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Synthesis, crystal structure, and Hirshfeld surface analysis of undecacarbonyl{tris[4-(methylsulfanyl)-phenyl]arsine}-*triangulo*-triosmium(0)

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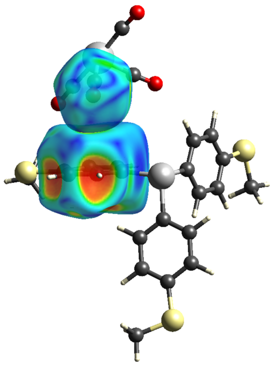
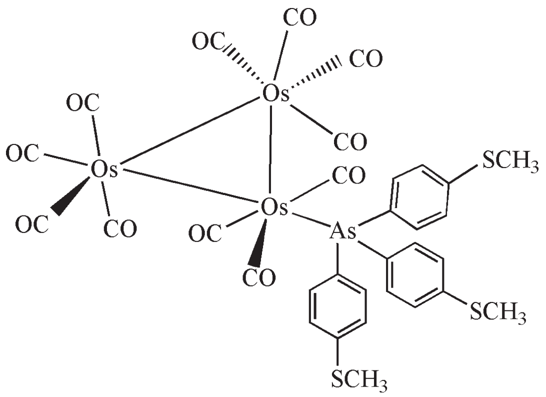
The title compound, $[Os_3(C_{21}H_{21}AsS_3)(CO)_{11}]$ or $[Os_3\{As(C_6H_4SCH_3)_3\}(CO)_{11}]$, comprises a triangle of Os atoms, two of which are bonded to four carbonyl ligands. The third Os atom is bound to three carbonyl ligands, and the arsine ligand $[As(C_6H_4SCH_3)_3]$ occupies the equatorial position. In the crystal, the molecules are linked by C—H⋯O hydrogen bonds. To further analyse the intermolecular interactions, a Hirshfeld surface analysis was performed. Two out of the three methylsulfanyl groups are disordered over two sites with final refinement occupancy ratios of 0.612 (12):0.388 (12) and 0.620 (9):0.380 (9).

1. Chemical context

The chemistry of triosmium carbonyl clusters with group 15 ligands has been extensively studied (Raithby, 2024). The majority of reported structures have focused on tertiary phosphine ligands (PR_3) with R = alkyl or aryl groups, with fewer examples involving tertiary arsine ligands ($AsPR_3$) (webCSD, accessed May 2025; Groom *et al.*, 2016). These ligands stabilize low oxidation states of metal centres and can be used to modify both the electronic and steric properties of resulting coordination compounds (Honaker *et al.*, 2007). Numerous triosmium carbonyl clusters containing one, two, or three PR_3 have been synthesized and fully characterised (Bruce *et al.*, 1988*a*,*b*; Biradha *et al.*, 2000). $Os_3(CO)_{11}(PR_3)$ is the most reported crystal structure among derivatives in this series, the earlier ones being $Os_3(CO)_{11}(PPh_3)$, and $Os_3(CO)_{11}\{PPh(OMe)_2\}$, which were prepared in refluxing toluene for more than 10 h (Bruce *et al.*, 1988*a*). Biradha and co-workers reported a series of $Os_3(CO)_{11}(PR_3)$ with R = F, OPh, Et, *p*-C_6H_4Me, *o*-C_6H_4Me, *p*-$C_6H_4(CF_3)$ and C_6H_{11} (Biradha *et al.*, 2000) by reacting $Os_3(CO)_{11}(CH_3CN)$ with PR_3 in dichloromethane for 15 min (Hansen *et al.*, 1998). According to these structures, the steric and electronic effects of PR_3 often result in variations of the Os—Os bond that is *cis* to PR_3 and the Os—P bond length (Biradha *et al.*, 2000). However, there are not many reactions conducted on $Os_3(CO)_{12}$ with $AsPR_3$. $Os_3(CO)_{11}(AsPh_3)$ is the only reported structure in this series (Oh *et al.*, 2015). Thus, we are currently exploring the reaction between $Os_3(CO)_{12}$ and the $AsPR_3$ ligand, focusing on how such ligands influence structural parameters within the triangular osmium cluster. We



anticipate that the resulting compound will serve as a representative example contributing to the broader understanding of this structural series $Os_3(CO)_{11}(P/AsR_3)$. Herein, we report the synthesis of $Os_3(CO)_{11}\{As(C_6H_4SCH_3)_3\}$, **1**, and its examination using single-crystal X-ray diffraction and Hirshfeld surface analysis.



2. Structural commentary

The molecular structure of **1** is shown in Fig. 1. The molecule comprises an Os_3 triangle with one Os centre being equatorially coordinated by the tris{4-(methylsulfanyl)phenyl}arsine ligand $[As(C_6H_4SCH_3)_3]$. The Os—Os bond lengths in the Os_3 triangle are not equivalent, with the Os1—Os2 bond [2.9150 (3) Å] being longer than the Os1—Os3 and Os2—Os3 bonds, at 2.8611 (3) and 2.8817 (4) Å, respectively. The longest Os—Os bond is *cis* to $As(C_6H_4SCH_3)_3$ and comparable with a similar Os—Os bond [2.9148 (7) Å] in $Os_3(CO)_{11}AsPh_3$ (Oh *et al.*, 2015). These observations are attributed to the steric and electronic effects of the arsine ligand on the Os—Os bonds. The Os—As bond length in **1** is 2.4603 (5) Å and almost similar to the related bond in $Os_3(CO)_{11}(AsPh_3)$ 2.4670 (9) Å (Oh *et al.*, 2015). The Os—C(CO) bond lengths are in the range 1.872 (6)–1.951 (7) Å. The equatorial Os—C≡O bond angles range from 175.7 (5) to 178.4 (5)°, whereas the axial Os—C≡O bond angles range from 174.3 (6) to 177.2 (5)°.

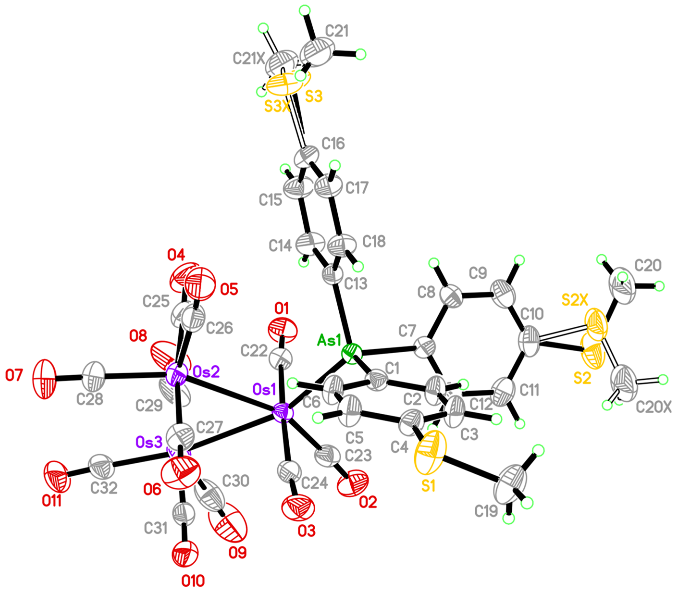


Figure 1
The molecular structure of **1** with 30% displacement ellipsoids.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$A\cdots$O10^{i}	0.93	2.55	3.41 (1)	154

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

3. Supramolecular features

In the crystal, C5—H5$A\cdots$O10 intermolecular interactions (Table 1, Fig. 2) lead to the formation of an inversion dimer between two molecules. This dimer is further consolidated by a short S3$\cdots$O10 contact [3.21 (2) Å, symmetry code: $\frac{1}{2}+x, \frac{3}{2}-y, \frac{1}{2}+z$].

4. Hirshfeld surface analysis

The major and minor components of the disorder in **1** were subjected to Hirshfeld surface analysis using *CrystalExplorer21* (Spackman *et al.*, 2021). This is based on the procedures described in the literature (Tan *et al.*, 2019) to better understand the nature of the intermolecular interactions that exist in the crystal.

The $d_{\rm norm}$ mapping reveals a relatively simple landscape of molecular interactions, with only a few red spots being observed on the Hirshfeld surfaces. For the major component, the red spots originated from H5*A*, O10, H21*B*, C20, S3, O7, H20*A*, and C21 (Fig. 3*a*), corresponding to the close contacts for C5—H5$A\cdots$O10, C21—H21$B\cdots$C20, S3$\cdots$O10, O7$\cdots$O7, and C20—H20$A\cdots$C21 (Table 2). The respective deviations of these contacts from the sum of the van der Waals radii are 0.20, 0.15, 0.11, 0.09 and 0.04 Å, reflecting the intensity of the corresponding red spots. For the minor component, red spots are detected on the disorder fragments of S3*X* and H21*D*,

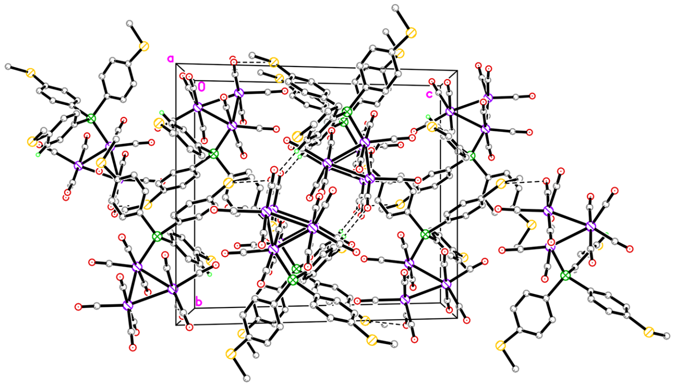


Figure 2
The crystal structure of the title compound viewed along the *c* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

Table 2

The d_{norm} contact distances (Å, adjusted to neutron values) for all identified interactions present in the major and minor components of **1** with respect to the corresponding sum of van der Waals radii of the relevant contact atoms.

Contact	d_{norm} Distance	ΣvdW radii	Δ(ΣvdW – d_{norm} distance)	Symmetry operation
Major				
C5–H5*A*···O10	2.41	2.61	0.20	$1 - x, 2 - y, 2 - z$
C20–H20*A*···C21	2.57	2.61	0.04	$-\frac{1}{2} + x, \frac{1}{2} - y, -\frac{1}{2} + z$
C21–H21*B*···C20	2.64	2.79	0.15	$\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$
S3···O10	3.21	3.32	0.11	$\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z$
O7···O7	2.95	3.04	0.09	$2 - x, 2 - y, 2 - z$
Minor				
C5–H5*A*···O10	2.41	2.61	0.20	$1 - x, 2 - y, 2 - z$
S3*X*···O10	3.13	3.32	0.19	$\frac{1}{2} + x, \frac{3}{2} - y, \frac{1}{2} + z$
O7···O7	2.95	3.04	0.09	$2 - x, 2 - y, 2 - z$
C21*X*–H21*D*···O1	2.55	2.61	0.06	$2 - x, 1 - y, 2 - z$

corresponding to S3*X*···O10 and C21*X*—H21*D*···O1 in addition to the intrinsic C5—H5*A*···O10 and O7···O7 close contacts for **1** (Fig. 3*b*). The deviations between the d_{norm} contact distance and the sum of the van der Waals radii for S3*X*···O10 and H21*D*···O1 are 0.19 and 0.06 Å, respectively (Table 3).

Apart from the close contacts indicated by red spots, another significant feature emerges from the shape-index mapping on the Hirshfeld surface. This mapping highlights a complementary intermolecular stacking interaction between C32—O11 and the C7–C12 ring (symmetry code: $\frac{3}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$), providing evidence of a lone pair···π interaction (Fig. 4). This finding aligns with the analysis from *PLATON* (Spek, 2020), which identified a contact distance of 3.867 (5) Å between O11 and the aromatic π-ring, along with a C≡O···π angle of 94.0 (4)°. Studies suggested that such interactions typically occur within a distance range of 3.0–4.5 Å, with angles varying between 60 and 160° (Caracelli *et al.*, 2016; Chen *et al.*, 2024), depending on the specific lone-pair donor and π-acceptor involved.

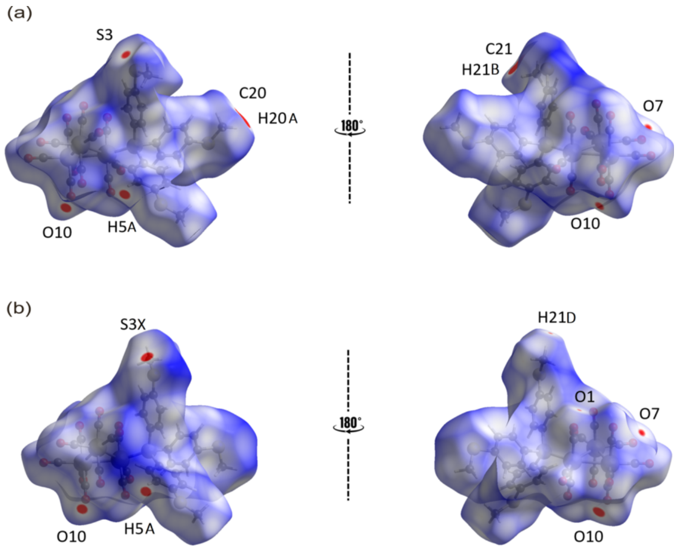


Figure 3

Two views of the d_{norm} map showing the atoms with close contacts, as indicated by the corresponding red spots, with varying intensities for (*a*) the major component and (*b*) the minor component of **1**.

The major and minor components of **1** were subjected to 2D fingerprint plot analysis to quantitatively assess close contacts within the structure. Both exhibit distinct shield- and paw-like fingerprint profiles, which, upon decomposition, reveal symmetrical H···O/O···H, H···H, H···C/C···H, O···S/S···O, O···O, and O···C/C···O interactions (Fig. 5), indicating homogeneous reciprocal contacts between internal-*X*···*Y*-external and external-*X*···*Y*-internal interfaces.

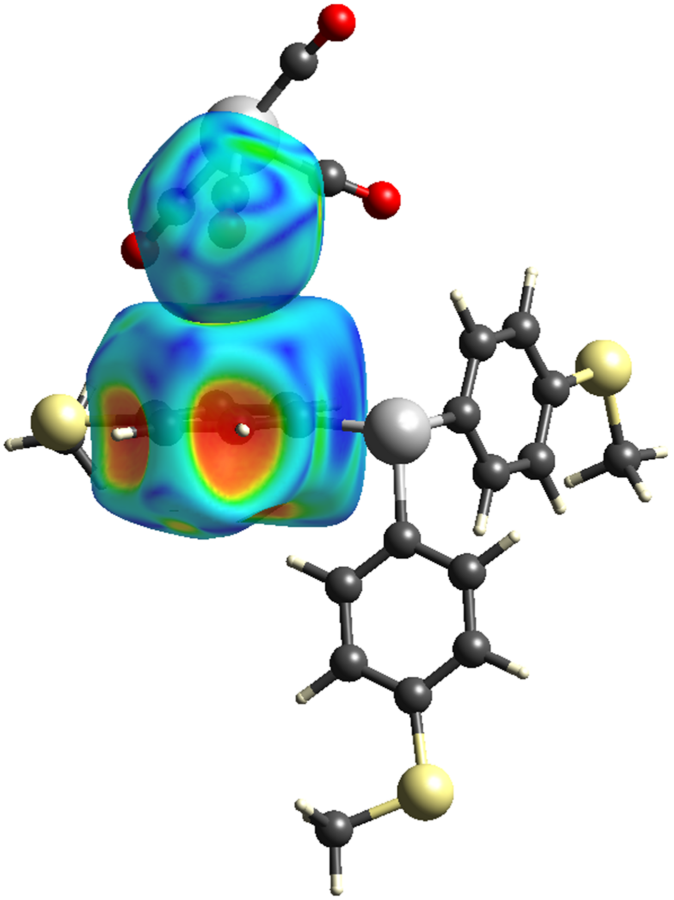


Figure 4

The partial Hirshfeld surface mapped with shape-index for C32–O11 (top) and the C7–C12 ring (bottom; $\frac{3}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$), showing the shape complementarity between the intermolecular stacking fragments of **1**. The remaining parts of the molecules were omitted for clarity.

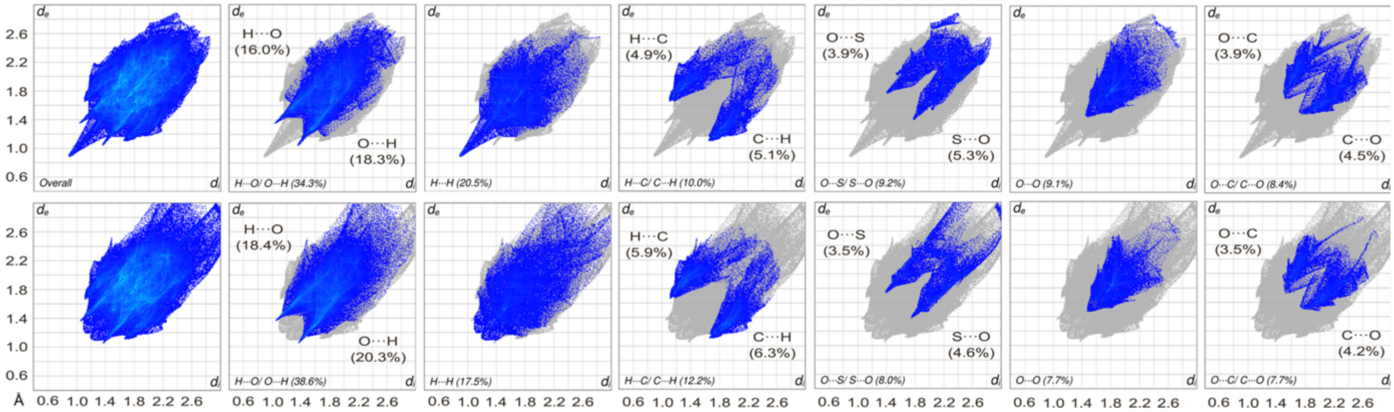


Figure 5
The comparison of the overall and prominent decomposed fingerprint print plots (> 5%) delineated into H···O/O···H, H···H, H···C/C···H, O···S/S···O, O···O, and O···C/C···O close contacts for the major (top) and minor (bottom) components of **1**.

Slight deviations are observed in the decomposed fingerprint plots of H···H and O···S/S···O. The major component features a distinct H···H peak at a $d_i + d_e$ of approximately 1.80 Å (H20*A*···H21*A*), whereas the minor component exhibits a broader profile with a larger $d_i + d_e$ of about 2.30 Å (H21*F*···H19*B*). In the pincer-like decomposed fingerprint plots of O···S/S···O, the reciprocal contacts correspond to O10···S3 ($d_i + d_e \simeq 3.21$ Å) in the major component and O10···S3*X* ($d_i + d_e \simeq 3.12$ Å) in the minor component. Other fingerprint plots remain consistent across both components, with close contact distributions being as follows: H···O/O···H (34.3% *vs* 38.6%), H···H (20.5% *vs* 17.5%), H···C/C···H (10.0% *vs* 12.2%), O···S/S···O (9.2% *vs* 8.0%), O···O (9.1% *vs* 7.7%), and O···C/C···O (8.4% *vs* 7.7%), while the remaining less prominent contacts contribute to approximately 4.1% to 4.2% (Fig. 6).

5. Database survey

A search of the Cambridge Structural Database (webCSD accessed May 2025; Groom *et al.*, 2016) for the title compound returned no relevant hits. However, a search with generalized tertiary arsine ligand (AsR_3) returned one hit [$Os_3(CO)_{11}(AsPh_3)$] [CSD refcode YUCXEB; Oh *et al.*, 2015). The structure of the title compound is very similar to that of $Ru_3(CO)_{11}\{As(C_6H_4SCH_3)_3\}$ (SUXQEI; Shawkataly *et al.*, 2010), in which tris{4-(methylsulfanyl)phenyl}arsine [$As(C_6H_4SCH_3)_3$] is equatorially bonded to the metal centre. The structure is consistent with literature precedents for complexes with the general formula $Os_3(CO)_{11}PR_3$ [HIYVUG (Hansen *et al.*, 1998), MASPEB, MASPIF and MASPUR (Biradha *et al.*, 2000), VADYEE (Bruce *et al.*, 1988*a*, VAWWUL (Ang *et al.*, 1989), YEDZOW and YEFCAN (Adams *et al.*, 1994)].

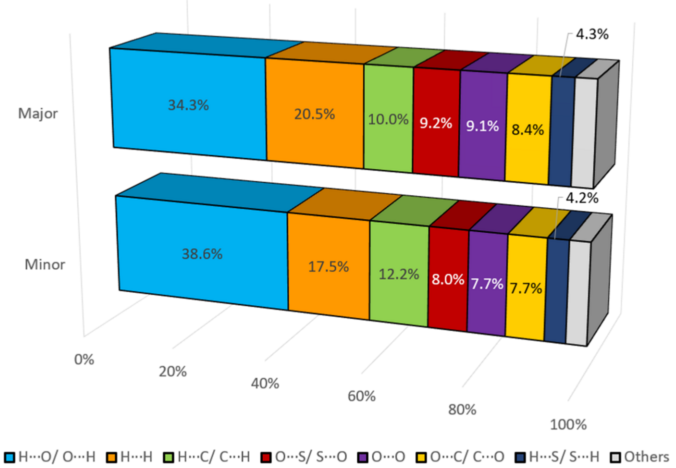


Figure 6
The percentage contributions of different close contacts to the Hirshfeld surfaces of the major and minor components of **1**.

6. Synthesis and crystallization

A solution of $Os_3(CO)_{11}(CH_3CN)$ (Nicholls *et al.*, 1990; Hansen *et al.*, 1998) (80 mg, 0.087 mmol) and $As(C_6H_4SCH_3)_3$ (60 mg, 0.13 mmol) in CH_2Cl_2 (25 ml) was stirred at room temperature for 60 min. The reaction was carried out under nitrogen-free oxygen using standard Schlenk techniques. The solution was dried in *vacuo*, and the residue was chromatographed by preparative thin-layer chromatography on silica gel with C_6H_{14}/CH_2Cl_2 (3:2) as the eluent. Chromatographic separation afforded two bands: the first yellow band was identified as the starting material $Os_3(CO)_{12}$. The desired product $Os_3(CO)_{11}\{As(C_6H_4SCH_3)_3\}$ was isolated as the second yellow band in 50% yield and recrystallized from CH_2Cl_2/CH_3OH (1:3). IR (ATR): ν(CO) 2107 *s*, 2051 *m*, 2006 *w*, 1974 *m*, 1942 *w* cm^{-1}.

7. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were positioned geometrically and refined using a riding model with C—H distances of 0.93 or 0.96 Å (for methyl groups) and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(C-methyl). Two out of the three methylsulfanyl groups were disordered over two sites with a final refinement occupancy ratios of 0.612 (12):0.388 (12) and

0.620 (9):0.380 (9). Anisotropic displacement parameters and rigid-body restraints were applied to the disordered components. Due to poor agreement, reflections 020, $\bar{4}33$, 680, $\bar{3}07$, and 379 were omitted from the final cycles of refinement. Maximum and minimum residual electron densities of 1.46 and -1.46 e Å^{-3} were observed at 0.83 Å from Os1 and 0.70 Å from Os3, respectively.

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Table 3
Experimental details.

Crystal data	
Chemical formula	$[Os_3(C_{21}H_{21}AsS_3)(CO)_{11}]$
M_r	1323.19
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	297
a, b, c (Å)	14.5019 (15), 15.3759 (16), 17.8575 (19)
β (°)	107.870 (2)
V (Å^3)	3789.8 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	11.12
Crystal size (mm)	0.41 × 0.15 × 0.09
Data collection	
Diffractometer	Bruker *APEX* Duo CCD area detector
Absorption correction	Multi-scan (*SADABS*; Krause et al., 2015)
$T_{\min}$, $T_{\max}$	0.024, 0.076
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	52142, 13246, 8766
$R_{\rm int}$	0.054
(sin $\theta/\lambda)_{\max}$ (Å^{-1})	0.749
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.081, 0.97
No. of reflections	13246
No. of parameters	482
No. of restraints	64
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	1.46, −1.46

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *SHELXTL* (Sheldrick, 2015*a*) and *PLATON* (Spek, 2020).

supporting information

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Synthesis, crystal structure, and Hirshfeld surface analysis of undecacarbonyl{tris[4-(methylsulfanyl)phenyl]arsine}-*triangulo*-triosmium(0)

Siti Syaida Sirat, Mohd Mustaqim Rosli, Sang Loon Tan, Ibrahim Abdul Razak and Omar bin Shawkataly

Computing details

Undecacarbonyl{tris[4-(methylsulfanyl)phenyl]arsine}-*triangulo*-triosmium(0)

Crystal data

$[Os_3(C_{21}H_{21}AsS_3)(CO)_{11}]$
M_r = 1323.19
Monoclinic, $P2_1/n$
a = 14.5019 (15) Å
b = 15.3759 (16) Å
c = 17.8575 (19) Å
β = 107.870 (2)°
V = 3789.8 (7) Å^3
Z = 4

$F(000)$ = 2440
D_x = 2.319 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9975 reflections
θ = 2.7–27.7°
μ = 11.12 mm^{-1}
T = 297 K
Plate, yellow
0.41 × 0.15 × 0.09 mm

Data collection

Bruker APEX Duo CCD area detector diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause et al., 2015)
T_{min} = 0.024, T_{max} = 0.076
52142 measured reflections

13246 independent reflections
8766 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 32.2°, θ_{min} = 2.7°
$h = -20 \rightarrow 21$
$k = -22 \rightarrow 23$
$l = -25 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.081
S = 0.97
13246 reflections
482 parameters
64 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 1.46 e Å^{-3}
$\Delta\rho_{min}$ = −1.46 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$	Occ. (<1)
Os1	0.64030 (2)	0.79000 (2)	0.83741 (2)	0.04272 (5)	
Os2	0.77751 (2)	0.87250 (2)	0.97335 (2)	0.05053 (6)	
Os3	0.75404 (2)	0.93459 (2)	0.81633 (2)	0.05645 (6)	
As1	0.58467 (3)	0.66988 (3)	0.90375 (2)	0.04018 (9)	
S1	0.26975 (11)	0.78176 (13)	1.07849 (11)	0.0909 (6)	
S2	0.3328 (6)	0.3694 (4)	0.6797 (4)	0.098 (2)	0.612 (12)
C20	0.3547 (12)	0.2721 (10)	0.7360 (9)	0.126 (4)	0.612 (12)
H20A	0.3099	0.2281	0.7089	0.189*	0.612 (12)
H20B	0.3465	0.2829	0.7865	0.189*	0.612 (12)
H20C	0.4197	0.2528	0.7429	0.189*	0.612 (12)
S2X	0.3528 (7)	0.3392 (6)	0.7063 (7)	0.089 (3)	0.388 (12)
C20X	0.252 (2)	0.3784 (14)	0.6533 (15)	0.126 (4)	0.388 (12)
H20D	0.2008	0.3392	0.6530	0.189*	0.388 (12)
H20E	0.2544	0.3862	0.6005	0.189*	0.388 (12)
H20F	0.2414	0.4336	0.6743	0.189*	0.388 (12)
S3	0.9056 (13)	0.4559 (13)	1.1746 (11)	0.102 (4)	0.620 (9)
C21	0.8517 (8)	0.4338 (9)	1.2521 (7)	0.104 (3)	0.620 (9)
H21A	0.8994	0.4082	1.2963	0.156*	0.620 (9)
H21B	0.7984	0.3943	1.2329	0.156*	0.620 (9)
H21C	0.8289	0.4872	1.2680	0.156*	0.620 (9)
S3X	0.905 (2)	0.4698 (19)	1.1841 (16)	0.083 (4)	0.380 (9)
C21X	0.9804 (14)	0.4194 (15)	1.1371 (12)	0.104 (3)	0.380 (9)
H21D	1.0389	0.4004	1.1757	0.156*	0.380 (9)
H21E	0.9960	0.4598	1.1019	0.156*	0.380 (9)
H21F	0.9474	0.3701	1.1079	0.156*	0.380 (9)
O1	0.7863 (3)	0.6672 (3)	0.7993 (2)	0.0725 (10)	
O2	0.5161 (3)	0.7732 (3)	0.6676 (2)	0.0875 (13)	
O3	0.4744 (3)	0.9005 (3)	0.8608 (3)	0.0838 (12)	
O4	0.9236 (3)	0.7338 (4)	0.9578 (3)	0.1041 (16)	
O5	0.7750 (4)	0.7808 (3)	1.1233 (3)	0.0938 (14)	
O6	0.6178 (4)	0.9914 (3)	0.9960 (3)	0.0998 (15)	
O7	0.9269 (3)	1.0144 (3)	1.0409 (3)	0.0917 (14)	
O8	0.9216 (5)	0.8158 (4)	0.8063 (4)	0.136 (2)	
O9	0.6690 (7)	0.9423 (4)	0.6384 (3)	0.152 (3)	
O10	0.5906 (3)	1.0542 (3)	0.8289 (2)	0.0752 (11)	
O11	0.8903 (3)	1.0898 (3)	0.8460 (3)	0.0991 (15)	
C1	0.4875 (3)	0.6994 (3)	0.9544 (3)	0.0444 (9)	
C2	0.4001 (3)	0.6577 (3)	0.9364 (3)	0.0555 (12)	
H2A	0.3860	0.6135	0.8992	0.067*	

C3	0.3318 (3)	0.6811 (4)	0.9734 (3)	0.0598 (12)
H3A	0.2727	0.6520	0.9605	0.072*
C4	0.3507 (3)	0.7467 (3)	1.0290 (3)	0.0520 (11)
C5	0.4391 (3)	0.7880 (3)	1.0464 (3)	0.0583 (12)
H5A	0.4534	0.8322	1.0838	0.070*
C6	0.5069 (3)	0.7657 (3)	1.0100 (3)	0.0538 (11)
H6A	0.5658	0.7951	1.0226	0.065*
C7	0.5209 (3)	0.5744 (3)	0.8363 (2)	0.0442 (9)
C8	0.5417 (4)	0.4876 (3)	0.8579 (3)	0.0527 (10)
H8A	0.5917	0.4744	0.9034	0.063*
C9	0.4893 (4)	0.4213 (4)	0.8128 (3)	0.0666 (14)
H9A	0.5053	0.3638	0.8272	0.080*
C10	0.4135 (4)	0.4392 (4)	0.7466 (3)	0.0651 (14)
C11	0.3932 (4)	0.5262 (4)	0.7243 (3)	0.0690 (14)
H11A	0.3424	0.5395	0.6794	0.083*
C12	0.4478 (4)	0.5918 (4)	0.7684 (3)	0.0582 (12)
H12A	0.4350	0.6492	0.7520	0.070*
C13	0.6804 (3)	0.6093 (3)	0.9873 (2)	0.0421 (9)
C14	0.7659 (4)	0.5830 (4)	0.9766 (3)	0.0617 (13)
H14A	0.7786	0.5965	0.9299	0.074*
C15	0.8332 (4)	0.5369 (4)	1.0342 (3)	0.0682 (14)
H15A	0.8899	0.5181	1.0252	0.082*
C16	0.8178 (3)	0.5182 (4)	1.1049 (3)	0.0589 (12)
C17	0.7331 (4)	0.5453 (3)	1.1170 (3)	0.0615 (13)
H17A	0.7214	0.5336	1.1644	0.074*
C18	0.6649 (4)	0.5903 (3)	1.0575 (3)	0.0559 (11)
H18A	0.6074	0.6080	1.0657	0.067*
C19	0.1568 (4)	0.7396 (5)	1.0225 (4)	0.090 (2)
H19A	0.1085	0.7550	1.0468	0.135*
H19B	0.1610	0.6774	1.0198	0.135*
H19C	0.1394	0.7634	0.9703	0.135*
C22	0.7360 (4)	0.7139 (3)	0.8156 (3)	0.0518 (10)
C23	0.5636 (4)	0.7775 (3)	0.7325 (3)	0.0603 (12)
C24	0.5387 (4)	0.8629 (3)	0.8546 (3)	0.0536 (11)
C25	0.8686 (4)	0.7860 (4)	0.9595 (3)	0.0687 (15)
C26	0.7747 (4)	0.8120 (4)	1.0660 (4)	0.0670 (14)
C27	0.6752 (4)	0.9480 (4)	0.9840 (3)	0.0648 (13)
C28	0.8726 (4)	0.9610 (4)	1.0160 (3)	0.0653 (13)
C29	0.8587 (6)	0.8578 (4)	0.8105 (5)	0.094 (2)
C30	0.7036 (7)	0.9381 (4)	0.7049 (4)	0.095 (2)
C31	0.6500 (4)	1.0078 (3)	0.8269 (3)	0.0557 (11)
C32	0.8418 (4)	1.0322 (4)	0.8361 (4)	0.0701 (15)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Os1	0.04402 (9)	0.04182 (9)	0.04327 (10)	0.00121 (7)	0.01478 (7)	0.00311 (6)
Os2	0.04408 (9)	0.05623 (11)	0.05050 (11)	−0.00492 (8)	0.01333 (7)	−0.00148 (8)

Os3	0.06879 (12)	0.04738 (10)	0.06249 (13)	−0.00426 (9)	0.03387 (10)	0.00544 (8)
As1	0.0409 (2)	0.0400 (2)	0.0403 (2)	0.00060 (16)	0.01330 (17)	−0.00004 (16)
S1	0.0575 (8)	0.1229 (15)	0.1047 (13)	−0.0127 (8)	0.0434 (8)	−0.0478 (11)
S2	0.127 (5)	0.084 (4)	0.081 (3)	−0.049 (4)	0.029 (3)	−0.031 (2)
C20	0.144 (9)	0.087 (7)	0.124 (9)	−0.049 (7)	0.006 (8)	−0.023 (6)
S2X	0.094 (4)	0.058 (5)	0.114 (7)	−0.028 (3)	0.028 (4)	−0.025 (3)
C20X	0.144 (9)	0.087 (7)	0.124 (9)	−0.049 (7)	0.006 (8)	−0.023 (6)
S3	0.070 (4)	0.142 (10)	0.075 (5)	0.025 (5)	−0.007 (3)	0.036 (5)
C21	0.074 (5)	0.134 (9)	0.090 (7)	0.001 (5)	0.005 (4)	0.032 (6)
S3X	0.079 (7)	0.097 (5)	0.066 (6)	0.032 (4)	0.014 (5)	0.027 (5)
C21X	0.074 (5)	0.134 (9)	0.090 (7)	0.001 (5)	0.005 (4)	0.032 (6)
O1	0.076 (2)	0.069 (2)	0.081 (3)	0.018 (2)	0.037 (2)	−0.0059 (19)
O2	0.089 (3)	0.111 (4)	0.047 (2)	0.008 (3)	−0.001 (2)	0.008 (2)
O3	0.067 (2)	0.075 (3)	0.117 (4)	0.022 (2)	0.040 (2)	0.009 (2)
O4	0.065 (2)	0.116 (4)	0.117 (4)	0.026 (3)	0.007 (3)	−0.020 (3)
O5	0.107 (3)	0.103 (3)	0.062 (3)	−0.028 (3)	0.013 (2)	0.019 (2)
O6	0.098 (3)	0.112 (4)	0.095 (3)	0.033 (3)	0.038 (3)	−0.018 (3)
O7	0.086 (3)	0.099 (3)	0.097 (3)	−0.044 (3)	0.038 (2)	−0.028 (3)
O8	0.134 (4)	0.092 (4)	0.239 (7)	0.029 (3)	0.141 (5)	0.042 (4)
O9	0.286 (9)	0.112 (4)	0.062 (4)	−0.028 (5)	0.059 (5)	−0.002 (3)
O10	0.065 (2)	0.065 (2)	0.083 (3)	0.003 (2)	0.005 (2)	−0.0114 (19)
O11	0.090 (3)	0.070 (3)	0.143 (4)	−0.025 (2)	0.043 (3)	0.016 (3)
C1	0.045 (2)	0.041 (2)	0.049 (2)	0.0043 (17)	0.0162 (18)	−0.0003 (17)
C2	0.048 (2)	0.059 (3)	0.061 (3)	−0.012 (2)	0.019 (2)	−0.019 (2)
C3	0.044 (2)	0.068 (3)	0.072 (3)	−0.018 (2)	0.024 (2)	−0.017 (2)
C4	0.042 (2)	0.060 (3)	0.057 (3)	0.003 (2)	0.019 (2)	−0.004 (2)
C5	0.052 (2)	0.063 (3)	0.067 (3)	−0.010 (2)	0.027 (2)	−0.022 (2)
C6	0.043 (2)	0.062 (3)	0.060 (3)	−0.012 (2)	0.020 (2)	−0.015 (2)
C7	0.047 (2)	0.048 (2)	0.038 (2)	0.0006 (18)	0.0132 (17)	−0.0042 (16)
C8	0.062 (3)	0.044 (2)	0.054 (3)	−0.001 (2)	0.021 (2)	−0.0018 (19)
C9	0.084 (4)	0.053 (3)	0.070 (4)	−0.008 (3)	0.036 (3)	−0.013 (2)
C10	0.069 (3)	0.067 (3)	0.067 (4)	−0.020 (3)	0.032 (3)	−0.028 (3)
C11	0.065 (3)	0.087 (4)	0.050 (3)	−0.010 (3)	0.010 (2)	−0.018 (3)
C12	0.067 (3)	0.058 (3)	0.047 (3)	−0.001 (2)	0.012 (2)	−0.001 (2)
C13	0.043 (2)	0.041 (2)	0.042 (2)	−0.0020 (16)	0.0122 (17)	−0.0006 (16)
C14	0.057 (3)	0.077 (4)	0.057 (3)	0.014 (2)	0.027 (2)	0.014 (2)
C15	0.052 (3)	0.083 (4)	0.074 (4)	0.019 (3)	0.025 (3)	0.017 (3)
C16	0.046 (2)	0.068 (3)	0.052 (3)	0.002 (2)	−0.001 (2)	0.005 (2)
C17	0.069 (3)	0.069 (3)	0.042 (3)	0.001 (3)	0.010 (2)	0.008 (2)
C18	0.057 (3)	0.065 (3)	0.049 (3)	0.012 (2)	0.021 (2)	0.010 (2)
C19	0.049 (3)	0.130 (6)	0.100 (5)	−0.005 (3)	0.037 (3)	−0.012 (4)
C22	0.056 (2)	0.055 (3)	0.047 (3)	0.000 (2)	0.020 (2)	−0.0001 (19)
C23	0.064 (3)	0.058 (3)	0.061 (3)	0.006 (2)	0.022 (3)	0.012 (2)
C24	0.052 (2)	0.047 (3)	0.064 (3)	0.002 (2)	0.020 (2)	0.004 (2)
C25	0.044 (2)	0.080 (4)	0.076 (4)	0.001 (3)	0.009 (2)	−0.012 (3)
C26	0.057 (3)	0.073 (4)	0.065 (4)	−0.017 (3)	0.010 (3)	0.001 (3)
C27	0.071 (3)	0.073 (4)	0.051 (3)	0.000 (3)	0.019 (3)	−0.003 (2)
C28	0.058 (3)	0.075 (4)	0.065 (3)	−0.015 (3)	0.022 (3)	−0.011 (3)

C29	0.106 (5)	0.061 (4)	0.152 (7)	0.002 (3)	0.094 (5)	0.016 (4)
C30	0.162 (7)	0.064 (4)	0.072 (5)	−0.015 (4)	0.054 (5)	−0.001 (3)
C31	0.059 (3)	0.050 (3)	0.054 (3)	−0.007 (2)	0.012 (2)	−0.002 (2)
C32	0.068 (3)	0.063 (3)	0.084 (4)	−0.003 (3)	0.029 (3)	0.016 (3)

Geometric parameters (Å, º)

Os1—C23	1.872 (6)	O3—C24	1.131 (6)
Os1—C22	1.944 (5)	O4—C25	1.139 (7)
Os1—C24	1.950 (5)	O5—C26	1.129 (7)
Os1—As1	2.4603 (5)	O6—C27	1.137 (7)
Os1—Os3	2.8611 (3)	O7—C28	1.130 (6)
Os1—Os2	2.9150 (3)	O8—C29	1.139 (7)
Os2—C26	1.910 (6)	O9—C30	1.142 (8)
Os2—C28	1.921 (6)	O10—C31	1.128 (6)
Os2—C27	1.939 (6)	O11—C32	1.112 (7)
Os2—C25	1.943 (6)	C1—C2	1.368 (6)
Os2—Os3	2.8817 (4)	C1—C6	1.389 (6)
Os3—C30	1.898 (8)	C2—C3	1.396 (7)
Os3—C32	1.929 (6)	C2—H2A	0.9300
Os3—C31	1.938 (6)	C3—C4	1.383 (7)
Os3—C29	1.951 (7)	C3—H3A	0.9300
As1—C13	1.936 (4)	C4—C5	1.377 (6)
As1—C7	1.943 (4)	C5—C6	1.379 (6)
As1—C1	1.948 (4)	C5—H5A	0.9300
S1—C4	1.757 (5)	C6—H6A	0.9300
S1—C19	1.760 (6)	C7—C12	1.369 (6)
S2—C10	1.759 (8)	C7—C8	1.397 (6)
S2—C20	1.775 (17)	C8—C9	1.376 (7)
C20—H20A	0.9600	C8—H8A	0.9300
C20—H20B	0.9600	C9—C10	1.372 (8)
C20—H20C	0.9600	C9—H9A	0.9300
S2X—C20X	1.59 (3)	C10—C11	1.400 (8)
S2X—C10	1.809 (10)	C11—C12	1.373 (7)
C20X—H20D	0.9600	C11—H11A	0.9300
C20X—H20E	0.9600	C12—H12A	0.9300
C20X—H20F	0.9600	C13—C14	1.372 (6)
S3—C16	1.765 (16)	C13—C18	1.372 (6)
S3—C21	1.82 (2)	C14—C15	1.377 (7)
C21—H21A	0.9600	C14—H14A	0.9300
C21—H21B	0.9600	C15—C16	1.380 (7)
C21—H21C	0.9600	C15—H15A	0.9300
S3X—C21X	1.75 (4)	C16—C17	1.375 (8)
S3X—C16	1.75 (3)	C17—C18	1.393 (7)
C21X—H21D	0.9600	C17—H17A	0.9300
C21X—H21E	0.9600	C18—H18A	0.9300
C21X—H21F	0.9600	C19—H19A	0.9600
O1—C22	1.124 (6)	C19—H19B	0.9600

O2—C23	1.155 (6)	C19—H19C	0.9600

C23—Os1—C22	88.8 (2)	H21D—C21X—H21F	109.5
C23—Os1—C24	88.3 (2)	H21E—C21X—H21F	109.5
C22—Os1—C24	176.7 (2)	C2—C1—C6	118.8 (4)
C23—Os1—As1	102.89 (16)	C2—C1—As1	122.1 (3)
C22—Os1—As1	90.24 (14)	C6—C1—As1	119.1 (3)
C24—Os1—As1	88.87 (14)	C1—C2—C3	120.6 (4)
C23—Os1—Os3	97.90 (16)	C1—C2—H2A	119.7
C22—Os1—Os3	88.04 (14)	C3—C2—H2A	119.7
C24—Os1—Os3	93.91 (14)	C4—C3—C2	120.9 (4)
As1—Os1—Os3	159.100 (13)	C4—C3—H3A	119.5
C23—Os1—Os2	157.23 (16)	C2—C3—H3A	119.5
C22—Os1—Os2	94.70 (14)	C5—C4—C3	117.7 (4)
C24—Os1—Os2	88.54 (15)	C5—C4—S1	117.7 (4)
As1—Os1—Os2	99.586 (13)	C3—C4—S1	124.7 (4)
Os3—Os1—Os2	59.847 (8)	C4—C5—C6	121.9 (4)
C26—Os2—C28	101.9 (2)	C4—C5—H5A	119.1
C26—Os2—C27	89.2 (2)	C6—C5—H5A	119.1
C28—Os2—C27	90.9 (2)	C5—C6—C1	120.1 (4)
C26—Os2—C25	88.5 (3)	C5—C6—H6A	120.0
C28—Os2—C25	95.8 (2)	C1—C6—H6A	120.0
C27—Os2—C25	173.2 (2)	C12—C7—C8	118.3 (4)
C26—Os2—Os3	167.70 (16)	C12—C7—As1	119.5 (3)
C28—Os2—Os3	90.40 (17)	C8—C7—As1	121.9 (3)
C27—Os2—Os3	91.81 (16)	C9—C8—C7	120.8 (5)
C25—Os2—Os3	89.11 (19)	C9—C8—H8A	119.6
C26—Os2—Os1	108.61 (16)	C7—C8—H8A	119.6
C28—Os2—Os1	149.54 (17)	C10—C9—C8	120.6 (5)
C27—Os2—Os1	89.70 (16)	C10—C9—H9A	119.7
C25—Os2—Os1	85.01 (16)	C8—C9—H9A	119.7
Os3—Os2—Os1	59.148 (8)	C9—C10—C11	118.7 (5)
C30—Os3—C32	101.0 (3)	C9—C10—S2	130.7 (5)
C30—Os3—C31	91.4 (3)	C11—C10—S2	110.6 (5)
C32—Os3—C31	91.2 (2)	C9—C10—S2X	109.6 (5)
C30—Os3—C29	91.0 (4)	C11—C10—S2X	131.7 (6)
C32—Os3—C29	90.0 (3)	C12—C11—C10	120.3 (5)
C31—Os3—C29	177.1 (3)	C12—C11—H11A	119.9
C30—Os3—Os1	96.2 (2)	C10—C11—H11A	119.9
C32—Os3—Os1	162.78 (18)	C7—C12—C11	121.2 (5)
C31—Os3—Os1	86.62 (15)	C7—C12—H12A	119.4
C29—Os3—Os1	91.50 (18)	C11—C12—H12A	119.4
C30—Os3—Os2	157.2 (2)	C14—C13—C18	118.2 (4)
C32—Os3—Os2	101.86 (18)	C14—C13—As1	120.0 (3)
C31—Os3—Os2	87.73 (15)	C18—C13—As1	121.8 (3)
C29—Os3—Os2	89.4 (2)	C13—C14—C15	120.8 (5)
Os1—Os3—Os2	61.005 (6)	C13—C14—H14A	119.6
C13—As1—C7	101.94 (18)	C15—C14—H14A	119.6

C13—As1—C1	101.79 (18)	C14—C15—C16	120.9 (5)
C7—As1—C1	100.94 (18)	C14—C15—H15A	119.5
C13—As1—Os1	117.92 (12)	C16—C15—H15A	119.5
C7—As1—Os1	115.62 (13)	C17—C16—C15	119.0 (4)
C1—As1—Os1	116.07 (12)	C17—C16—S3X	117.6 (10)
C4—S1—C19	104.5 (3)	C15—C16—S3X	123.1 (10)
C10—S2—C20	99.4 (6)	C17—C16—S3	122.7 (7)
S2—C20—H20A	109.5	C15—C16—S3	118.2 (7)
S2—C20—H20B	109.5	C16—C17—C18	119.3 (5)
H20A—C20—H20B	109.5	C16—C17—H17A	120.3
S2—C20—H20C	109.5	C18—C17—H17A	120.3
H20A—C20—H20C	109.5	C13—C18—C17	121.7 (5)
H20B—C20—H20C	109.5	C13—C18—H18A	119.1
C20X—S2X—C10	99.1 (9)	C17—C18—H18A	119.1
S2X—C20X—H20D	109.5	S1—C19—H19A	109.5
S2X—C20X—H20E	109.5	S1—C19—H19B	109.5
H20D—C20X—H20E	109.5	H19A—C19—H19B	109.5
S2X—C20X—H20F	109.5	S1—C19—H19C	109.5
H20D—C20X—H20F	109.5	H19A—C19—H19C	109.5
H20E—C20X—H20F	109.5	H19B—C19—H19C	109.5
C16—S3—C21	104.6 (10)	O1—C22—Os1	175.3 (4)
S3—C21—H21A	109.5	O2—C23—Os1	177.4 (5)
S3—C21—H21B	109.5	O3—C24—Os1	174.4 (5)
H21A—C21—H21B	109.5	O4—C25—Os2	174.3 (6)
S3—C21—H21C	109.5	O5—C26—Os2	175.7 (5)
H21A—C21—H21C	109.5	O6—C27—Os2	175.0 (5)
H21B—C21—H21C	109.5	O7—C28—Os2	178.4 (5)
C21X—S3X—C16	101.8 (16)	O8—C29—Os3	177.2 (5)
S3X—C21X—H21D	109.5	O9—C30—Os3	176.4 (8)
S3X—C21X—H21E	109.5	O10—C31—Os3	174.9 (5)
H21D—C21X—H21E	109.5	O11—C32—Os3	177.9 (6)
S3X—C21X—H21F	109.5		

C6—C1—C2—C3	−0.3 (8)	C9—C10—C11—C12	−0.6 (8)
As1—C1—C2—C3	−179.5 (4)	S2—C10—C11—C12	−179.9 (5)
C1—C2—C3—C4	0.1 (9)	S2X—C10—C11—C12	175.7 (7)
C2—C3—C4—C5	0.0 (8)	C8—C7—C12—C11	2.9 (7)
C2—C3—C4—S1	179.5 (4)	As1—C7—C12—C11	−171.9 (4)
C19—S1—C4—C5	163.2 (5)	C10—C11—C12—C7	−2.2 (8)
C19—S1—C4—C3	−16.3 (6)	C18—C13—C14—C15	1.6 (8)
C3—C4—C5—C6	0.3 (8)	As1—C13—C14—C15	−177.4 (5)
S1—C4—C5—C6	−179.3 (4)	C13—C14—C15—C16	−2.0 (9)
C4—C5—C6—C1	−0.5 (8)	C14—C15—C16—C17	1.0 (9)
C2—C1—C6—C5	0.6 (8)	C14—C15—C16—S3X	−173.2 (14)
As1—C1—C6—C5	179.7 (4)	C14—C15—C16—S3	178.0 (9)
C12—C7—C8—C9	−0.9 (7)	C21X—S3X—C16—C17	163.8 (12)
As1—C7—C8—C9	173.8 (4)	C21X—S3X—C16—C15	−22 (2)
C7—C8—C9—C10	−1.9 (8)	C21—S3—C16—C17	4.3 (15)

C8—C9—C10—C11	2.6 (8)	C21—S3—C16—C15	−172.7 (8)
C8—C9—C10—S2	−178.3 (5)	C15—C16—C17—C18	0.3 (8)
C8—C9—C10—S2X	−174.5 (6)	S3X—C16—C17—C18	174.9 (13)
C20—S2—C10—C9	15.4 (10)	S3—C16—C17—C18	−176.6 (9)
C20—S2—C10—C11	−165.3 (8)	C14—C13—C18—C17	−0.3 (7)
C20X—S2X—C10—C9	161.1 (12)	As1—C13—C18—C17	178.7 (4)
C20X—S2X—C10—C11	−15.4 (15)	C16—C17—C18—C13	−0.7 (8)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*A*···O10^{i}	0.93	2.55	3.41 (1)	154

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