

# A molybdenum tris(dithiolene) complex coordinates to three bound cobalt centers in three different ways

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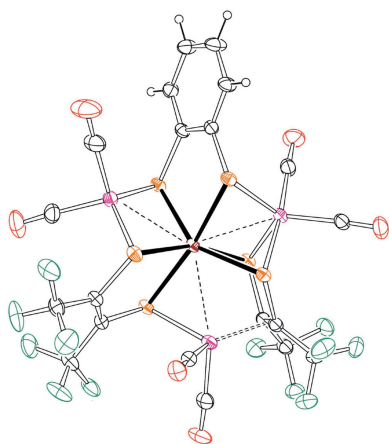
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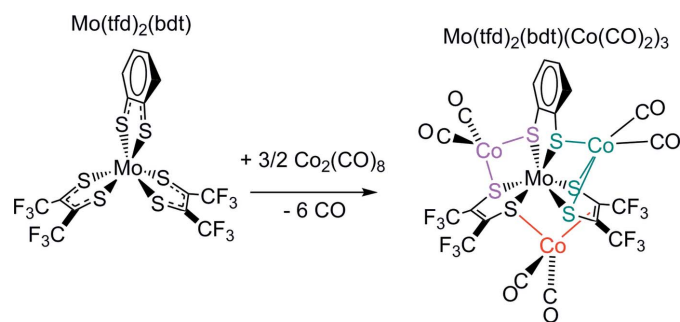
The synthesis and structural characterization of the molecular compound ( $\mu_3$ -benzene-1,2-dithiolato)hexacarbonylbis( $\mu_3$ -1,1,1,4,4,4-hexafluorobut-2-ene-2,3-dithiolato)tricobaltmolybdenum,  $[\text{Co}_3\text{Mo}(\text{C}_4\text{F}_6\text{S}_2)_2(\text{C}_6\text{H}_4\text{S}_2)(\text{CO})_6]$  or  $\text{Mo}(\text{tfd})_2(\text{bdt})(\text{Co}(\text{CO})_2)_3$  (tfd is 1,1,1,4,4,4-hexafluorobut-2-ene-2,3-dithiolate and bdt is benzene-1,2-dithiolate), are reported. The structure of the molecule contains the molybdenum tris(dithiolene) complex  $\text{Mo}(\text{tfd})_2(\text{bdt})$  coordinated as a multi-dentate ligand to three cobalt dicarbonyl units. Each of the three cobalt centers is relatively close to molybdenum, with  $\text{Co}\cdots\text{Mo}$  distances of 2.7224 (7), 2.8058 (7), and 2.6320 (6) Å. Additionally, each of the cobalt centers is bound *via* main-group donor atoms, but each one in a different way: the first cobalt atom is coordinated by two sulfur atoms from different dithiolenes (bdt and tfd). The second cobalt atom is coordinated by one sulfur from one tfd and two olefinic carbons from another tfd. The third cobalt is coordinated by one sulfur from bdt and two sulfurs from tfd. This is, to the best of our knowledge, the first structurally characterized example of a molybdenum (tris)dithiolene complex that coordinates to cobalt. The F atoms of two of the  $-\text{CF}_3$  groups were refined as disordered over two sets of sites with ratios of refined occupancies of 0.703 (7):0.297 (7) and 0.72 (2):0.28 (2).

## 1. Chemical context

Sulfur removal from crude petroleum is performed on a large industrial scale through a process called hydrodesulfurization. This involves use of hydrogen gas (the sulfur is removed as  $\text{H}_2\text{S}$ ) and addition of a catalyst, typically cobalt-doped  $\text{MoS}_2$  (Hinnemann *et al.*, 2008).  $\text{MoS}_2$  is not a molecular compound but rather possesses an extended structure, consisting of close-packed sulfur layers between which molybdenum is sandwiched (Dickinson & Pauling, 1923). The coordination geometry around molybdenum is trigonal prismatic. Several attempts to model  $\text{MoS}_2$  using molecular compounds have been made, often using dithiolene ( $\text{S}_2\text{C}_2\text{R}_2$ ) ligands, where some examples also contain the hydrodesulfurization-relevant addition of cobalt. Complexes containing molybdenum, cobalt, and one or two (but not three) dithiolenes are known. A molybdenum bis(dithiolene) that coordinates to two cobalt centers has been characterized crystallographically (Nihei *et al.*, 1999; Murata *et al.*, 2006). The study reports  $[\text{Mo}(\text{bdt})_2(\text{CO})_2(\text{CpCo})_2]$ , where bdt = *o*- $\text{C}_6\text{H}_4\text{S}_2$  and Cp = *cyclo*- $\text{C}_5\text{H}_5$ . The methylated analog  $[\text{Mo}(\text{bdt})_2(\text{CO})_2(\text{Cp}^*\text{Co})_2]$ , where  $\text{Cp}^*$  = *cyclo*- $\text{C}_5\text{Me}_5$  was also structurally characterized (Muratsugu *et al.*, 2011). An analogous  $[\text{Mo}(\text{ddd})_2(\text{CO})_2(\text{CpCo})_2]$  was reported by a different group, where ddd is the unusual di-

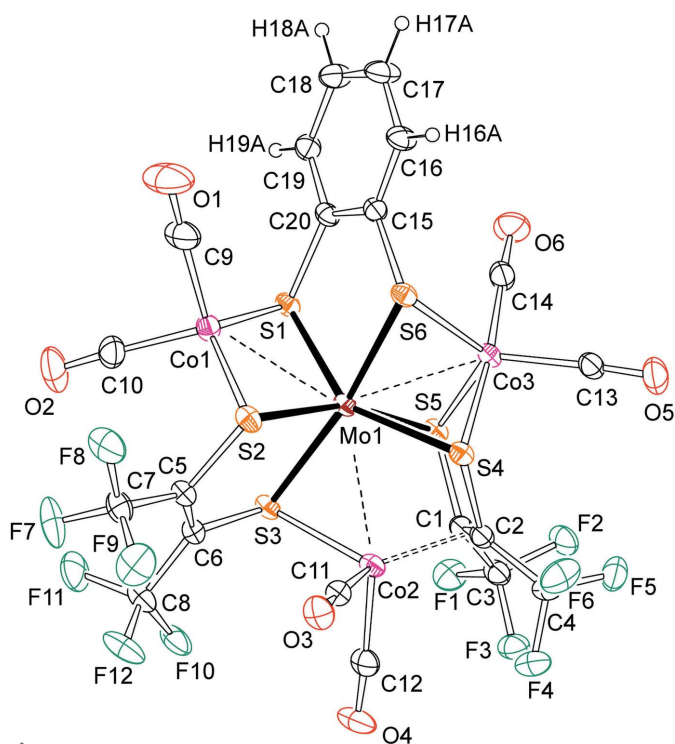


thiolene 1,2-dicarba-*closo*-dodecaborane-1,2-disulfide (Chen *et al.*, 2007). The above contribution also reported a molybdenum mono(dithiolene) complex coordinated to a cobalt fragment, namely  $[\text{Mo}(\text{ddd})\text{(CO)}_2(\text{py})_2(\text{Cp}^*\text{Co})]$ , where  $\text{py}$  = pyridine. Coordinating to cobalt a molybdenum tris(dithiolene), that is a compound where three dithiolenes are bound to molybdenum, would be interesting, because molybdenum tris(dithiolene)s mimic  $\text{MoS}_2$  particularly well. Similar to  $\text{MoS}_2$ , they contain molybdenum coordinated to six sulfur atoms, and, also, depending on the oxidation state of the compound, the environment of molybdenum can sometimes be trigonal prismatic (Beswick *et al.*, 2004). However, we could not find any structurally characterized example for how a molybdenum tris(dithiolene) complex can act as ligand for cobalt. Such an example is provided here. In 2007, the mixed dithiolene complex  $\text{Mo}(\text{tfd})_2(\text{bdt})$  [ $\text{tfd} = \text{S}_2\text{C}_2(\text{CF}_3)_2$ ], an unsymmetrical tris(dithiolene), was reported for the first time (Harrison *et al.*, 2007). Later, this complex, which contains two different dithiolenes, was used to create structural models for the active sites of  $\text{MoS}_2$  hydrodesulfurization catalysts, albeit cobalt-free ones (Nguyen *et al.*, 2010). In this current work, we have successfully linked three cobalt centers to one  $\text{Mo}(\text{tfd})_2(\text{bdt})$  molecule. Surprisingly, each of the three cobalt-containing units [each one is a  $\text{Co}(\text{CO})_2$  fragment] is bound to the molybdenum tris(dithiolene) center in a different way.



## 2. Structural commentary

An anisotropic displacement plot showing the structure of the  $\text{Mo}(\text{tfd})_2(\text{bdt})(\text{Co}(\text{CO})_2)_3$  molecule is shown in Fig. 1. A good starting point for the structural description is considering the core  $\text{Mo}(\text{tfd})_2(\text{bdt})$  substructure first. Molybdenum is coordinated by six sulfur atoms, four from the two  $\text{tfd}$  ligands, two from the one  $\text{bdt}$  ligand. The  $\text{Mo}-\text{S}$  distances are fairly normal, ranging from 2.413 (1) Å ( $\text{Mo1}-\text{S5}$ ) to 2.457 (1) Å ( $\text{Mo1}-\text{S4}$ ). The appearance of the structure is ‘approximately octahedral’. A more quantitative measure is obtained using the  $X-M-X_{\text{trans}}$  criterion (Beswick *et al.*, 2004; Nguyen *et al.*, 2010), which indicates that the geometry around molybdenum is 71% octahedral (29% trigonal prismatic). The intra-ring C–C distance in the  $\text{tfd}$  ligand that is not  $\pi$ -coordinated to cobalt (C5–C6) is 1.335 (6) Å, indicating that description as an ene-dithiolate is appropriate (Hosking *et al.*, 2009). The intra-ring C–C distance in the  $\text{tfd}$  ligand that is  $\pi$ -coordinated to cobalt (C1–C2) is much longer, at 1.439 (6) Å, but this elongation is expected as an effect of  $\pi$ -coordination to cobalt



**Figure 1**  
A view of the molecular structure of  $\text{Mo}(\text{tfd})_2(\text{bdt})(\text{Co}(\text{CO})_2)_3$ . Anisotropic displacement ellipsoids in this plot, generated with ORTEP-3 (Farrugia, 2012), are shown at the 30% level. Hydrogen atoms are shown as spheres of arbitrary radius. For the disordered fluorines on C7 and C8 only one orientation (major component) is shown.

(Co2). At this point it makes sense to discuss the way in which the  $\text{Mo}(\text{tfd})_2(\text{bdt})$  substructure coordinates to the three cobalt dicarbonyl fragments. Co1 is coordinated by two sulfurs from different dithiolenes ( $\text{bdt}$  and  $\text{tfd}$ ) at bond lengths of 2.225 (1) Å ( $\text{Co1}-\text{S1}$ ) and 2.241 (1) Å ( $\text{Co1}-\text{S2}$ ), respectively. The  $\text{C}_2\text{S}_2$  environment of Co1 is nearly tetrahedral, with very slight distortions. The  $\text{S1}-\text{Co1}-\text{S2}$  angle is slightly wide, at 115.44 (5)°, the  $\text{C9}-\text{Co1}-\text{C10}$  angle is slightly narrow, at 98.4 (3)°. Co2, in contrast, is coordinated by one sulfur from one  $\text{tfd}$  and two olefinic carbons from another  $\text{tfd}$ , where bond lengths are 2.256 (1) Å ( $\text{Co2}-\text{S3}$ ), 2.010 (4) Å ( $\text{Co2}-\text{C1}$ ), and 1.970 (4) Å ( $\text{Co2}-\text{C2}$ ). The coordination geometry of Co2 (not including Mo1 here) is, again, approximately tetrahedral, where the largest deviation from tetrahedral geometry are  $\text{C11}-\text{Co2}-\text{C12}$ , at 96.3 (2)° and the comparably wide ‘bite’ of the chelating substructure, with  $\text{C11}-\text{Co2}-\text{S3}$  measuring 119.7°, where C11 is the mid-point between C11 and C12. Another sulfur atom, S4, is relatively close to Co2, but the interatomic distance, at 2.767 (1) Å, is considerably longer than the  $\text{Co2}-\text{S3}$  bond, such that S4 is almost certainly not bonded. Finally, Co3 is coordinated by one sulfur from  $\text{bdt}$  and two sulfurs from  $\text{tfd}$ , at distances of 2.234 (1) Å ( $\text{Co3}-\text{S4}$ ), 2.239 (1) Å ( $\text{Co3}-\text{S5}$ ), and 2.275 (1) Å ( $\text{Co3}-\text{S6}$ ). Co3 is surrounded by these three sulfurs and two carbons in an approximately trigonal-bipyramidal fashion. C14 and S4 occupy axial positions, with the  $\text{C14}-\text{Co3}-\text{S4}$  angle being 174.3 (2)°. The three angles in the trigonal plane are 115.38 (4)° ( $\text{S5}-\text{Co3}-\text{S6}$ ), 118.6 (2)° ( $\text{S5}-\text{Co3}-\text{C13}$ ), and

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C17-H17A\cdots O6^i$	0.95	2.57	3.353 (7)	140
$C17-H17A\cdots F11^{ii}$	0.95	2.62	3.461 (9)	148
$C17-H17A\cdots F10A^{ii}$	0.95	2.55	3.29 (2)	135

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

124.0 (2)° ( $S6-Co3-C13$ ). While there is no doubt that the three cobalt atoms are bound by the heteroatoms (sulfur, carbon) of the  $Mo(tfd)_2(bdt)$  structure, each of the three cobalt atoms is also close to the central molybdenum, and these metal-metal contacts could possibly be bonding as well. The relevant distances are 2.7224 (7) Å ( $Co1-Mo1$ ), 2.8058 (7) Å ( $Co2-Mo1$ ), and 2.6320 (6) Å ( $Co3-Mo1$ ). Such Mo-Co distances are typically considered of a range compatible with Mo-Co bonds (Chen *et al.*, 2007; Curtis *et al.*, 1997; Murata *et al.*, 2006; Muratsugu *et al.*, 2011).

### 3. Supramolecular features

Molecules of  $Mo(tfd)_2(bdt)(Co(CO)_2)_3$  pack, without any solvent in the crystal, *via* contacting van der Waals surfaces. The packing pattern is shown in Fig. 2. Hydrogen atom H17A forms close intermolecular contacts to an oxygen atom from a neighboring carbonyl and to a fluorine atom of the major disorder component (F11), as well as to a fluorine atom of the minor disorder component (F10A). Details can be found in Table 1.

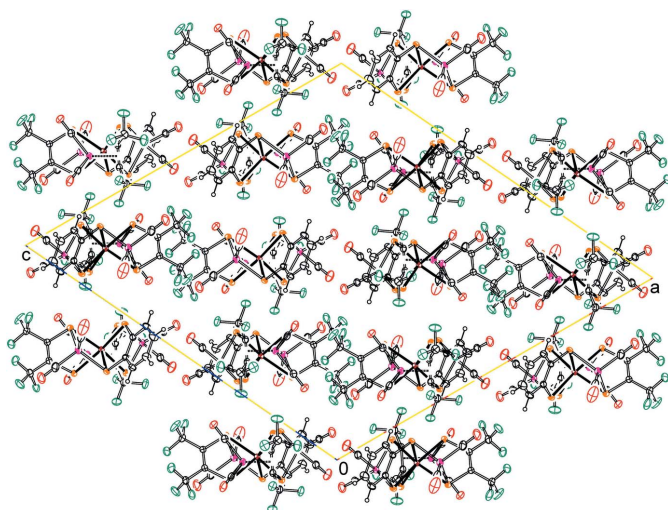
### 4. Database survey

The Cambridge Crystallographic Database (version 5.40, including updates up to May 2019; Groom *et al.*, 2016) was searched. The search was performed as a substructure search containing the most general dithiolene S-C-C-S substructure

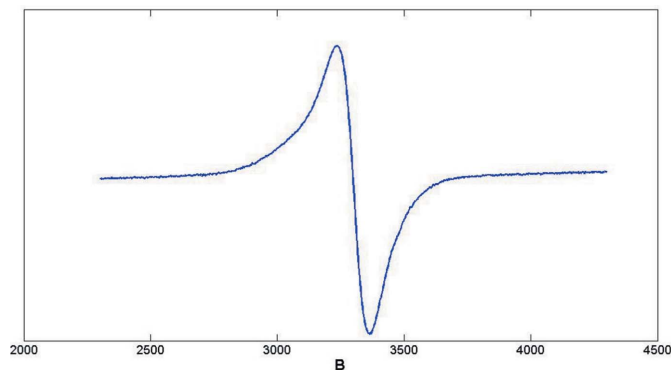
(with any kind of bond allowed in the chain), plus a molybdenum and a cobalt atom. Since no specific requirement was imposed with regard to whether or in which way cobalt or molybdenum are bonded to the S-C-C-S structure, hits that do not contain a molybdenum dithiolene complex coordinated to cobalt where manually removed as follows. Seven hits were retrieved: EYUHIQ, JOQWIV, JOQWIV01, SEVMIQ, SEVMOW, TASDAT, OQAMEZ. Out of these, TASDAT and OQAMEZ are not relevant here, since they do not contain a molybdenum dithiolene unit that is directly bonded to cobalt. They contain, respectively, a cobalt-based counter-cation for an anionic molybdenum complex and a nickel bis(dithiolene) anion as a counter-anion for a molybdenum/cobalt sulfido cluster. The structures EYUHIQ, JOQWIV, JOQWIV01, SEVMIQ and SEVMOW are relevant, since they contain at least one molybdenum dithiolene unit that is directly bonded to cobalt. These structures are all discussed above in the *Chemical context* (Nihei *et al.*, 1999; Murata *et al.*, 2006; Muratsugu *et al.*, 2011; Chen *et al.*, 2007).

### 5. Synthesis and crystallization

$Mo(tfd)_2(bdt)(Co(CO)_2)_3$  was prepared from  $Mo(tfd)_2(bdt)$  (Harrison *et al.*, 2007) and dicobaltoctacarbonyl (obtained from Sigma-Aldrich) as summarized in the Scheme, using air-free conditions and rigorously dried solvents. 48 mg of  $Mo(tfd)_2(bdt)$  (0.0697 mmol) were dissolved in 18 mL of hexane (dried over Na/benzophenone). 60 mg (0.175 mmol) of  $(Co)_2(CO)_8$  dissolved in 2 mL of hexane were added and the mixture was shaken. The mixture was stored overnight at 243 K in the freezer of a nitrogen-filled glovebox. The supernatant was decanted off, and the black crystals of  $Mo(tfd)_2(bdt)(Co(CO)_2)_3$  were washed twice with 5 mL of cold hexane. Total yield 27 mg (0.026 mmol, 37%). Analysis calculated for  $Mo_1S_6C_{20}H_4F_{12}Co_3O_6$ : C, 23.25; H, 0.39; O, 9.29; S, 18.62. Found: C, 23.70; H, 0.44; O, 9.70; S, 18.80.  $^1H$  NMR (400 MHz,  $C_6D_6$ ):  $\delta$  6.38 (*m*), 7.02 (*m*). The compound is paramagnetic. An estimate of the magnetic moment in solution (Evans method) yielded *ca* 0.9 BM, consistent with one unpaired electron. An EPR spectrum was also obtained, shown in Fig. 3.



**Figure 2**  
Packing of molecules of  $Mo(tfd)_2(bdt)(Co(CO)_2)_3$ , viewed along the *b* axis.



**Figure 3**  
X-band EPR spectrum of  $Mo(tfd)_2(bdt)(Co(CO)_2)_3$  in hexane at 298 K;  $g = 2.010$ .

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were placed in calculated positions and included in a riding-motion approximation with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The F atoms of the  $-\text{CF}_3$  groups containing C7 and C8 were refined as disordered over two sets of sites with ratios of refined occupancies of 0.703 (7):0.297 (7) and 0.72 (2):0.28 (2), respectively.

## Acknowledgements

We thank Professors Wolfgang Kaim and Biprajit Sarkar (University of Stuttgart) for the use of their EPR spectrometer for the spectrum shown in Fig. 3.

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Table 2

Experimental details.

Crystal data	
Chemical formula	$[\text{Co}_3\text{Mo}(\text{C}_4\text{F}_6\text{S}_2)_2(\text{C}_6\text{H}_4\text{S}_2)(\text{CO})_6]$
$M_r$	1033.32
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	150
$a, b, c$ (Å)	22.7465 (5), 12.8779 (5), 23.6033 (6)
$\beta$ (°)	115.3840 (16)
$V$ (Å <sup>3</sup> )	6246.5 (3)
$Z$	8
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	2.47
Crystal size (mm)	0.32 × 0.12 × 0.10
Data collection	
Diffractometer	Nonius KappaCCD
Absorption correction	Multi-scan (SORTAV; Blessing, 1995)
$T_{\text{min}}, T_{\text{max}}$	0.686, 0.798
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	21250, 7102, 5019
$R_{\text{int}}$	0.046
$(\sin \theta/\lambda)_{\text{max}}$ (Å <sup>-1</sup> )	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.045, 0.112, 1.07
No. of reflections	7102
No. of parameters	489
No. of restraints	210
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	1.09, -0.74

Computer programs: COLLECT (Nonius, 2002), DENZO-SMN (Otwinowski & Minor, 1997), SIR92 (Altomare *et al.*, 1994), SHELXL2018 (Sheldrick, 2015), PLATON (Spek, 2009) and SHELXTL (Sheldrick, 2008).

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## supporting information

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## A molybdenum tris(dithiolene) complex coordinates to three bound cobalt centers in three different ways

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### Computing details

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

( $\mu_3$ -Benzene-1,2-dithiolato)hexacarbonylbis( $\mu_3$ -1,1,1,4,4,4-hexafluorobut-2-ene-2,3-dithiolato)tricobaltmolybdenum

### Crystal data

[Co<sub>3</sub>Mo(C<sub>4</sub>F<sub>6</sub>S<sub>2</sub>)<sub>2</sub>(C<sub>6</sub>H<sub>4</sub>S<sub>2</sub>)(CO)<sub>6</sub>]

$M_r = 1033.32$

Monoclinic, *C2/c*

$a = 22.7465$  (5) Å

$b = 12.8779$  (5) Å

$c = 23.6033$  (6) Å

$\beta = 115.3840$  (16)°

$V = 6246.5$  (3) Å<sup>3</sup>

$Z = 8$

$F(000) = 3992$

$D_x = 2.198$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 21250 reflections

$\theta = 3.0$ – $27.5^\circ$

$\mu = 2.47$  mm<sup>-1</sup>

$T = 150$  K

Needle, dark red

$0.32 \times 0.12 \times 0.10$  mm

### Data collection

Nonius KappaCCD

diffractometer

Radiation source: fine-focus sealed tube

Detector resolution: 9 pixels mm<sup>-1</sup>

$\varphi$  scans and  $\omega$  scans with  $\kappa$  offsets

Absorption correction: multi-scan

(SORTAV; Blessing, 1995)

$T_{\min} = 0.686$ ,  $T_{\max} = 0.798$

21250 measured reflections

7102 independent reflections

5019 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.0^\circ$

$h = -29 \rightarrow 29$

$k = -16 \rightarrow 16$

$l = -30 \rightarrow 30$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.045$

$wR(F^2) = 0.112$

$S = 1.07$

7102 reflections

489 parameters

210 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

$$w = 1/[\sigma^2(F_o^2) + (0.054P)^2 + 5.1797P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 1.09 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.74 \text{ e } \text{\AA}^{-3}$$

*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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Mo1	0.37011 (2)	0.67610 (3)	0.12477 (2)	0.02586 (11)	
Co1	0.32882 (3)	0.85549 (5)	0.15702 (3)	0.03548 (16)	
Co2	0.33267 (3)	0.47117 (5)	0.13309 (3)	0.03083 (16)	
Co3	0.45749 (3)	0.63936 (5)	0.08184 (3)	0.02962 (15)	
S1	0.32447 (5)	0.82941 (9)	0.06212 (5)	0.0297 (2)	
S2	0.36985 (5)	0.72385 (9)	0.22479 (5)	0.0331 (3)	
S3	0.26312 (5)	0.60667 (9)	0.10435 (5)	0.0296 (2)	
S4	0.45637 (5)	0.54398 (9)	0.16042 (5)	0.0301 (2)	
S5	0.35447 (5)	0.58534 (9)	0.02990 (5)	0.0295 (2)	
S6	0.47364 (5)	0.76648 (9)	0.15395 (5)	0.0307 (3)	
F1	0.26591 (12)	0.4072 (2)	-0.02994 (12)	0.0493 (7)	
F2	0.35969 (14)	0.3736 (2)	-0.02658 (12)	0.0484 (7)	
F3	0.32346 (13)	0.2830 (2)	0.02808 (12)	0.0456 (7)	
F4	0.41197 (15)	0.2522 (2)	0.14259 (14)	0.0581 (8)	
F5	0.46739 (15)	0.3033 (2)	0.09356 (15)	0.0588 (8)	
F6	0.49947 (14)	0.3377 (2)	0.19160 (14)	0.0635 (9)	
F7	0.2282 (2)	0.7313 (7)	0.2705 (2)	0.074 (2)	0.703 (7)
F8	0.3246 (3)	0.7860 (5)	0.3117 (3)	0.0698 (18)	0.703 (7)
F9	0.3064 (4)	0.6287 (4)	0.3225 (2)	0.0766 (19)	0.703 (7)
F7A	0.2573 (8)	0.7953 (11)	0.2754 (6)	0.072 (4)	0.297 (7)
F8A	0.3435 (5)	0.7165 (15)	0.3305 (4)	0.063 (3)	0.297 (7)
F9A	0.2537 (7)	0.6372 (10)	0.2967 (5)	0.063 (3)	0.297 (7)
F10	0.1632 (4)	0.5120 (8)	0.1246 (4)	0.055 (2)	0.72 (2)
F11	0.1431 (3)	0.6580 (6)	0.1565 (6)	0.066 (2)	0.72 (2)
F12	0.1944 (4)	0.5381 (9)	0.2222 (3)	0.068 (2)	0.72 (2)
F10A	0.1475 (9)	0.558 (2)	0.1103 (7)	0.057 (4)	0.28 (2)
F11A	0.1543 (10)	0.6471 (14)	0.1877 (12)	0.056 (4)	0.28 (2)
F12A	0.1972 (10)	0.4990 (14)	0.2037 (10)	0.057 (4)	0.28 (2)
O1	0.3951 (3)	1.0559 (4)	0.2075 (3)	0.112 (2)	
O2	0.19536 (19)	0.9067 (4)	0.1404 (2)	0.0771 (13)	
O3	0.37570 (16)	0.4528 (3)	0.26994 (14)	0.0486 (9)	
O4	0.23791 (19)	0.2999 (3)	0.09880 (16)	0.0587 (11)	
O5	0.56008 (17)	0.5074 (3)	0.07720 (17)	0.0586 (10)	
O6	0.4473 (2)	0.7725 (3)	-0.02293 (17)	0.0610 (10)	
C1	0.35680 (19)	0.4568 (3)	0.06092 (19)	0.0304 (10)	
C2	0.41017 (19)	0.4338 (4)	0.1204 (2)	0.0323 (10)	

C3	0.3269 (2)	0.3798 (4)	0.0090 (2)	0.0372 (11)
C4	0.4467 (2)	0.3306 (4)	0.1367 (2)	0.0423 (12)
C5	0.29505 (19)	0.6793 (4)	0.22259 (18)	0.0309 (10)
C6	0.25188 (19)	0.6280 (3)	0.17312 (19)	0.0304 (10)
C7	0.2880 (2)	0.7059 (4)	0.2817 (2)	0.0437 (12)
C8	0.1880 (2)	0.5842 (4)	0.1692 (2)	0.0435 (12)
C9	0.3691 (3)	0.9805 (5)	0.1880 (3)	0.0646 (17)
C10	0.2465 (3)	0.8898 (4)	0.1474 (2)	0.0495 (13)
C11	0.3593 (2)	0.4622 (4)	0.2178 (2)	0.0354 (10)
C12	0.2757 (2)	0.3625 (4)	0.1124 (2)	0.0409 (11)
C13	0.5214 (2)	0.5607 (4)	0.0791 (2)	0.0370 (11)
C14	0.4513 (2)	0.7229 (4)	0.0182 (2)	0.0410 (11)
C15	0.45531 (19)	0.8839 (3)	0.11004 (19)	0.0296 (9)
C16	0.5057 (2)	0.9503 (4)	0.1170 (2)	0.0398 (11)
H16A	0.549037	0.934569	0.146045	0.048*
C17	0.4928 (2)	1.0394 (4)	0.0814 (2)	0.0512 (14)
H17A	0.527525	1.083894	0.085070	0.061*
C18	0.4294 (2)	1.0649 (4)	0.0401 (2)	0.0442 (12)
H18A	0.420821	1.127055	0.016168	0.053*
C19	0.3788 (2)	0.9995 (4)	0.0339 (2)	0.0347 (10)
H19A	0.335466	1.016576	0.005600	0.042*
C20	0.39134 (19)	0.9089 (3)	0.06908 (19)	0.0291 (9)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mo1	0.02129 (18)	0.0321 (2)	0.02433 (19)	-0.00421 (15)	0.00990 (15)	-0.00087 (15)
Co1	0.0354 (3)	0.0368 (4)	0.0387 (3)	-0.0013 (3)	0.0202 (3)	-0.0033 (3)
Co2	0.0325 (3)	0.0345 (4)	0.0287 (3)	-0.0072 (3)	0.0162 (3)	-0.0013 (2)
Co3	0.0259 (3)	0.0351 (4)	0.0308 (3)	-0.0016 (3)	0.0149 (2)	0.0027 (3)
S1	0.0216 (5)	0.0358 (6)	0.0311 (5)	-0.0030 (4)	0.0107 (4)	0.0019 (5)
S2	0.0278 (5)	0.0441 (7)	0.0269 (5)	-0.0067 (5)	0.0112 (4)	-0.0048 (5)
S3	0.0242 (5)	0.0394 (7)	0.0261 (5)	-0.0077 (5)	0.0117 (4)	-0.0025 (5)
S4	0.0286 (5)	0.0344 (6)	0.0283 (5)	-0.0017 (5)	0.0130 (4)	0.0029 (5)
S5	0.0275 (5)	0.0357 (6)	0.0269 (5)	-0.0036 (5)	0.0133 (4)	-0.0001 (5)
S6	0.0229 (5)	0.0362 (7)	0.0304 (5)	-0.0045 (4)	0.0088 (4)	0.0008 (5)
F1	0.0445 (15)	0.0509 (18)	0.0423 (15)	-0.0106 (14)	0.0088 (13)	-0.0117 (13)
F2	0.0626 (17)	0.0540 (19)	0.0453 (15)	-0.0151 (15)	0.0391 (14)	-0.0152 (13)
F3	0.0604 (17)	0.0358 (16)	0.0460 (15)	-0.0124 (13)	0.0281 (13)	-0.0079 (12)
F4	0.0690 (19)	0.0357 (17)	0.074 (2)	-0.0050 (15)	0.0343 (17)	0.0094 (15)
F5	0.073 (2)	0.0481 (19)	0.072 (2)	0.0172 (16)	0.0474 (18)	0.0034 (15)
F6	0.0556 (19)	0.0473 (19)	0.0605 (19)	0.0085 (15)	-0.0008 (16)	0.0074 (15)
F7	0.043 (3)	0.130 (6)	0.055 (3)	0.008 (3)	0.027 (2)	-0.032 (4)
F8	0.092 (4)	0.085 (4)	0.054 (3)	-0.038 (4)	0.051 (3)	-0.038 (3)
F9	0.124 (5)	0.081 (4)	0.033 (3)	0.019 (4)	0.041 (3)	0.012 (3)
F7A	0.097 (8)	0.077 (8)	0.052 (6)	0.022 (7)	0.042 (6)	-0.017 (6)
F8A	0.061 (6)	0.106 (9)	0.028 (5)	-0.005 (7)	0.025 (5)	-0.006 (6)
F9A	0.083 (8)	0.081 (7)	0.038 (6)	-0.025 (7)	0.038 (5)	-0.011 (5)

F10	0.045 (4)	0.069 (5)	0.063 (4)	-0.029 (3)	0.035 (3)	-0.024 (3)
F11	0.030 (3)	0.084 (4)	0.084 (5)	0.006 (2)	0.024 (3)	-0.006 (4)
F12	0.062 (3)	0.099 (5)	0.053 (3)	-0.032 (4)	0.035 (3)	0.005 (4)
F10A	0.031 (6)	0.087 (10)	0.052 (7)	-0.023 (7)	0.017 (5)	-0.012 (7)
F11A	0.044 (7)	0.067 (7)	0.072 (9)	-0.008 (6)	0.039 (7)	-0.017 (7)
F12A	0.055 (6)	0.065 (8)	0.063 (8)	-0.014 (7)	0.036 (6)	0.005 (7)
O1	0.183 (5)	0.076 (4)	0.116 (4)	-0.071 (4)	0.102 (4)	-0.047 (3)
O2	0.058 (2)	0.107 (4)	0.082 (3)	0.038 (3)	0.045 (2)	0.027 (3)
O3	0.053 (2)	0.063 (3)	0.0311 (18)	0.0045 (18)	0.0197 (16)	0.0060 (16)
O4	0.078 (3)	0.063 (3)	0.051 (2)	-0.042 (2)	0.043 (2)	-0.0207 (19)
O5	0.052 (2)	0.068 (3)	0.069 (2)	0.020 (2)	0.0381 (19)	0.012 (2)
O6	0.091 (3)	0.053 (2)	0.054 (2)	-0.002 (2)	0.045 (2)	0.0113 (19)
C1	0.031 (2)	0.030 (2)	0.034 (2)	-0.0034 (19)	0.0177 (19)	-0.0025 (19)
C2	0.033 (2)	0.034 (3)	0.035 (2)	-0.0041 (19)	0.0195 (19)	-0.0018 (19)
C3	0.039 (3)	0.041 (3)	0.037 (2)	-0.007 (2)	0.022 (2)	-0.003 (2)
C4	0.048 (3)	0.032 (3)	0.047 (3)	-0.007 (2)	0.021 (2)	0.000 (2)
C5	0.027 (2)	0.039 (3)	0.028 (2)	-0.0028 (19)	0.0126 (18)	0.0002 (19)
C6	0.027 (2)	0.036 (3)	0.031 (2)	0.0008 (19)	0.0146 (19)	0.0010 (19)
C7	0.044 (3)	0.061 (3)	0.032 (2)	-0.001 (3)	0.022 (2)	-0.006 (2)
C8	0.036 (2)	0.059 (3)	0.044 (3)	-0.010 (2)	0.024 (2)	-0.002 (2)
C9	0.098 (5)	0.056 (4)	0.065 (4)	-0.029 (4)	0.059 (4)	-0.022 (3)
C10	0.058 (3)	0.049 (3)	0.052 (3)	0.010 (3)	0.034 (3)	0.003 (3)
C11	0.036 (2)	0.034 (3)	0.039 (3)	-0.001 (2)	0.019 (2)	0.000 (2)
C12	0.053 (3)	0.046 (3)	0.032 (2)	-0.009 (3)	0.026 (2)	-0.008 (2)
C13	0.034 (2)	0.042 (3)	0.040 (3)	0.003 (2)	0.020 (2)	0.009 (2)
C14	0.039 (3)	0.045 (3)	0.045 (3)	-0.001 (2)	0.024 (2)	-0.005 (2)
C15	0.029 (2)	0.032 (3)	0.030 (2)	-0.0031 (18)	0.0144 (19)	-0.0032 (18)
C16	0.026 (2)	0.040 (3)	0.048 (3)	-0.008 (2)	0.011 (2)	0.003 (2)
C17	0.045 (3)	0.042 (3)	0.064 (3)	-0.017 (2)	0.021 (3)	0.005 (3)
C18	0.043 (3)	0.035 (3)	0.050 (3)	-0.004 (2)	0.016 (2)	0.009 (2)
C19	0.029 (2)	0.036 (3)	0.037 (2)	-0.002 (2)	0.012 (2)	-0.003 (2)
C20	0.026 (2)	0.034 (3)	0.029 (2)	-0.0074 (18)	0.0129 (18)	-0.0057 (19)

*Geometric parameters (Å, °)*

Mo1—S5	2.4134 (11)	F6—C4	1.339 (5)
Mo1—S1	2.4179 (11)	F7—C7	1.312 (6)
Mo1—S3	2.4391 (10)	F8—C7	1.324 (6)
Mo1—S2	2.4420 (11)	F9—C7	1.321 (6)
Mo1—S6	2.4461 (11)	F7A—C7	1.322 (10)
Mo1—S4	2.4571 (11)	F8A—C7	1.300 (10)
Mo1—Co3	2.6320 (6)	F9A—C7	1.324 (9)
Mo1—Co1	2.7224 (7)	F10—C8	1.333 (7)
Mo1—Co2	2.8058 (7)	F11—C8	1.332 (7)
Co1—C10	1.840 (5)	F12—C8	1.336 (7)
Co1—C9	1.842 (6)	F10A—C8	1.341 (12)
Co1—S1	2.2247 (12)	F11A—C8	1.312 (12)
Co1—S2	2.2414 (13)	F12A—C8	1.329 (12)



Co2—C12	1.825 (5)	O1—C9	1.127 (7)
Co2—C11	1.827 (5)	O2—C10	1.125 (6)
Co2—C2	1.970 (4)	O3—C11	1.130 (5)
Co2—C1	2.010 (4)	O4—C12	1.122 (5)
Co2—S3	2.2556 (13)	O5—C13	1.131 (5)
Co2—S4	2.7671 (11)	O6—C14	1.133 (6)
Co3—C13	1.796 (5)	C1—C2	1.439 (6)
Co3—C14	1.803 (5)	C1—C3	1.494 (6)
Co3—S4	2.2338 (12)	C2—C4	1.528 (7)
Co3—S5	2.2395 (11)	C5—C6	1.335 (6)
Co3—S6	2.2749 (13)	C5—C7	1.509 (6)
S1—C20	1.782 (4)	C6—C8	1.524 (6)
S2—C5	1.775 (4)	C15—C16	1.383 (6)
S3—C6	1.770 (4)	C15—C20	1.396 (6)
S4—C2	1.777 (4)	C16—C17	1.377 (7)
S5—C1	1.801 (4)	C16—H16A	0.9500
S6—C15	1.779 (4)	C17—C18	1.390 (7)
F1—C3	1.341 (5)	C17—H17A	0.9500
F2—C3	1.344 (5)	C18—C19	1.381 (6)
F3—C3	1.339 (5)	C18—H18A	0.9500
F4—C4	1.324 (5)	C19—C20	1.389 (6)
F5—C4	1.340 (6)	C19—H19A	0.9500
S5—Mo1—S1	88.52 (4)	C2—S4—Co3	102.26 (15)
S5—Mo1—S3	84.34 (4)	C2—S4—Mo1	99.62 (14)
S1—Mo1—S3	92.75 (4)	Co3—S4—Mo1	68.07 (3)
S5—Mo1—S2	163.43 (4)	C2—S4—Co2	45.16 (13)
S1—Mo1—S2	101.96 (4)	Co3—S4—Co2	111.42 (4)
S3—Mo1—S2	82.39 (4)	Mo1—S4—Co2	64.65 (3)
S5—Mo1—S6	103.47 (4)	C1—S5—Co3	102.78 (13)
S1—Mo1—S6	83.85 (4)	C1—S5—Mo1	95.79 (14)
S3—Mo1—S6	171.36 (4)	Co3—S5—Mo1	68.78 (3)
S2—Mo1—S6	90.52 (4)	C15—S6—Co3	104.69 (14)
S5—Mo1—S4	76.17 (4)	C15—S6—Mo1	106.48 (13)
S1—Mo1—S4	147.71 (4)	Co3—S6—Mo1	67.65 (3)
S3—Mo1—S4	113.36 (4)	C2—C1—C3	124.1 (4)
S2—Mo1—S4	100.13 (4)	C2—C1—S5	116.8 (3)
S6—Mo1—S4	72.66 (4)	C3—C1—S5	110.6 (3)
S5—Mo1—Co3	52.48 (3)	C2—C1—Co2	67.3 (2)
S1—Mo1—Co3	96.23 (3)	C3—C1—Co2	124.2 (3)
S3—Mo1—Co3	135.41 (3)	S5—C1—Co2	106.8 (2)
S2—Mo1—Co3	137.11 (3)	C1—C2—C4	124.4 (4)
S6—Mo1—Co3	53.08 (3)	C1—C2—S4	114.4 (3)
S4—Mo1—Co3	51.93 (3)	C4—C2—S4	115.3 (3)
S5—Mo1—Co1	137.65 (3)	C1—C2—Co2	70.3 (2)
S1—Mo1—Co1	50.87 (3)	C4—C2—Co2	126.8 (3)
S3—Mo1—Co1	86.08 (3)	S4—C2—Co2	95.1 (2)
S2—Mo1—Co1	51.09 (3)	F3—C3—F1	106.5 (3)

S6—Mo1—Co1	85.61 (3)	F3—C3—F2	106.4 (4)
S4—Mo1—Co1	144.34 (3)	F1—C3—F2	106.0 (3)
Co3—Mo1—Co1	131.93 (2)	F3—C3—C1	114.4 (4)
S5—Mo1—Co2	71.40 (3)	F1—C3—C1	111.2 (4)
S1—Mo1—Co2	138.35 (3)	F2—C3—C1	111.9 (4)
S3—Mo1—Co2	50.35 (3)	F4—C4—F6	106.2 (4)
S2—Mo1—Co2	92.44 (3)	F4—C4—F5	107.4 (4)
S6—Mo1—Co2	135.42 (3)	F6—C4—F5	107.0 (4)
S4—Mo1—Co2	63.03 (3)	F4—C4—C2	113.9 (4)
Co3—Mo1—Co2	99.20 (2)	F6—C4—C2	110.4 (4)
Co1—Mo1—Co2	128.84 (2)	F5—C4—C2	111.5 (4)
C10—Co1—C9	98.4 (3)	C6—C5—C7	126.2 (4)
C10—Co1—S1	107.95 (16)	C6—C5—S2	121.5 (3)
C9—Co1—S1	109.32 (18)	C7—C5—S2	112.3 (3)
C10—Co1—S2	111.11 (17)	C5—C6—C8	124.2 (4)
C9—Co1—S2	113.2 (2)	C5—C6—S3	122.6 (3)
S1—Co1—S2	115.44 (5)	C8—C6—S3	113.3 (3)
C10—Co1—Mo1	128.61 (18)	F7—C7—F9	108.1 (5)
C9—Co1—Mo1	132.8 (2)	F8A—C7—F7A	105.8 (10)
S1—Co1—Mo1	57.46 (3)	F7—C7—F8	105.8 (5)
S2—Co1—Mo1	57.97 (3)	F9—C7—F8	105.4 (5)
C12—Co2—C11	96.3 (2)	F8A—C7—F9A	107.0 (9)
C12—Co2—C2	110.5 (2)	F7A—C7—F9A	105.6 (10)
C11—Co2—C2	104.60 (18)	F8A—C7—C5	113.3 (6)
C12—Co2—C1	97.04 (18)	F7—C7—C5	112.5 (4)
C11—Co2—C1	146.99 (18)	F9—C7—C5	112.2 (4)
C2—Co2—C1	42.40 (16)	F7A—C7—C5	110.7 (6)
C12—Co2—S3	100.76 (17)	F8—C7—C5	112.3 (4)
C11—Co2—S3	103.81 (15)	F9A—C7—C5	113.8 (6)
C2—Co2—S3	134.51 (14)	F11A—C8—F12A	105.5 (11)
C1—Co2—S3	103.14 (13)	F11—C8—F10	107.2 (5)
C12—Co2—S4	148.89 (16)	F11—C8—F12	107.0 (6)
C11—Co2—S4	86.51 (14)	F10—C8—F12	105.6 (6)
C2—Co2—S4	39.76 (13)	F11A—C8—F10A	105.2 (11)
C1—Co2—S4	66.97 (12)	F12A—C8—F10A	106.5 (11)
S3—Co2—S4	108.66 (4)	F11A—C8—C6	115.3 (9)
C12—Co2—Mo1	154.70 (16)	F12A—C8—C6	111.9 (9)
C11—Co2—Mo1	99.65 (15)	F11—C8—C6	111.6 (5)
C2—Co2—Mo1	84.29 (13)	F10—C8—C6	112.1 (5)
C1—Co2—Mo1	79.96 (12)	F12—C8—C6	112.9 (5)
S3—Co2—Mo1	56.37 (3)	F10A—C8—C6	111.8 (9)
S4—Co2—Mo1	52.32 (3)	O1—C9—Co1	178.5 (8)
C13—Co3—C14	94.7 (2)	O2—C10—Co1	177.0 (6)
C13—Co3—S4	91.03 (14)	O3—C11—Co2	177.4 (4)
C14—Co3—S4	174.25 (15)	O4—C12—Co2	176.0 (5)
C13—Co3—S5	118.60 (16)	O5—C13—Co3	176.9 (4)
C14—Co3—S5	92.28 (15)	O6—C14—Co3	177.6 (5)
S4—Co3—S5	84.38 (4)	C16—C15—C20	120.3 (4)

C13—Co3—S6	124.00 (15)	C16—C15—S6	118.8 (3)
C14—Co3—S6	97.07 (16)	C20—C15—S6	120.9 (3)
S4—Co3—S6	80.22 (4)	C17—C16—C15	119.5 (4)
S5—Co3—S6	115.38 (4)	C17—C16—H16A	120.2
C13—Co3—Mo1	150.72 (14)	C15—C16—H16A	120.2
C14—Co3—Mo1	114.26 (15)	C16—C17—C18	120.8 (4)
S4—Co3—Mo1	60.00 (3)	C16—C17—H17A	119.6
S5—Co3—Mo1	58.74 (3)	C18—C17—H17A	119.6
S6—Co3—Mo1	59.27 (3)	C19—C18—C17	119.7 (4)
C20—S1—Co1	98.78 (14)	C19—C18—H18A	120.1
C20—S1—Mo1	106.69 (15)	C17—C18—H18A	120.1
Co1—S1—Mo1	71.67 (4)	C18—C19—C20	120.1 (4)
C5—S2—Co1	97.05 (15)	C18—C19—H19A	120.0
C5—S2—Mo1	106.85 (14)	C20—C19—H19A	120.0
Co1—S2—Mo1	70.94 (3)	C19—C20—C15	119.6 (4)
C6—S3—Co2	101.70 (15)	C19—C20—S1	118.7 (3)
C6—S3—Mo1	106.61 (14)	C15—C20—S1	121.8 (3)
Co2—S3—Mo1	73.29 (3)		
Co3—S5—C1—C2	20.2 (3)	Co2—S3—C6—C5	79.7 (4)
Mo1—S5—C1—C2	-49.3 (3)	Mo1—S3—C6—C5	3.9 (4)
Co3—S5—C1—C3	-129.4 (3)	Co2—S3—C6—C8	-101.5 (3)
Mo1—S5—C1—C3	161.1 (3)	Mo1—S3—C6—C8	-177.3 (3)
Co3—S5—C1—Co2	92.78 (16)	C6—C5—C7—F8A	153.6 (10)
Mo1—S5—C1—Co2	23.27 (17)	S2—C5—C7—F8A	-26.0 (11)
C3—C1—C2—C4	4.9 (7)	C6—C5—C7—F7	-37.8 (8)
S5—C1—C2—C4	-140.2 (4)	S2—C5—C7—F7	142.6 (5)
Co2—C1—C2—C4	121.8 (4)	C6—C5—C7—F9	84.4 (7)
C3—C1—C2—S4	156.5 (3)	S2—C5—C7—F9	-95.2 (5)
S5—C1—C2—S4	11.4 (4)	C6—C5—C7—F7A	-87.7 (11)
Co2—C1—C2—S4	-86.6 (3)	S2—C5—C7—F7A	92.7 (10)
C3—C1—C2—Co2	-116.9 (4)	C6—C5—C7—F8	-157.0 (6)
S5—C1—C2—Co2	98.0 (3)	S2—C5—C7—F8	23.4 (6)
Co3—S4—C2—C1	-37.5 (3)	C6—C5—C7—F9A	31.1 (11)
Mo1—S4—C2—C1	32.0 (3)	S2—C5—C7—F9A	-148.5 (9)
Co2—S4—C2—C1	70.6 (3)	C5—C6—C8—F11A	45.7 (14)
Co3—S4—C2—C4	116.8 (3)	S3—C6—C8—F11A	-133.1 (14)
Mo1—S4—C2—C4	-173.7 (3)	C5—C6—C8—F12A	-74.8 (13)
Co2—S4—C2—C4	-135.1 (4)	S3—C6—C8—F12A	106.4 (13)
Co3—S4—C2—Co2	-108.11 (14)	C5—C6—C8—F11	78.1 (8)
Mo1—S4—C2—Co2	-38.65 (16)	S3—C6—C8—F11	-100.7 (7)
C2—C1—C3—F3	36.6 (6)	C5—C6—C8—F10	-161.6 (7)
S5—C1—C3—F3	-176.6 (3)	S3—C6—C8—F10	19.6 (8)
Co2—C1—C3—F3	-47.6 (5)	C5—C6—C8—F12	-42.4 (9)
C2—C1—C3—F1	157.2 (4)	S3—C6—C8—F12	138.8 (7)
S5—C1—C3—F1	-55.9 (4)	C5—C6—C8—F10A	165.8 (14)
Co2—C1—C3—F1	73.1 (5)	S3—C6—C8—F10A	-13.0 (14)
C2—C1—C3—F2	-84.5 (5)	Co3—S6—C15—C16	-108.6 (3)

S5—C1—C3—F2	62.4 (4)	Mo1—S6—C15—C16	-179.2 (3)
Co2—C1—C3—F2	-168.6 (3)	Co3—S6—C15—C20	71.1 (4)
C1—C2—C4—F4	-69.7 (6)	Mo1—S6—C15—C20	0.5 (4)
S4—C2—C4—F4	138.9 (3)	C20—C15—C16—C17	-2.5 (7)
Co2—C2—C4—F4	20.4 (6)	S6—C15—C16—C17	177.3 (4)
C1—C2—C4—F6	170.9 (4)	C15—C16—C17—C18	2.0 (8)
S4—C2—C4—F6	19.5 (5)	C16—C17—C18—C19	-0.9 (8)
Co2—C2—C4—F6	-99.0 (4)	C17—C18—C19—C20	0.3 (7)
C1—C2—C4—F5	52.1 (6)	C18—C19—C20—C15	-0.8 (7)
S4—C2—C4—F5	-99.3 (4)	C18—C19—C20—S1	177.5 (4)
Co2—C2—C4—F5	142.3 (3)	C16—C15—C20—C19	1.9 (6)
Co1—S2—C5—C6	73.6 (4)	S6—C15—C20—C19	-177.9 (3)
Mo1—S2—C5—C6	1.4 (4)	C16—C15—C20—S1	-176.3 (3)
Co1—S2—C5—C7	-106.8 (3)	S6—C15—C20—S1	3.9 (5)
Mo1—S2—C5—C7	-178.9 (3)	Co1—S1—C20—C19	-111.0 (3)
C7—C5—C6—C8	-2.0 (7)	Mo1—S1—C20—C19	175.6 (3)
S2—C5—C6—C8	177.6 (3)	Co1—S1—C20—C15	67.2 (4)
C7—C5—C6—S3	176.7 (4)	Mo1—S1—C20—C15	-6.2 (4)
S2—C5—C6—S3	-3.7 (6)		

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C17—H17A...O6 <sup>i</sup>	0.95	2.57	3.353 (7)	140
C17—H17A...F11 <sup>ii</sup>	0.95	2.62	3.461 (9)	148
C17—H17A...F10A <sup>ii</sup>	0.95	2.55	3.29 (2)	135

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