991); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Siemens, 1995); software used to prepare material for publication: *SHELXTL-Plus*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2423).

References

Couldwell, C., Prout, K., Robey, D., Taylor, R. & Rossotti, F. J. C. (1978). *Acta Cryst.* B**34**, 1491–1499.
Fait, J. (1991). *XSCANS*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Henderson, W. & Nicholson, B. K. (1995). *Acta Cryst.* C**51**, 37–40.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1994). *XEMP*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1995). *SHELXTL-Plus*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

supplementary materials

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Hexaaquazinc(II) D-camphor-10-sulfonate

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Comment

The title compound was prepared as part of an ongoing research project to develop new materials for the zinc-catalyzed production of polycarbonates from CO_2 and epoxides (ethylene oxide, propylene oxide *etc*.). Two analogous metal salts of *D*-camphor-10-sulfonic acid have been structurally characterized previously (copper: Couldwell *et al.*, 1978; nickel: Henderson & Nicholson, 1995). Here we present the crystal structure of $[Zn(H_2O)_6]$.

The three metal salts of D-camphor-10 sulfonic acid are isomorphous. The lattice of the title compound consists of $[Zn(H_2O)_6]$ cations and two crystallographically independent *D*-camphor-sulfonate anions. The cation is essentially octahedral, with Zn—O distances ranging from 2.048 (2) to 2.099 (2) Å and O—Zn—O angles between 82.99 (11) and 96.47 (6)°. No coordination of either the sulfonate or the ketone O atoms of the anions is observed.

The two independent D-camphor-10 sulfonate anions show only small differences in bond parameters. As in the lattices of the related nickel and copper compounds, the water sphere and the O atoms of the sulfonate groups are involved in a complex hydrogen bonding network. In contrast to the structure of the nickel complex, in which all H atoms were reported to take part in hydrogen bonds, we find that two water H atoms (H01 & H03) of the title compound do not form hydrogen bonds. This may be associated with the difficulty in localizing H atoms in pseudosymmetric structures, a problem that surprisingly was not mentioned in the earlier reports (see X-ray details).

Experimental

The title compound was prepared by saturating a hot aqueous solution of *D*-camphor-10-sulfonic acid with zinc oxide, followed by filtration and slow evaporation at ambient temperature.

Refinement

All H atoms were refined with a riding model with O—H = 0.84 Å, C—H ranging from 0.98–1.00Å and U(H) = 1.2 U_{eq}(C,*O*) or U(H) = 1.5 $U_{eq}(C_{methyl})$. It is probable that X-ray data alone cannot provide unambiguous positions for all H.

Figures

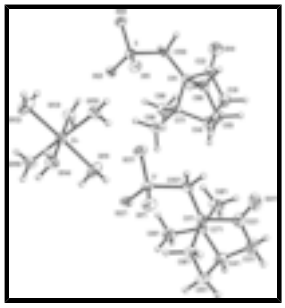


Fig. 1. The molecule of the title compound in the crystal. Thermal ellipsoids represent 50% probability levels. H-Atom radii are arbitrary.
Fig. 2. The hydrogen-bond network.

Hexaaquazinc(II) *D*-camphor-10-sulfonate

Crystal data

$[Zn(H_2O)_6](C_{10}H_{15}O_4S)_2$	F_{000} = 672
M_r = 636.03	D_x = 1.484 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P2yb	Cell parameters from 66 reflections
a = 11.7293 (14) Å	θ = 3–12.5º
b = 7.0854 (8) Å	μ = 1.07 mm^{-1}
c = 17.169 (2) Å	T = 173 (2) K
β = 93.841 (10)º	Plate, colourless
V = 1423.7 (3) Å^3	0.60 × 0.60 × 0.20 mm
Z = 2	

Data collection

Siemens P4 diffractometer	R_{int} = 0.023
Radiation source: fine-focus sealed tube	θ_{max} = 28.8º
Monochromator: graphite	θ_{min} = 3.0º
T = 173(2) K	h = −15→15
ω scans	k = −9→9
Absorption correction: empirical (using intensity measurements) (Siemens, 1994)	l = 0→22
T_{min} = 0.565, T_{max} = 0.814	3 standard reflections
7590 measured reflections	every 247 reflections
7364 independent reflections	intensity decay: none
5903 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.087$

$S = 0.97$

7364 reflections

334 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.005$

$\Delta\rho_{max} = 0.51$ e Å^{-3}

$\Delta\rho_{min} = -0.47$ e Å^{-3}

Extinction correction: none

Absolute structure: Flack (1983), 3392 Friedel pairs

Flack parameter: −0.005 (10)

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 $F^2 > 2$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}
Zn	0.24152 (2)	0.23602 (6)	0.494431 (14)	0.01905 (7)
O11	0.35940 (15)	0.2373 (4)	0.58803 (11)	0.0380 (4)
H01	0.4241	0.2623	0.5725	0.046*
H02	0.3635	0.1211	0.5973	0.046*
O12	0.12659 (17)	0.2322 (4)	0.39833 (12)	0.0437 (5)
H03	0.0773	0.1569	0.4132	0.052*
H04	0.0907	0.3348	0.3941	0.052*
O13	0.1539 (2)	0.4604 (3)	0.54210 (15)	0.0260 (5)
H05	0.0868	0.4420	0.5548	0.031*
H06	0.1535	0.5749	0.5296	0.031*
O14	0.32956 (19)	0.0144 (3)	0.44599 (15)	0.0263 (6)
H07	0.3961	0.0090	0.4308	0.032*
H08	0.3149	−0.0984	0.4564	0.032*
O15	0.1528 (2)	0.0204 (3)	0.54855 (15)	0.0265 (5)
H09	0.1738	−0.0927	0.5527	0.032*
H10	0.0843	0.0168	0.5597	0.032*
O16	0.3304 (2)	0.4525 (3)	0.44272 (16)	0.0316 (6)
H11	0.3119	0.5651	0.4333	0.038*
H12	0.3971	0.4458	0.4281	0.038*
S	−0.08148 (4)	0.23795 (13)	0.66721 (3)	0.01718 (10)
O1	−0.0216 (2)	0.0609 (3)	0.65366 (14)	0.0227 (5)

O2	−0.01836 (19)	0.4015 (3)	0.64225 (14)	0.0237 (5)
O3	−0.19981 (12)	0.2363 (4)	0.63493 (9)	0.0248 (3)
C1	0.00787 (17)	0.2248 (5)	0.82661 (12)	0.0186 (4)
C2	−0.0241 (2)	0.2782 (4)	0.90868 (15)	0.0279 (7)
C3	0.0859 (2)	0.2888 (5)	0.96047 (16)	0.0353 (8)
H3A	0.0855	0.1982	1.0044	0.042*
H3B	0.0994	0.4177	0.9814	0.042*
C4	0.17475 (19)	0.2344 (6)	0.90275 (13)	0.0268 (5)
H4	0.2548	0.2727	0.9193	0.032*
C5	0.1589 (2)	0.0215 (4)	0.88764 (16)	0.0280 (6)
H5A	0.1549	−0.0490	0.9372	0.034*
H5B	0.2219	−0.0302	0.8585	0.034*
C6	0.0428 (2)	0.0126 (4)	0.83773 (16)	0.0226 (5)
H6A	−0.0152	−0.0576	0.8655	0.027*
H6B	0.0522	−0.0489	0.7868	0.027*
C7	0.1269 (2)	0.3230 (4)	0.82407 (15)	0.0203 (5)
C8	0.1166 (3)	0.5399 (4)	0.8263 (2)	0.0358 (7)
H8A	0.1923	0.5953	0.8383	0.043*
H8B	0.0655	0.5766	0.8665	0.043*
H8C	0.0855	0.5857	0.7753	0.043*
C9	0.1999 (2)	0.2681 (4)	0.75685 (14)	0.0260 (7)
H9A	0.2798	0.3017	0.7704	0.031*
H9B	0.1725	0.3356	0.7094	0.031*
H9C	0.1940	0.1318	0.7478	0.031*
O4	−0.11982 (18)	0.3062 (4)	0.92834 (12)	0.0454 (6)
C10	−0.09305 (19)	0.2637 (4)	0.76947 (13)	0.0199 (6)
H11A	−0.1178	0.3950	0.7786	0.024*
H11B	−0.1561	0.1804	0.7839	0.024*
S'	0.40990 (4)	−0.26391 (13)	0.65060 (3)	0.01825 (10)
O1'	0.4675 (2)	−0.4357 (3)	0.62698 (15)	0.0253 (5)
O2'	0.46865 (19)	−0.0944 (3)	0.62639 (15)	0.0234 (5)
O3'	0.28824 (12)	−0.2646 (4)	0.62623 (9)	0.0255 (3)
C1'	0.53121 (17)	−0.2603 (5)	0.79946 (12)	0.0202 (4)
C2'	0.5312 (3)	−0.3858 (4)	0.87247 (17)	0.0281 (6)
C3'	0.6312 (3)	−0.3214 (4)	0.92760 (18)	0.0368 (8)
H3'1	0.6872	−0.4244	0.9381	0.044*
H3'2	0.6048	−0.2750	0.9777	0.044*
C4'	0.6823 (2)	−0.1597 (4)	0.88023 (16)	0.0271 (6)
H4'	0.7314	−0.0691	0.9121	0.033*
C5'	0.74126 (19)	−0.2540 (6)	0.81366 (15)	0.0301 (5)
H5'1	0.7911	−0.3587	0.8333	0.036*
H5'2	0.7876	−0.1618	0.7861	0.036*
C6'	0.6400 (2)	−0.3285 (4)	0.75948 (16)	0.0245 (6)
H6'1	0.6419	−0.4679	0.7560	0.029*
H6'2	0.6421	−0.2750	0.7063	0.029*
C7'	0.5732 (2)	−0.0704 (4)	0.83839 (15)	0.0218 (5)
C8'	0.4922 (3)	0.0105 (5)	0.8950 (2)	0.0334 (8)
H8'1	0.4646	−0.0911	0.9276	0.040*
H8'2	0.4271	0.0699	0.8658	0.040*

H8'3	0.5324	0.1049	0.9283	0.040*
C9'	0.6006 (2)	0.0861 (4)	0.78097 (17)	0.0288 (6)
H9'1	0.5295	0.1317	0.7541	0.035*
H9'2	0.6509	0.0361	0.7425	0.035*
H9'3	0.6389	0.1905	0.8095	0.035*
O4'	0.4641 (2)	−0.5084 (3)	0.88454 (15)	0.0405 (6)
C10'	0.41553 (17)	−0.2650 (6)	0.75433 (12)	0.0228 (4)
H11C	0.3713	−0.1549	0.7711	0.027*
H11D	0.3751	−0.3795	0.7707	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn	0.01953 (12)	0.01708 (11)	0.02041 (12)	−0.00012 (19)	0.00036 (9)	0.0005 (2)
O11	0.0426 (10)	0.0213 (8)	0.0473 (11)	0.0010 (15)	−0.0189 (8)	0.0040 (15)
O12	0.0539 (11)	0.0211 (9)	0.0518 (11)	−0.0047 (15)	−0.0287 (9)	0.0055 (16)
O13	0.0290 (13)	0.0186 (12)	0.0311 (13)	−0.0012 (10)	0.0072 (11)	−0.0011 (10)
O14	0.0218 (13)	0.0234 (12)	0.0346 (15)	0.0021 (10)	0.0082 (11)	−0.0007 (11)
O15	0.0228 (12)	0.0240 (13)	0.0340 (14)	−0.0006 (10)	0.0104 (10)	0.0037 (10)
O16	0.0298 (14)	0.0245 (13)	0.0416 (17)	0.0063 (11)	0.0107 (12)	0.0131 (12)
S	0.0163 (2)	0.0165 (2)	0.0185 (2)	0.0004 (4)	−0.00026 (17)	−0.0013 (4)
O1	0.0243 (12)	0.0192 (11)	0.0241 (11)	0.0017 (9)	−0.0010 (9)	−0.0046 (8)
O2	0.0225 (12)	0.0206 (11)	0.0281 (12)	−0.0026 (9)	0.0027 (9)	0.0058 (9)
O3	0.0186 (7)	0.0275 (8)	0.0273 (8)	−0.0018 (13)	−0.0051 (6)	0.0003 (13)
C1	0.0178 (9)	0.0216 (12)	0.0163 (9)	0.0030 (14)	0.0007 (7)	0.0024 (14)
C2	0.0317 (13)	0.0301 (18)	0.0220 (12)	0.0004 (10)	0.0032 (10)	−0.0047 (10)
C3	0.0382 (16)	0.047 (2)	0.0205 (13)	−0.0005 (12)	−0.0004 (11)	−0.0061 (11)
C4	0.0231 (10)	0.0327 (12)	0.0238 (10)	−0.0050 (19)	−0.0048 (8)	0.0032 (19)
C5	0.0281 (14)	0.0294 (15)	0.0258 (14)	0.0030 (11)	−0.0045 (11)	0.0048 (11)
C6	0.0255 (13)	0.0179 (12)	0.0244 (13)	−0.0023 (10)	0.0007 (10)	0.0045 (10)
C7	0.0160 (11)	0.0205 (12)	0.0240 (13)	−0.0019 (9)	−0.0008 (10)	−0.0005 (10)
C8	0.0377 (17)	0.0240 (15)	0.0445 (18)	−0.0064 (13)	−0.0055 (14)	−0.0038 (13)
C9	0.0216 (11)	0.033 (2)	0.0238 (11)	−0.0013 (11)	0.0026 (9)	0.0045 (11)
O4	0.0312 (11)	0.0763 (18)	0.0298 (11)	0.0040 (11)	0.0112 (9)	−0.0116 (10)
C10	0.0163 (9)	0.0250 (17)	0.0184 (10)	0.0023 (10)	0.0013 (8)	−0.0009 (10)
S'	0.0153 (2)	0.0172 (2)	0.0220 (2)	−0.0003 (4)	−0.00066 (18)	0.0007 (4)
O1'	0.0248 (13)	0.0203 (12)	0.0303 (13)	−0.0014 (10)	−0.0029 (11)	−0.0057 (10)
O2'	0.0178 (12)	0.0217 (11)	0.0310 (13)	−0.0031 (9)	0.0034 (10)	0.0036 (10)
O3'	0.0167 (7)	0.0271 (8)	0.0319 (8)	−0.0018 (12)	−0.0040 (6)	−0.0023 (14)
C1'	0.0187 (9)	0.0208 (10)	0.0211 (9)	−0.0035 (16)	0.0008 (8)	0.0005 (17)
C2'	0.0327 (15)	0.0248 (14)	0.0263 (14)	−0.0019 (12)	−0.0011 (12)	0.0016 (11)
C3'	0.0413 (17)	0.0409 (18)	0.0265 (14)	−0.0017 (13)	−0.0091 (13)	0.0050 (11)
C4'	0.0248 (13)	0.0277 (15)	0.0278 (14)	−0.0003 (11)	−0.0062 (11)	−0.0025 (11)
C5'	0.0202 (10)	0.0333 (14)	0.0360 (12)	0.0044 (17)	−0.0044 (9)	−0.0015 (19)
C6'	0.0180 (12)	0.0269 (13)	0.0284 (13)	0.0027 (9)	−0.0003 (11)	−0.0052 (10)
C7'	0.0182 (12)	0.0244 (14)	0.0231 (13)	−0.0024 (10)	0.0029 (10)	−0.0052 (10)
C8'	0.0277 (15)	0.0366 (17)	0.0367 (18)	−0.0037 (13)	0.0086 (14)	−0.0138 (14)
C9'	0.0255 (14)	0.0249 (14)	0.0358 (16)	−0.0052 (11)	0.0012 (12)	−0.0010 (12)

O4'	0.0471 (15)	0.0360 (13)	0.0381 (14)	−0.0126 (11)	−0.0002 (11)	0.0105 (10)
C10'	0.0178 (9)	0.0294 (11)	0.0215 (10)	−0.0022 (17)	0.0032 (8)	−0.0002 (18)

Geometric parameters (Å, °)

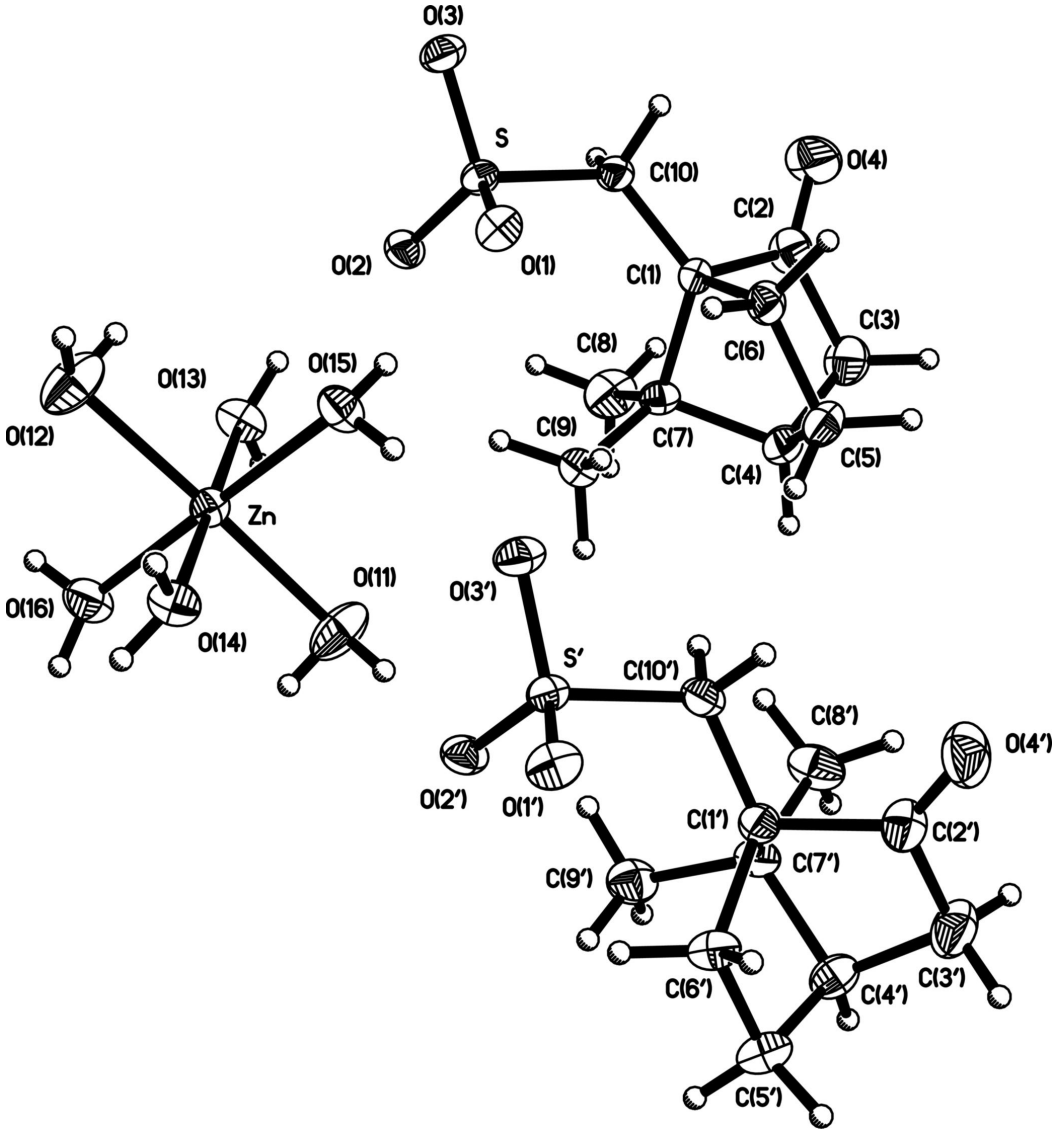
Zn—O11	2.0485 (17)	C7—C8	1.543 (4)
Zn—O12	2.0597 (17)	C8—H8A	0.9800
Zn—O14	2.083 (2)	C8—H8B	0.9800
Zn—O16	2.086 (2)	C8—H8C	0.9800
Zn—O13	2.090 (2)	C9—H9A	0.9800
Zn—O15	2.100 (2)	C9—H9B	0.9800
O11—H01	0.8405	C9—H9C	0.9800
O11—H02	0.8387	C10—H11A	0.9900
O12—H03	0.8394	C10—H11B	0.9900
O12—H04	0.8407	S'—O2'	1.459 (2)
O13—H05	0.8401	S'—O3'	1.4600 (14)
O13—H06	0.8394	S'—O1'	1.462 (2)
O14—H07	0.8404	S'—C10'	1.778 (2)
O14—H08	0.8397	C1'—C10'	1.517 (3)
O15—H09	0.8403	C1'—C2'	1.537 (4)
O15—H10	0.8391	C1'—C6'	1.566 (3)
O16—H11	0.8392	C1'—C7'	1.567 (4)
O16—H12	0.8396	C2'—O4'	1.200 (4)
S—O2	1.455 (2)	C2'—C3'	1.527 (4)
S—O3	1.4596 (14)	C3'—C4'	1.549 (4)
S—O1	1.464 (2)	C3'—H3'1	0.9900
S—C10	1.779 (2)	C3'—H3'2	0.9900
C1—C10	1.511 (3)	C4'—C5'	1.529 (4)
C1—C2	1.530 (3)	C4'—C7'	1.559 (4)
C1—C7	1.563 (3)	C4'—H4'	1.0000
C1—C6	1.566 (4)	C5'—C6'	1.551 (3)
C2—O4	1.210 (3)	C5'—H5'1	0.9900
C2—C3	1.519 (4)	C5'—H5'2	0.9900
C3—C4	1.535 (4)	C6'—H6'1	0.9900
C3—H3A	0.9900	C6'—H6'2	0.9900
C3—H3B	0.9900	C7'—C8'	1.517 (4)
C4—C5	1.540 (5)	C7'—C9'	1.532 (4)
C4—C7	1.560 (3)	C8'—H8'1	0.9800
C4—H4	1.0000	C8'—H8'2	0.9800
C5—C6	1.561 (3)	C8'—H8'3	0.9800
C5—H5A	0.9900	C9'—H9'1	0.9800
C5—H5B	0.9900	C9'—H9'2	0.9800
C6—H6A	0.9900	C9'—H9'3	0.9800
C6—H6B	0.9900	C10'—H11C	0.9900
C7—C9	1.533 (3)	C10'—H11D	0.9900
O11—Zn—O12	178.36 (9)	H8A—C8—H8B	109.5
O11—Zn—O14	89.42 (10)	C7—C8—H8C	109.5
O12—Zn—O14	89.18 (11)	H8A—C8—H8C	109.5
O11—Zn—O16	90.03 (11)	H8B—C8—H8C	109.5

O12—Zn—O16	89.28 (11)	C7—C9—H9A	109.5
O14—Zn—O16	96.27 (6)	C7—C9—H9B	109.5
O11—Zn—O13	90.77 (11)	H9A—C9—H9B	109.5
O12—Zn—O13	90.62 (11)	C7—C9—H9C	109.5
O14—Zn—O13	179.36 (12)	H9A—C9—H9C	109.5
O16—Zn—O13	83.13 (11)	H9B—C9—H9C	109.5
O11—Zn—O15	89.10 (11)	C1—C10—S	120.91 (16)
O12—Zn—O15	91.61 (11)	C1—C10—H11A	107.1
O14—Zn—O15	84.37 (11)	S—C10—H11A	107.1
O16—Zn—O15	178.92 (12)	C1—C10—H11B	107.1
O13—Zn—O15	96.24 (6)	S—C10—H11B	107.1
Zn—O11—H01	109.1	H11A—C10—H11B	106.8
Zn—O11—H02	99.9	O2'—S'—O3'	113.11 (15)
H01—O11—H02	103.0	O2'—S'—O1'	111.75 (9)
Zn—O12—H03	101.0	O3'—S'—O1'	112.23 (15)
Zn—O12—H04	110.8	O2'—S'—C10'	107.61 (17)
H03—O12—H04	103.0	O3'—S'—C10'	104.89 (9)
Zn—O13—H05	118.5	O1'—S'—C10'	106.69 (17)
Zn—O13—H06	128.9	C10'—C1'—C2'	110.8 (2)
H05—O13—H06	103.2	C10'—C1'—C6'	119.8 (2)
Zn—O14—H07	130.8	C2'—C1'—C6'	102.9 (2)
Zn—O14—H08	121.2	C10'—C1'—C7'	118.8 (3)
H07—O14—H08	103.3	C2'—C1'—C7'	99.55 (19)
Zn—O15—H09	125.5	C6'—C1'—C7'	102.11 (19)
Zn—O15—H10	129.3	O4'—C2'—C3'	126.5 (3)
H09—O15—H10	103.4	O4'—C2'—C1'	126.6 (3)
Zn—O16—H11	130.6	C3'—C2'—C1'	106.9 (2)
Zn—O16—H12	126.0	C2'—C3'—C4'	101.7 (2)
H11—O16—H12	103.3	C2'—C3'—H3'1	111.4
O2—S—O3	112.59 (15)	C4'—C3'—H3'1	111.4
O2—S—O1	112.13 (10)	C2'—C3'—H3'2	111.4
O3—S—O1	112.77 (16)	C4'—C3'—H3'2	111.4
O2—S—C10	106.45 (14)	H3'1—C3'—H3'2	109.3
O3—S—C10	104.01 (10)	C5'—C4'—C3'	106.2 (3)
O1—S—C10	108.28 (14)	C5'—C4'—C7'	103.4 (2)
C10—C1—C2	108.9 (2)	C3'—C4'—C7'	102.0 (2)
C10—C1—C7	124.3 (2)	C5'—C4'—H4'	114.6
C2—C1—C7	100.9 (2)	C3'—C4'—H4'	114.6
C10—C1—C6	116.2 (2)	C7'—C4'—H4'	114.6
C2—C1—C6	101.7 (2)	C4'—C5'—C6'	103.34 (19)
C7—C1—C6	101.77 (19)	C4'—C5'—H5'1	111.1
O4—C2—C3	126.6 (3)	C6'—C5'—H5'1	111.1
O4—C2—C1	125.9 (2)	C4'—C5'—H5'2	111.1
C3—C2—C1	107.5 (2)	C6'—C5'—H5'2	111.1
C2—C3—C4	101.3 (2)	H5'1—C5'—H5'2	109.1
C2—C3—H3A	111.5	C5'—C6'—C1'	104.2 (2)
C4—C3—H3A	111.5	C5'—C6'—H6'1	110.9
C2—C3—H3B	111.5	C1'—C6'—H6'1	110.9
C4—C3—H3B	111.5	C5'—C6'—H6'2	110.9

H3A—C3—H3B	109.3	C1'—C6'—H6'2	110.9
C3—C4—C5	106.0 (2)	H6'1—C6'—H6'2	108.9
C3—C4—C7	103.7 (2)	C8'—C7'—C9'	107.8 (2)
C5—C4—C7	102.5 (2)	C8'—C7'—C4'	112.8 (2)
C3—C4—H4	114.4	C9'—C7'—C4'	112.9 (2)
C5—C4—H4	114.4	C8'—C7'—C1'	113.9 (2)
C7—C4—H4	114.4	C9'—C7'—C1'	114.9 (2)
C4—C5—C6	102.9 (2)	C4'—C7'—C1'	94.2 (2)
C4—C5—H5A	111.2	C7'—C8'—H8'1	109.5
C6—C5—H5A	111.2	C7'—C8'—H8'2	109.5
C4—C5—H5B	111.2	H8'1—C8'—H8'2	109.5
C6—C5—H5B	111.2	C7'—C8'—H8'3	109.5
H5A—C5—H5B	109.1	H8'1—C8'—H8'3	109.5
C5—C6—C1	103.9 (2)	H8'2—C8'—H8'3	109.5
C5—C6—H6A	111.0	C7'—C9'—H9'1	109.5
C1—C6—H6A	111.0	C7'—C9'—H9'2	109.5
C5—C6—H6B	111.0	H9'1—C9'—H9'2	109.5
C1—C6—H6B	111.0	C7'—C9'—H9'3	109.5
H6A—C6—H6B	109.0	H9'1—C9'—H9'3	109.5
C9—C7—C8	108.6 (2)	H9'2—C9'—H9'3	109.5
C9—C7—C4	111.3 (2)	C1'—C10'—S'	118.91 (14)
C8—C7—C4	113.8 (3)	C1'—C10'—H11C	107.6
C9—C7—C1	116.9 (2)	S'—C10'—H11C	107.6
C8—C7—C1	111.8 (2)	C1'—C10'—H11D	107.6
C4—C7—C1	93.85 (19)	S'—C10'—H11D	107.6
C7—C8—H8A	109.5	H11C—C10'—H11D	107.0
C7—C8—H8B	109.5		
C10—C1—C2—O4	15.3 (4)	C10'—C1'—C2'—O4'	18.1 (5)
C7—C1—C2—O4	147.5 (3)	C6'—C1'—C2'—O4'	−111.2 (3)
C6—C1—C2—O4	−107.9 (3)	C7'—C1'—C2'—O4'	144.0 (3)
C10—C1—C2—C3	−164.9 (2)	C10'—C1'—C2'—C3'	−160.6 (3)
C7—C1—C2—C3	−32.7 (3)	C6'—C1'—C2'—C3'	70.2 (3)
C6—C1—C2—C3	71.9 (2)	C7'—C1'—C2'—C3'	−34.7 (3)
O4—C2—C3—C4	178.5 (3)	O4'—C2'—C3'—C4'	−178.8 (3)
C1—C2—C3—C4	−1.3 (3)	C1'—C2'—C3'—C4'	−0.2 (3)
C2—C3—C4—C5	−72.1 (3)	C2'—C3'—C4'—C5'	−72.4 (3)
C2—C3—C4—C7	35.4 (3)	C2'—C3'—C4'—C7'	35.5 (3)
C3—C4—C5—C6	71.2 (2)	C3'—C4'—C5'—C6'	70.7 (3)
C7—C4—C5—C6	−37.2 (2)	C7'—C4'—C5'—C6'	−36.3 (3)
C4—C5—C6—C1	2.5 (2)	C4'—C5'—C6'—C1'	2.4 (3)
C10—C1—C6—C5	170.7 (2)	C10'—C1'—C6'—C5'	165.4 (3)
C2—C1—C6—C5	−71.2 (2)	C2'—C1'—C6'—C5'	−71.2 (3)
C7—C1—C6—C5	32.7 (2)	C7'—C1'—C6'—C5'	31.7 (3)
C3—C4—C7—C9	−175.0 (2)	C5'—C4'—C7'—C8'	172.5 (3)
C5—C4—C7—C9	−64.9 (3)	C3'—C4'—C7'—C8'	62.3 (3)
C3—C4—C7—C8	61.9 (3)	C5'—C4'—C7'—C9'	−64.9 (3)
C5—C4—C7—C8	172.0 (2)	C3'—C4'—C7'—C9'	−175.1 (2)
C3—C4—C7—C1	−54.1 (3)	C5'—C4'—C7'—C1'	54.3 (2)
C5—C4—C7—C1	56.1 (2)	C3'—C4'—C7'—C1'	−55.8 (2)

C10—C1—C7—C9	−70.6 (4)	C10'—C1'—C7'—C8'	57.0 (3)
C2—C1—C7—C9	167.4 (2)	C2'—C1'—C7'—C8'	−63.2 (3)
C6—C1—C7—C9	62.8 (3)	C6'—C1'—C7'—C8'	−168.8 (2)
C10—C1—C7—C8	55.5 (3)	C10'—C1'—C7'—C9'	−68.1 (3)
C2—C1—C7—C8	−66.5 (3)	C2'—C1'—C7'—C9'	171.7 (2)
C6—C1—C7—C8	−171.1 (2)	C6'—C1'—C7'—C9'	66.1 (3)
C10—C1—C7—C4	173.1 (3)	C10'—C1'—C7'—C4'	174.2 (2)
C2—C1—C7—C4	51.1 (3)	C2'—C1'—C7'—C4'	54.0 (2)
C6—C1—C7—C4	−53.5 (2)	C6'—C1'—C7'—C4'	−51.5 (2)
C2—C1—C10—S	174.2 (2)	C2'—C1'—C10'—S'	−142.1 (3)
C7—C1—C10—S	55.8 (4)	C6'—C1'—C10'—S'	−22.6 (5)
C6—C1—C10—S	−71.7 (3)	C7'—C1'—C10'—S'	103.6 (3)
O2—S—C10—C1	−75.9 (3)	O2'—S'—C10'—C1'	−58.0 (3)
O3—S—C10—C1	165.0 (3)	O3'—S'—C10'—C1'	−178.7 (3)
O1—S—C10—C1	44.9 (3)	O1'—S'—C10'—C1'	62.1 (3)

Fig. 1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