

μ -Glycine- $\kappa^2O:O'$ -di- μ -sulfido-bis[(glycinato- κ^2N,O)oxidomolybdenum(V)]

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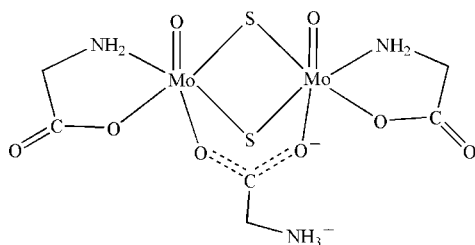
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(C-C) = 0.023$ Å; R factor = 0.087; wR factor = 0.178; data-to-parameter ratio = 13.3.

In the title compound, $[Mo_2(C_2H_4NO_2)_2O_2S_2(C_2H_5NO_2)]$, the two Mo^V atoms are bridged by two μ_2 -S atoms and one glycine ligand in an $O:O'$ -bidentate mode. In addition, each Mo^V atom is bonded to one terminal oxygen ligand and chelated by one N,O -bidentate glycinate ligand, resulting in a distorted octahedral coordination. A complex hydrogen-bonding network is constructed by intermolecular $N-H \cdots O$ hydrogen bonds.

Related literature

For related structures, see: Spivack & Dori (1975); Li *et al.* (2005); Liu *et al.* (2000); Lin *et al.* (1998).

**Experimental***Crystal data*

$[Mo_2(C_2H_4NO_2)_2O_2S_2(C_2H_5NO_2)]$
 $M_r = 511.19$

Monoclinic, $P2_1/c$
 $a = 13.1258$ (13) Å
 $b = 10.8384$ (10) Å
 $c = 10.5850$ (10) Å
 $\beta = 106.597$ (2)°

$V = 1443.1$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 2.07$ mm⁻¹
 $T = 295$ K
 $0.20 \times 0.15 \times 0.10$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{min} = 0.483$, $T_{max} = 0.813$

4358 measured reflections
 2519 independent reflections
 1620 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.086$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.087$
 $wR(F^2) = 0.178$
 $S = 1.11$
 2519 reflections

190 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 1.16$ e Å⁻³
 $\Delta\rho_{min} = -1.10$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N1-H1A \cdots O3^i$	0.90	2.09	2.975 (16)	167
$N1-H1B \cdots O5^{ii}$	0.90	2.10	2.882 (16)	144
$N2-H2A \cdots O3^{iii}$	0.90	2.13	2.958 (16)	153
$N3-H3A \cdots O1^{iv}$	0.89	2.33	3.119 (17)	148
$N3-H3B \cdots O6^v$	0.89	1.94	2.825 (16)	172
$N3-H3E \cdots O1^{vi}$	0.89	2.08	2.934 (17)	160

Symmetry codes: (i) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (ii) $x, y - 1, z$; (iii) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $-x + 2, y + \frac{1}{2}, -z + \frac{3}{2}$; (v) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (vi) $-x + 2, -y + 1, -z + 1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXTL* (Siemens, 1996); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2039).

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supplementary materials

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μ_2 -Glycine- μ_2 -O:O'-di- μ_2 -sulfido-bis[(glycinato- μ_2 -N,O)oxido-molybdenum(V)]

Y. M. Li, Y. H. Li and C. P. Zhai

Comment

Dimolybdenum complexes containing $[\text{Mo}_2\text{O}_2(\mu\text{-S})_2]$ have attracted many chemists' attention, not only because the $[\text{Mo}_2\text{O}_2(\mu\text{-S})_2]$ unit has special stability but also because it may be employed as a starting material to react with many transition metals. Some $[\text{Mo}_2\text{O}_2(\mu\text{-S})_2]$ structural compounds based on amino-acid have been isolated and structurally characterized (Spivack & Dori, 1975; Li *et al.*, 2005). The crystal structure of our new neutral dimolybdenum glycinato complex is similar to the compound $[\text{Mo}_2\text{O}_4(\text{C}_2\text{H}_4\text{NO}_2)_2(\text{C}_2\text{H}_5\text{NO}_2)]$ (Liu *et al.*, 2000).

The title structure consists of the neutral $\text{Mo}_2\text{O}_2(\mu\text{-S})_2(\text{C}_2\text{H}_5\text{NO}_2)(\text{C}_2\text{H}_4\text{NO}_2)_2$ (Fig. 1). In the structure, the two molybdenum atoms are not crystallographically equivalent, which are linked by two μ_2 -S ligand and one glycine ($^+\text{H}_3\text{NCH}_2\text{COO}^-$) ligand in an *O:O'*-bidentate mode. Each Mo^{V} atom is also bonded to one terminal oxygen atom and chelated by one *N,O*-glycine ($\text{NH}_2\text{CH}_2\text{COO}^-$) ligand, resulting in a distorted octahedral coordination. The $\text{Mo}\cdots\text{Mo}$ separation is 2.788 (2) Å, which is shorter than the $\text{Mo}\cdots\text{Mo}$ distance (2.848 (1) Å) in the histidinato complex (Spivack & Dori, 1975). The $\text{Mo}-\text{S}$, $\text{Mo}-\text{N}$, $\text{Mo}-\text{O}$ and $\text{Mo}=\text{O}$ bond lengths are 2.304 (5)—2.336 (4) Å, 2.195 (12)—2.225 (11) Å, 2.091 (11)—2.328 (9) Å and 1.668 (11)—1.696 (10) Å, respectively.

A three-dimensional network is constructed by six classic intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 1 and Fig. 2).

Experimental

The title compound was prepared by adding a solution of glycine (0.075 g, 1 mmol) in 5 ml H_2O to a solution of $(\text{Et}_4\text{N})_2\text{Mo}_2\text{S}_2\text{O}_2(\text{edt})_2$ (0.366 g, 0.5 mmol) in 5 ml DMF. After stirring about 10 min, the solution was filtered. Orange block crystals of the title compound were obtained by slow evaporation of the orange filtrate for several weeks. $(\text{Et}_4\text{N})_2\text{Mo}_2\text{S}_2\text{O}_2(\text{edt})_2$ was synthesized by the literature (Lin *et al.*, 1998).

Refinement

All H atoms were positioned geometrically and treated as riding atoms (including free rotation about the $\text{C}-\text{NH}_3^+$ bond), with $\text{C}-\text{H} = 0.97$ Å and $\text{N}-\text{H} = 0.89-0.90$ Å, with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C}, \text{N})$ (1.5 for $-\text{NH}_3^+$ groups). R_{int} value of 0.086 and R of 0.0869 indicate a low structure quality.

Figures

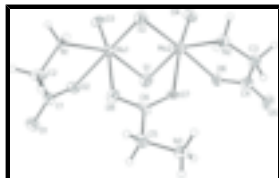


Fig. 1. The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

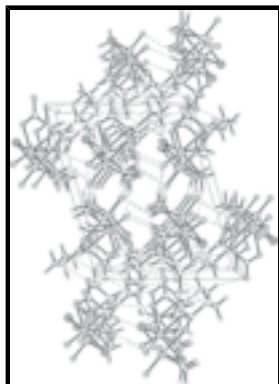


Fig. 2. A view of the crystal packing along the *b* axis. Hydrogen bonds are shown as dashed lines.

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Crystal data

$[\text{Mo}_2(\text{C}_2\text{H}_4\text{NO}_2)_2\text{O}_2\text{S}_2(\text{C}_2\text{H}_5\text{NO}_2)]$

$M_r = 511.19$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 13.1258 (13) \text{ \AA}$

$b = 10.8384 (10) \text{ \AA}$

$c = 10.5850 (10) \text{ \AA}$

$\beta = 106.597 (2)^\circ$

$V = 1443.1 (2) \text{ \AA}^3$

$Z = 4$

$F_{000} = 1000$

$D_x = 2.353 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 45 reflections

$\theta = 2.5\text{--}25.0^\circ$

$\mu = 2.07 \text{ mm}^{-1}$

$T = 295 \text{ K}$

Block, orange

$0.20 \times 0.15 \times 0.10 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 295 \text{ K}$

ϕ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.483$, $T_{\max} = 0.813$

4358 measured reflections

2519 independent reflections

1620 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.086$

$\theta_{\max} = 25.0^\circ$

$\theta_{\min} = 2.5^\circ$

$h = -15 \rightarrow 13$

$k = -12 \rightarrow 7$

$l = -7 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.087$	H-atom parameters constrained
$wR(F^2) = 0.178$	$w = 1/[\sigma^2(F_o^2) + (0.0001P)^2 + 52.2323P]$
$S = 1.11$	where $P = (F_o^2 + 2F_c^2)/3$
2519 reflections	$(\Delta/\sigma)_{\max} < 0.001$
190 parameters	$\Delta\rho_{\max} = 1.16 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -1.10 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

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 ($\text{\AA}^2$)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mo1	0.72243 (11)	0.35843 (13)	0.32342 (13)	0.0272 (4)
Mo2	0.64096 (11)	0.59751 (13)	0.30419 (13)	0.0281 (4)
S1	0.7788 (4)	0.5267 (4)	0.2284 (5)	0.0513 (13)
S2	0.5926 (3)	0.4310 (4)	0.4150 (4)	0.0355 (10)
O1	1.0118 (9)	0.1842 (12)	0.4619 (12)	0.051 (3)
O2	0.8716 (8)	0.2768 (10)	0.3310 (10)	0.034 (3)
O3	0.6503 (8)	0.2828 (10)	0.1868 (10)	0.036 (3)
O4	0.5367 (8)	0.6025 (11)	0.1700 (10)	0.040 (3)
O5	0.7134 (10)	0.9688 (11)	0.3142 (13)	0.051 (3)
O6	0.7004 (8)	0.7698 (10)	0.2716 (10)	0.033 (3)
O7	0.7740 (7)	0.6195 (10)	0.5025 (10)	0.030 (3)
O8	0.8358 (9)	0.4270 (10)	0.5171 (10)	0.035 (3)
N1	0.7391 (10)	0.1977 (10)	0.4585 (12)	0.027 (3)
H1A	0.7119	0.2171	0.5250	0.032*
H1B	0.7018	0.1336	0.4143	0.032*
N2	0.5774 (10)	0.7223 (11)	0.4264 (12)	0.030 (3)
H2A	0.5061	0.7154	0.4028	0.036*
H2B	0.6023	0.6992	0.5113	0.036*

supplementary materials

N3	0.9018 (10)	0.6917 (13)	0.7315 (12)	0.035 (3)
H3A	0.9475	0.7059	0.8101	0.053*
H3B	0.8358	0.7047	0.7355	0.053*
H3E	0.9156	0.7423	0.6722	0.053*
C1	0.9187 (14)	0.2111 (16)	0.4302 (18)	0.040 (4)
C2	0.8498 (12)	0.1619 (18)	0.5123 (16)	0.043 (5)
H2C	0.8547	0.0726	0.5158	0.052*
H2D	0.8763	0.1929	0.6016	0.052*
C3	0.6054 (14)	0.8498 (15)	0.4143 (17)	0.040 (4)
H3C	0.6394	0.8823	0.5016	0.047*
H3D	0.5409	0.8968	0.3775	0.047*
C4	0.6778 (13)	0.8681 (16)	0.3302 (14)	0.034 (4)
C5	0.9124 (13)	0.5617 (16)	0.6923 (17)	0.042 (4)
H5A	0.9843	0.5468	0.6884	0.050*
H5B	0.8980	0.5061	0.7569	0.050*
C6	0.8361 (12)	0.5390 (16)	0.5617 (14)	0.029 (4)

Atomic displacement parameters ($\text{\AA}^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0314 (8)	0.0282 (8)	0.0244 (7)	−0.0040 (6)	0.0116 (6)	−0.0006 (6)
Mo2	0.0289 (8)	0.0300 (8)	0.0281 (7)	0.0000 (6)	0.0128 (6)	0.0005 (6)
S1	0.062 (3)	0.035 (3)	0.061 (3)	0.000 (2)	0.024 (3)	−0.004 (2)
S2	0.039 (3)	0.035 (3)	0.038 (2)	−0.0018 (19)	0.019 (2)	0.0015 (19)
O1	0.032 (7)	0.057 (9)	0.062 (9)	0.005 (6)	0.010 (6)	0.015 (7)
O2	0.026 (6)	0.046 (7)	0.035 (6)	0.002 (5)	0.017 (5)	0.003 (6)
O3	0.037 (7)	0.039 (7)	0.032 (6)	−0.012 (5)	0.012 (5)	−0.001 (5)
O4	0.035 (7)	0.052 (8)	0.037 (6)	0.004 (6)	0.016 (5)	0.007 (6)
O5	0.058 (9)	0.030 (7)	0.078 (10)	−0.009 (6)	0.038 (8)	−0.005 (7)
O6	0.038 (7)	0.025 (6)	0.043 (7)	0.005 (5)	0.023 (6)	0.006 (5)
O7	0.015 (5)	0.038 (7)	0.030 (6)	−0.004 (5)	−0.004 (4)	−0.006 (5)
O8	0.046 (7)	0.033 (7)	0.028 (6)	−0.004 (5)	0.012 (5)	0.002 (5)
N1	0.044 (8)	0.007 (6)	0.037 (7)	−0.003 (6)	0.023 (6)	−0.002 (5)
N2	0.032 (8)	0.031 (8)	0.030 (7)	0.001 (6)	0.012 (6)	0.001 (6)
N3	0.031 (8)	0.053 (10)	0.024 (7)	−0.003 (7)	0.011 (6)	−0.007 (6)
C1	0.033 (11)	0.037 (11)	0.053 (12)	0.010 (8)	0.015 (9)	0.002 (9)
C2	0.028 (10)	0.067 (14)	0.033 (10)	−0.012 (9)	0.004 (8)	0.000 (9)
C3	0.047 (11)	0.030 (10)	0.050 (11)	0.000 (8)	0.028 (9)	−0.005 (8)
C4	0.035 (9)	0.040 (11)	0.021 (8)	−0.003 (8)	−0.003 (7)	0.003 (8)
C5	0.034 (10)	0.045 (11)	0.047 (11)	0.007 (8)	0.012 (8)	−0.011 (9)
C6	0.017 (8)	0.049 (11)	0.021 (8)	0.012 (8)	0.003 (7)	0.004 (8)

Geometric parameters ($\text{\AA}$, $^\circ$)

Mo1—O3	1.696 (10)	N1—C2	1.454 (19)
Mo1—O2	2.129 (10)	N1—H1A	0.9000
Mo1—N1	2.225 (11)	N1—H1B	0.9000
Mo1—O8	2.286 (11)	N2—C3	1.44 (2)
Mo1—S1	2.304 (5)	N2—H2A	0.9000

Mo1—S2	2.325 (4)	N2—H2B	0.9000
Mo1—Mo2	2.788 (2)	N3—C5	1.49 (2)
Mo2—O4	1.668 (11)	N3—H3A	0.8900
Mo2—O6	2.091 (11)	N3—H3B	0.8900
Mo2—N2	2.195 (12)	N3—H3E	0.8900
Mo2—S1	2.310 (5)	C1—C2	1.52 (2)
Mo2—O7	2.328 (9)	C2—H2C	0.9700
Mo2—S2	2.336 (4)	C2—H2D	0.9700
O1—C1	1.206 (19)	C3—C4	1.49 (2)
O2—C1	1.274 (19)	C3—H3C	0.9700
O5—C4	1.219 (19)	C3—H3D	0.9700
O6—C4	1.308 (19)	C5—C6	1.48 (2)
O7—C6	1.235 (17)	C5—H5A	0.9700
O8—C6	1.303 (19)	C5—H5B	0.9700
O3—Mo1—O2	96.6 (5)	C6—O8—Mo1	124.2 (9)
O3—Mo1—N1	95.6 (5)	C2—N1—Mo1	111.4 (9)
O2—Mo1—N1	74.3 (4)	C2—N1—H1A	109.3
O3—Mo1—O8	169.5 (5)	Mo1—N1—H1A	109.3
O2—Mo1—O8	75.2 (4)	C2—N1—H1B	109.3
N1—Mo1—O8	76.0 (4)	Mo1—N1—H1B	109.3
O3—Mo1—S1	100.4 (4)	H1A—N1—H1B	108.0
O2—Mo1—S1	86.5 (3)	C3—N2—Mo2	112.8 (9)
N1—Mo1—S1	156.3 (4)	C3—N2—H2A	109.0
O8—Mo1—S1	85.8 (3)	Mo2—N2—H2A	109.0
O3—Mo1—S2	102.8 (4)	C3—N2—H2B	109.0
O2—Mo1—S2	154.2 (3)	Mo2—N2—H2B	109.0
N1—Mo1—S2	86.9 (3)	H2A—N2—H2B	107.8
O8—Mo1—S2	83.3 (3)	C5—N3—H3A	109.5
S1—Mo1—S2	106.19 (17)	C5—N3—H3B	109.5
O3—Mo1—Mo2	106.1 (4)	H3A—N3—H3B	109.5
O2—Mo1—Mo2	135.9 (3)	C5—N3—H3E	109.5
N1—Mo1—Mo2	137.7 (3)	H3A—N3—H3E	109.5
O8—Mo1—Mo2	84.3 (3)	H3B—N3—H3E	109.5
S1—Mo1—Mo2	52.90 (13)	O1—C1—O2	125.3 (16)
S2—Mo1—Mo2	53.45 (11)	O1—C1—C2	118.6 (16)
O4—Mo2—O6	94.9 (5)	O2—C1—C2	116.1 (14)
O4—Mo2—N2	97.1 (5)	N1—C2—C1	112.0 (14)
O6—Mo2—N2	76.7 (4)	N1—C2—H2C	109.2
O4—Mo2—S1	104.4 (4)	C1—C2—H2C	109.2
O6—Mo2—S1	82.7 (3)	N1—C2—H2D	109.2
N2—Mo2—S1	151.3 (4)	C1—C2—H2D	109.2
O4—Mo2—O7	170.5 (5)	H2C—C2—H2D	107.9
O6—Mo2—O7	80.7 (4)	N2—C3—C4	113.7 (13)
N2—Mo2—O7	73.7 (4)	N2—C3—H3C	108.8
S1—Mo2—O7	83.5 (3)	C4—C3—H3C	108.8
O4—Mo2—S2	100.2 (4)	N2—C3—H3D	108.8
O6—Mo2—S2	160.1 (3)	C4—C3—H3D	108.8
N2—Mo2—S2	88.7 (3)	H3C—C3—H3D	107.7
S1—Mo2—S2	105.66 (17)	O5—C4—O6	121.1 (15)

supplementary materials

O7—Mo2—S2	82.4 (3)	O5—C4—C3	122.5 (16)
O4—Mo2—Mo1	107.2 (4)	O6—C4—C3	116.4 (14)
O6—Mo2—Mo1	133.5 (3)	C6—C5—N3	109.0 (14)
N2—Mo2—Mo1	137.1 (3)	C6—C5—H5A	109.9
S1—Mo2—Mo1	52.73 (13)	N3—C5—H5A	109.9
O7—Mo2—Mo1	81.7 (3)	C6—C5—H5B	109.9
S2—Mo2—Mo1	53.08 (11)	N3—C5—H5B	109.9
Mo1—S1—Mo2	74.36 (16)	H5A—C5—H5B	108.3
Mo1—S2—Mo2	73.47 (13)	O7—C6—O8	122.7 (14)
C1—O2—Mo1	119.2 (10)	O7—C6—C5	122.0 (15)
C4—O6—Mo2	120.2 (10)	O8—C6—C5	115.2 (14)
C6—O7—Mo2	127.0 (10)		

Hydrogen-bond geometry ($\text{\AA}$, $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ O3 ⁱ	0.90	2.09	2.975 (16)	167
N1—H1B $\cdots$ O5 ⁱⁱ	0.90	2.10	2.882 (16)	144
N2—H2A $\cdots$ O3 ⁱⁱⁱ	0.90	2.13	2.958 (16)	153
N3—H3A $\cdots$ O1 ^{iv}	0.89	2.33	3.119 (17)	148
N3—H3B $\cdots$ O6 ^v	0.89	1.94	2.825 (16)	172
N3—H3E $\cdots$ O1 ^{vi}	0.89	2.08	2.934 (17)	160

Symmetry codes: (i) $x, -y+1/2, z+1/2$; (ii) $x, y-1, z$; (iii) $-x+1, y+1/2, -z+1/2$; (iv) $-x+2, y+1/2, -z+3/2$; (v) $x, -y+3/2, z+1/2$; (vi) $-x+2, -y+1, -z+1$.

Fig. 1

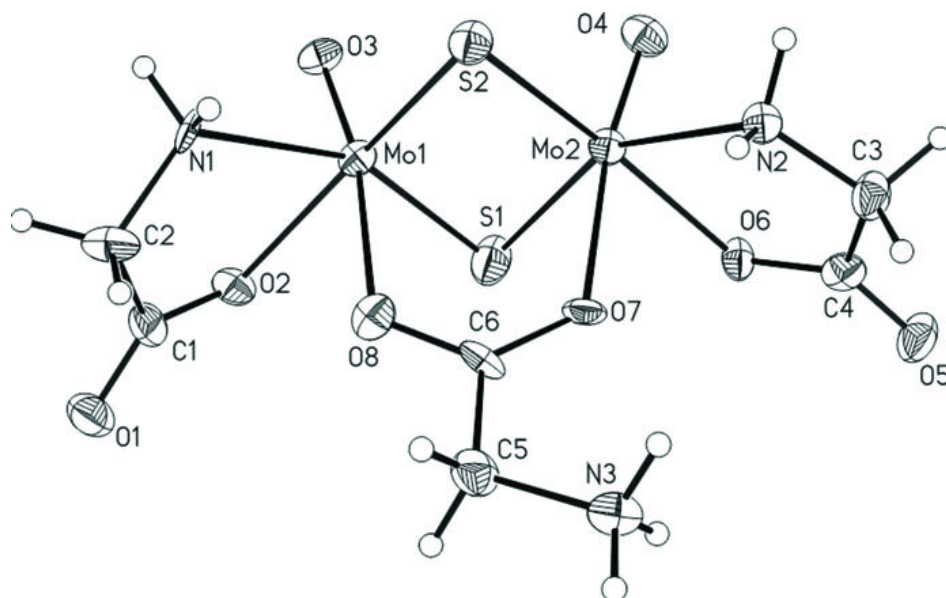


Fig. 2

