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# *trans*-Acetyldicarbonyl($\eta^5$-cyclopentadienyl)[tris(furan-2-yl)phosphane-$\kappa P$]-molybdenum(II)

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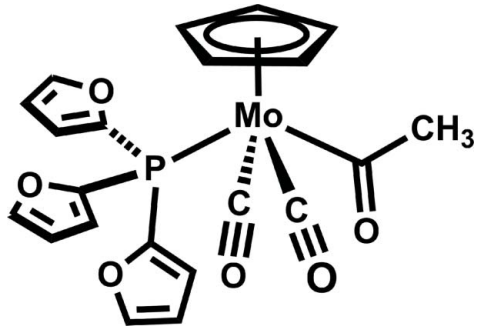
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.035; $wR$ factor = 0.075; data-to-parameter ratio = 17.3.

The title compound, $[Mo(C_5H_5)(C_2H_3O)(C_{12}H_9O_3P)(CO)_2]$, was prepared by reaction of $[Mo(C_5H_5)(CO)_3(CH_3)]$ with tris(furan-2-yl)phosphane. The $Mo^{II}$ atom exhibits a four-legged piano-stool coordination geometry with the acetyl and phosphine ligands *trans* to each other. The O atom of the acetyl ligand points down, away from the Cp ring. In the crystal, molecules form centrosymmetrical dimers *via* $\pi$–$\pi$ interactions between furyl rings [the centroid–centroid distance is 3.396 (4) Å]. The dimers are linked by C—H···O hydrogen bonds into layers parallel to (100).

## Related literature

For synthetic details for a related complex, see: Gladysz *et al.* (1979). For related structures, see: Churchill & Fennessey (1968); Barnett *et al.* (1972); Michelini-Rodriguez *et al.* (1993); Adams *et al.* (1997, 2000); Whited *et al.* (2012).




## Experimental

### Crystal data

$[Mo(C_5H_5)(C_2H_3O)(C_{12}H_9O_3P)(CO)_2]$
$M_r$ = 492.28
Monoclinic, $P2_1/c$
$a$ = 8.050 (2) Å
$b$ = 15.762 (4) Å
$c$ = 16.073 (4) Å
$\beta$ = 102.852 (8)°
$V$ = 1988.4 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.78 mm$^{-1}$
$T$ = 173 K
0.24 × 0.17 × 0.15 mm

### Data collection

Rigaku XtaLAB mini diffractometer
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
$T_{min}$ = 0.709, $T_{max}$ = 0.890
16222 measured reflections
4539 independent reflections
3799 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.044

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.075
$S$ = 1.06
4539 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.52 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Mo1—P1 | 2.4189 (8) | Mo1—C7 | 2.359 (3) |
| Mo1—C1 | 2.253 (4) | Mo1—C8 | 2.374 (4) |
| Mo1—C3 | 1.968 (3) | Mo1—C9 | 2.382 (4) |
| Mo1—C4 | 1.982 (3) | O1—C1 | 1.227 (4) |
| Mo1—C5 | 2.341 (4) | O2—C3 | 1.150 (4) |
| Mo1—C6 | 2.332 (4) | O3—C4 | 1.148 (4) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8···O1$^{i}$ | 1.00 | 2.38 | 3.324 (4) | 158 |
| C11—H11···O1$^{i}$ | 0.95 | 2.40 | 3.166 (5) | 137 |

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

Data collection: *CrystalClear* (Rigaku Americas and Rigaku, 2011); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku Americas and Rigaku, 2010); 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: KQ2007).

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# supporting information

*Acta Cryst.* (2013). E**69**, m475–m476 [doi:10.1107/S160053681302059X]

# *trans*-Acetyldicarbonyl($\eta^5$-cyclopentadienyl)[tris(furan-2-yl)phosphane-$\kappa P$]molybdenum(II)

**Matthew T. Whited, Julia G. Bakker-Arkema, Julia E. Greenwald, Lucas A. Morrill and Daron E. Janzen**

## S1. Comment

Synthesis of the title complex, $[Mo(C_5H_5)(C_2H_3O)(CO)_2(C_{12}H_{12}O_3P)]$ (**I**), has not previously been reported, though several analogues containing various phosphine ligands have been reported and their reactivity studied (Adams *et al.*, 1997; Barnett *et al.*, 1972). The most closely related complexes, for which structural information is available, contain a triphenylphosphine or methyldiphenylphosphine ligand (Churchill & Fennessey, 1968; Whited *et al.*, 2012).

The molecular structure of **I** consists of a Mo(II) atom coordinated to a cyclopentadienyl ring in an $\eta^5$ fashion, two CO ligands, one tris(furan-2-yl)phosphane ligand, and one acetyl ligand (Fig. 1, Table 1). The orientation of the CO ligands can be described as *trans* (Fig. 2). The Mo—Cp centroid distance is 2.029 (2) Å.

In the crystal, the molecules of **I** form centrosymmetrical dimers *via* the $\pi$—$\pi$ interactions between furyl rings (the centroid-to-centroid distance is 3.396 (4) Å, Fig. 3).

There are several particularly short intermolecular distances involving H atoms. One short contact (2.38 Å) is present between O1 of the acetyl carbonyl on one Mo complex and H8 of a Cp ring on another (Table 2). Another short contact (2.40 Å) involves O1 of the acetyl group of one Mo complex and H11 of a furyl group on another (Table 2). These contacts between the acetyl carbonyl and hydrogen atoms may contribute to the unusual geometry adopted by the acetyl ligand, where the carbonyl points down, away from the Cp ring. In related structures reported by this laboratory (Whited *et al.*, 2012) and others (Churchill & Fennessey, 1968; Michelini-Rodriguez *et al.*, 1993; Adams *et al.*, 1997, 2000), the carbonyl points up toward the Cp ring. These hydrogen-bonding interactions lead to the formation of layers parallel to (100), as shown in Fig. 4.

## S2. Experimental

**$CpMo(CO)_3(CH_3)$**. This compound was prepared by a modification of the method used by Gladysz *et al.* (1979), as previously reported by Whited *et al.* (2012).

**$CpMo(CO)_2(P(2\text{-}Fur)_3)(COCH_3)$ (I)**. In an inert-atmosphere glove box, $CpMo(CO)_3(CH_3)$ (30.6 mg, 0.118 mmol) was dissolved in 2 ml acetonitrile. In a separate vial, tris(furan-2-yl)phosphane (42.0 mg, 0.181 mmol) was dissolved in 2 ml acetonitrile. The vials were combined and the resulting solution was stirred for 1 week. Solvent was removed *in vacuo*, leaving an orange oil that was triturated with pentane (5 mL) and isolated by filtration to afford the desired product in pure form as a yellow powder (21.6 mg, 37.2%), as confirmed by IR and NMR ($^1$H, $^{13}$C, and $^{31}$P) spectral analyses. Crystalline material was obtained as yellow-orange prisms by vapor diffusion of pentane into a concentrated solution of **I** in diethyl ether at 233 K.

### S3. Refinement

H-atoms were treated in calculated positions and refined in the riding model approximation with distances of C—H = 0.95, 1.00 and 0.98 Å for the furanyl, cyclopentadienyl and methyl groups, respectively, and with $U_{iso}$(H) = $k$×$U_{eq}$(C), $k$ = 1.2 for furanyl and cyclopentadienyl groups and 1.5 for methyl groups. Methyl group H atoms were allowed to rotate in order to find the best rotameric conformation. The maximum and minimum electron densities in the final difference Fourier map are located 0.98 and 0.77 Å, respectively, from atom Mo1.

Eight low-angle reflections were rejected from the high-quality data set due to the arrangement of the instrument with a conservatively sized beam stop and a fixed-position detector. The large number of reflections in this data set (and the Fourier-transform relationship of intensities to atoms) ensures that no particular bias was thereby introduced into this routine structure determination.

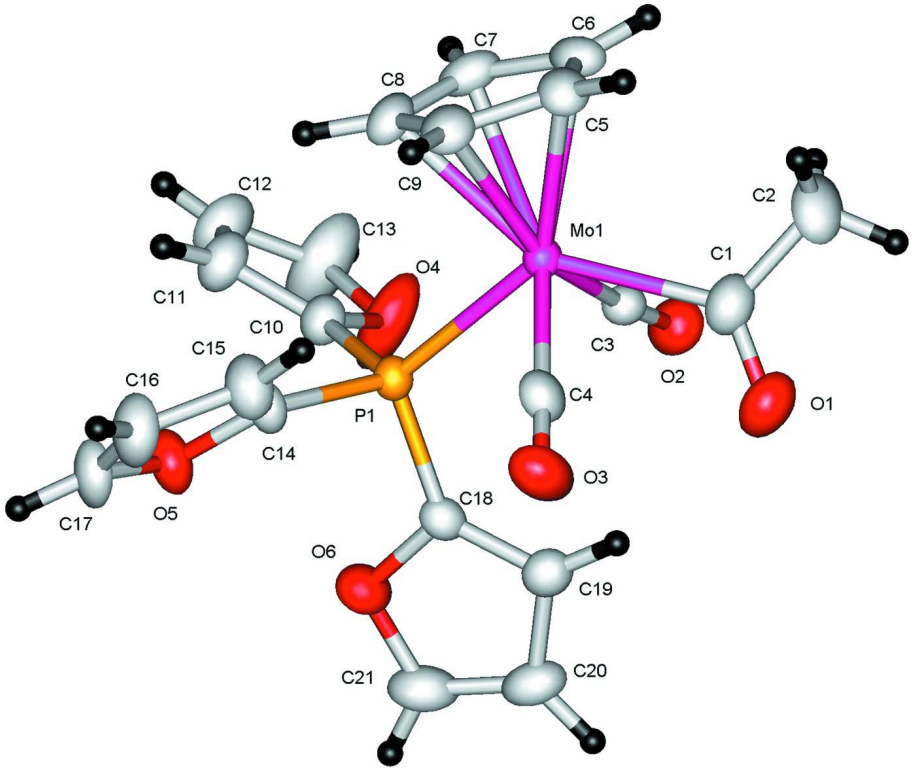


**Figure 1**

Molecular structure of **I** (50% probability ellipsoids for non-H atoms). H atoms are presented as small spheres of arbitrary radius.

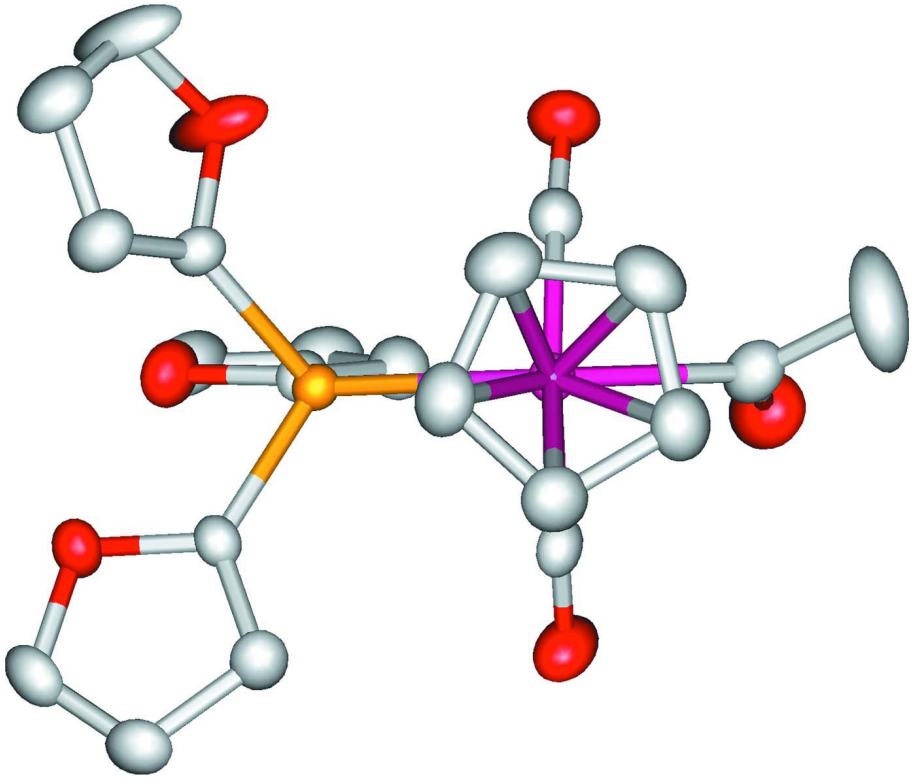

**Figure 2**

View of **I** perpendicular to Cp least-squares plane showing *trans* CO orientation.

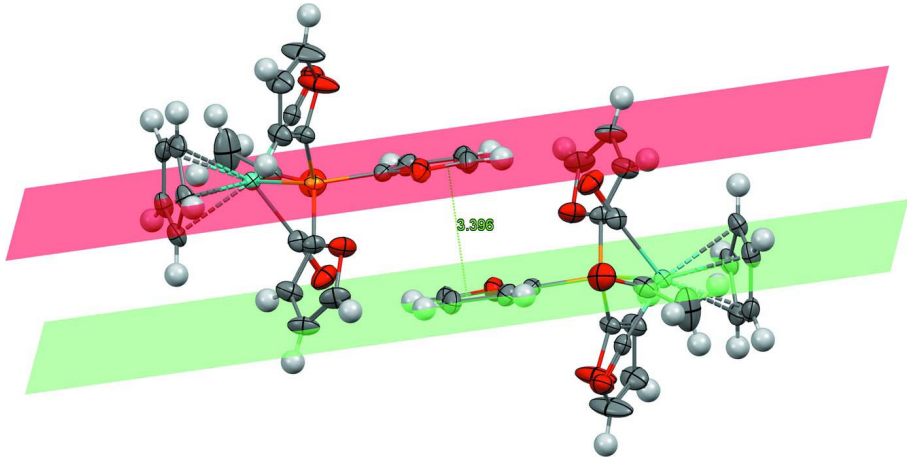


**Figure 3**

The centrosymmetrical dimers of **I**.

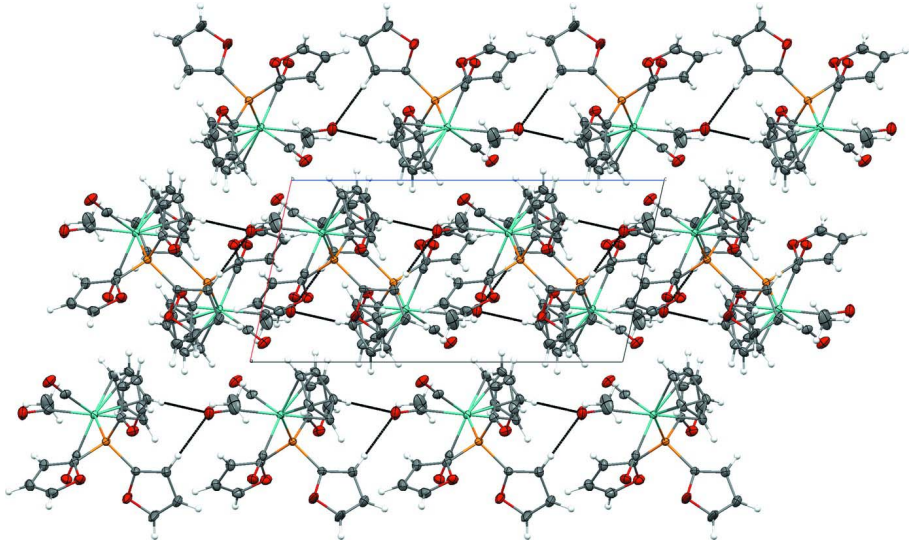

**Figure 4**

Crystal packing of **I** along the *b* axis showing the layers parallel to (100). Dashed lines indicate the intermolecular C—H···O hydrogen bonds.

### *trans*-Acetyldicarbonyl($\eta^5$-cyclopentadienyl)[tris(furan-2-yl)phosphane-$\kappa P$]molybdenum(II)

*Crystal data*

$[Mo(C_5H_5)(C_2H_3O)(C_{12}H_9O_3P)(CO)_2]$
$M_r$ = 492.28
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 8.050 (2) Å
$b$ = 15.762 (4) Å
$c$ = 16.073 (4) Å
$\beta$ = 102.852 (8)°
$V$ = 1988.4 (9) Å$^3$
$Z$ = 4
$F(000)$ = 992.00
$D_x$ = 1.644 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71075 Å
Cell parameters from 13392 reflections
$\theta$ = 3.2–27.6°
$\mu$ = 0.78 mm$^{-1}$
$T$ = 173 K
Prism, orange
0.24 × 0.17 × 0.15 mm

*Data collection*

Rigaku XtaLAB mini diffractometer
Detector resolution: 6.827 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
$T_{min}$ = 0.709, $T_{max}$ = 0.890
16222 measured reflections
4539 independent reflections
3799 reflections with $F^2 > 2\sigma(F^2)$
$R_{int}$ = 0.044
$\theta_{max}$ = 27.5°
$h$ = −10→9
$k$ = −20→20
$l$ = −20→20

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.075
$S$ = 1.06
4539 reflections
263 parameters
0 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

$w = 1/[\sigma^2(F_o^2) + (0.025P)^2 + 1.9823P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.55$ e Å$^{-3}$
$\Delta\rho_{min} = -0.52$ e Å$^{-3}$

*Special details*

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

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Mo1 | 0.28931 (3) | 0.203772 (14) | 0.114671 (14) | 0.01996 (7) |
| P1 | 0.43789 (8) | 0.33427 (4) | 0.16296 (4) | 0.02053 (15) |
| O1 | 0.2805 (4) | 0.17390 (16) | −0.07804 (14) | 0.0472 (6) |
| O2 | 0.6441 (3) | 0.15779 (14) | 0.07963 (13) | 0.0357 (5) |
| O3 | 0.1064 (3) | 0.33025 (14) | −0.02625 (14) | 0.0419 (6) |
| O4 | 0.7480 (3) | 0.2905 (2) | 0.25444 (14) | 0.0615 (9) |
| O5 | 0.3794 (3) | 0.49098 (13) | 0.22768 (13) | 0.0345 (5) |
| O6 | 0.6466 (3) | 0.45252 (13) | 0.11535 (13) | 0.0334 (5) |
| C1 | 0.2624 (4) | 0.1388 (2) | −0.01250 (19) | 0.0338 (7) |
| C2 | 0.2310 (7) | 0.0460 (3) | −0.0174 (3) | 0.0706 (14) |
| C3 | 0.5144 (4) | 0.17806 (17) | 0.09207 (16) | 0.0243 (6) |
| C4 | 0.1775 (4) | 0.28439 (17) | 0.02493 (18) | 0.0282 (7) |
| C5 | 0.0773 (4) | 0.11426 (19) | 0.14393 (19) | 0.0331 (7) |
| C6 | 0.2380 (4) | 0.08037 (19) | 0.18492 (19) | 0.0354 (7) |
| C7 | 0.3150 (4) | 0.1382 (2) | 0.24888 (18) | 0.0356 (7) |
| C8 | 0.2035 (4) | 0.2073 (2) | 0.24670 (18) | 0.0333 (7) |
| C9 | 0.0548 (4) | 0.19244 (19) | 0.18202 (19) | 0.0325 (7) |
| C10 | 0.6004 (4) | 0.32891 (18) | 0.26045 (17) | 0.0247 (6) |
| C11 | 0.6050 (4) | 0.3458 (2) | 0.34274 (18) | 0.0342 (7) |
| C12 | 0.7657 (5) | 0.3184 (3) | 0.39118 (19) | 0.0423 (9) |
| C13 | 0.8462 (5) | 0.2861 (4) | 0.3364 (3) | 0.0703 (15) |
| C14 | 0.3049 (4) | 0.41841 (17) | 0.18893 (17) | 0.0254 (6) |
| C15 | 0.1340 (4) | 0.4247 (2) | 0.17555 (19) | 0.0354 (7) |
| C16 | 0.0987 (5) | 0.5054 (2) | 0.2072 (2) | 0.0406 (8) |
| C17 | 0.2480 (5) | 0.5421 (2) | 0.2373 (2) | 0.0393 (8) |
| C18 | 0.5519 (4) | 0.38037 (17) | 0.08986 (16) | 0.0237 (6) |
| C19 | 0.5672 (4) | 0.35793 (19) | 0.01093 (18) | 0.0315 (7) |
| C20 | 0.6773 (4) | 0.4186 (2) | −0.0150 (2) | 0.0374 (8) |
| C21 | 0.7201 (4) | 0.4734 (2) | 0.0491 (2) | 0.0392 (8) |
| H2A | 0.1192 | 0.0339 | −0.0055 | 0.0847* |
| H2B | 0.3196 | 0.0170 | 0.0247 | 0.0847* |
| H2C | 0.2336 | 0.0256 | −0.0747 | 0.0847* |
| H5 | −0.0110 | 0.0843 | 0.1003 | 0.0397* |
| H6 | 0.2812 | 0.0224 | 0.1758 | 0.0425* |
| H7 | 0.4236 | 0.1288 | 0.2922 | 0.0427* |
| H8 | 0.2210 | 0.2559 | 0.2877 | 0.0399* |
| H9 | −0.0506 | 0.2280 | 0.1698 | 0.0390* |

| | | | | |
|---|---|---|---|---|
| H11 | 0.5168 | 0.3715 | 0.3646 | 0.0410* |
| H12 | 0.8064 | 0.3227 | 0.4512 | 0.0507* |
| H13 | 0.9576 | 0.2626 | 0.3511 | 0.0844* |
| H15 | 0.0529 | 0.3833 | 0.1500 | 0.0425* |
| H16 | −0.0105 | 0.5285 | 0.2068 | 0.0487* |
| H17 | 0.2620 | 0.5969 | 0.2624 | 0.0471* |
| H19 | 0.5147 | 0.3108 | −0.0213 | 0.0378* |
| H20 | 0.7128 | 0.4196 | −0.0675 | 0.0449* |
| H21 | 0.7925 | 0.5210 | 0.0490 | 0.0470* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Mo1 | 0.01978 (12) | 0.02049 (12) | 0.01972 (11) | −0.00095 (9) | 0.00462 (8) | −0.00145 (9) |
| P1 | 0.0182 (4) | 0.0218 (4) | 0.0205 (4) | 0.0010 (3) | 0.0019 (3) | −0.0024 (3) |
| O1 | 0.0551 (16) | 0.0590 (16) | 0.0275 (12) | 0.0048 (13) | 0.0091 (11) | −0.0021 (11) |
| O2 | 0.0297 (12) | 0.0416 (13) | 0.0372 (12) | 0.0077 (10) | 0.0102 (10) | 0.0013 (10) |
| O3 | 0.0439 (14) | 0.0342 (12) | 0.0386 (13) | −0.0032 (11) | −0.0101 (11) | 0.0062 (10) |
| O4 | 0.0363 (14) | 0.120 (3) | 0.0239 (11) | 0.0383 (15) | −0.0028 (10) | −0.0109 (13) |
| O5 | 0.0311 (11) | 0.0289 (11) | 0.0408 (12) | 0.0030 (9) | 0.0017 (10) | −0.0134 (9) |
| O6 | 0.0317 (12) | 0.0309 (11) | 0.0359 (12) | −0.0088 (9) | 0.0038 (9) | −0.0006 (9) |
| C1 | 0.0271 (16) | 0.0452 (19) | 0.0288 (16) | −0.0002 (14) | 0.0053 (13) | −0.0068 (14) |
| C2 | 0.108 (4) | 0.050 (3) | 0.065 (3) | −0.035 (3) | 0.044 (3) | −0.029 (2) |
| C3 | 0.0289 (15) | 0.0229 (14) | 0.0211 (13) | −0.0022 (12) | 0.0057 (11) | 0.0016 (11) |
| C4 | 0.0254 (15) | 0.0255 (15) | 0.0310 (15) | −0.0065 (12) | 0.0003 (12) | −0.0062 (12) |
| C5 | 0.0334 (17) | 0.0321 (16) | 0.0370 (16) | −0.0103 (13) | 0.0148 (13) | −0.0029 (13) |
| C6 | 0.0445 (19) | 0.0270 (16) | 0.0406 (17) | 0.0012 (14) | 0.0218 (15) | 0.0086 (13) |
| C7 | 0.0347 (17) | 0.048 (2) | 0.0257 (15) | 0.0015 (15) | 0.0112 (13) | 0.0113 (14) |
| C8 | 0.0359 (17) | 0.0427 (18) | 0.0249 (14) | −0.0079 (15) | 0.0147 (13) | −0.0057 (13) |
| C9 | 0.0267 (15) | 0.0382 (17) | 0.0363 (16) | −0.0044 (13) | 0.0150 (13) | 0.0002 (13) |
| C10 | 0.0189 (13) | 0.0305 (15) | 0.0243 (14) | 0.0023 (11) | 0.0039 (11) | −0.0020 (11) |
| C11 | 0.0296 (16) | 0.0474 (19) | 0.0258 (15) | 0.0029 (14) | 0.0068 (13) | −0.0042 (13) |
| C12 | 0.0366 (18) | 0.064 (3) | 0.0228 (15) | 0.0043 (16) | −0.0011 (13) | 0.0006 (15) |
| C13 | 0.039 (2) | 0.138 (5) | 0.0272 (17) | 0.041 (3) | −0.0083 (16) | −0.006 (3) |
| C14 | 0.0267 (15) | 0.0216 (14) | 0.0265 (14) | 0.0027 (12) | 0.0028 (11) | −0.0060 (11) |
| C15 | 0.0245 (15) | 0.0375 (18) | 0.0432 (18) | 0.0015 (14) | 0.0052 (13) | −0.0118 (14) |
| C16 | 0.0329 (17) | 0.047 (2) | 0.0402 (18) | 0.0157 (15) | 0.0039 (14) | −0.0132 (15) |
| C17 | 0.047 (2) | 0.0330 (17) | 0.0368 (17) | 0.0138 (15) | 0.0060 (15) | −0.0141 (14) |
| C18 | 0.0226 (14) | 0.0218 (13) | 0.0249 (13) | −0.0017 (11) | 0.0012 (11) | 0.0012 (11) |
| C19 | 0.0364 (17) | 0.0312 (16) | 0.0269 (15) | 0.0001 (14) | 0.0069 (13) | 0.0021 (12) |
| C20 | 0.0359 (17) | 0.0452 (19) | 0.0335 (16) | 0.0007 (15) | 0.0124 (14) | 0.0131 (15) |
| C21 | 0.0298 (17) | 0.0414 (19) | 0.0445 (19) | −0.0075 (15) | 0.0045 (14) | 0.0147 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Mo1—P1 | 2.4189 (8) | C10—C11 | 1.342 (4) |
| Mo1—C1 | 2.253 (4) | C11—C12 | 1.421 (5) |
| Mo1—C3 | 1.968 (3) | C12—C13 | 1.307 (6) |

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|---|---|---|---|
| Mo1—C4 | 1.982 (3) | C14—C15 | 1.348 (5) |
| Mo1—C5 | 2.341 (4) | C15—C16 | 1.422 (5) |
| Mo1—C6 | 2.332 (4) | C16—C17 | 1.325 (5) |
| Mo1—C7 | 2.359 (3) | C18—C19 | 1.349 (4) |
| Mo1—C8 | 2.374 (4) | C19—C20 | 1.427 (5) |
| Mo1—C9 | 2.382 (4) | C20—C21 | 1.330 (5) |
| P1—C10 | 1.806 (3) | C2—H2A | 0.980 |
| P1—C14 | 1.810 (3) | C2—H2B | 0.980 |
| P1—C18 | 1.797 (3) | C2—H2C | 0.980 |
| O1—C1 | 1.227 (4) | C5—H5 | 1.000 |
| O2—C3 | 1.150 (4) | C6—H6 | 1.000 |
| O3—C4 | 1.148 (4) | C7—H7 | 1.000 |
| O4—C10 | 1.356 (4) | C8—H8 | 1.000 |
| O4—C13 | 1.379 (4) | C9—H9 | 1.000 |
| O5—C14 | 1.375 (4) | C11—H11 | 0.950 |
| O5—C17 | 1.365 (4) | C12—H12 | 0.950 |
| O6—C18 | 1.380 (4) | C13—H13 | 0.950 |
| O6—C21 | 1.368 (5) | C15—H15 | 0.950 |
| C1—C2 | 1.484 (6) | C16—H16 | 0.950 |
| C5—C6 | 1.419 (5) | C17—H17 | 0.950 |
| C5—C9 | 1.406 (5) | C19—H19 | 0.950 |
| C6—C7 | 1.410 (5) | C20—H20 | 0.950 |
| C7—C8 | 1.406 (5) | C21—H21 | 0.950 |
| C8—C9 | 1.420 (4) | | |

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|---|---|---|---|
| P1···O3 | 3.573 (3) | C2···H5$^{xiii}$ | 2.8413 |
| O1···O2 | 3.428 (3) | C2···H11$^{i}$ | 3.5382 |
| O1···O3 | 3.041 (4) | C3···H9$^{iv}$ | 3.5348 |
| O1···C3 | 2.956 (4) | C3···H17$^{v}$ | 2.9114 |
| O1···C4 | 2.659 (4) | C4···H12$^{ii}$ | 3.4063 |
| O2···O4 | 3.453 (4) | C4···H13$^{ii}$ | 3.0478 |
| O2···C1 | 3.114 (4) | C4···H21$^{vi}$ | 3.3179 |
| O2···C18 | 3.597 (4) | C5···H2A$^{xiii}$ | 3.3681 |
| O2···C19 | 3.354 (4) | C5···H2C$^{xiii}$ | 3.3355 |
| O3···C1 | 3.258 (4) | C5···H12$^{ii}$ | 3.5118 |
| O3···C15 | 3.531 (4) | C5···H16$^{ix}$ | 2.9065 |
| O4···O6 | 3.373 (4) | C5···H17$^{ix}$ | 3.4107 |
| O4···C3 | 3.362 (4) | C6···H16$^{ix}$ | 2.9100 |
| O4···C18 | 3.105 (4) | C7···H16$^{ix}$ | 3.2069 |
| O5···O6 | 3.160 (4) | C7···H17$^{v}$ | 3.5114 |
| O5···C10 | 3.091 (4) | C8···H13$^{viii}$ | 2.9953 |
| O5···C11 | 3.234 (4) | C8···H16$^{ix}$ | 3.3813 |
| O5···C18 | 3.353 (4) | C9···H13$^{viii}$ | 3.1884 |
| O6···C10 | 3.124 (4) | C9···H16$^{ix}$ | 3.2067 |
| O6···C14 | 3.271 (4) | C9···H17$^{ix}$ | 3.2533 |
| C2···C3 | 3.294 (5) | C10···H6$^{vii}$ | 3.2903 |
| C2···C5 | 3.293 (6) | C11···H2B$^{vii}$ | 3.4072 |
| C2···C6 | 3.285 (6) | C11···H6$^{vii}$ | 2.9657 |

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|---|---|---|---|
| C3···C10 | 3.553 (4) | C11···H19$^{x}$ | 3.4790 |
| C3···C18 | 3.204 (4) | C12···H2B$^{vii}$ | 3.5370 |
| C3···C19 | 3.188 (5) | C12···H6$^{vii}$ | 3.3854 |
| C4···C14 | 3.356 (4) | C12···H19$^{x}$ | 3.3869 |
| C4···C15 | 3.355 (5) | C13···H8$^{iv}$ | 3.3152 |
| C4···C18 | 3.326 (4) | C13···H9$^{iv}$ | 3.1123 |
| C4···C19 | 3.398 (5) | C13···H17$^{v}$ | 3.3987 |
| C8···C14 | 3.597 (5) | C14···H20$^{vi}$ | 3.1976 |
| C11···C14 | 3.255 (4) | C15···H20$^{vi}$ | 3.3925 |
| O1···C8$^{i}$ | 3.324 (4) | C15···H21$^{viii}$ | 3.3930 |
| O1···C11$^{i}$ | 3.166 (5) | C16···H2C$^{x}$ | 3.4656 |
| O1···C13$^{ii}$ | 3.518 (5) | C16···H5$^{xii}$ | 3.5488 |
| O2···C2$^{iii}$ | 3.574 (5) | C16···H20$^{vi}$ | 3.2027 |
| O2···C5$^{iv}$ | 3.479 (4) | C16···H21$^{viii}$ | 3.1327 |
| O2···C9$^{iv}$ | 3.394 (4) | C17···H2C$^{x}$ | 3.2303 |
| O2···C12$^{i}$ | 3.405 (5) | C17···H7$^{vii}$ | 3.1047 |
| O2···C17$^{v}$ | 3.406 (4) | C17···H20$^{vi}$ | 2.8803 |
| O3···C13$^{ii}$ | 3.250 (5) | C18···H21$^{vi}$ | 3.5115 |
| O3···C21$^{vi}$ | 3.449 (4) | C19···H7$^{i}$ | 3.4546 |
| O4···C9$^{iv}$ | 3.335 (5) | C19···H21$^{vi}$ | 3.4225 |
| O5···C6$^{vii}$ | 3.395 (4) | C20···H7$^{i}$ | 3.3946 |
| O5···C7$^{vii}$ | 3.342 (4) | C20···H15$^{iv}$ | 3.5936 |
| O6···C20$^{vi}$ | 3.414 (4) | C21···H15$^{iv}$ | 3.1450 |
| C2···O2$^{iii}$ | 3.574 (5) | C21···H16$^{iv}$ | 3.0711 |
| C5···O2$^{viii}$ | 3.479 (4) | H2A···C2$^{xiii}$ | 3.1828 |
| C5···C16$^{ix}$ | 3.491 (5) | H2A···C5$^{xiii}$ | 3.3681 |
| C6···O5$^{v}$ | 3.395 (4) | H2A···H2A$^{xiii}$ | 2.2378 |
| C7···O5$^{v}$ | 3.342 (4) | H2A···H2B$^{xiii}$ | 3.5677 |
| C8···O1$^{x}$ | 3.324 (4) | H2A···H2C$^{xiii}$ | 3.4984 |
| C9···O2$^{viii}$ | 3.394 (4) | H2A···H5$^{xiii}$ | 2.4410 |
| C9···O4$^{viii}$ | 3.335 (5) | H2A···H12$^{v}$ | 3.4606 |
| C11···O1$^{x}$ | 3.166 (5) | H2A···H12$^{ii}$ | 3.3393 |
| C12···O2$^{x}$ | 3.405 (5) | H2B···O2$^{iii}$ | 3.2721 |
| C13···O1$^{xi}$ | 3.518 (5) | H2B···C11$^{v}$ | 3.4072 |
| C13···O3$^{xi}$ | 3.250 (5) | H2B···C12$^{v}$ | 3.5370 |
| C15···C21$^{viii}$ | 3.579 (4) | H2B···H2A$^{xiii}$ | 3.5677 |
| C16···C5$^{xii}$ | 3.491 (5) | H2B···H2B$^{iii}$ | 3.2227 |
| C16···C21$^{viii}$ | 3.543 (5) | H2B···H2C$^{iii}$ | 3.5712 |
| C17···O2$^{vii}$ | 3.406 (4) | H2B···H5$^{xiii}$ | 3.2452 |
| C18···C21$^{vi}$ | 3.595 (4) | H2B···H11$^{v}$ | 3.0188 |
| C19···C21$^{vi}$ | 3.515 (5) | H2B···H12$^{v}$ | 3.2762 |
| C20···O6$^{vi}$ | 3.414 (4) | H2C···O2$^{iii}$ | 3.0612 |
| C20···C21$^{vi}$ | 3.557 (5) | H2C···C5$^{xiii}$ | 3.3355 |
| C21···O3$^{vi}$ | 3.449 (4) | H2C···C16$^{i}$ | 3.4656 |
| C21···C15$^{iv}$ | 3.579 (4) | H2C···C17$^{i}$ | 3.2303 |
| C21···C16$^{iv}$ | 3.543 (5) | H2C···H2A$^{xiii}$ | 3.4984 |
| C21···C18$^{vi}$ | 3.595 (4) | H2C···H2B$^{iii}$ | 3.5712 |
| C21···C19$^{vi}$ | 3.515 (5) | H2C···H5$^{xiii}$ | 2.4602 |

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|---|---|---|---|
| C21···C20$^{vi}$ | 3.557 (5) | H2C···H11$^{i}$ | 3.1246 |
| Mo1···H2A | 3.4052 | H2C···H17$^{i}$ | 3.3020 |
| Mo1···H2B | 3.3128 | H5···O2$^{viii}$ | 2.9591 |
| Mo1···H15 | 3.5256 | H5···C2$^{xiii}$ | 2.8413 |
| Mo1···H19 | 3.5603 | H5···C16$^{ix}$ | 3.5488 |
| P1···H8 | 3.1866 | H5···H2A$^{xiii}$ | 2.4410 |
| P1···H11 | 3.2156 | H5···H2B$^{xiii}$ | 3.2452 |
| P1···H15 | 3.1555 | H5···H2C$^{xiii}$ | 2.4602 |
| P1···H19 | 3.1787 | H5···H12$^{ii}$ | 2.9127 |
| O1···H2A | 2.9305 | H5···H16$^{ix}$ | 3.1909 |
| O1···H2B | 2.9517 | H5···H17$^{ix}$ | 3.3139 |
| O1···H2C | 2.3698 | H6···O5$^{v}$ | 2.8696 |
| O1···H19 | 2.8766 | H6···O6$^{v}$ | 3.4567 |
| O2···H2B | 3.3917 | H6···C10$^{v}$ | 3.2903 |
| O2···H19 | 2.9626 | H6···C11$^{v}$ | 2.9657 |
| O3···H15 | 3.0736 | H6···C12$^{v}$ | 3.3854 |
| O3···H19 | 3.2846 | H6···H11$^{v}$ | 3.0322 |
| O4···H11 | 3.1144 | H6···H16$^{ix}$ | 3.1850 |
| O4···H12 | 3.1337 | H7···O5$^{v}$ | 2.7503 |
| O5···H11 | 2.9209 | H7···O6$^{v}$ | 3.2600 |
| O5···H15 | 3.1445 | H7···C17$^{v}$ | 3.1047 |
| O5···H16 | 3.1378 | H7···C19$^{x}$ | 3.4546 |
| O6···H19 | 3.1475 | H7···C20$^{x}$ | 3.3946 |
| O6···H20 | 3.1439 | H7···H17$^{v}$ | 2.9010 |
| C1···H5 | 3.2622 | H7···H19$^{x}$ | 3.0750 |
| C1···H6 | 3.5136 | H7···H20$^{x}$ | 2.9593 |
| C1···H19 | 3.4091 | H8···O1$^{x}$ | 2.3768 |
| C2···H5 | 3.0620 | H8···O3$^{x}$ | 3.5861 |
| C2···H6 | 3.0642 | H8···C1$^{x}$ | 3.5639 |
| C3···H2B | 3.0535 | H8···C13$^{viii}$ | 3.3152 |
| C3···H6 | 3.5333 | H8···H13$^{viii}$ | 2.5503 |
| C3···H7 | 3.5392 | H8···H19$^{x}$ | 3.5900 |
| C3···H19 | 2.7741 | H9···O2$^{viii}$ | 2.7898 |
| C4···H9 | 3.3890 | H9···O4$^{viii}$ | 2.5358 |
| C4···H15 | 2.8933 | H9···C3$^{viii}$ | 3.5348 |
| C4···H19 | 2.9982 | H9···C13$^{viii}$ | 3.1123 |
| C5···H2A | 2.8007 | H9···H12$^{ii}$ | 3.5362 |
| C5···H2B | 3.3893 | H9···H13$^{viii}$ | 2.9508 |
| C5···H7 | 3.2477 | H9···H17$^{ix}$ | 3.0301 |
| C5···H8 | 3.2364 | H11···O1$^{x}$ | 2.4000 |
| C6···H2A | 3.0845 | H11···O2$^{x}$ | 3.4100 |
| C6···H2B | 2.9686 | H11···C1$^{x}$ | 3.1494 |
| C6···H8 | 3.2410 | H11···C2$^{x}$ | 3.5382 |
| C6···H9 | 3.2593 | H11···H2B$^{vii}$ | 3.0188 |
| C7···H5 | 3.2448 | H11···H2C$^{x}$ | 3.1246 |
| C7···H9 | 3.2588 | H11···H6$^{vii}$ | 3.0322 |
| C8···H5 | 3.2368 | H11···H19$^{x}$ | 3.4104 |
| C8···H6 | 3.2403 | H12···O2$^{x}$ | 2.6951 |

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|---|---|---|---|
| C8···H15 | 3.2779 | H12···O3$^{xi}$ | 3.3742 |
| C9···H6 | 3.2549 | H12···C4$^{xi}$ | 3.4063 |
| C9···H7 | 3.2582 | H12···C5$^{xi}$ | 3.5118 |
| C9···H15 | 3.0516 | H12···H2A$^{vii}$ | 3.4606 |
| C10···H7 | 3.5430 | H12···H2A$^{xi}$ | 3.3393 |
| C10···H8 | 3.3826 | H12···H2B$^{vii}$ | 3.2762 |
| C10···H12 | 3.1464 | H12···H5$^{xi}$ | 2.9127 |
| C10···H13 | 3.1018 | H12···H9$^{xi}$ | 3.5362 |
| C11···H8 | 3.3365 | H12···H19$^{x}$ | 3.2551 |
| C11···H13 | 3.1033 | H13···O1$^{xi}$ | 2.7818 |
| C13···H11 | 3.0967 | H13···O3$^{xi}$ | 2.5324 |
| C14···H8 | 3.1651 | H13···C1$^{xi}$ | 3.2942 |
| C14···H11 | 3.0477 | H13···C4$^{xi}$ | 3.0478 |
| C14···H16 | 3.1411 | H13···C8$^{iv}$ | 2.9953 |
| C14···H17 | 3.1002 | H13···C9$^{iv}$ | 3.1884 |
| C15···H8 | 3.2035 | H13···H8$^{iv}$ | 2.5503 |
| C15···H9 | 3.4305 | H13···H9$^{iv}$ | 2.9508 |
| C15···H17 | 3.1200 | H13···H17$^{v}$ | 3.4406 |
| C17···H15 | 3.1177 | H15···O4$^{viii}$ | 3.5809 |
| C18···H20 | 3.1487 | H15···O6$^{viii}$ | 3.3749 |
| C18···H21 | 3.1083 | H15···C20$^{viii}$ | 3.5936 |
| C19···H21 | 3.1265 | H15···C21$^{viii}$ | 3.1450 |
| C21···H19 | 3.1235 | H15···H21$^{viii}$ | 3.1980 |
| H2A···H5 | 2.3253 | H16···O6$^{viii}$ | 3.0672 |
| H2A···H6 | 2.9215 | H16···C5$^{xii}$ | 2.9065 |
| H2B···H5 | 3.3341 | H16···C6$^{xii}$ | 2.9100 |
| H2B···H6 | 2.5171 | H16···C7$^{xii}$ | 3.2069 |
| H5···H6 | 2.5858 | H16···C8$^{xii}$ | 3.3813 |
| H5···H9 | 2.5780 | H16···C9$^{xii}$ | 3.2067 |
| H6···H7 | 2.5833 | H16···C21$^{viii}$ | 3.0711 |
| H7···H8 | 2.5739 | H16···H5$^{xii}$ | 3.1909 |
| H8···H9 | 2.5930 | H16···H6$^{xii}$ | 3.1850 |
| H8···H11 | 3.0352 | H16···H21$^{viii}$ | 2.6784 |
| H8···H15 | 3.0715 | H17···O2$^{vii}$ | 2.6622 |
| H9···H15 | 2.6274 | H17···O4$^{vii}$ | 3.0622 |
| H11···H12 | 2.5539 | H17···C3$^{vii}$ | 2.9114 |
| H12···H13 | 2.4165 | H17···C5$^{xii}$ | 3.4107 |
| H15···H16 | 2.5576 | H17···C7$^{vii}$ | 3.5114 |
| H16···H17 | 2.4292 | H17···C9$^{xii}$ | 3.2533 |
| H19···H20 | 2.5627 | H17···C13$^{vii}$ | 3.3987 |
| H20···H21 | 2.4355 | H17···H2C$^{x}$ | 3.3020 |
| O1···H8$^{i}$ | 2.3768 | H17···H5$^{xii}$ | 3.3139 |
| O1···H11$^{i}$ | 2.4000 | H17···H7$^{vii}$ | 2.9010 |
| O1···H13$^{ii}$ | 2.7818 | H17···H9$^{xii}$ | 3.0301 |
| O2···H2B$^{iii}$ | 3.2721 | H17···H13$^{vii}$ | 3.4406 |
| O2···H2C$^{iii}$ | 3.0612 | H17···H20$^{vi}$ | 3.1945 |
| O2···H5$^{iv}$ | 2.9591 | H19···C11$^{i}$ | 3.4790 |
| O2···H9$^{iv}$ | 2.7898 | H19···C12$^{i}$ | 3.3869 |

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|---|---|---|---|
| O2···H11$^{i}$ | 3.4100 | H19···H7$^{i}$ | 3.0750 |
| O2···H12$^{i}$ | 2.6951 | H19···H8$^{i}$ | 3.5900 |
| O2···H17$^{v}$ | 2.6622 | H19···H11$^{i}$ | 3.4104 |
| O3···H8$^{i}$ | 3.5861 | H19···H12$^{i}$ | 3.2551 |
| O3···H12$^{ii}$ | 3.3742 | H19···H21$^{vi}$ | 3.5859 |
| O3···H13$^{ii}$ | 2.5324 | H20···O3$^{iv}$ | 3.3953 |
| O3···H20$^{viii}$ | 3.3953 | H20···O5$^{vi}$ | 2.8838 |
| O3···H21$^{vi}$ | 2.5352 | H20···O6$^{vi}$ | 3.4695 |
| O4···H9$^{iv}$ | 2.5358 | H20···C14$^{vi}$ | 3.1976 |
| O4···H15$^{iv}$ | 3.5809 | H20···C15$^{vi}$ | 3.3925 |
| O4···H17$^{v}$ | 3.0622 | H20···C16$^{vi}$ | 3.2027 |
| O5···H6$^{vii}$ | 2.8696 | H20···C17$^{vi}$ | 2.8803 |
| O5···H7$^{vii}$ | 2.7503 | H20···H7$^{i}$ | 2.9593 |
| O5···H20$^{vi}$ | 2.8838 | H20···H17$^{vi}$ | 3.1945 |
| O6···H6$^{vii}$ | 3.4567 | H21···O3$^{vi}$ | 2.5352 |
| O6···H7$^{vii}$ | 3.2600 | H21···C4$^{vi}$ | 3.3179 |
| O6···H15$^{iv}$ | 3.3749 | H21···C15$^{iv}$ | 3.3930 |
| O6···H16$^{iv}$ | 3.0672 | H21···C16$^{iv}$ | 3.1327 |
| O6···H20$^{vi}$ | 3.4695 | H21···C18$^{vi}$ | 3.5115 |
| C1···H8$^{i}$ | 3.5639 | H21···C19$^{vi}$ | 3.4225 |
| C1···H11$^{i}$ | 3.1494 | H21···H15$^{iv}$ | 3.1980 |
| C1···H13$^{ii}$ | 3.2942 | H21···H16$^{iv}$ | 2.6784 |
| C2···H2A$^{xiii}$ | 3.1828 | H21···H19$^{vi}$ | 3.5859 |

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|---|---|---|---|
| P1—Mo1—C1 | 128.21 (9) | C7—C8—C9 | 108.7 (3) |
| P1—Mo1—C3 | 79.89 (8) | Mo1—C9—C5 | 71.1 (2) |
| P1—Mo1—C4 | 78.48 (8) | Mo1—C9—C8 | 72.30 (19) |
| P1—Mo1—C5 | 141.13 (8) | C5—C9—C8 | 107.1 (3) |
| P1—Mo1—C6 | 133.02 (8) | P1—C10—O4 | 115.9 (2) |
| P1—Mo1—C7 | 98.20 (8) | P1—C10—C11 | 134.6 (3) |
| P1—Mo1—C8 | 85.10 (8) | O4—C10—C11 | 109.1 (3) |
| P1—Mo1—C9 | 107.65 (8) | C10—C11—C12 | 107.5 (3) |
| C1—Mo1—C3 | 69.24 (11) | C11—C12—C13 | 106.1 (3) |
| C1—Mo1—C4 | 72.24 (12) | O4—C13—C12 | 111.0 (4) |
| C1—Mo1—C5 | 88.91 (12) | P1—C14—O5 | 119.6 (2) |
| C1—Mo1—C6 | 93.91 (12) | P1—C14—C15 | 130.7 (3) |
| C1—Mo1—C7 | 126.97 (12) | O5—C14—C15 | 109.7 (3) |
| C1—Mo1—C8 | 146.42 (12) | C14—C15—C16 | 106.7 (3) |
| C1—Mo1—C9 | 116.88 (11) | C15—C16—C17 | 106.4 (3) |
| C3—Mo1—C4 | 106.58 (12) | O5—C17—C16 | 111.4 (3) |
| C3—Mo1—C5 | 130.94 (11) | P1—C18—O6 | 117.9 (2) |
| C3—Mo1—C6 | 100.79 (12) | P1—C18—C19 | 132.5 (3) |
| C3—Mo1—C7 | 100.46 (11) | O6—C18—C19 | 109.6 (3) |
| C3—Mo1—C8 | 129.25 (10) | C18—C19—C20 | 106.9 (3) |
| C3—Mo1—C9 | 157.46 (11) | C19—C20—C21 | 106.3 (3) |
| C4—Mo1—C5 | 107.42 (11) | O6—C21—C20 | 111.3 (3) |
| C4—Mo1—C6 | 141.87 (11) | C1—C2—H2A | 109.475 |
| C4—Mo1—C7 | 151.60 (13) | C1—C2—H2B | 109.476 |

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|---|---|---|---|
| C4—Mo1—C8 | 117.41 (12) | C1—C2—H2C | 109.471 |
| C4—Mo1—C9 | 95.82 (12) | H2A—C2—H2B | 109.480 |
| C5—Mo1—C6 | 35.35 (11) | H2A—C2—H2C | 109.467 |
| C5—Mo1—C7 | 58.13 (11) | H2B—C2—H2C | 109.459 |
| C5—Mo1—C8 | 57.63 (11) | Mo1—C5—H5 | 125.465 |
| C5—Mo1—C9 | 34.61 (11) | C6—C5—H5 | 125.462 |
| C6—Mo1—C7 | 34.99 (11) | C9—C5—H5 | 125.463 |
| C6—Mo1—C8 | 57.89 (11) | Mo1—C6—H6 | 125.921 |
| C6—Mo1—C9 | 58.25 (11) | C5—C6—H6 | 125.931 |
| C7—Mo1—C8 | 34.57 (11) | C7—C6—H6 | 125.919 |
| C7—Mo1—C9 | 57.92 (11) | Mo1—C7—H7 | 125.887 |
| C8—Mo1—C9 | 34.73 (10) | C6—C7—H7 | 125.888 |
| Mo1—P1—C10 | 116.72 (10) | C8—C7—H7 | 125.885 |
| Mo1—P1—C14 | 114.92 (10) | Mo1—C8—H8 | 125.541 |
| Mo1—P1—C18 | 114.96 (9) | C7—C8—H8 | 125.535 |
| C10—P1—C14 | 100.70 (13) | C9—C8—H8 | 125.540 |
| C10—P1—C18 | 102.09 (13) | Mo1—C9—H9 | 126.321 |
| C14—P1—C18 | 105.58 (13) | C5—C9—H9 | 126.319 |
| C10—O4—C13 | 106.3 (3) | C8—C9—H9 | 126.314 |
| C14—O5—C17 | 105.8 (3) | C10—C11—H11 | 126.232 |
| C18—O6—C21 | 105.9 (3) | C12—C11—H11 | 126.226 |
| Mo1—C1—O1 | 124.6 (3) | C11—C12—H12 | 126.961 |
| Mo1—C1—C2 | 118.5 (3) | C13—C12—H12 | 126.951 |
| O1—C1—C2 | 116.8 (3) | O4—C13—H13 | 124.493 |
| Mo1—C3—O2 | 175.7 (3) | C12—C13—H13 | 124.484 |
| Mo1—C4—O3 | 177.1 (3) | C14—C15—H15 | 126.643 |
| Mo1—C5—C6 | 71.96 (19) | C16—C15—H15 | 126.650 |
| Mo1—C5—C9 | 74.30 (19) | C15—C16—H16 | 126.781 |
| C6—C5—C9 | 108.7 (3) | C17—C16—H16 | 126.780 |
| Mo1—C6—C5 | 72.69 (18) | O5—C17—H17 | 124.313 |
| Mo1—C6—C7 | 73.56 (19) | C16—C17—H17 | 124.310 |
| C5—C6—C7 | 107.6 (3) | C18—C19—H19 | 126.546 |
| Mo1—C7—C6 | 71.45 (18) | C20—C19—H19 | 126.540 |
| Mo1—C7—C8 | 73.29 (18) | C19—C20—H20 | 126.865 |
| C6—C7—C8 | 107.9 (3) | C21—C20—H20 | 126.858 |
| Mo1—C8—C7 | 72.14 (19) | O6—C21—H21 | 124.340 |
| Mo1—C8—C9 | 72.97 (19) | C20—C21—H21 | 124.322 |

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| P1—Mo1—C1—O1 | −21.0 (3) | C8—Mo1—C5—C6 | −78.82 (14) |
| P1—Mo1—C1—C2 | 155.15 (13) | C8—Mo1—C5—C9 | 37.38 (11) |
| C1—Mo1—P1—C10 | −123.99 (11) | C5—Mo1—C9—C5 | 0.00 (12) |
| C1—Mo1—P1—C14 | 118.42 (11) | C5—Mo1—C9—C8 | 115.8 (2) |
| C1—Mo1—P1—C18 | −4.46 (11) | C9—Mo1—C5—C6 | −116.2 (2) |
| C3—Mo1—P1—C10 | −70.77 (9) | C9—Mo1—C5—C9 | 0.00 (12) |
| C3—Mo1—P1—C14 | 171.65 (8) | C6—Mo1—C7—C6 | 0.00 (15) |
| C3—Mo1—P1—C18 | 48.76 (8) | C6—Mo1—C7—C8 | −116.1 (3) |
| C4—Mo1—P1—C10 | 179.83 (10) | C7—Mo1—C6—C5 | 115.0 (3) |
| C4—Mo1—P1—C14 | 62.25 (10) | C7—Mo1—C6—C7 | 0.00 (15) |

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| C4—Mo1—P1—C18 | −60.64 (10) | C6—Mo1—C8—C7 | 37.45 (12) |
| P1—Mo1—C5—C6 | −97.48 (14) | C6—Mo1—C8—C9 | −79.32 (14) |
| P1—Mo1—C5—C9 | 18.72 (19) | C8—Mo1—C6—C5 | 77.99 (15) |
| C5—Mo1—P1—C10 | 76.30 (12) | C8—Mo1—C6—C7 | −36.99 (12) |
| C5—Mo1—P1—C14 | −41.29 (12) | C6—Mo1—C9—C5 | −37.63 (11) |
| C5—Mo1—P1—C18 | −164.17 (11) | C6—Mo1—C9—C8 | 78.21 (13) |
| P1—Mo1—C6—C5 | 121.66 (9) | C9—Mo1—C6—C5 | 36.82 (12) |
| P1—Mo1—C6—C7 | 6.7 (2) | C9—Mo1—C6—C7 | −78.17 (15) |
| C6—Mo1—P1—C10 | 24.61 (13) | C7—Mo1—C8—C7 | 0.00 (14) |
| C6—Mo1—P1—C14 | −92.97 (12) | C7—Mo1—C8—C9 | −116.8 (3) |
| C6—Mo1—P1—C18 | 144.14 (12) | C8—Mo1—C7—C6 | 116.1 (3) |
| P1—Mo1—C7—C6 | −175.07 (11) | C8—Mo1—C7—C8 | 0.00 (13) |
| P1—Mo1—C7—C8 | 68.84 (12) | C7—Mo1—C9—C5 | −79.11 (14) |
| C7—Mo1—P1—C10 | 28.47 (10) | C7—Mo1—C9—C8 | 36.73 (12) |
| C7—Mo1—P1—C14 | −89.11 (9) | C9—Mo1—C7—C6 | 79.19 (15) |
| C7—Mo1—P1—C18 | 148.00 (9) | C9—Mo1—C7—C8 | −36.89 (12) |
| P1—Mo1—C8—C7 | −112.11 (11) | C8—Mo1—C9—C5 | −115.8 (3) |
| P1—Mo1—C8—C9 | 131.13 (12) | C8—Mo1—C9—C8 | −0.00 (14) |
| C8—Mo1—P1—C10 | 60.56 (8) | C9—Mo1—C8—C7 | 116.8 (3) |
| C8—Mo1—P1—C14 | −57.03 (8) | C9—Mo1—C8—C9 | −0.00 (13) |
| C8—Mo1—P1—C18 | −179.91 (8) | Mo1—P1—C10—O4 | 74.1 (2) |
| P1—Mo1—C9—C5 | −167.80 (8) | Mo1—P1—C10—C11 | −96.6 (3) |
| P1—Mo1—C9—C8 | −51.96 (12) | Mo1—P1—C14—O5 | 171.31 (15) |
| C9—Mo1—P1—C10 | 87.32 (8) | Mo1—P1—C14—C15 | −9.8 (3) |
| C9—Mo1—P1—C14 | −30.26 (8) | Mo1—P1—C18—O6 | −176.72 (13) |
| C9—Mo1—P1—C18 | −153.15 (8) | Mo1—P1—C18—C19 | 2.5 (3) |
| C3—Mo1—C1—O1 | −78.4 (3) | C10—P1—C14—O5 | 45.0 (3) |
| C3—Mo1—C1—C2 | 97.7 (2) | C10—P1—C14—C15 | −136.2 (3) |
| C4—Mo1—C1—O1 | 37.8 (3) | C14—P1—C10—O4 | −160.81 (19) |
| C4—Mo1—C1—C2 | −146.1 (3) | C14—P1—C10—C11 | 28.5 (3) |
| C1—Mo1—C5—C6 | 98.33 (14) | C10—P1—C18—O6 | −49.4 (2) |
| C1—Mo1—C5—C9 | −145.47 (13) | C10—P1—C18—C19 | 129.9 (3) |
| C5—Mo1—C1—O1 | 146.5 (3) | C18—P1—C10—O4 | −52.1 (3) |
| C5—Mo1—C1—C2 | −37.42 (19) | C18—P1—C10—C11 | 137.2 (3) |
| C1—Mo1—C6—C5 | −82.56 (14) | C14—P1—C18—O6 | 55.5 (2) |
| C1—Mo1—C6—C7 | 162.46 (14) | C14—P1—C18—C19 | −125.2 (3) |
| C6—Mo1—C1—O1 | −178.5 (3) | C18—P1—C14—O5 | −60.9 (2) |
| C6—Mo1—C1—C2 | −2.4 (2) | C18—P1—C14—C15 | 117.9 (3) |
| C1—Mo1—C7—C6 | −22.1 (2) | C10—O4—C13—C12 | 0.9 (5) |
| C1—Mo1—C7—C8 | −138.20 (13) | C13—O4—C10—P1 | −174.4 (3) |
| C7—Mo1—C1—O1 | −166.0 (2) | C13—O4—C10—C11 | −1.4 (4) |
| C7—Mo1—C1—C2 | 10.1 (3) | C14—O5—C17—C16 | 0.1 (3) |
| C1—Mo1—C8—C7 | 74.4 (3) | C17—O5—C14—P1 | 178.9 (2) |
| C1—Mo1—C8—C9 | −42.4 (3) | C17—O5—C14—C15 | −0.2 (3) |
| C8—Mo1—C1—O1 | 150.83 (19) | C18—O6—C21—C20 | −0.3 (3) |
| C8—Mo1—C1—C2 | −33.1 (3) | C21—O6—C18—P1 | 179.48 (19) |
| C1—Mo1—C9—C5 | 39.45 (16) | C21—O6—C18—C19 | 0.1 (3) |
| C1—Mo1—C9—C8 | 155.29 (12) | Mo1—C5—C6—Mo1 | 0.0 |

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|---|---|---|---|
| C9—Mo1—C1—O1 | 125.3 (3) | Mo1—C5—C6—C7 | 65.80 (19) |
| C9—Mo1—C1—C2 | −58.6 (2) | Mo1—C5—C9—Mo1 | 0.0 |
| C3—Mo1—C5—C6 | 37.40 (19) | Mo1—C5—C9—C8 | −63.79 (19) |
| C3—Mo1—C5—C9 | 153.60 (11) | C6—C5—C9—Mo1 | 64.2 (3) |
| C3—Mo1—C6—C5 | −152.15 (13) | C6—C5—C9—C8 | 0.4 (4) |
| C3—Mo1—C6—C7 | 92.86 (14) | C9—C5—C6—Mo1 | −65.8 (3) |
| C3—Mo1—C7—C6 | −93.92 (14) | C9—C5—C6—C7 | 0.0 (4) |
| C3—Mo1—C7—C8 | 150.00 (13) | Mo1—C6—C7—Mo1 | 0.0 |
| C3—Mo1—C8—C7 | −39.42 (19) | Mo1—C6—C7—C8 | 64.70 (19) |
| C3—Mo1—C8—C9 | −156.19 (12) | C5—C6—C7—Mo1 | −65.2 (3) |
| C3—Mo1—C9—C5 | −61.2 (3) | C5—C6—C7—C8 | −0.5 (4) |
| C3—Mo1—C9—C8 | 54.6 (4) | Mo1—C7—C8—Mo1 | 0.0 |
| C4—Mo1—C5—C6 | 169.32 (13) | Mo1—C7—C8—C9 | 64.30 (19) |
| C4—Mo1—C5—C9 | −74.48 (14) | C6—C7—C8—Mo1 | −63.5 (3) |
| C4—Mo1—C6—C5 | −16.6 (3) | C6—C7—C8—C9 | 0.8 (4) |
| C4—Mo1—C6—C7 | −131.62 (17) | Mo1—C8—C9—Mo1 | 0.0 |
| C4—Mo1—C7—C6 | 104.0 (3) | Mo1—C8—C9—C5 | 62.99 (19) |
| C4—Mo1—C7—C8 | −12.1 (3) | C7—C8—C9—Mo1 | −63.8 (3) |
| C4—Mo1—C8—C7 | 173.56 (11) | C7—C8—C9—C5 | −0.8 (4) |
| C4—Mo1—C8—C9 | 56.80 (17) | P1—C10—C11—C12 | 172.5 (3) |
| C4—Mo1—C9—C5 | 112.47 (13) | O4—C10—C11—C12 | 1.4 (4) |
| C4—Mo1—C9—C8 | −131.70 (13) | C10—C11—C12—C13 | −0.8 (4) |
| C5—Mo1—C6—C5 | 0.00 (14) | C11—C12—C13—O4 | −0.0 (5) |
| C5—Mo1—C6—C7 | −115.0 (3) | P1—C14—C15—C16 | −178.7 (2) |
| C6—Mo1—C5—C6 | 0.00 (14) | O5—C14—C15—C16 | 0.2 (3) |
| C6—Mo1—C5—C9 | 116.2 (3) | C14—C15—C16—C17 | −0.1 (4) |
| C5—Mo1—C7—C6 | 38.14 (13) | C15—C16—C17—O5 | −0.0 (4) |
| C5—Mo1—C7—C8 | −77.95 (15) | P1—C18—C19—C20 | −179.13 (19) |
| C7—Mo1—C5—C6 | −37.74 (12) | O6—C18—C19—C20 | 0.1 (3) |
| C7—Mo1—C5—C9 | 78.46 (14) | C18—C19—C20—C21 | −0.3 (4) |
| C5—Mo1—C8—C7 | 79.52 (14) | C19—C20—C21—O6 | 0.4 (4) |
| C5—Mo1—C8—C9 | −37.25 (12) | | |

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) *x*−1, −*y*+1/2, *z*−1/2; (iii) −*x*+1, −*y*, −*z*; (iv) *x*+1, *y*, *z*; (v) −*x*+1, *y*−1/2, −*z*+1/2; (vi) −*x*+1, −*y*+1, −*z*; (vii) −*x*+1, *y*+1/2, −*z*+1/2; (viii) *x*−1, *y*, *z*; (ix) −*x*, *y*−1/2, −*z*+1/2; (x) *x*, −*y*+1/2, *z*+1/2; (xi) *x*+1, −*y*+1/2, *z*+1/2; (xii) −*x*, *y*+1/2, −*z*+1/2; (xiii) −*x*, −*y*, −*z*.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8···O1$^{x}$ | 1.00 | 2.38 | 3.324 (4) | 158 |
| C11—H11···O1$^{x}$ | 0.95 | 2.40 | 3.166 (5) | 137 |

Symmetry code: (x) *x*, −*y*+1/2, *z*+1/2.