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## Structure Reports

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Nitrosyltris(pyridine-2-thiolato- $\kappa^2N,S$ )-molybdenum(II) dihydrate

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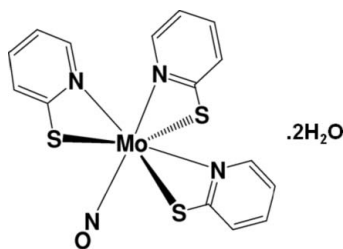
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(C-C) = 0.008$  Å; disorder in solvent or counterion;  $R$  factor = 0.039;  $wR$  factor = 0.126; data-to-parameter ratio = 17.6.

In the title compound,  $[Mo(C_5H_4NS)_3(NO)] \cdot 2H_2O$ , the Mo atom is coordinated by a nitrosyl ligand and three mono-anionic  $N,S$ -bidentate ligands in a distorted  $MoN_4S_3$  pentagonal-bipyramidal molecular geometry. The pyridine N atom of one pyridine-2-thiolate (pyt) ligand is coordinated to the Mo atom in the *trans* position relative to the NO ligand [ $N(\text{pyt})-Mo-N(\text{NO}) = 170.62(19)^\circ$ ]. The compound has  $C_s$  symmetry, with a mirror plane that includes one pyt ring and the NO group. The  $S-Mo-N(\text{NO})$  and  $N(\text{pyt})-Mo-N(\text{NO})$  angles [ $97.24(12)$  and  $91.87(8)^\circ$ , respectively] are large relative to the ideal angles of  $90^\circ$ . In the crystal, the molecules pack in a zigzag arrangement. The cavities between the molecules are occupied by disordered water molecules of crystallization.

## Related literature

For the synthesis and chemistry of similar nitrosyl, pyridine-thiolato, or pyrimidinethiolato derivative complexes, see: Halpenny & Mascharak (2009); Rose *et al.* (2007); Cini *et al.* (2003); Murya *et al.* (2006); Kunkely & Vogler (2003); Ford *et al.* (1998); Proust *et al.* (1994); Ardon & Cohen (1993); Calderon *et al.* (1969); Yonemura *et al.* (2006, 2001); Bucher *et al.* (2008).



## Experimental

## Crystal data

$[Mo(C_5H_4NS)_3(NO)] \cdot 2H_2O$   
 $M_r = 492.44$   
 Orthorhombic,  $Pnma$   
 $a = 15.7519(16)$  Å  
 $b = 14.8889(14)$  Å  
 $c = 9.0535(12)$  Å

$V = 2123.3(4)$  Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.93$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.45 \times 0.40 \times 0.25$  mm

## Data collection

Rigaku AFC-7S diffractometer  
 Absorption correction:  $\psi$  scan  
 (North *et al.*, 1968)  
 $T_{min} = 0.727$ ,  $T_{max} = 0.792$   
 3681 measured reflections  
 2540 independent reflections

2088 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.023$   
 3 standard reflections  
 every 150 reflections  
 intensity decay: 1.3%

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.039$   
 $wR(F^2) = 0.126$   
 $S = 1.13$   
 2540 reflections

144 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{max} = 1.14$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.64$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Mo1—S1	2.5240 (12)	Mo1—N2	2.228 (3)
Mo1—S2	2.4815 (16)	Mo1—N3	1.777 (5)
Mo1—N1	2.218 (5)		
S1—Mo1—S2	138.29 (3)	S1 <sup>1</sup> —Mo1—S2	138.29 (3)
S1—Mo1—N1	90.40 (10)	N1—Mo1—N2	86.66 (8)
S1—Mo1—N3	97.24 (12)	N1—Mo1—N3	170.62 (19)
S2—Mo1—N2	80.58 (7)	N2—Mo1—N3	91.87 (8)

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

Data collection: *WinAFC* (Rigaku/MSK, 2000); cell refinement: *WinAFC*; data reduction: *CrystalStructure* (Rigaku/MSK, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); 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: SU2152).

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**supplementary materials**

*Acta Cryst.* (2009). E65, m1463-m1464 [ doi:10.1107/S1600536809043712 ]

## Nitrosyltris(pyridine-2-thiolato- $\kappa^2N,S$ )molybdenum(II) dihydrate

T. Yonemura

### Comment

In recent years, pyridinethiolate- or pyrimidinethiolate-type ligands and their complexes have been investigated as anti-metabolite and antiviral agents, as well as for their unique photochemical properties (Halpenny & Mascharak, 2009; Rose *et al.*, 2007; Cini *et al.*, 2003). For example, attempts to regulate NO *in vivo* have prompted studies of NO scavengers and NO-releasing drugs. Although some photoinduced NO-releasing reactions of mononitrosyl complexes have been reported, relatively little is known about the analogous reactions of dinitrosyl complexes in this respect (Maurya *et al.*, 2006; Kunkely & Vogler, 2003; Ford *et al.*, 1998). We previously reported on the preparation, characterization and interesting photo-dimerization reactions of some dinitrosyl-molybdenum complexes containing thiolate ligands, which were accompanied by NO cleavage (Yonemura *et al.*, 2001, 2006). This highlighted the need to further study the reactivities and properties of these dinitrosyl-molybdenum complexes. That communication described a novel reaction of dinitrosyl-molybdenum [Mo(bidentate-*N,S*)<sub>2</sub>(NO)<sub>2</sub>]-type complexes with PPh<sub>3</sub> (Yonemura, *et al.*, 2006). This reaction, which uses pyridine-2-thiolate (pyt) as a thiolate ligand, was shown to form [Mo(py<sub>3</sub>)(NO)], [ $\{(ON)Mo(py)_2\}_2(\mu-OH)_2$ ], and Ph<sub>3</sub>PO. In this paper, we report on the structure of [Mo(py<sub>3</sub>)(NO)] Dihydrate.

In the title compound the molybdenum atom is coordinated to a nitrosyl ligand and three monoanionic *N,S*- bidentate ligands, producing a distorted MoN<sub>5</sub>S<sub>2</sub> pentagonal bipyramidal molecular geometry (Fig. 1 and Table 1). The geometrical parameters are available in the archived CIF. This complex is derived from the elimination of one NO ligand from [Mo(py<sub>2</sub>)(NO)<sub>2</sub>] and the introduction of a third pyt ligand, giving rise to a Mo atom surrounded by three pyt ligands and one NO ligand. The complex adopts a seven-coordinate structure with a distorted pentagonal bipyramidal coordination geometry about the Mo atom. Both the N and S atoms of two pyt ligands and an S atom of the third pyt ligand occupy the equatorial positions of the complex. The remaining N-atom of the third pyt ligand occupies one of the axial sites. The NO ligand occupies the other axial site in its linear mode [Mo1—N3—O1 = 179.6 (4)°], indicating that the NO ligand is coordinated as NO<sup>+</sup> (Proust *et al.*, 1994; Ardon & Cohen, 1993; Calderon *et al.*, 1969). Therefore, the oxidation state of the molybdenum atom in the title compound is formally +II; that is, the molybdenum atom is oxidized from 0 to +II.

The Mo—S distances are 2.5240 (12) and 2.4815 (16) Å, compared to 2.497 (3) and 2.477 (3) Å in complex [Mo(py<sub>2</sub>)(NO)<sub>2</sub>] (Yonemura *et al.*, 2001), and 2.4870 (7) Å in [Mo(aet)<sub>2</sub>(NO)<sub>2</sub>] (Bucher *et al.*, 2008). In this latter complex, the Mo—N<sub>2</sub> distance (2.228 (3) Å), corresponding to the N *trans* to the NO ligand, is almost the same as the other Mo—N distance in the title compound (Mo1—N1 = 2.218 (5) Å). The Mo1—NO distance (1.777 (5) Å) in the title compound is significantly shorter than those in complexes [Mo(py<sub>2</sub>)(NO)<sub>2</sub>] (1.814 (8) and 1.84 (1) Å), and [Mo(aet)<sub>2</sub>(NO)<sub>2</sub>] (1.828 (2) and 1.837 (2) Å). However, the Mo1—NO distance is almost the same as that in complex [ $\{(ON)Mo(py)_2\}_2(\mu-OH)_2$ ], that is 1.756 (2) Å (Yonemura *et al.*, 2001). The S1—Mo1—N3(NO) and N1—Mo1—N3(NO) angles (97.24 (12) and 91.87 (8)°, respectively) are large compared to the corresponding angles (95.71 (6), 94.48 (7) and 86.36 (8), 88.12 (8)°, respectively) in [ $\{(ON)Mo(py)_2\}_2(\mu-OH)_2$ ].

## supplementary materials

In the crystal the molecules pack in a zigzag arrangement (Fig. 2). The cavities between the molecules are occupied by disordered water molecules of crystallization.

### Experimental

A solution of  $[\text{Mo}(\text{pyt})_2(\text{NO})_2]$  (0.25 g, 0.65 mmol) in *N,N*-dimethylformamide (DMF) and  $\text{PPh}_3$  (0.37 g, 1.41 mmol) in tetrahydrofuran (THF) was stirred at rt for 4 days to produce an orange solution. Yellow precipitates of  $[\{(\text{ON})\text{Mo}(\text{pyt})_2\}_2(\mu\text{-OH})_2]$  and  $[\text{Mo}(\text{pyt})_3(\text{NO})]$  were obtained by allowing the reaction solution to stand in a refrigerator for a few days. The resulting orange-yellow crystals were collected by filtration. The filtrate was then poured into water, and the precipitate produced was collected by filtration and recrystallized from an acetone solution to give orange-yellow crystals of the title compound (23% yield). Anal. Calcd for  $[\text{Mo}(\text{pyt})_3(\text{NO})] = \text{C}_{16}\text{H}_{16}\text{MoN}_4\text{O}_2\text{S}_3$ : C 25.53, H 1.55, N 22.13%, Found: C 25.70, H 1.61, N 21.98%. IR [KBr;  $\nu_{\text{max}}$ ,  $\text{cm}^{-1}$ ]: 1644 (NO), 1582, 1551(CC, CN), 1447, 1420 (NC, CH), 1260 (CS).  $^{13}\text{C}$  NMR (acetone- $d_6$ ):  $\delta$  176.5, 149.1, 148.2, 140.3, 140.1, 126.8, 126.5, 119.9, 118.7.

### Refinement

The water molecules of solvent of crystallization are disordered with occupancies of 0.5 each, and it was not possible to locate their H-atoms. The C-bound H-atom were included in calculated positions and treated as riding: C—H = 0.93 Å, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

### Figures

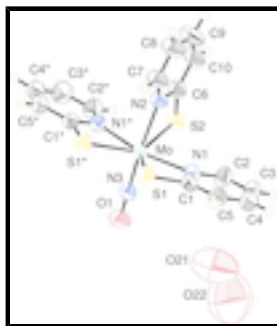


Fig. 1. A view of the molecular structure of the title compound, showing the atom-labelling scheme and 50% probability displacement ellipsoids. Atoms related by the mirror symmetry are marked by \*; symmetry operation:  $x, -y+1/2, z$ .

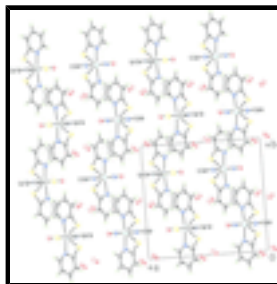


Fig. 2. Crystal packing diagram of the title compound viewed along the  $c$  axis (some H-atoms have been omitted for clarity).

Nitrosyltris(pyridine-2-thiolato- $\kappa^2N,S$ )molybdenum(II) dihydrate

Crystal data

$[\text{Mo}(\text{C}_5\text{H}_4\text{NS})_3(\text{NO})]\cdot 2\text{H}_2\text{O}$	$F_{000} = 992.00$
$M_r = 492.44$	$D_x = 1.540 \text{ Mg m}^{-3}$
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation, $\lambda = 0.71069 \text{ \AA}$
Hall symbol: $-P\ 2ac\ 2n$	Cell parameters from 25 reflections
$a = 15.7519 (16) \text{ \AA}$	$\theta = 15.4\text{--}17.4^\circ$
$b = 14.8889 (14) \text{ \AA}$	$\mu = 0.93 \text{ mm}^{-1}$
$c = 9.0535 (12) \text{ \AA}$	$T = 296 \text{ K}$
$V = 2123.3 (4) \text{ \AA}^3$	Prismatic, orange
$Z = 4$	$0.45 \times 0.40 \times 0.25 \text{ mm}$

Data collection

Rigaku AFC-7S diffractometer	$R_{\text{int}} = 0.023$
$T = 296 \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
$\omega$ - $2\theta$ scans	$h = 0 \rightarrow 20$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	$k = -10 \rightarrow 19$
$T_{\text{min}} = 0.727$ , $T_{\text{max}} = 0.792$	$l = -11 \rightarrow 6$
3681 measured reflections	3 standard reflections
2540 independent reflections	every 150 reflections
2088 reflections with $F^2 > 2\sigma(F^2)$	intensity decay: $-1.3\%$

Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2 + 2.5132P]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.126$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.13$	$\Delta\rho_{\text{max}} = 1.14 \text{ e \AA}^{-3}$
2540 reflections	$\Delta\rho_{\text{min}} = -0.64 \text{ e \AA}^{-3}$
144 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008)
H-atom parameters constrained	Extinction coefficient: $0.0029 (5)$

Special details

**Geometry.** Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**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).

## supplementary materials

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### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Mo1	0.17875 (3)	0.25000	0.95698 (4)	0.0359 (1)	
S1	0.07755 (7)	0.15176 (7)	1.10056 (12)	0.0512 (3)	
S2	0.25067 (10)	0.25000	0.71312 (17)	0.0516 (4)	
O1	0.3191 (3)	0.25000	1.1749 (5)	0.0667 (14)	
N1	0.0907 (3)	0.25000	0.7658 (5)	0.0427 (12)	
N2	0.1905 (2)	0.1024 (2)	0.9222 (3)	0.0427 (9)	
N3	0.2627 (3)	0.25000	1.0881 (5)	0.0423 (12)	
C1	0.1292 (2)	0.0662 (2)	1.0080 (4)	0.0420 (10)	
C2	0.1159 (3)	-0.0257 (2)	1.0145 (4)	0.0520 (12)	
C3	0.1680 (3)	-0.0801 (3)	0.9319 (5)	0.0627 (14)	
C4	0.2315 (3)	-0.0437 (3)	0.8467 (5)	0.0653 (16)	
C5	0.2415 (2)	0.0478 (3)	0.8434 (5)	0.0560 (12)	
C6	0.1452 (4)	0.25000	0.6512 (6)	0.0477 (14)	
C7	0.0065 (4)	0.25000	0.7415 (8)	0.0570 (17)	
C8	-0.0257 (5)	0.25000	0.5987 (9)	0.077 (3)	
C9	0.0308 (6)	0.25000	0.4820 (8)	0.080 (3)	
C10	0.1160 (5)	0.25000	0.5066 (7)	0.066 (2)	
O21	-0.0333 (11)	0.4696 (10)	0.609 (2)	0.258 (12)	0.500
O22	0.0678 (7)	0.5119 (9)	0.5891 (12)	0.128 (5)	0.500
H1	0.07300	-0.04980	1.07300	0.0630*	
H2	0.16030	-0.14210	0.93360	0.0750*	
H3	0.26730	-0.08070	0.79200	0.0780*	
H4	0.28430	0.07260	0.78550	0.0670*	
H5	-0.03070	0.25000	0.82130	0.0690*	
H6	-0.08390	0.25000	0.58200	0.0920*	
H7	0.01040	0.25000	0.38570	0.0960*	
H8	0.15400	0.25000	0.42800	0.0790*	
H9	-0.01120	0.48460	0.54280	0.3170*	0.500
H10	-0.05690	0.48240	0.65730	0.3170*	0.500
H11	0.02840	0.51090	0.60270	0.1900*	0.500
H12	0.08240	0.49480	0.49830	0.1900*	0.500

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mo1	0.0365 (2)	0.0382 (2)	0.0330 (2)	0.0000	0.0017 (2)	0.0000
S1	0.0579 (5)	0.0446 (5)	0.0510 (5)	-0.0049 (4)	0.0178 (4)	-0.0019 (4)
S2	0.0495 (7)	0.0588 (8)	0.0464 (7)	0.0000	0.0145 (6)	0.0000
O1	0.066 (2)	0.074 (3)	0.060 (2)	0.0000	-0.025 (2)	0.0000
N1	0.045 (2)	0.049 (2)	0.034 (2)	0.0000	-0.0012 (18)	0.0000
N2	0.0440 (16)	0.0440 (17)	0.0401 (15)	0.0014 (13)	0.0003 (12)	-0.0030 (13)
N3	0.044 (2)	0.042 (2)	0.041 (2)	0.0000	-0.0001 (19)	0.0000
C1	0.0457 (19)	0.0416 (18)	0.0387 (17)	0.0002 (15)	-0.0037 (15)	-0.0016 (14)
C2	0.063 (2)	0.044 (2)	0.049 (2)	-0.0051 (19)	-0.0008 (19)	0.0026 (17)

C3	0.085 (3)	0.039 (2)	0.064 (2)	0.004 (2)	-0.011 (2)	-0.0020 (19)
C4	0.072 (3)	0.051 (2)	0.073 (3)	0.017 (2)	0.007 (2)	-0.008 (2)
C5	0.054 (2)	0.056 (2)	0.058 (2)	0.0076 (19)	0.0063 (19)	-0.004 (2)
C6	0.057 (3)	0.047 (2)	0.039 (2)	0.0000	0.005 (2)	0.0000
C7	0.047 (3)	0.068 (3)	0.056 (3)	0.0000	-0.003 (2)	0.0000
C8	0.070 (4)	0.099 (6)	0.061 (4)	0.0000	-0.023 (3)	0.0000
C9	0.095 (6)	0.103 (6)	0.043 (3)	0.0000	-0.019 (3)	0.0000
C10	0.084 (5)	0.079 (4)	0.034 (2)	0.0000	0.006 (3)	0.0000
O21	0.213 (18)	0.132 (13)	0.43 (3)	0.100 (12)	-0.21 (2)	-0.171 (17)
O22	0.104 (7)	0.164 (11)	0.117 (7)	0.009 (7)	-0.024 (6)	0.001 (8)

*Geometric parameters (Å, °)*

Mo1—S1	2.5240 (12)	N2—C5	1.347 (5)
Mo1—S2	2.4815 (16)	C1—C2	1.386 (4)
Mo1—N1	2.218 (5)	C2—C3	1.374 (6)
Mo1—N2	2.228 (3)	C3—C4	1.375 (7)
Mo1—N3	1.777 (5)	C4—C5	1.372 (6)
Mo1—S1 <sup>i</sup>	2.5240 (12)	C6—C10	1.388 (9)
Mo1—N2 <sup>i</sup>	2.228 (3)	C7—C8	1.389 (11)
S1—C1	1.728 (3)	C8—C9	1.381 (12)
S2—C6	1.753 (6)	C9—C10	1.360 (12)
O1—N3	1.186 (7)	C2—H1	0.9300
O21—O22	1.72 (2)	C3—H2	0.9300
O21—H10	0.6000	C4—H3	0.9300
O21—H9	0.7300	C5—H4	0.9300
O22—H12	0.8900	C7—H5	0.9300
O22—H11	0.6300	C8—H6	0.9300
N1—C6	1.347 (7)	C9—H7	0.9300
N1—C7	1.344 (8)	C10—H8	0.9300
N2—C1	1.351 (4)		
S1—Mo1—S2	138.29 (3)	Mo1—N3—O1	179.6 (4)
S1—Mo1—N1	90.40 (10)	N2—C1—C2	121.8 (3)
S1—Mo1—N2	63.49 (8)	S1—C1—N2	108.7 (2)
S1—Mo1—N3	97.24 (12)	S1—C1—C2	129.5 (3)
S1—Mo1—S1 <sup>i</sup>	70.83 (4)	C1—C2—C3	118.0 (4)
S1—Mo1—N2 <sup>i</sup>	134.18 (8)	C2—C3—C4	120.5 (4)
S2—Mo1—N1	65.87 (13)	C3—C4—C5	119.2 (4)
S2—Mo1—N2	80.58 (7)	N2—C5—C4	121.3 (4)
S2—Mo1—N3	104.75 (15)	N1—C6—C10	121.0 (6)
S1 <sup>i</sup> —Mo1—S2	138.29 (3)	S2—C6—N1	111.0 (4)
S2—Mo1—N2 <sup>i</sup>	80.58 (7)	S2—C6—C10	128.0 (5)
N1—Mo1—N2	86.66 (8)	N1—C7—C8	120.8 (6)
N1—Mo1—N3	170.62 (19)	C7—C8—C9	118.5 (7)
S1 <sup>i</sup> —Mo1—N1	90.40 (10)	C8—C9—C10	120.7 (7)
N1—Mo1—N2 <sup>i</sup>	86.66 (8)	C6—C10—C9	118.8 (6)
N2—Mo1—N3	91.87 (8)	C1—C2—H1	121.00



## supplementary materials

S1 <sup>i</sup> —Mo1—N2	134.18 (8)	C3—C2—H1	121.00
N2—Mo1—N2 <sup>i</sup>	161.13 (11)	C2—C3—H2	120.00
S1 <sup>i</sup> —Mo1—N3	97.24 (12)	C4—C3—H2	120.00
N2 <sup>i</sup> —Mo1—N3	91.87 (8)	C5—C4—H3	120.00
S1 <sup>i</sup> —Mo1—N2 <sup>i</sup>	63.49 (8)	C3—C4—H3	120.00
Mo1—S1—C1	83.12 (11)	N2—C5—H4	119.00
Mo1—S2—C6	81.48 (19)	C4—C5—H4	119.00
H9—O21—H10	142.00	N1—C7—H5	120.00
H11—O22—H12	115.00	C8—C7—H5	120.00
Mo1—N1—C6	101.7 (4)	C7—C8—H6	121.00
C6—N1—C7	120.2 (5)	C9—C8—H6	121.00
Mo1—N1—C7	138.1 (4)	C8—C9—H7	120.00
Mo1—N2—C5	136.0 (3)	C10—C9—H7	120.00
C1—N2—C5	119.3 (3)	C9—C10—H8	121.00
Mo1—N2—C1	104.6 (2)	C6—C10—H8	121.00
S2—Mo1—S1—C1	32.54 (14)	Mo1—S1—C1—N2	1.4 (2)
N1—Mo1—S1—C1	85.19 (14)	Mo1—S1—C1—C2	-179.6 (4)
N2—Mo1—S1—C1	-0.87 (14)	Mo1—S2—C6—N1	0.00
N3—Mo1—S1—C1	-89.34 (15)	Mo1—S2—C6—C10	180.00
S1 <sup>i</sup> —Mo1—S1—C1	175.48 (12)	Mo1—N1—C6—S2	0.00
N2 <sup>i</sup> —Mo1—S1—C1	170.92 (16)	Mo1—N1—C6—C10	180.00
S1—Mo1—S2—C6	60.58 (6)	C7—N1—C6—S2	180.00
N1—Mo1—S2—C6	0.00	C7—N1—C6—C10	0.00
N2—Mo1—S2—C6	90.55 (8)	Mo1—N1—C7—C8	180.00
N3—Mo1—S2—C6	-180.00	C6—N1—C7—C8	0.00
S1—Mo1—N1—C6	-144.58 (2)	Mo1—N2—C1—S1	-1.6 (3)
S1—Mo1—N1—C7	35.42 (2)	Mo1—N2—C1—C2	179.3 (3)
S2—Mo1—N1—C6	0.00	C5—N2—C1—S1	177.5 (3)
S2—Mo1—N1—C7	180.00	C5—N2—C1—C2	-1.6 (5)
N2—Mo1—N1—C6	-81.17 (8)	Mo1—N2—C5—C4	179.9 (3)
N2—Mo1—N1—C7	98.83 (8)	C1—N2—C5—C4	1.1 (6)
S1—Mo1—N2—C1	1.14 (19)	S1—C1—C2—C3	-178.1 (3)
S1—Mo1—N2—C5	-177.8 (4)	N2—C1—C2—C3	0.8 (6)
S2—Mo1—N2—C1	-157.1 (2)	C1—C2—C3—C4	0.4 (6)
S2—Mo1—N2—C5	24.1 (3)	C2—C3—C4—C5	-0.9 (7)
N1—Mo1—N2—C1	-91.0 (2)	C3—C4—C5—N2	0.2 (7)
N1—Mo1—N2—C5	90.1 (4)	S2—C6—C10—C9	180.00
N3—Mo1—N2—C1	98.3 (3)	N1—C6—C10—C9	0.00
N3—Mo1—N2—C5	-80.6 (4)	N1—C7—C8—C9	0.00
S1 <sup>i</sup> —Mo1—N2—C1	-3.7 (3)	C7—C8—C9—C10	0.00
S1 <sup>i</sup> —Mo1—N2—C5	177.4 (3)	C8—C9—C10—C6	0.00

Symmetry codes: (i)  $x, -y+1/2, z$ .

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O21—H9 $\cdots$ O22	0.73	1.37	1.72 (2)	106

C5—H4...S2

0.93

2.77

3.237 (5)

112

Fig. 1

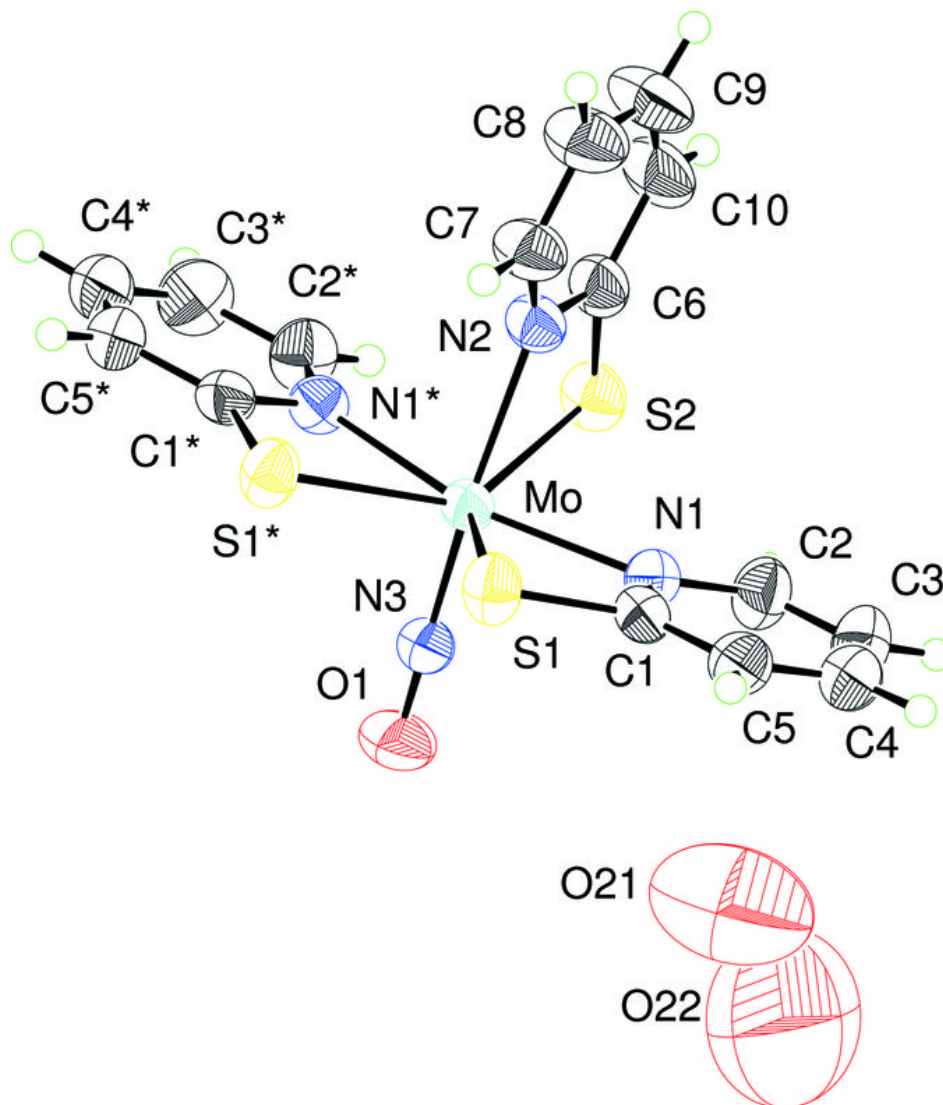


Fig. 2

