Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Dibromidobis(*N*,*N*-diethyldithiocarbamato-$\kappa^2S,S'$)tetra-$\mu_3$-sulfidodicopper(I)dimolybdenum(V) isopropanol disolvate

**Qing Zhang* and Min Liu**

College of Chemistry and Chemical Engineering, Jiangxi Science and Technology Normal University, Nanchang 330013, People's Republic of China
Correspondence e-mail: jxstnu2008@yahoo.cn

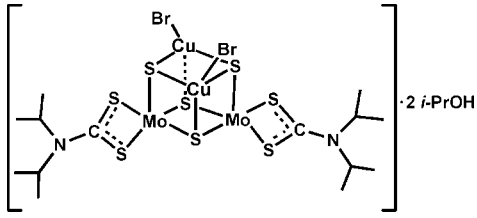
Received 22 September 2008; accepted 28 October 2008

Key indicators: single-crystal X-ray study; $T$ = 291 K; mean $\sigma$(C–C) = 0.013 Å; disorder in main residue; $R$ factor = 0.055; $wR$ factor = 0.121; data-to-parameter ratio = 19.0.

The molecule of the title compound, $[Cu_2Mo_2Br_2(C_7H_{14}NS_2)_2S_4]\cdot 2C_3H_7OH$, comprises one $[(i\text{-}C_3H_7)_2NCS_2]_2Mo_2S_4$ unit and two CuBr units held together by six Cu—$\mu_3$-S bonds, thus forming a cubane-like $Mo_2S_4Cu_2$ core. Intramolecular O—H···S hydrogen bonds may stabilize the structure. Two methyl groups of the two independent solvent molecules are disordered over two positions and were refined with occupancies of 0.733 (12) and 0.267 (12).

## Related literature

For sulfido-bridged dinuclear complexes with an $M_2S_4$ core ($M$ = Mo, W), see: Hidai *et al.* (1999); Lang *et al.* (2003); Curtis *et al.* (1997); Stiefel *et al.* (1985); Wu *et al.* (1990).




## Experimental

### Crystal data

$[Cu_2Mo_2Br_2(C_7H_{14}NS_2)_2S_4]\cdot 2C_3H_8O$
$M_r$ = 1079.91
Triclinic, $P\overline{1}$
$a$ = 12.515 (3) Å
$b$ = 12.734 (3) Å
$c$ = 12.759 (3) Å
$\alpha$ = 107.76 (3)°
$\beta$ = 108.26 (3)°
$\gamma$ = 90.12 (3)°
$V$ = 1828.2 (9) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 4.48 mm$^{-1}$
$T$ = 291 (2) K
0.30 × 0.29 × 0.20 mm

### Data collection

Rigaku Mercury diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
$T_{min}$ = 0.284, $T_{max}$ = 0.408
17918 measured reflections
6703 independent reflections
5814 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.032

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.121
$S$ = 1.12
6703 reflections
353 parameters
10 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.90 e Å$^{-3}$
$\Delta\rho_{min}$ = −2.13 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2$D$···S5 | 0.82 | 2.47 | 3.199 (8) | 149 |
| O2—H2$D$···S6 | 0.82 | 2.59 | 3.258 (8) | 139 |

Data collection: *CrystalClear* (Rigaku/MSC, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge Jiangxi Science and Technology Normal University for funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2539).

## References

Curtis, M. D., Druker, S. H., Goossen, L. & Kampf, J. W. (1997). *Organometallics*, **16**, 231–235.
Hidai, M., Ikada, T., Kuwata, S. & Mizobe, Y. (1999). *Inorg. Chem.* **38**, 64–69.
Jacobson, R. (1998). Private communication to the Rigaku Corporation, Tokyo, Japan.
Lang, J.-P., Wei, Z.-H., Xu, Q.-F., Li, H.-X. & Chen, J.-X. (2003). *J. Organomet. Chem.* **87**, 197–202.
Rigaku/MSC (2001). *CrystalClear*. Rigaku/MSC, The Woodlands, Texas, USA.
Rigaku/MSC (2004). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Stiefel, E. I., Halbert, T. R. & Cohen, S. A. (1985). *Organometallics*, **4**, 1689–1690.
Wu, X.-T., Zhu, N.-Y. & Zheng, Y.-F. (1990). *J. Chem. Soc. Chem. Commun.* pp. 780–781.

# supporting information

*Acta Cryst.* (2008). E**64**, m1540 [doi:10.1107/S1600536808035241]

# Dibromidobis(*N*,*N*-diethyldithiocarbamato-$\kappa^2S,S'$)tetra-$\mu_3$-sulfido-dicopper(I)dimolybdenum(V) isopropanol disolvate

**Qing Zhang and Min Liu**

## S1. Comment

In the past decades, chemistry of the sulfido-bridged dinuclear complexes with an $M_2S_4$ core (M = Mo, W) and various transition metals has been intensively investigated. For example, precursors $[(dtc)_2Mo_2S_2(\mu\text{-}S)_2]$ (dtc = $S_2CNEt_2$) (Hidai *et al.*, 1999; Lang *et al.*, 2003) and $[Cp^x{}_2Mo_2S_2(\mu\text{-}S)_2]$ ($Cp^x$ = pentamethyl-, pentaethyl- or pentabutyl-cyclopentadienyl) (Curtis *et al.*, 1997; Stiefel *et al.*, 1985) and $[Et_4N]_2[(edt)_2Mo_2S_2(\mu\text{-}S)_2]$ (edt = ethanedithiolate) (Wu *et al.*, 1990) were shown to react with transition metals to form both incomplete $[Mo_2MS_4]$ and complete $[Mo_2M_2S_4]$ cubane-like clusters. We report herein the formation of a complete cubane-like $[Mo_2Cu_2S_4]$ by using $[(i\text{-}C_3H_7)_2NCS_2]_2Mo_2S_4$ as the starting material to react with two equivalents of CuBr.

The title molecule contains one $[(i\text{-}C_3H_7)_2NCS_2]_2Mo_2S_4$ moiety and two CuBr units, which are assembled into a distorted $Mo_2Cu_2S_4$ cubane-like core (Fig. 1). The formal oxidation states for each Mo and Cu remain + 5 and + 1, respectively. Each Mo center is coordinated by three $\mu_3$-S atoms, and the two S atoms of an $[(i\text{-}C_3H_7)_2NCS_2]$ group, forming a distorted square pyramidal geometry, while each Cu atom is tetrahedrally coordinated by three $\mu_3$-S atoms and a terminal bromide. The Mo-S bonds are in the range of 2.1621 (19)-2.4465 (18) Å, due to the different S atoms coordinated. The Cu-S(terminal) bonds [average value: 2.436 (2) Å] are longer than the other Cu-S bonds [average value: 2.211 (2) Å]. The Mo···Mo [2.7874 (10) Å] and Mo···Cu [average value: 2.8114 (15) Å] distances and the Cu-Br bonds [average value: 2.2812 (15) Å] have normal values. Intramolecular O-H···S hydrogen bonds (Table 1) may be effective in the stabilization of the structure.

## S2. Experimental

For the preparation of the title compound, $[(i\text{-}C_3H_7)_2NCS_2]_2Mo_2S_4$ (0.49 g, 0.5 mmol), and CuBr (0.144 g, 1.0 mmol) were added into $CH_2Cl_2$ solution (20 ml). The mixture was stirred at room temperature for 0.5 h, and the dark-red suspension gradually turned into dark red solution, and then filtered. The filtrate was layered with isopropyl alcohol (30 ml) to produce dark red crystals in 4 d.

## S3. Refinement

The C15, C16 and C19 methyl groups in di-isopropyl alcohol solvate were disordered over two positions. During the refinement process the disordered atoms were refined with occupancies of 0.733 (12) for C15, H15A, H15B, H15C, C16, H16A, H16B, H16C, C19, H19A, H19B, H19C and 0.267 (12) for C15A, H15D, H15E, H15F, C16A, H16D, H16E, H16F, C19A, H19D, H19E, H19F, respectively. The C15 and C15A atoms were refined isotropically. H atoms were positioned geometrically, with O-H = 0.82 Å (for OH) and C-H = 0.98 and 0.96 Å for methine and methyl H, respectively, and constrained to ride on their parent atoms with $U_{iso}(H) = xU_{eq}(C,O)$, where x = 1.2 for methine H and x = 1.5 for all other H atoms.

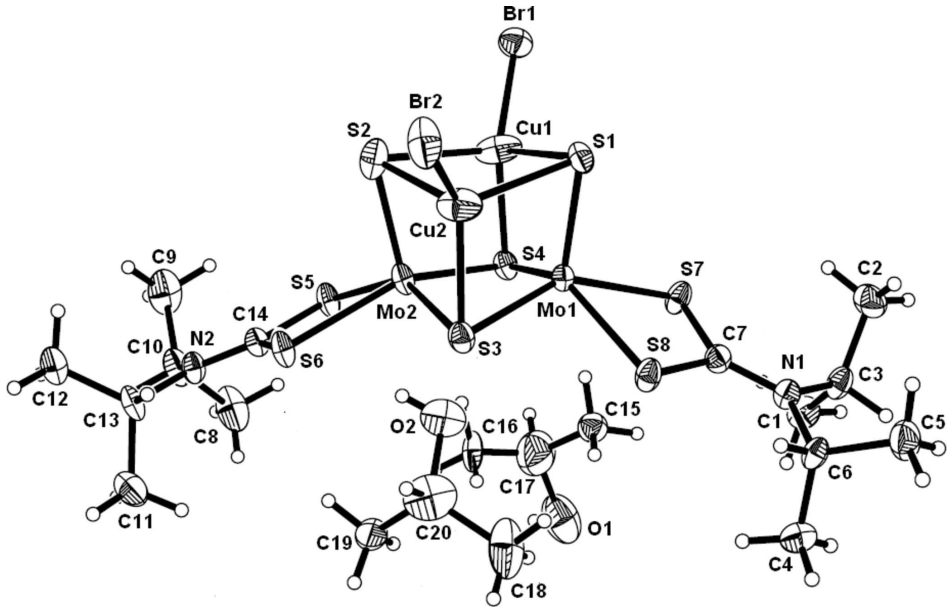



**Figure 1**

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

**(I)**

*Crystal data*

$[Cu_2Mo_2Br_2(C_7H_{14}NS_2)_2S_4]\cdot 2C_3H_8O$
$M_r = 1079.91$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 12.515\ (3)$ Å
$b = 12.734\ (3)$ Å
$c = 12.759\ (3)$ Å
$\alpha = 107.76\ (3)°$
$\beta = 108.26\ (3)°$
$\gamma = 90.12\ (3)°$
$V = 1828.2\ (9)$ Å$^3$
$Z = 2$
$F(000) = 1068$
$D_x = 1.962$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6125 reflections
$\theta = 3.3–25.4°$
$\mu = 4.48$ mm$^{-1}$
$T = 291$ K
Block, dark red
0.30 × 0.29 × 0.20 mm

*Data collection*

Rigaku Mercury diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (Jacobson, 1998)
$T_{min} = 0.284$, $T_{max} = 0.408$
17918 measured reflections
6703 independent reflections
5814 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 25.4°$, $\theta_{min} = 3.3°$
$h = -15\rightarrow15$
$k = -15\rightarrow15$
$l = -15\rightarrow15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.121$
$S = 1.12$
6703 reflections
353 parameters
10 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2 + 11.7921P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 1.90$ e Å$^{-3}$
$\Delta\rho_{min} = -2.13$ e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Mo1 | 1.00881 (5) | 0.18736 (4) | 0.39883 (5) | 0.02348 (15) | |
| Mo2 | 1.16712 (5) | 0.20599 (5) | 0.29120 (5) | 0.02768 (16) | |
| Cu1 | 1.12203 (10) | 0.00501 (8) | 0.33253 (10) | 0.0544 (3) | |
| Cu2 | 1.23373 (9) | 0.24097 (8) | 0.53604 (10) | 0.0517 (3) | |
| Br1 | 1.13513 (7) | −0.18080 (6) | 0.29790 (7) | 0.0441 (2) | |
| Br2 | 1.37543 (7) | 0.30267 (8) | 0.71075 (7) | 0.0535 (3) | |
| S1 | 1.09552 (15) | 0.10190 (15) | 0.51854 (15) | 0.0308 (4) | |
| S2 | 1.29693 (17) | 0.12006 (18) | 0.3783 (2) | 0.0473 (5) | |
| S3 | 1.13192 (15) | 0.34620 (14) | 0.44228 (15) | 0.0301 (4) | |
| S4 | 1.00310 (14) | 0.07858 (14) | 0.21230 (14) | 0.0281 (4) | |
| S5 | 1.17527 (16) | 0.15164 (14) | 0.09288 (15) | 0.0323 (4) | |
| S6 | 1.28036 (15) | 0.35219 (14) | 0.27486 (15) | 0.0311 (4) | |
| S7 | 0.81395 (14) | 0.10577 (14) | 0.33380 (16) | 0.0327 (4) | |
| S8 | 0.90078 (15) | 0.32398 (14) | 0.48497 (16) | 0.0325 (4) | |
| O1 | 0.6199 (7) | 0.1776 (6) | −0.1619 (6) | 0.087 (2) | |
| H1D | 0.6271 | 0.1595 | −0.2265 | 0.131* | |
| O2 | 1.0055 (6) | 0.3083 (5) | 0.1913 (6) | 0.0697 (19) | |
| H2D | 1.0646 | 0.2930 | 0.1781 | 0.104* | |
| N1 | 0.6852 (5) | 0.2439 (4) | 0.4372 (5) | 0.0284 (12) | |
| N2 | 1.3096 (5) | 0.3023 (5) | 0.0653 (5) | 0.0293 (13) | |
| C1 | 0.5412 (6) | 0.1342 (7) | 0.2459 (6) | 0.0413 (18) | |
| H1A | 0.5335 | 0.2023 | 0.2279 | 0.062* | |
| H1B | 0.4691 | 0.0901 | 0.2127 | 0.062* | |
| H1C | 0.5947 | 0.0940 | 0.2140 | 0.062* | |
| C2 | 0.5971 (7) | 0.0577 (6) | 0.4167 (8) | 0.046 (2) | |

| | | | | | |
|---|---|---|---|---|---|
| H2A | 0.6226 | 0.0806 | 0.5003 | 0.069* | |
| H2B | 0.6520 | 0.0160 | 0.3886 | 0.069* | |
| H2C | 0.5260 | 0.0122 | 0.3862 | 0.069* | |
| C3 | 0.5824 (6) | 0.1597 (6) | 0.3769 (7) | 0.0349 (16) | |
| H3A | 0.5220 | 0.1956 | 0.4033 | 0.042* | |
| C4 | 0.6128 (7) | 0.4224 (6) | 0.4354 (7) | 0.0429 (19) | |
| H4A | 0.6557 | 0.4262 | 0.3859 | 0.064* | |
| H4B | 0.6087 | 0.4959 | 0.4831 | 0.064* | |
| H4C | 0.5377 | 0.3876 | 0.3883 | 0.064* | |
| C5 | 0.6097 (8) | 0.3443 (7) | 0.5956 (8) | 0.050 (2) | |
| H5A | 0.6503 | 0.3014 | 0.6423 | 0.075* | |
| H5B | 0.5345 | 0.3081 | 0.5516 | 0.075* | |
| H5C | 0.6056 | 0.4169 | 0.6454 | 0.075* | |
| C6 | 0.6703 (6) | 0.3545 (6) | 0.5132 (6) | 0.0298 (15) | |
| H6A | 0.7460 | 0.3928 | 0.5609 | 0.036* | |
| C7 | 0.7831 (6) | 0.2252 (5) | 0.4229 (6) | 0.0287 (15) | |
| C8 | 1.1642 (8) | 0.2257 (9) | −0.1322 (7) | 0.063 (3) | |
| H8A | 1.1360 | 0.2969 | −0.1193 | 0.094* | |
| H8B | 1.1222 | 0.1780 | −0.1100 | 0.094* | |
| H8C | 1.1559 | 0.1935 | −0.2132 | 0.094* | |
| C9 | 1.3407 (9) | 0.1315 (7) | −0.0753 (8) | 0.061 (3) | |
| H9A | 1.4192 | 0.1456 | −0.0281 | 0.091* | |
| H9B | 1.3342 | 0.0982 | −0.1557 | 0.091* | |
| H9C | 1.3022 | 0.0820 | −0.0518 | 0.091* | |
| C10 | 1.2881 (7) | 0.2392 (6) | −0.0598 (6) | 0.0401 (19) | |
| H10A | 1.3274 | 0.2847 | −0.0889 | 0.048* | |
| C11 | 1.3276 (8) | 0.4937 (7) | 0.0623 (9) | 0.056 (2) | |
| H11A | 1.2572 | 0.5032 | 0.0775 | 0.084* | |
| H11B | 1.3132 | 0.4691 | −0.0203 | 0.084* | |
| H11C | 1.3750 | 0.5630 | 0.0975 | 0.084* | |
| C12 | 1.4996 (7) | 0.3893 (7) | 0.0935 (7) | 0.046 (2) | |
| H12A | 1.5341 | 0.3352 | 0.1281 | 0.069* | |
| H12B | 1.5484 | 0.4578 | 0.1287 | 0.069* | |
| H12C | 1.4879 | 0.3629 | 0.0113 | 0.069* | |
| C13 | 1.3864 (6) | 0.4082 (6) | 0.1130 (6) | 0.0337 (16) | |
| H13A | 1.4011 | 0.4361 | 0.1974 | 0.040* | |
| C14 | 1.2634 (6) | 0.2720 (5) | 0.1317 (6) | 0.0281 (15) | |
| C15 | 0.7206 (16) | 0.1461 (12) | 0.0386 (12) | 0.041 (3)* | 0.733 (12) |
| H15A | 0.7706 | 0.0973 | 0.0688 | 0.061* | 0.733 (12) |
| H15B | 0.6436 | 0.1170 | 0.0193 | 0.061* | 0.733 (12) |
| H15C | 0.7353 | 0.2182 | 0.0964 | 0.061* | 0.733 (12) |
| C15A | 0.722 (4) | 0.186 (5) | 0.057 (3) | 0.041 (3)* | 0.267 (12) |
| H15D | 0.7931 | 0.2152 | 0.1172 | 0.061* | 0.267 (12) |
| H15E | 0.6914 | 0.1219 | 0.0661 | 0.061* | 0.267 (12) |
| H15F | 0.6700 | 0.2418 | 0.0613 | 0.061* | 0.267 (12) |
| C16 | 0.8461 (8) | 0.2073 (9) | −0.0314 (8) | 0.039 (3) | 0.733 (12) |
| H16A | 0.8528 | 0.2791 | 0.0251 | 0.058* | 0.733 (12) |
| H16B | 0.8590 | 0.2158 | −0.0989 | 0.058* | 0.733 (12) |

| | | | | | |
|---|---|---|---|---|---|
| H16C | 0.9012 | 0.1639 | 0.0017 | 0.058* | 0.733 (12) |
| C16A | 0.750 (3) | 0.181 (5) | 0.0666 (18) | 0.039 (3) | 0.267 (12) |
| H16D | 0.8166 | 0.1527 | 0.1055 | 0.058* | 0.267 (12) |
| H16E | 0.6846 | 0.1478 | 0.0724 | 0.058* | 0.267 (12) |
| H16F | 0.7567 | 0.2603 | 0.1025 | 0.058* | 0.267 (12) |
| C17 | 0.7390 (11) | 0.1546 (12) | −0.0634 (10) | 0.092 (4) | |
| H17 | 0.7484 | 0.0778 | −0.1029 | 0.111* | |
| C18 | 0.8873 (8) | 0.4760 (11) | 0.2435 (8) | 0.080 (4) | |
| H18A | 0.8899 | 0.5548 | 0.2593 | 0.120* | |
| H18B | 0.8831 | 0.4585 | 0.3103 | 0.120* | |
| H18C | 0.8218 | 0.4401 | 0.1775 | 0.120* | |
| C19 | 1.0116 (11) | 0.4568 (14) | 0.1142 (12) | 0.059 (4) | 0.733 (12) |
| H19A | 1.0792 | 0.4282 | 0.1019 | 0.088* | 0.733 (12) |
| H19B | 1.0174 | 0.5354 | 0.1280 | 0.088* | 0.733 (12) |
| H19C | 0.9474 | 0.4214 | 0.0464 | 0.088* | 0.733 (12) |
| C19A | 0.991 (3) | 0.388 (4) | 0.100 (4) | 0.059 (4) | 0.267 (12) |
| H19D | 0.9542 | 0.4360 | 0.0569 | 0.088* | 0.267 (12) |
| H19E | 0.9475 | 0.3167 | 0.0671 | 0.088* | 0.267 (12) |
| H19F | 1.0654 | 0.3808 | 0.0950 | 0.088* | 0.267 (12) |
| C20 | 0.9974 (10) | 0.4343 (10) | 0.2164 (10) | 0.083 (3) | |
| H20 | 1.0628 | 0.4732 | 0.2846 | 0.099* | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mo1 | 0.0218 (3) | 0.0244 (3) | 0.0245 (3) | −0.0001 (2) | 0.0092 (2) | 0.0066 (2) |
| Mo2 | 0.0320 (3) | 0.0283 (3) | 0.0232 (3) | −0.0066 (2) | 0.0126 (2) | 0.0052 (2) |
| Cu1 | 0.0570 (7) | 0.0372 (6) | 0.0485 (6) | 0.0155 (5) | −0.0029 (5) | 0.0061 (5) |
| Cu2 | 0.0422 (6) | 0.0401 (6) | 0.0523 (6) | −0.0043 (4) | −0.0116 (5) | 0.0145 (5) |
| Br1 | 0.0499 (5) | 0.0361 (4) | 0.0474 (5) | 0.0070 (4) | 0.0162 (4) | 0.0146 (4) |
| Br2 | 0.0384 (5) | 0.0843 (7) | 0.0297 (4) | −0.0176 (4) | 0.0042 (3) | 0.0146 (4) |
| S1 | 0.0307 (9) | 0.0365 (9) | 0.0284 (9) | −0.0022 (7) | 0.0110 (7) | 0.0139 (8) |
| S2 | 0.0355 (11) | 0.0513 (12) | 0.0539 (13) | −0.0013 (9) | 0.0220 (10) | 0.0076 (10) |
| S3 | 0.0314 (9) | 0.0260 (9) | 0.0325 (9) | −0.0032 (7) | 0.0133 (8) | 0.0061 (7) |
| S4 | 0.0302 (9) | 0.0285 (9) | 0.0240 (8) | −0.0036 (7) | 0.0095 (7) | 0.0057 (7) |
| S5 | 0.0387 (10) | 0.0319 (9) | 0.0249 (9) | −0.0102 (7) | 0.0161 (8) | 0.0017 (7) |
| S6 | 0.0368 (10) | 0.0311 (9) | 0.0244 (8) | −0.0107 (7) | 0.0157 (7) | 0.0019 (7) |
| S7 | 0.0233 (9) | 0.0280 (9) | 0.0390 (10) | −0.0016 (7) | 0.0123 (8) | −0.0022 (8) |
| S8 | 0.0265 (9) | 0.0267 (9) | 0.0405 (10) | −0.0028 (7) | 0.0152 (8) | 0.0015 (8) |
| O1 | 0.117 (7) | 0.081 (5) | 0.064 (5) | −0.019 (5) | 0.042 (5) | 0.010 (4) |
| O2 | 0.081 (5) | 0.060 (4) | 0.067 (4) | 0.012 (4) | 0.020 (4) | 0.024 (4) |
| N1 | 0.026 (3) | 0.026 (3) | 0.029 (3) | −0.002 (2) | 0.008 (2) | 0.003 (2) |
| N2 | 0.033 (3) | 0.033 (3) | 0.023 (3) | −0.002 (2) | 0.016 (2) | 0.004 (2) |
| C1 | 0.033 (4) | 0.042 (4) | 0.039 (4) | 0.000 (3) | 0.004 (3) | 0.007 (4) |
| C2 | 0.039 (5) | 0.041 (4) | 0.057 (5) | −0.007 (4) | 0.011 (4) | 0.021 (4) |
| C3 | 0.022 (4) | 0.035 (4) | 0.043 (4) | 0.000 (3) | 0.012 (3) | 0.004 (3) |
| C4 | 0.046 (5) | 0.037 (4) | 0.044 (5) | 0.011 (4) | 0.014 (4) | 0.012 (4) |
| C5 | 0.060 (6) | 0.044 (5) | 0.057 (5) | 0.005 (4) | 0.037 (5) | 0.011 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C6 | 0.027 (4) | 0.032 (4) | 0.028 (4) | 0.004 (3) | 0.012 (3) | 0.001 (3) |
| C7 | 0.033 (4) | 0.026 (3) | 0.028 (4) | 0.003 (3) | 0.014 (3) | 0.006 (3) |
| C8 | 0.057 (6) | 0.090 (7) | 0.031 (5) | −0.026 (5) | −0.002 (4) | 0.022 (5) |
| C9 | 0.077 (7) | 0.053 (5) | 0.049 (5) | −0.005 (5) | 0.041 (5) | −0.010 (4) |
| C10 | 0.053 (5) | 0.045 (4) | 0.020 (4) | −0.012 (4) | 0.016 (3) | 0.002 (3) |
| C11 | 0.064 (6) | 0.043 (5) | 0.074 (6) | 0.002 (4) | 0.032 (5) | 0.026 (5) |
| C12 | 0.045 (5) | 0.044 (5) | 0.051 (5) | −0.007 (4) | 0.022 (4) | 0.014 (4) |
| C13 | 0.040 (4) | 0.032 (4) | 0.031 (4) | −0.012 (3) | 0.016 (3) | 0.008 (3) |
| C14 | 0.029 (4) | 0.028 (4) | 0.027 (4) | −0.002 (3) | 0.010 (3) | 0.007 (3) |
| C16 | 0.020 (5) | 0.068 (7) | 0.018 (4) | −0.017 (5) | 0.002 (4) | 0.005 (4) |
| C16A | 0.020 (5) | 0.068 (7) | 0.018 (4) | −0.017 (5) | 0.002 (4) | 0.005 (4) |
| C17 | 0.089 (9) | 0.125 (11) | 0.087 (9) | 0.027 (8) | 0.045 (7) | 0.051 (8) |
| C18 | 0.056 (6) | 0.154 (11) | 0.031 (5) | −0.012 (7) | 0.010 (4) | 0.034 (6) |
| C19 | 0.047 (7) | 0.092 (12) | 0.072 (8) | 0.031 (8) | 0.028 (6) | 0.065 (10) |
| C19A | 0.047 (7) | 0.092 (12) | 0.072 (8) | 0.031 (8) | 0.028 (6) | 0.065 (10) |
| C20 | 0.093 (9) | 0.084 (8) | 0.054 (6) | 0.015 (7) | 0.010 (6) | 0.011 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Mo1—Mo2 | 2.7874 (10) | C8—H8B | 0.9600 |
| Mo1—Cu1 | 2.7715 (14) | C8—H8C | 0.9600 |
| Mo1—Cu2 | 2.7618 (16) | C9—C10 | 1.508 (12) |
| Mo1—S1 | 2.1621 (19) | C9—H9A | 0.9600 |
| Mo1—S3 | 2.3535 (19) | C9—H9B | 0.9600 |
| Mo1—S4 | 2.3386 (19) | C9—H9C | 0.9600 |
| Mo1—S7 | 2.4310 (19) | C10—N2 | 1.486 (8) |
| Mo1—S8 | 2.4160 (19) | C10—H10A | 0.9800 |
| Mo2—Cu1 | 2.8547 (14) | C11—C13 | 1.510 (11) |
| Mo2—Cu2 | 2.8582 (15) | C11—H11A | 0.9600 |
| Mo2—S2 | 2.166 (2) | C11—H11B | 0.9600 |
| Mo2—S3 | 2.352 (2) | C11—H11C | 0.9600 |
| Mo2—S4 | 2.356 (2) | C12—C13 | 1.522 (10) |
| Mo2—S5 | 2.4465 (18) | C12—H12A | 0.9600 |
| Mo2—S6 | 2.4349 (18) | C12—H12B | 0.9600 |
| Cu1—Br1 | 2.2867 (14) | C12—H12C | 0.9600 |
| Cu1—S1 | 2.444 (2) | C13—N2 | 1.497 (8) |
| Cu1—S2 | 2.437 (2) | C13—H13A | 0.9800 |
| Cu1—S4 | 2.213 (2) | C14—N2 | 1.306 (8) |
| Cu2—Br2 | 2.2756 (16) | C15—H15A | 0.9600 |
| Cu2—S1 | 2.383 (2) | C15—H15B | 0.9600 |
| Cu2—S2 | 2.481 (3) | C15—H15C | 0.9600 |
| Cu2—S3 | 2.209 (2) | C15A—H15D | 0.9600 |
| S5—C14 | 1.731 (7) | C15A—H15E | 0.9600 |
| S6—C14 | 1.744 (7) | C15A—H15F | 0.9600 |
| S7—C7 | 1.726 (7) | C16—H16A | 0.9600 |
| S8—C7 | 1.741 (7) | C16—H16B | 0.9600 |
| O1—H1D | 0.8200 | C16—H16C | 0.9600 |
| O2—H2D | 0.8200 | C16A—H16D | 0.9600 |

| | | | |
|---|---|---|---|
| C1—C3 | 1.515 (10) | C16A—H16E | 0.9600 |
| C1—H1A | 0.9600 | C16A—H16F | 0.9600 |
| C1—H1B | 0.9600 | C17—C16 | 1.378 (15) |
| C1—H1C | 0.9600 | C17—C15 | 1.425 (17) |
| C2—C3 | 1.525 (10) | C17—C15A | 1.544 (19) |
| C2—H2A | 0.9600 | C17—C16A | 1.547 (18) |
| C2—H2B | 0.9600 | C17—O1 | 1.715 (15) |
| C2—H2C | 0.9600 | C17—H17 | 0.9800 |
| C3—N1 | 1.505 (8) | C18—H18A | 0.9600 |
| C3—H3A | 0.9800 | C18—H18B | 0.9600 |
| C4—C6 | 1.526 (10) | C18—H18C | 0.9600 |
| C4—H4A | 0.9600 | C19—H19A | 0.9600 |
| C4—H4B | 0.9600 | C19—H19B | 0.9600 |
| C4—H4C | 0.9600 | C19—H19C | 0.9600 |
| C5—C6 | 1.510 (10) | C19A—H19D | 0.9600 |
| C5—H5A | 0.9600 | C19A—H19E | 0.9600 |
| C5—H5B | 0.9600 | C19A—H19F | 0.9600 |
| C5—H5C | 0.9600 | C20—C19A | 1.40 (4) |
| C6—N1 | 1.497 (8) | C20—C19 | 1.479 (17) |
| C6—H6A | 0.9800 | C20—O2 | 1.546 (13) |
| C7—N1 | 1.306 (8) | C20—C18 | 1.579 (12) |
| C8—C10 | 1.513 (12) | C20—H20 | 0.9800 |
| C8—H8A | 0.9600 | | |

| | | | |
|---|---|---|---|
| S1—Mo1—S4 | 107.30 (7) | C10—C8—H8B | 109.5 |
| S1—Mo1—S3 | 105.60 (7) | H8A—C8—H8B | 109.5 |
| S4—Mo1—S3 | 104.32 (7) | C10—C8—H8C | 109.5 |
| S1—Mo1—S8 | 110.87 (7) | H8A—C8—H8C | 109.5 |
| S4—Mo1—S8 | 137.84 (7) | H8B—C8—H8C | 109.5 |
| S3—Mo1—S8 | 82.15 (6) | C6—C5—H5A | 109.5 |
| S1—Mo1—S7 | 102.40 (7) | C6—C5—H5B | 109.5 |
| S4—Mo1—S7 | 83.56 (7) | H5A—C5—H5B | 109.5 |
| S3—Mo1—S7 | 146.89 (7) | C6—C5—H5C | 109.5 |
| S8—Mo1—S7 | 71.52 (6) | H5A—C5—H5C | 109.5 |
| S1—Mo1—Cu2 | 56.33 (6) | H5B—C5—H5C | 109.5 |
| S4—Mo1—Cu2 | 107.39 (6) | C3—C2—H2A | 109.5 |
| S3—Mo1—Cu2 | 50.40 (6) | C3—C2—H2B | 109.5 |
| S8—Mo1—Cu2 | 108.24 (6) | H2A—C2—H2B | 109.5 |
| S7—Mo1—Cu2 | 157.85 (6) | C3—C2—H2C | 109.5 |
| S1—Mo1—Cu1 | 57.82 (6) | H2A—C2—H2C | 109.5 |
| S4—Mo1—Cu1 | 50.46 (5) | H2B—C2—H2C | 109.5 |
| S3—Mo1—Cu1 | 106.97 (6) | C3—C1—H1A | 109.5 |
| S8—Mo1—Cu1 | 166.67 (6) | C3—C1—H1B | 109.5 |
| S7—Mo1—Cu1 | 102.73 (6) | H1A—C1—H1B | 109.5 |
| Cu2—Mo1—Cu1 | 72.36 (5) | C3—C1—H1C | 109.5 |
| S1—Mo1—Mo2 | 101.97 (5) | H1A—C1—H1C | 109.5 |
| S4—Mo1—Mo2 | 53.87 (5) | H1B—C1—H1C | 109.5 |
| S3—Mo1—Mo2 | 53.66 (5) | C6—C4—H4A | 109.5 |

| | | | |
|---|---|---|---|
| S8—Mo1—Mo2 | 130.76 (5) | C6—C4—H4B | 109.5 |
| S7—Mo1—Mo2 | 135.61 (5) | H4A—C4—H4B | 109.5 |
| Cu2—Mo1—Mo2 | 62.00 (4) | C6—C4—H4C | 109.5 |
| Cu1—Mo1—Mo2 | 61.80 (4) | H4A—C4—H4C | 109.5 |
| S2—Mo2—S3 | 105.05 (8) | H4B—C4—H4C | 109.5 |
| S2—Mo2—S4 | 104.02 (8) | N2—C13—C11 | 109.8 (6) |
| S3—Mo2—S4 | 103.81 (7) | N2—C13—C12 | 111.4 (6) |
| S2—Mo2—S6 | 101.58 (8) | C11—C13—C12 | 112.6 (6) |
| S3—Mo2—S6 | 85.72 (6) | N2—C13—H13A | 107.6 |
| S4—Mo2—S6 | 149.13 (7) | C11—C13—H13A | 107.6 |
| S2—Mo2—S5 | 103.59 (8) | C12—C13—H13A | 107.6 |
| S3—Mo2—S5 | 146.24 (7) | N1—C7—S7 | 126.4 (5) |
| S4—Mo2—S5 | 86.05 (7) | N1—C7—S8 | 123.9 (5) |
| S6—Mo2—S5 | 71.31 (7) | S7—C7—S8 | 109.6 (4) |
| S2—Mo2—Mo1 | 98.63 (6) | N2—C10—C9 | 111.9 (6) |
| S3—Mo2—Mo1 | 53.70 (5) | N2—C10—C8 | 112.6 (7) |
| S4—Mo2—Mo1 | 53.29 (5) | C9—C10—C8 | 113.5 (7) |
| S6—Mo2—Mo1 | 138.23 (5) | N2—C10—H10A | 106.1 |
| S5—Mo2—Mo1 | 137.45 (5) | C9—C10—H10A | 106.1 |
| S2—Mo2—Cu1 | 56.09 (6) | C8—C10—H10A | 106.1 |
| S3—Mo2—Cu1 | 104.42 (5) | N1—C6—C5 | 112.3 (6) |
| S4—Mo2—Cu1 | 49.13 (5) | N1—C6—C4 | 108.4 (6) |
| S6—Mo2—Cu1 | 156.98 (6) | C5—C6—C4 | 113.6 (6) |
| S5—Mo2—Cu1 | 106.21 (6) | N1—C6—H6A | 107.4 |
| Mo1—Mo2—Cu1 | 58.83 (4) | C5—C6—H6A | 107.4 |
| S2—Mo2—Cu2 | 57.22 (7) | C4—C6—H6A | 107.4 |
| S3—Mo2—Cu2 | 49.00 (5) | N1—C3—C1 | 112.6 (6) |
| S4—Mo2—Cu2 | 103.90 (6) | N1—C3—C2 | 112.3 (6) |
| S6—Mo2—Cu2 | 104.35 (6) | C1—C3—C2 | 114.5 (6) |
| S5—Mo2—Cu2 | 159.79 (6) | N1—C3—H3A | 105.5 |
| Mo1—Mo2—Cu2 | 58.56 (4) | C1—C3—H3A | 105.5 |
| Cu1—Mo2—Cu2 | 69.75 (5) | C2—C3—H3A | 105.5 |
| S4—Cu1—Br1 | 124.95 (7) | N2—C14—S5 | 126.6 (5) |
| S4—Cu1—S2 | 100.02 (9) | N2—C14—S6 | 123.5 (5) |
| Br1—Cu1—S2 | 116.22 (8) | S5—C14—S6 | 109.9 (4) |
| S4—Cu1—S1 | 102.17 (8) | C16—C17—C15 | 108.4 (12) |
| Br1—Cu1—S1 | 114.44 (7) | C16—C17—C15A | 100 (2) |
| S2—Cu1—S1 | 93.70 (8) | C16—C17—C16A | 90.1 (16) |
| S4—Cu1—Mo1 | 54.58 (5) | C16—C17—O1 | 125.5 (10) |
| Br1—Cu1—Mo1 | 148.85 (6) | C15—C17—O1 | 113.2 (11) |
| S2—Cu1—Mo1 | 92.75 (7) | C15A—C17—O1 | 108.3 (18) |
| S1—Cu1—Mo1 | 48.48 (5) | C16A—C17—O1 | 121 (2) |
| S4—Cu1—Mo2 | 53.62 (6) | C16—C17—H17 | 102.0 |
| Br1—Cu1—Mo2 | 150.08 (6) | C15—C17—H17 | 102.0 |
| S2—Cu1—Mo2 | 47.51 (6) | C15A—C17—H17 | 120.4 |
| S1—Cu1—Mo2 | 93.37 (6) | C16A—C17—H17 | 115.2 |
| Mo1—Cu1—Mo2 | 59.37 (3) | O1—C17—H17 | 102.0 |
| S3—Cu2—Br2 | 125.87 (7) | C19A—C20—O2 | 72.2 (18) |

| | | | |
|---|---|---|---|
| S3—Cu2—S1 | 103.11 (8) | C19—C20—O2 | 104.5 (10) |
| Br2—Cu2—S1 | 115.75 (7) | C19A—C20—C18 | 118.1 (18) |
| S3—Cu2—S2 | 99.62 (9) | C19—C20—C18 | 113.8 (9) |
| Br2—Cu2—S2 | 112.85 (8) | O2—C20—C18 | 115.1 (10) |
| S1—Cu2—S2 | 94.10 (8) | C19A—C20—H20 | 129.3 |
| S3—Cu2—Mo1 | 55.17 (5) | C19—C20—H20 | 107.7 |
| Br2—Cu2—Mo1 | 153.00 (6) | O2—C20—H20 | 107.7 |
| S1—Cu2—Mo1 | 49.02 (5) | C18—C20—H20 | 107.7 |
| S2—Cu2—Mo1 | 92.04 (7) | C20—C18—H18A | 109.5 |
| S3—Cu2—Mo2 | 53.47 (6) | C20—C18—H18B | 109.5 |
| Br2—Cu2—Mo2 | 146.41 (6) | H18A—C18—H18B | 109.5 |
| S1—Cu2—Mo2 | 94.60 (6) | C20—C18—H18C | 109.5 |
| S2—Cu2—Mo2 | 47.21 (6) | H18A—C18—H18C | 109.5 |
| Mo1—Cu2—Mo2 | 59.44 (4) | H18B—C18—H18C | 109.5 |
| Cu1—S4—Mo1 | 74.96 (6) | C7—N1—C6 | 120.0 (5) |
| Cu1—S4—Mo2 | 77.26 (7) | C7—N1—C3 | 123.1 (6) |
| Mo1—S4—Mo2 | 72.84 (6) | C6—N1—C3 | 116.9 (5) |
| C14—S6—Mo2 | 89.4 (2) | C14—N2—C10 | 124.0 (6) |
| C7—S7—Mo1 | 89.2 (2) | C14—N2—C13 | 120.0 (5) |
| C7—S8—Mo1 | 89.3 (2) | C10—N2—C13 | 116.0 (5) |
| Mo2—S2—Cu1 | 76.40 (7) | C17—O1—H1D | 109.5 |
| Mo2—S2—Cu2 | 75.57 (7) | C20—O2—H2D | 109.5 |
| Cu1—S2—Cu2 | 83.22 (8) | C17—C15—H15A | 109.5 |
| Mo1—S1—Cu2 | 74.65 (6) | C17—C15—H15B | 109.5 |
| Mo1—S1—Cu1 | 73.70 (6) | C17—C15—H15C | 109.5 |
| Cu2—S1—Cu1 | 85.16 (7) | C20—C19—H19A | 109.5 |
| C14—S5—Mo2 | 89.3 (2) | C20—C19—H19B | 109.5 |
| Cu2—S3—Mo2 | 77.53 (7) | H19A—C19—H19B | 109.5 |
| Cu2—S3—Mo1 | 74.43 (6) | C20—C19—H19C | 109.5 |
| Mo2—S3—Mo1 | 72.65 (6) | H19A—C19—H19C | 109.5 |
| C10—C9—H9A | 109.5 | H19B—C19—H19C | 109.5 |
| C10—C9—H9B | 109.5 | C17—C16—H16A | 109.5 |
| H9A—C9—H9B | 109.5 | C17—C16—H16B | 109.5 |
| C10—C9—H9C | 109.5 | C17—C16—H16C | 109.5 |
| H9A—C9—H9C | 109.5 | C20—C19A—H19D | 109.5 |
| H9B—C9—H9C | 109.5 | C20—C19A—H19E | 109.5 |
| C13—C12—H12A | 109.5 | H19D—C19A—H19E | 109.5 |
| C13—C12—H12B | 109.5 | C20—C19A—H19F | 109.5 |
| H12A—C12—H12B | 109.5 | H19D—C19A—H19F | 109.5 |
| C13—C12—H12C | 109.5 | H19E—C19A—H19F | 109.5 |
| H12A—C12—H12C | 109.5 | C17—C15A—H15D | 109.5 |
| H12B—C12—H12C | 109.5 | C17—C15A—H15E | 109.5 |
| C13—C11—H11A | 109.5 | H15D—C15A—H15E | 109.5 |
| C13—C11—H11B | 109.5 | C17—C15A—H15F | 109.5 |
| H11A—C11—H11B | 109.5 | H15D—C15A—H15F | 109.5 |
| C13—C11—H11C | 109.5 | H15E—C15A—H15F | 109.5 |
| H11A—C11—H11C | 109.5 | C17—C16A—H16D | 109.5 |
| H11B—C11—H11C | 109.5 | C17—C16A—H16E | 109.5 |

| | | | |
|---|---|---|---|
| C10—C8—H8A | 109.5 | C17—C16A—H16F | 109.5 |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O2—H2*D*···S5 | 0.82 | 2.47 | 3.199 (8) | 149 |
| O2—H2*D*···S6 | 0.82 | 2.59 | 3.258 (8) | 139 |