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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*]

Takashi Shibahara,* Shinobu Ogasahara and Genta Sakane

Department of Chemistry, Okayama University of Science, Ridai-cho, Okayama 700-0005, Japan
Correspondence e-mail: shiba@chem.ous.ac.jp

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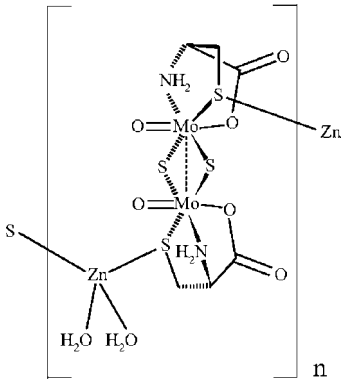
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.003 Å; R factor = 0.020; wR factor = 0.049; data-to-parameter ratio = 21.8.

The title compound, $[Mo_2Zn(C_3H_5NO_2S)_2O_2S_2(H_2O)_2]$, 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-sulfide 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

$[Mo_2Zn(C_3H_5NO_2S)_2O_2S_2(H_2O)_2]$
M_r = 627.69
Monoclinic, $P2_1$
a = 8.6881 (11) Å
b = 10.3529 (8) Å
c = 9.8686 (11) Å
β = 108.2022 (14)°
V = 843.23 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 3.40 mm^{-1}
T = 93.1 K
0.35 × 0.30 × 0.10 mm

Data collection

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

Refinement

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

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—H···A	D—H	H···A	D···A	D—H···A
O7—H11···O3^{ii}	0.84	2.03	2.832 (2)	161
O8—H13···O5^{ii}	0.84	1.77	2.604 (2)	171
O8—H14···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*.

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

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.

Brown, D. H. & Jeffreys, J. A. D. (1973). *J. Chem. Soc. Dalton Trans.* pp. 732–735.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Hong, M.-C., Shi, J., Huang, Z. & Liu, H. (1983). *Jiegou Huaxue*, **2**, 153–156.

Jacobson, R. (1998). Private communication to Rigaku Corporation, Tokyo, Japan.

Kay, A. & Mitchell, P. C. H. (1970). *J. Chem. Soc. A*, pp. 2421–2428.

Knox, J. R. & Prout, C. K. (1969). *Acta Cryst.* B**25**, 1857–1866.

Lee, M. S., Gippert, G. P., Soman, K. V., Case, D. A. & Wright, P. E. (1989). *Science*, **245**, 635–637.

Liu, H. & Williams, G. J. B. (1981). *Acta Cryst.* B**37**, 2065–2067.

Rigaku (1999). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.

Rigaku (2007). *CrystalStructure*. Rigaku Americas Corporation, The Woodlands, Texas, USA.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Shibahara, T., Kuroya, H., Matsumoto, K. & Ooi, S. (1987). *Bull. Chem. Soc. Jpn*, **60**, 2277–2279.

Xing, Y.-H., Xu, J.-Q., Li, D.-M., Sun, H.-R., Bu, W.-M., Ye, L., Yang, G.-D. & Fan, Y.-G. (1998). *Synth. React. Inorg. Met. Org. Chem.* **28**, 1493–1503.

supporting information

Acta Cryst. (2008). E**64**, m605–m606 [doi:10.1107/S1600536808007757]

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*]

Takashi Shibahara, Shinobu Ogasahara and Genta Sakane

S1. Comment

Molybdenum and *L*-cysteine are important components of many enzymes. X-ray structures of sulfur/oxygen-bridged dinuclear molybdenum complexes with *L*-cysteine ligands: $Na_2[Mo_2(\mu\text{-}S)_2O_2(cys)_2].4H_2O$ (Brown & Jeffreys, 1973; Hong *et al.*, 1983); $K_2[Mo_2S_2O_2(cys)_2].4H_2O.CH_3OH$ (Xing *et al.*, 1998), $Ca[Mo_2(\mu\text{-}S)(\mu\text{-}O)O_2(cys)_2].3H_2O$ (Shibahara *et al.*, 1987), and $Na_2[Mo_2O_4(cys)_2].5H_2O$ (Knox & Prout, 1969; Kay & Mitchell, 1970; Liu & Williams, 1981), have been reported, where alkaline or alkaline earth metals are counter cations, and the existence of metal-oxygen (cysteine oxygen) bonds has been reported. Seeking another crystal structure type, we used Zn^{2+}ion, as the counter ion. The present structural study of the complex compound $Zn[Mo_2O_2S_2(cys)_2].2H_2O$ (I) reveals the existence of Zn—S(cysteine sulfur) bonds, which result in polymerization; this type of Zn—S bond has been found in zinc finger proteins. The asymmetric unit of I is shown in Fig. 1 and a view of part of a one-dimensional polymeric chain of I is shown in Fig. 2. The zinc ion bridges the molybdenum complex anions: the coordination of the cysteine sulfur in the complex anion to the zinc ion results in the formation of one dimensional chains, where the zinc forms a tetrahedral structure by the additional coordination of two water molecules. The one dimensional chains are connected to each other by hydrogen bonds. Intra-chain hydrogen bonds also exist. The dimensions of the molybdenum complex and of the zinc tetrahedron are listed in Table 1, and the hydrogen bonds are listed in Table 2. The Zn—S(cysteine) distances (2.3599 (6), 2.3072 (6) Å) are close to that in ZnS (2.35 Å). The distances and angles within the complex are very close to those reported in the sodium and potassium salts in the di-μ-sulfide species.

S2. Experimental

The title compound was prepared by the addition of $ZnCl_2$ to a diluted aqueous solution of $Na_2[Mo_2O_2S_2(cys)_2].4H_2O$. A crystal suitable for single-crystal X-ray diffraction was selected directly from the prepared sample.

S3. Refinement

H atoms bonded to C, N, and O (H_2O) atoms were located in a difference map and refined with distance restraints of C—H = 0.99 (1), N—H = 0.92 (1), and O—H, 0.84 (1) Å, and with U_{iso}(H) = 1.2U_{eq}(C, N, O). The absolute structure was confirmed by the value of Flack parameter (0.003 (7)).

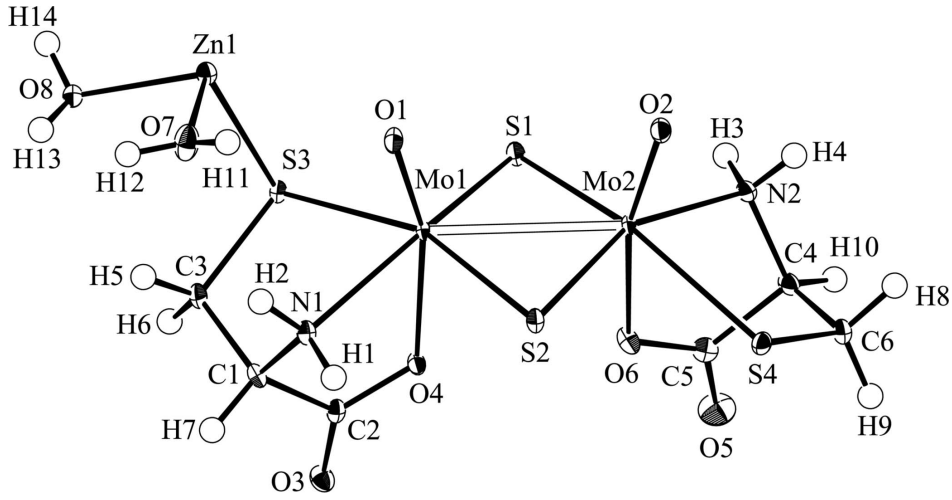

Figure 1

The asymmetric unit of I with atom labels and 50% probability displacement ellipsoids for non-H atoms.

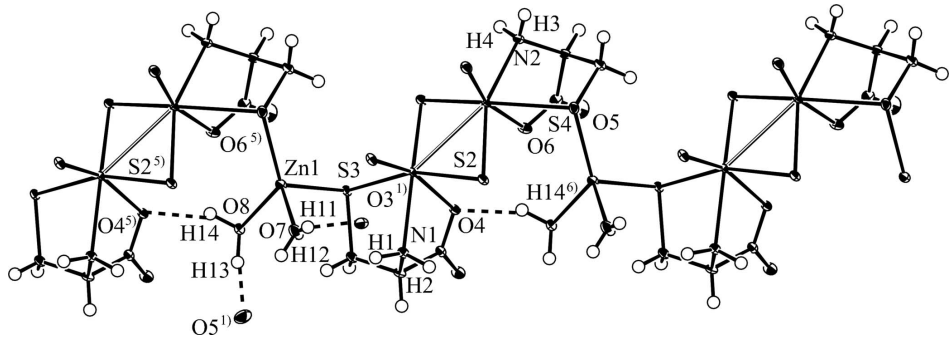

Figure 2

A view of part of a one-dimensional polymeric chain with hydrogen bonds (dashed lines).

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

Crystal data

$[Mo_2Zn(C_3H_5NO_2S)_2O_2S_2(H_2O)_2]$
M_r = 627.69
Monoclinic, $P2_1$
Hall symbol: P 2yb
a = 8.6881 (11) Å
b = 10.3529 (8) Å
c = 9.8686 (11) Å
β = 108.2022 (14)°
V = 843.23 (16) Å^3
Z = 2
$F(000)$ = 612.00
D_x = 2.472 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71070 Å
Cell parameters from 3004 reflections
θ = 5.5–30.0°
μ = 3.41 mm^{-1}
T = 93 K
Platelet, orange
0.35 × 0.30 × 0.10 mm

Data collection

Rigaku Mercury diffractometer
Detector resolution: 14.63 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.382, T_{max} = 0.727
9357 measured reflections

4556 independent reflections
4549 reflections with $F^2 > 2\sigma(F^2)$
$R_{int} = 0.019$
$\theta_{max} = 30.0°$
$h = -12 \rightarrow 11$
$k = -14 \rightarrow 14$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.049$
$S = 1.02$
4556 reflections
209 parameters
15 restraints
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 0.5406P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.94$ e Å^{-3}
Absolute structure: Flack (1983), with 2010 Friedel pairs
Absolute structure parameter: 0.002 (7)

Special details

Geometry. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0\ \sigma > F^2$) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Mo1	−0.056910 (19)	0.591229 (16)	0.808774 (16)	0.00615 (4)
Mo2	0.113206 (19)	0.533750 (19)	0.613333 (16)	0.00647 (4)
Zn1	−0.46728 (3)	0.59442 (3)	0.84366 (3)	0.01008 (4)
S1	−0.07812 (7)	0.40574 (6)	0.67221 (6)	0.00917 (8)
S2	0.16158 (6)	0.70395 (5)	0.77534 (6)	0.00880 (8)
S3	−0.22984 (6)	0.46976 (5)	0.93439 (5)	0.00813 (8)
S4	0.39318 (6)	0.59322 (6)	0.60271 (5)	0.01009 (8)
O1	−0.2167 (2)	0.68209 (17)	0.71583 (17)	0.0104 (2)
O2	0.00101 (19)	0.60344 (18)	0.45909 (16)	0.0111 (2)
O3	0.2203 (2)	0.45050 (18)	1.21945 (17)	0.0125 (3)
O4	0.13324 (19)	0.49461 (16)	0.98677 (16)	0.0089 (2)
O5	0.4690 (2)	0.2383 (2)	0.7999 (2)	0.0217 (3)
O6	0.2865 (2)	0.39663 (18)	0.77426 (17)	0.0125 (3)
O7	−0.3954 (2)	0.77830 (18)	0.9006 (2)	0.0182 (3)
O8	−0.54704 (19)	0.55572 (18)	1.00931 (17)	0.0136 (3)
N1	−0.0163 (2)	0.70357 (19)	1.01408 (19)	0.0087 (3)
N2	0.1744 (2)	0.3658 (2)	0.4962 (2)	0.0102 (3)
C1	0.0084 (2)	0.6095 (2)	1.1320 (2)	0.0092 (3)
C2	0.1322 (2)	0.5110 (2)	1.1161 (2)	0.0083 (3)
C3	−0.1525 (2)	0.5421 (2)	1.1147 (2)	0.0099 (3)
C4	0.3455 (2)	0.3284 (2)	0.5675 (2)	0.0112 (3)
C5	0.3694 (2)	0.3165 (2)	0.7269 (2)	0.0116 (4)
C6	0.4534 (2)	0.4378 (2)	0.5447 (2)	0.0130 (4)
H1	0.0683	0.7596	1.0256	0.010*
H2	−0.1027	0.7551	1.0124	0.010*

H3	0.1090	0.2957	0.4919	0.012*
H4	0.1624	0.3890	0.4039	0.012*
H5	−0.2299	0.6042	1.1334	0.012*
H6	−0.1366	0.4727	1.1869	0.012*
H7	0.0460	0.6482	1.2291	0.011*
H8	0.4318	0.4416	0.4403	0.016*
H9	0.5706	0.4243	0.5928	0.016*
H10	0.3821	0.2458	0.5359	0.013*
H11	−0.3638	0.8290	0.8487	0.022*
H12	−0.4303	0.8035	0.9659	0.022*
H13	−0.5293	0.6197	1.0646	0.016*
H14	−0.6424	0.5281	0.9816	0.016*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.00760 (7)	0.00633 (8)	0.00567 (7)	0.00053 (6)	0.00374 (5)	0.00047 (6)
Mo2	0.00756 (7)	0.00729 (8)	0.00565 (7)	0.00067 (6)	0.00364 (5)	0.00022 (6)
Zn1	0.01030 (10)	0.01118 (12)	0.00928 (10)	0.00082 (10)	0.00382 (8)	−0.00105 (9)
S1	0.0114 (2)	0.0085 (2)	0.0091 (2)	−0.00148 (18)	0.00549 (17)	−0.00119 (17)
S2	0.0109 (2)	0.0077 (2)	0.0098 (2)	−0.00074 (18)	0.00601 (17)	−0.00107 (17)
S3	0.0087 (2)	0.0085 (2)	0.0086 (2)	−0.00003 (18)	0.00480 (16)	−0.00014 (17)
S4	0.0088 (2)	0.0127 (2)	0.0098 (2)	−0.0003 (2)	0.00436 (16)	0.00152 (19)
O1	0.0111 (6)	0.0117 (8)	0.0102 (6)	0.0024 (5)	0.0060 (5)	0.0015 (5)
O2	0.0113 (6)	0.0135 (8)	0.0097 (6)	0.0019 (6)	0.0048 (5)	0.0014 (6)
O3	0.0152 (7)	0.0123 (8)	0.0101 (6)	0.0030 (6)	0.0039 (5)	0.0014 (6)
O4	0.0102 (6)	0.0099 (7)	0.0074 (6)	0.0011 (5)	0.0041 (5)	0.0002 (5)
O5	0.0216 (8)	0.0185 (9)	0.0221 (8)	0.0064 (7)	0.0027 (7)	0.0083 (7)
O6	0.0166 (7)	0.0129 (8)	0.0087 (6)	0.0010 (6)	0.0049 (5)	−0.0004 (5)
O7	0.0217 (9)	0.0131 (8)	0.0250 (8)	−0.0031 (7)	0.0146 (7)	−0.0054 (7)
O8	0.0096 (6)	0.0217 (10)	0.0103 (6)	−0.0025 (5)	0.0045 (5)	−0.0045 (6)
N1	0.0111 (7)	0.0069 (8)	0.0096 (7)	0.0002 (6)	0.0053 (6)	0.0004 (6)
N2	0.0096 (7)	0.0125 (9)	0.0084 (7)	0.0010 (6)	0.0026 (6)	−0.0032 (6)
C1	0.0131 (8)	0.0086 (10)	0.0067 (7)	0.0002 (7)	0.0043 (6)	−0.0005 (7)
C2	0.0099 (8)	0.0060 (10)	0.0107 (8)	−0.0019 (6)	0.0058 (6)	−0.0008 (6)
C3	0.0118 (8)	0.0109 (9)	0.0088 (7)	−0.0005 (7)	0.0060 (6)	0.0001 (7)
C4	0.0114 (8)	0.0130 (10)	0.0088 (8)	0.0038 (7)	0.0024 (6)	−0.0032 (7)
C5	0.0126 (9)	0.0095 (10)	0.0124 (9)	−0.0007 (7)	0.0034 (7)	0.0003 (7)
C6	0.0117 (9)	0.0186 (11)	0.0099 (8)	0.0019 (7)	0.0052 (7)	−0.0024 (8)

Geometric parameters (Å, º)

Mo1—O1	1.6905 (17)	O5—C5	1.238 (3)
Mo1—O4	2.2366 (16)	O6—C5	1.279 (3)
Mo1—N1	2.2662 (19)	O7—H11	0.837
Mo1—S1	2.3201 (6)	O7—H12	0.835
Mo1—S2	2.3378 (6)	O8—H13	0.841
Mo1—S3	2.5572 (6)	O8—H14	0.838

Mo1—Mo2	2.8354 (3)	N1—C1	1.481 (3)
Mo2—O2	1.6914 (16)	N1—H1	0.915
Mo2—N2	2.2419 (19)	N1—H2	0.917
Mo2—O6	2.3044 (18)	N2—C4	1.484 (3)
Mo2—S2	2.3276 (6)	N2—H3	0.914
Mo2—S1	2.3368 (6)	N2—H4	0.915
Mo2—S4	2.5428 (6)	C1—C3	1.523 (3)
Zn1—O8	2.0052 (17)	C1—C2	1.526 (3)
Zn1—O7	2.0275 (19)	C1—H7	0.995
Zn1—S4^{i}	2.3072 (6)	C3—H5	0.989
Zn1—S3	2.3599 (6)	C3—H6	0.991
S3—C3	1.852 (2)	C4—C5	1.527 (3)
S4—C6	1.838 (3)	C4—C6	1.531 (4)
S4—Zn1^{ii}	2.3072 (6)	C4—H10	0.996
O3—C2	1.237 (3)	C6—H8	0.989
O4—C2	1.290 (2)	C6—H9	0.989

O1—Mo1—O4	162.73 (7)	C6—S4—Zn1^{ii}	102.50 (7)
O1—Mo1—N1	94.11 (7)	C6—S4—Mo2	99.79 (8)
O4—Mo1—N1	69.93 (6)	Zn1^{ii}—S4—Mo2	99.22 (2)
O1—Mo1—S1	104.04 (6)	C2—O4—Mo1	119.10 (14)
O4—Mo1—S1	89.50 (4)	C5—O6—Mo2	117.99 (14)
N1—Mo1—S1	154.97 (5)	Zn1—O7—H11	123.4
O1—Mo1—S2	102.18 (6)	Zn1—O7—H12	110.6
O4—Mo1—S2	84.32 (4)	H11—O7—H12	122.9
N1—Mo1—S2	87.91 (5)	Zn1—O8—H13	109.3
S1—Mo1—S2	104.59 (2)	Zn1—O8—H14	111.1
O1—Mo1—S3	91.69 (6)	H13—O8—H14	116.3
O4—Mo1—S3	78.52 (4)	C1—N1—Mo1	107.99 (13)
N1—Mo1—S3	76.70 (5)	C1—N1—H1	113.9
S1—Mo1—S3	85.55 (2)	Mo1—N1—H1	109.3
S2—Mo1—S3	160.022 (19)	C1—N1—H2	108.3
O1—Mo1—Mo2	105.18 (6)	Mo1—N1—H2	112.6
O4—Mo1—Mo2	91.51 (4)	H1—N1—H2	104.8
N1—Mo1—Mo2	138.35 (5)	C4—N2—Mo2	108.76 (13)
S1—Mo1—Mo2	52.760 (15)	C4—N2—H3	109.3
S2—Mo1—Mo2	52.411 (14)	Mo2—N2—H3	113.3
S3—Mo1—Mo2	137.441 (15)	C4—N2—H4	109.0
O2—Mo2—N2	91.69 (8)	Mo2—N2—H4	109.8
O2—Mo2—O6	162.14 (7)	H3—N2—H4	106.6
N2—Mo2—O6	70.64 (6)	N1—C1—C3	108.11 (17)
O2—Mo2—S2	103.00 (6)	N1—C1—C2	107.01 (16)
N2—Mo2—S2	156.97 (5)	C3—C1—C2	109.49 (18)
O6—Mo2—S2	93.10 (5)	N1—C1—H7	114.5
O2—Mo2—S1	102.18 (6)	C3—C1—H7	107.9
N2—Mo2—S1	89.44 (5)	C2—C1—H7	109.8
O6—Mo2—S1	80.89 (5)	O3—C2—O4	123.7 (2)
S2—Mo2—S1	104.38 (2)	O3—C2—C1	121.88 (18)

O2—Mo2—S4	98.59 (6)	O4—C2—C1	114.38 (18)
N2—Mo2—S4	77.44 (5)	C1—C3—S3	109.75 (13)
O6—Mo2—S4	75.53 (5)	C1—C3—H5	109.6
S2—Mo2—S4	82.83 (2)	S3—C3—H5	112.2
S1—Mo2—S4	155.71 (2)	C1—C3—H6	109.6
O2—Mo2—Mo1	104.26 (5)	S3—C3—H6	109.0
N2—Mo2—Mo1	140.49 (5)	H5—C3—H6	106.7
O6—Mo2—Mo1	91.59 (4)	N2—C4—C5	107.66 (18)
S2—Mo2—Mo1	52.737 (15)	N2—C4—C6	107.82 (19)
S1—Mo2—Mo1	52.226 (15)	C5—C4—C6	108.60 (18)
S4—Mo2—Mo1	133.300 (15)	N2—C4—H10	116.5
O8—Zn1—O7	96.70 (7)	C5—C4—H10	107.4
O8—Zn1—S4^{i}	129.42 (5)	C6—C4—H10	108.7
O7—Zn1—S4^{i}	107.94 (6)	O5—C5—O6	125.6 (2)
O8—Zn1—S3	93.73 (5)	O5—C5—C4	119.9 (2)
O7—Zn1—S3	104.55 (6)	O6—C5—C4	114.4 (2)
S4^{i}—Zn1—S3	120.25 (2)	C4—C6—S4	110.80 (15)
Mo1—S1—Mo2	75.014 (19)	C4—C6—H8	104.8
Mo2—S2—Mo1	74.853 (18)	S4—C6—H8	108.1
C3—S3—Zn1	98.94 (7)	C4—C6—H9	114.2
C3—S3—Mo1	100.08 (7)	S4—C6—H9	109.0
Zn1—S3—Mo1	97.09 (2)	H8—C6—H9	109.7

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H11···O3^{iii}	0.84	2.03	2.832 (2)	161
O7—H11···O4^{iii}	0.84	2.75	3.139 (2)	110
O7—H12···O5^{iii}	0.84	2.53	3.239 (3)	144
O7—H12···O6^{iii}	0.84	2.66	3.285 (2)	133
O7—H12···O8^{iv}	0.84	2.64	3.093 (2)	116
O8—H13···O5^{iii}	0.84	1.77	2.604 (2)	171
O8—H14···O4^{i}	0.84	2.00	2.789 (2)	158
O8—H14···O6^{i}	0.84	2.37	2.844 (2)	116
N1—H2···O4^{iii}	0.92	2.49	3.179 (2)	132
N1—H2···O7	0.92	2.45	3.224 (2)	143
N2—H3···O2^{v}	0.91	2.32	3.212 (2)	164
N2—H4···O1^{v}	0.92	2.56	2.934 (2)	105
N2—H4···O3^{vi}	0.92	2.13	3.011 (2)	161

Symmetry codes: (i) $x-1, y, z$; (iii) $-x, y+1/2, -z+2$; (iv) $-x-1, y+1/2, -z+2$; (v) $-x, y-1/2, -z+1$; (vi) $x, y, z-1$.