

catena-Poly[[diaquazinc(II)]- μ -L-cysteinato(2-)- κ^4 S:S,N,O-[di- μ -sulfido-bis[oxidomolybdate(V)](Mo—Mo)]- μ -L-cysteinato(2-)- κ^4 S,N,O:S]

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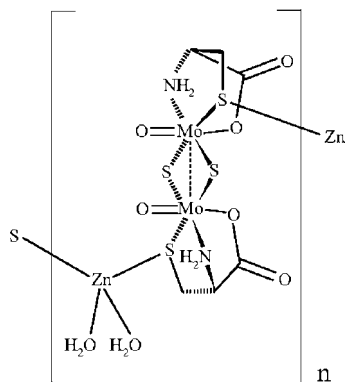
Received 6 March 2008; accepted 21 March 2008

Key indicators: single-crystal X-ray study; $T = 93$ K; mean $\sigma(\text{C—C}) = 0.003$ Å; R factor = 0.020; wR factor = 0.049; data-to-parameter ratio = 21.8.

The title compound, $[\text{Mo}_2\text{Zn}(\text{C}_3\text{H}_5\text{NO}_2\text{S})_2\text{O}_2\text{S}_2(\text{H}_2\text{O})_2]$, forms a one-dimensional chain. The cysteine S atom of the dinuclear molybdenum complex anion coordinates to the zinc ion, which has a tetrahedral environment by the additional coordination of two water molecules. The one-dimensional chains are connected to each other by hydrogen bonds. The Zn—S(cysteine) distances [2.3599 (6) and 2.3072 (6) Å] are close to the value in ZnS (2.35 Å). The distances and angles within the complex are very close to those reported for the sodium and potassium di- μ -sulfido species.

Related literature

For related literature, see: Brown & Jeffreys (1973); Hong *et al.* (1983); Kay & Mitchell (1970); Knox & Prout (1969); Shibahara *et al.* (1987); Lee *et al.* (1989); Liu & Williams (1981); Xing *et al.* (1998).



Experimental

Crystal data

$[\text{Mo}_2\text{Zn}(\text{C}_3\text{H}_5\text{NO}_2\text{S})_2\text{O}_2\text{S}_2(\text{H}_2\text{O})_2]$	$V = 843.23$ (16) Å ³
$M_r = 627.69$	$Z = 2$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 8.6881$ (11) Å	$\mu = 3.40$ mm ⁻¹
$b = 10.3529$ (8) Å	$T = 93.1$ K
$c = 9.8686$ (11) Å	$0.35 \times 0.30 \times 0.10$ mm
$\beta = 108.2022$ (14)°	

Data collection

Rigaku Mercury diffractometer	9357 measured reflections
Absorption correction: multi-scan (Jacobson, 1998)	4556 independent reflections
$T_{\min} = 0.382$, $T_{\max} = 0.727$	4549 reflections with $F^2 > 2\sigma(F^2)$
	$R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.019$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.049$	$\Delta\rho_{\text{max}} = 0.47$ e Å ⁻³
$S = 1.02$	$\Delta\rho_{\text{min}} = -0.94$ e Å ⁻³
4556 reflections	Absolute structure: Flack (1983), with 2010 Friedel pairs
209 parameters	Flack parameter: 0.002 (7)
15 restraints	

Table 1

Selected geometric parameters (Å, °).

Mo1—S1	2.3201 (6)	Mo2—S4	2.5428 (6)
Mo1—S2	2.3378 (6)	Zn1—O8	2.0052 (17)
Mo1—S3	2.5572 (6)	Zn1—O7	2.0275 (19)
Mo1—Mo2	2.8354 (3)	Zn1—S4 ⁱ	2.3072 (6)
Mo2—S2	2.3276 (6)	Zn1—S3	2.3599 (6)
Mo2—S1	2.3368 (6)		
O8—Zn1—O7	96.70 (7)	O8—Zn1—S3	93.73 (5)
O8—Zn1—S4 ⁱ	129.42 (5)	O7—Zn1—S3	104.55 (6)
O7—Zn1—S4 ⁱ	107.94 (6)	S4 ⁱ —Zn1—S3	120.25 (2)

Symmetry code: (i) $x - 1, y, z$.

Table 2

Hydrogen-bond geometry (Å, °).

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
O7—H11 \cdots O3 ⁱⁱ	0.84	2.03	2.832 (2)	161
O8—H13 \cdots O5 ⁱⁱ	0.84	1.77	2.604 (2)	171
O8—H14 \cdots O4 ⁱ	0.84	2.00	2.789 (2)	158

Symmetry codes: (i) $x - 1, y, z$; (ii) $-x, y + \frac{1}{2}, -z + 2$.

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku, 2007); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure*; software used to prepare material for publication: *CrystalStructure*.

This work was partly supported by a Special Grant for Cooperative Research administered by the Japan Private School Promotion Foundation.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WK2080).

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