

# Nonacarbonyl-1 $\kappa^3$ C,2 $\kappa^3$ C,3 $\kappa^3$ C- $\mu$ -bis-(diphenylarsino)methane-1:2 $\kappa^2$ As:As'-[tris(2-chloroethyl) phosphite-3 $\kappa^3$ P]-triangulo-triruthenium(0)

Omar bin Shawkataly,<sup>a\*</sup> Imthyaz Ahmed Khan,<sup>a</sup>  
Siti Syaida Sirat,<sup>a</sup> Chin Sing Yeap<sup>b</sup>§ and Hoong-Kun Fun<sup>b¶</sup>

<sup>a</sup>Chemical Sciences Programme, School of Distance Education, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and <sup>b</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia  
Correspondence e-mail: omarsa@usm.my

Received 25 June 2010; accepted 3 July 2010

Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.016$  Å;  $R$  factor = 0.080;  $wR$  factor = 0.184; data-to-parameter ratio = 19.7.

In the title triangulo-triruthenium(0) compound,  $[\text{Ru}_3(\text{C}_{25}\text{H}_{22}\text{As}_2)(\text{C}_6\text{H}_{12}\text{Cl}_3\text{O}_3\text{P})(\text{CO})_9]$ , the bis(diphenylarsino)methane ligand bridges an Ru—Ru bond and the monodentate phosphine ligand bonds to the third Ru atom. Both the arsine and phosphine ligands are equatorial with respect to the  $\text{Ru}_3$  triangle. In addition, each Ru atom carries one equatorial and two axial terminal carbonyl ligands. In the crystal packing, the molecules are linked by intermolecular C—H $\cdots$ O hydrogen bonds into a three-dimensional framework. Weak intermolecular C—H $\cdots$  $\pi$  interactions further stabilize the crystal structure.

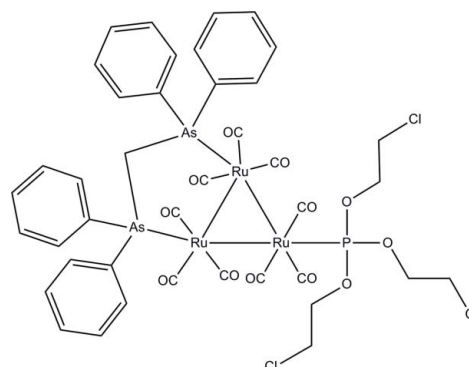
## Related literature

For general background to triangulo-triruthenium derivatives, see: Bruce *et al.* (1985, 1988*a,b*). For related structures, see: Shawkataly *et al.* (1998, 2004, 2010). For the synthesis of  $\mu$ -bis(diphenylarsino)methanedecacarbonyltriruthenium(0), see: Bruce *et al.* (1983). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).

\* Thomson Reuters ResearcherID: B-6034-2009. On secondment to: Multimedia University, Melaka Campus, Jalan Ayer Keroh Lama, 74750 Melaka, Malaysia.

§ Thomson Reuters ResearcherID: A-5523-2009.

¶ Thomson Reuters ResearcherID: A-3561-2009. Additional correspondence author, e-mail: hkfun@usm.my.



## Experimental

### Crystal data

$[\text{Ru}_3(\text{C}_{25}\text{H}_{22}\text{As}_2)(\text{C}_6\text{H}_{12}\text{Cl}_3\text{O}_3\text{P})(\text{CO})_9]$

$M_r = 1297.04$

Orthorhombic,  $Pbca$

$a = 14.9105$  (5) Å

$b = 21.3468$  (7) Å

$c = 28.7377$  (9) Å

$V = 9147.0$  (5) Å<sup>3</sup>

$Z = 8$

Mo  $K\alpha$  radiation

$\mu = 2.68$  mm<sup>-1</sup>

$T = 100$  K

$0.47 \times 0.18 \times 0.09$  mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer  
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)  
 $T_{\min} = 0.365$ ,  $T_{\max} = 0.798$

55092 measured reflections  
10492 independent reflections  
8686 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.047$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.080$   
 $wR(F^2) = 0.184$   
 $S = 1.28$   
10492 reflections

532 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 1.40$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -2.28$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$Cg1$  and  $Cg2$  are the centroids of the C1—C6 and C20—C25 benzene rings, respectively.

| $D-H\cdots A$                        | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------------|-------|-------------|-------------|---------------|
| C19—H19A $\cdots$ O6 <sup>i</sup>    | 0.93  | 2.57        | 3.275 (14)  | 133           |
| C27—H27B $\cdots$ O9 <sup>ii</sup>   | 0.97  | 2.47        | 3.231 (15)  | 135           |
| C30—H30A $\cdots$ O5 <sup>iii</sup>  | 0.97  | 2.56        | 3.297 (15)  | 133           |
| C4—H4A $\cdots$ Cg1 <sup>iv</sup>    | 0.93  | 2.77        | 3.468 (11)  | 133           |
| C9—H9A $\cdots$ Cg2 <sup>v</sup>     | 0.93  | 2.89        | 3.684 (12)  | 144           |
| C18—H18A $\cdots$ Cg1 <sup>vi</sup>  | 0.93  | 2.71        | 3.505 (12)  | 145           |
| C24—H24A $\cdots$ Cg2 <sup>vii</sup> | 0.93  | 2.69        | 3.473 (11)  | 142           |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

The authors would like to thank the Malaysian Government and Universiti Sains Malaysia (USM) for the Research grant

1001/PJJAUH/811115. SSS thanks USM for Research Officer position. IAK is grateful to USM for a Visiting Researcher position. HKF and CSY thank USM for the Research University Golden Goose grant 1001/PFIZIK/811012. CSY also thanks USM for the award of a USM Fellowship.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5029).

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## supporting information

*Acta Cryst.* (2010). E66, m929–m930 [https://doi.org/10.1107/S1600536810026267]

## Nonacarbonyl- $1\kappa^3C,2\kappa^3C,3\kappa^3C$ - $\mu$ -bis(diphenylarsino)methane- $1:2\kappa^2As:As'$ -[tris-(2-chloroethyl) phosphite- $3\kappa P$ ]-*triangulo*-triruthenium(0)

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### S1. Comment

*Triangulo*-triruthenium clusters are known for their interesting structural variations and related catalytic activity. A large number of substituted derivatives,  $Ru_3(CO)_{12-n}L_n$  ( $L =$  group 15 ligand) have been reported (Bruce, *et al.*, 1988*a,b*; Bruce *et al.*, 1985). As part of our study of the substitution of transition metal-carbonyl clusters with mixed-ligand complexes, we have published several structures of *triangulo*-triruthenium-carbonyl clusters containing mixed P/As and P/Sb ligands (Shawkataly *et al.*, 1998, 2004, 2010). Herein we report the synthesis and structure of the title compound.

The bond lengths and angles of title compound (Fig. 1) are comparable to those found in a related structure (Shawkataly *et al.*, 2010). The bis(diphenylarsino)methane ligand bridges the Ru1—Ru2 bond and the monodentate phosphine ligand bonds to the Ru3 atom. Both the phosphine and arsine ligands are equatorial with respect to the  $Ru_3$  triangle.

Additionally, each Ru atom carries one equatorial and two axial terminal carbonyl ligands. The dihedral angles between the two benzene rings (C1–C6/C7–C12 and C14–C19/C20–C25) are 85.4 (5) and 87.3 (5)° for the two diphenylarsino groups respectively.

In the crystal packing (Fig. 2), the molecules are linked by intermolecular C19—H19A $\cdots$ O6, C27—H27B $\cdots$ O9 and C30—H30A $\cdots$ O5 hydrogen bonds into a three-dimensional framework. Weak intermolecular C—H $\cdots$  $\pi$  interactions further stabilize the crystal structure (Table 1).

### S2. Experimental

All manipulations were performed under a dry, oxygen-free dinitrogen atmosphere using standard Schlenk techniques. All solvents were dried over sodium and distilled from sodium benzophenone ketyl under nitrogen. Tris(2-chloroethyl)phosphite (Aldrich) was used as received and  $\mu$ -bis(diphenylarsino)methanedecacarbonyltriruthenium(0) (Bruce *et al.*, 1983) was prepared by a reported procedure. The title compound was obtained by refluxing equimolar quantities of  $Ru_3(CO)_{10}(\mu-Ph_2AsCH_2AsPh_2)$  and tris(2-chloroethyl)phosphite in hexane under nitrogen atmosphere. Crystals suitable for X-ray diffraction were grown by slow solvent / solvent diffusion of  $CH_3OH$  into  $CH_2Cl_2$ .

### S3. Refinement

All hydrogen atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å and  $U_{iso}(H) = 1.2U_{eq}(C)$ . The same  $U^{ij}$  parameters were used for the atoms C17/C1/C20/C7. The maximum and minimum residual electron density peaks of 1.40 and -2.28 e Å<sup>-3</sup>, respectively, were located 0.79 Å and 1.42 Å from the RU1 and C36 atoms, respectively.

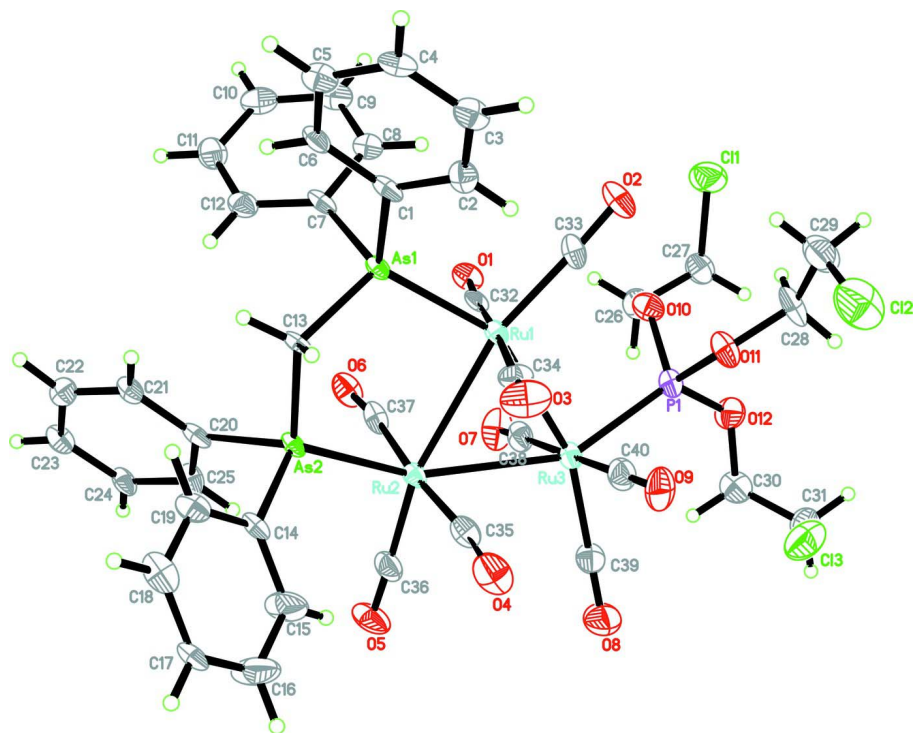
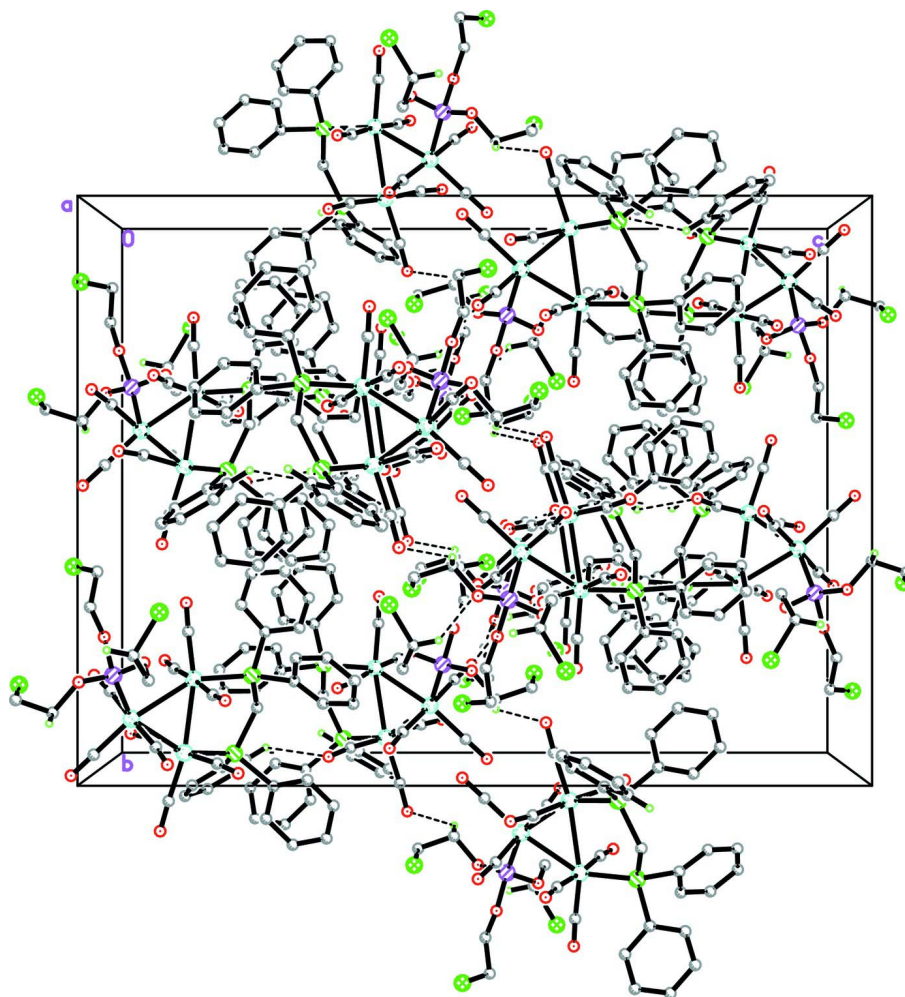


Figure 1

The molecular structure of the title compound with 50% probability ellipsoids for non-H atoms.



**Figure 2**

The crystal packing of the title compound, viewed down the  $a$  axis, showing the molecules linked into a 3-D framework. Hydrogen atoms not involved in the hydrogen-bonding (dashed lines) have been omitted for clarity.

**Nonacarbonyl- $1\kappa^3C,2\kappa^3C,3\kappa^3C$ - $\mu$ -bis(diphenylarsino)methane- $1:2\kappa^2As:As'$ -[tris(2-chloroethyl) phosphite- $3\kappa P$ ]-triangulo-triruthenium(0)**

*Crystal data*

$[Ru_3(C_{25}H_{22}As_2)(C_6H_{12}Cl_3O_3P)(CO)_9]$

$M_r = 1297.04$

Orthorhombic,  $Pbca$

Hall symbol:  $-P\ 2ac\ 2ab$

$a = 14.9105\ (5)\ \text{\AA}$

$b = 21.3468\ (7)\ \text{\AA}$

$c = 28.7377\ (9)\ \text{\AA}$

$V = 9147.0\ (5)\ \text{\AA}^3$

$Z = 8$

$F(000) = 5072$

$D_x = 1.884\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 9974 reflections

$\theta = 2.2\text{--}30.0^\circ$

$\mu = 2.68\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Block, red

$0.47 \times 0.18 \times 0.09\ \text{mm}$

*Data collection*

Bruker SMART APEXII CCD area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2009)

$T_{\min} = 0.365$ ,  $T_{\max} = 0.798$

55092 measured reflections

10492 independent reflections

8686 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.047$

$\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 2.0^\circ$

$h = -19 \rightarrow 19$

$k = -24 \rightarrow 27$

$l = -37 \rightarrow 28$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.080$

$wR(F^2) = 0.184$

$S = 1.28$

10492 reflections

532 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

$w = 1/[\sigma^2(F_o^2) + 274.9171P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.40 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -2.28 \text{ e } \text{\AA}^{-3}$

*Special details*

**Experimental.** The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

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

|     | $x$          | $y$          | $z$          | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| Ru1 | 0.21161 (5)  | 0.32808 (4)  | 0.36287 (3)  | 0.01629 (17)                     |
| Ru2 | 0.24882 (5)  | 0.45825 (4)  | 0.37688 (3)  | 0.01781 (17)                     |
| Ru3 | 0.13426 (6)  | 0.39328 (4)  | 0.43926 (3)  | 0.01984 (18)                     |
| As1 | 0.29465 (6)  | 0.32478 (4)  | 0.29063 (3)  | 0.0149 (2)                       |
| As2 | 0.36319 (6)  | 0.46579 (4)  | 0.31669 (3)  | 0.0157 (2)                       |
| Cl1 | -0.1760 (2)  | 0.20128 (17) | 0.38798 (12) | 0.0469 (8)                       |
| Cl2 | 0.1764 (3)   | 0.1315 (2)   | 0.51607 (17) | 0.0651 (11)                      |
| Cl3 | 0.0908 (3)   | 0.33271 (19) | 0.58014 (12) | 0.0515 (9)                       |
| P1  | 0.03663 (18) | 0.31463 (13) | 0.45706 (10) | 0.0220 (5)                       |
| O1  | 0.0321 (5)   | 0.3570 (3)   | 0.3155 (3)   | 0.0248 (16)                      |
| O2  | 0.1464 (6)   | 0.1935 (4)   | 0.3698 (3)   | 0.0343 (19)                      |
| O3  | 0.3930 (6)   | 0.3016 (5)   | 0.4095 (3)   | 0.042 (2)                        |
| O4  | 0.3881 (6)   | 0.4318 (4)   | 0.4543 (3)   | 0.043 (2)                        |
| O5  | 0.2262 (6)   | 0.5934 (4)   | 0.4072 (3)   | 0.042 (2)                        |

|      |             |            |            |             |
|------|-------------|------------|------------|-------------|
| O6   | 0.1079 (5)  | 0.4855 (4) | 0.3018 (3) | 0.0314 (18) |
| O7   | -0.0137 (6) | 0.4633 (4) | 0.3861 (3) | 0.039 (2)   |
| O8   | 0.1295 (7)  | 0.4908 (4) | 0.5165 (3) | 0.047 (2)   |
| O9   | 0.2772 (6)  | 0.3235 (4) | 0.4958 (3) | 0.038 (2)   |
| O10  | -0.0249 (5) | 0.2907 (4) | 0.4148 (3) | 0.0279 (17) |
| O11  | 0.0830 (5)  | 0.2504 (4) | 0.4713 (3) | 0.0301 (18) |
| O12  | -0.0405 (5) | 0.3227 (4) | 0.4958 (3) | 0.0320 (18) |
| C1   | 0.3636 (7)  | 0.2498 (5) | 0.2759 (4) | 0.0209 (10) |
| C2   | 0.3736 (7)  | 0.2020 (5) | 0.3078 (4) | 0.023 (2)   |
| H2A  | 0.3465      | 0.2052     | 0.3369     | 0.028*      |
| C3   | 0.4249 (7)  | 0.1481 (5) | 0.2966 (4) | 0.026 (2)   |
| H3A  | 0.4326      | 0.1159     | 0.3181     | 0.032*      |
| C4   | 0.4632 (7)  | 0.1445 (5) | 0.2528 (4) | 0.025 (2)   |
| H4A  | 0.4964      | 0.1093     | 0.2449     | 0.030*      |
| C5   | 0.4535 (7)  | 0.1918 (5) | 0.2209 (4) | 0.024 (2)   |
| H5A  | 0.4807      | 0.1887     | 0.1918     | 0.028*      |
| C6   | 0.4033 (7)  | 0.2442 (5) | 0.2319 (4) | 0.022 (2)   |
| H6A  | 0.3958      | 0.2759     | 0.2100     | 0.026*      |
| C7   | 0.2258 (6)  | 0.3321 (5) | 0.2337 (4) | 0.0209 (10) |
| C8   | 0.1547 (7)  | 0.2896 (5) | 0.2294 (4) | 0.024 (2)   |
| H8A  | 0.1413      | 0.2628     | 0.2539     | 0.028*      |
| C9   | 0.1037 (7)  | 0.2870 (5) | 0.1886 (4) | 0.029 (2)   |
| H9A  | 0.0571      | 0.2583     | 0.1856     | 0.035*      |
| C10  | 0.1238 (7)  | 0.3274 (6) | 0.1532 (4) | 0.029 (2)   |
| H10A | 0.0896      | 0.3264     | 0.1262     | 0.035*      |
| C11  | 0.1936 (8)  | 0.3698 (5) | 0.1567 (4) | 0.030 (2)   |
| H11A | 0.2059      | 0.3969     | 0.1323     | 0.036*      |
| C12  | 0.2454 (8)  | 0.3717 (5) | 0.1970 (4) | 0.024 (2)   |
| H12A | 0.2931      | 0.3995     | 0.1993     | 0.029*      |
| C13  | 0.3935 (6)  | 0.3858 (4) | 0.2876 (4) | 0.0155 (18) |
| H13A | 0.4457      | 0.3683     | 0.3030     | 0.019*      |
| H13B | 0.4090      | 0.3930     | 0.2552     | 0.019*      |
| C14  | 0.4795 (7)  | 0.4968 (5) | 0.3366 (4) | 0.021 (2)   |
| C15  | 0.4857 (9)  | 0.5300 (7) | 0.3778 (5) | 0.046 (4)   |
| H15A | 0.4354      | 0.5359     | 0.3965     | 0.055*      |
| C16  | 0.5688 (9)  | 0.5547 (8) | 0.3910 (5) | 0.055 (5)   |
| H16A | 0.5735      | 0.5770     | 0.4187     | 0.066*      |
| C17  | 0.6439 (7)  | 0.5466 (4) | 0.3639 (4) | 0.0209 (10) |
| H17A | 0.6989      | 0.5628     | 0.3732     | 0.025*      |
| C18  | 0.6363 (8)  | 0.5143 (5) | 0.3227 (4) | 0.031 (3)   |
| H18A | 0.6865      | 0.5098     | 0.3038     | 0.037*      |
| C19  | 0.5559 (7)  | 0.4884 (5) | 0.3089 (4) | 0.024 (2)   |
| H19A | 0.5524      | 0.4655     | 0.2814     | 0.029*      |
| C20  | 0.3436 (7)  | 0.5224 (4) | 0.2645 (4) | 0.0209 (10) |
| C21  | 0.3840 (6)  | 0.5139 (5) | 0.2209 (4) | 0.019 (2)   |
| H21A | 0.4181      | 0.4783     | 0.2151     | 0.023*      |
| C22  | 0.3731 (6)  | 0.5589 (5) | 0.1862 (4) | 0.022 (2)   |
| H22A | 0.3978      | 0.5519     | 0.1570     | 0.026*      |

|      |              |            |            |           |
|------|--------------|------------|------------|-----------|
| C23  | 0.3264 (7)   | 0.6135 (4) | 0.1943 (4) | 0.022 (2) |
| H23A | 0.3219       | 0.6442     | 0.1715     | 0.026*    |
| C24  | 0.2863 (7)   | 0.6216 (5) | 0.2374 (4) | 0.022 (2) |
| H24A | 0.2530       | 0.6576     | 0.2431     | 0.027*    |
| C25  | 0.2949 (7)   | 0.5764 (5) | 0.2724 (4) | 0.027 (2) |
| H25A | 0.2677       | 0.5828     | 0.3011     | 0.033*    |
| C26  | -0.1120 (8)  | 0.3167 (6) | 0.4048 (4) | 0.034 (3) |
| H26A | -0.1172      | 0.3248     | 0.3717     | 0.041*    |
| H26B | -0.1189      | 0.3563     | 0.4211     | 0.041*    |
| C27  | -0.1841 (8)  | 0.2726 (6) | 0.4197 (4) | 0.032 (3) |
| H27A | -0.2423      | 0.2915     | 0.4144     | 0.038*    |
| H27B | -0.1784      | 0.2641     | 0.4528     | 0.038*    |
| C28  | 0.0311 (9)   | 0.1978 (6) | 0.4858 (5) | 0.042 (3) |
| H28A | -0.0234      | 0.1956     | 0.4674     | 0.050*    |
| H28B | 0.0142       | 0.2029     | 0.5182     | 0.050*    |
| C29  | 0.0825 (10)  | 0.1385 (6) | 0.4802 (5) | 0.045 (3) |
| H29A | 0.1019       | 0.1352     | 0.4481     | 0.054*    |
| H29B | 0.0426       | 0.1036     | 0.4864     | 0.054*    |
| C30  | -0.0498 (8)  | 0.3739 (6) | 0.5280 (4) | 0.032 (3) |
| H30A | -0.1113      | 0.3888     | 0.5279     | 0.039*    |
| H30B | -0.0113      | 0.4082     | 0.5185     | 0.039*    |
| C31  | -0.0249 (10) | 0.3533 (7) | 0.5760 (4) | 0.042 (3) |
| H31A | -0.0613      | 0.3174     | 0.5846     | 0.050*    |
| H31B | -0.0378      | 0.3868     | 0.5978     | 0.050*    |
| C32  | 0.0983 (7)   | 0.3500 (4) | 0.3339 (4) | 0.021 (2) |
| C33  | 0.1725 (7)   | 0.2440 (5) | 0.3684 (4) | 0.024 (2) |
| C34  | 0.3240 (8)   | 0.3135 (5) | 0.3939 (4) | 0.027 (2) |
| C35  | 0.3336 (7)   | 0.4384 (6) | 0.4253 (4) | 0.030 (3) |
| C36  | 0.2369 (7)   | 0.5416 (5) | 0.3969 (4) | 0.029 (2) |
| C37  | 0.1579 (7)   | 0.4715 (5) | 0.3307 (4) | 0.024 (2) |
| C38  | 0.0446 (8)   | 0.4367 (5) | 0.4036 (4) | 0.027 (2) |
| C39  | 0.1298 (8)   | 0.4546 (5) | 0.4874 (4) | 0.029 (2) |
| C40  | 0.2281 (7)   | 0.3489 (6) | 0.4725 (4) | 0.029 (2) |

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

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Ru1 | 0.0141 (3)  | 0.0125 (3)  | 0.0223 (4)  | 0.0005 (3)   | 0.0010 (3)   | 0.0020 (3)   |
| Ru2 | 0.0153 (3)  | 0.0145 (4)  | 0.0236 (4)  | -0.0007 (3)  | 0.0036 (3)   | -0.0003 (3)  |
| Ru3 | 0.0196 (4)  | 0.0174 (4)  | 0.0225 (4)  | 0.0016 (3)   | 0.0041 (3)   | 0.0026 (3)   |
| As1 | 0.0125 (4)  | 0.0089 (4)  | 0.0231 (5)  | 0.0008 (3)   | 0.0007 (4)   | 0.0007 (4)   |
| As2 | 0.0133 (4)  | 0.0085 (4)  | 0.0251 (5)  | 0.0000 (4)   | 0.0029 (4)   | 0.0003 (4)   |
| Cl1 | 0.0447 (18) | 0.0480 (19) | 0.0480 (19) | -0.0177 (16) | 0.0021 (15)  | -0.0110 (16) |
| Cl2 | 0.059 (2)   | 0.050 (2)   | 0.086 (3)   | 0.0054 (19)  | -0.023 (2)   | 0.012 (2)    |
| Cl3 | 0.060 (2)   | 0.060 (2)   | 0.0340 (16) | 0.0100 (19)  | -0.0097 (15) | -0.0030 (16) |
| P1  | 0.0208 (13) | 0.0198 (13) | 0.0254 (13) | 0.0000 (10)  | 0.0029 (10)  | 0.0038 (10)  |
| O1  | 0.017 (4)   | 0.023 (4)   | 0.034 (4)   | 0.000 (3)    | -0.004 (3)   | -0.001 (3)   |
| O2  | 0.033 (4)   | 0.018 (4)   | 0.052 (5)   | -0.002 (3)   | 0.003 (4)    | 0.007 (4)    |



|     |           |            |           |              |            |            |
|-----|-----------|------------|-----------|--------------|------------|------------|
| O3  | 0.027 (4) | 0.050 (6)  | 0.049 (5) | 0.009 (4)    | -0.017 (4) | -0.011 (4) |
| O4  | 0.031 (5) | 0.043 (5)  | 0.054 (6) | -0.009 (4)   | -0.021 (4) | 0.015 (4)  |
| O5  | 0.041 (5) | 0.024 (5)  | 0.062 (6) | -0.008 (4)   | 0.023 (4)  | -0.019 (4) |
| O6  | 0.024 (4) | 0.026 (4)  | 0.044 (5) | -0.001 (3)   | -0.007 (4) | 0.010 (4)  |
| O7  | 0.031 (4) | 0.044 (5)  | 0.043 (5) | 0.017 (4)    | 0.006 (4)  | 0.014 (4)  |
| O8  | 0.060 (6) | 0.035 (5)  | 0.045 (5) | -0.004 (5)   | 0.011 (5)  | -0.011 (4) |
| O9  | 0.041 (5) | 0.042 (5)  | 0.033 (4) | 0.005 (4)    | -0.006 (4) | 0.018 (4)  |
| O10 | 0.020 (4) | 0.027 (4)  | 0.036 (4) | -0.004 (3)   | -0.001 (3) | -0.003 (3) |
| O11 | 0.024 (4) | 0.023 (4)  | 0.043 (5) | -0.002 (3)   | 0.007 (3)  | 0.007 (4)  |
| O12 | 0.028 (4) | 0.038 (5)  | 0.030 (4) | -0.003 (4)   | 0.010 (3)  | -0.003 (4) |
| C1  | 0.017 (2) | 0.011 (2)  | 0.035 (3) | -0.0042 (18) | 0.001 (2)  | -0.002 (2) |
| C2  | 0.017 (5) | 0.027 (5)  | 0.026 (5) | -0.004 (4)   | -0.003 (4) | 0.003 (4)  |
| C3  | 0.029 (6) | 0.020 (5)  | 0.031 (6) | 0.003 (4)    | -0.011 (5) | 0.003 (4)  |
| C4  | 0.025 (5) | 0.016 (5)  | 0.034 (6) | 0.002 (4)    | -0.005 (4) | -0.008 (4) |
| C5  | 0.017 (5) | 0.021 (5)  | 0.033 (6) | 0.004 (4)    | 0.001 (4)  | -0.005 (4) |
| C6  | 0.025 (5) | 0.010 (4)  | 0.030 (5) | -0.002 (4)   | 0.003 (4)  | 0.001 (4)  |
| C7  | 0.017 (2) | 0.011 (2)  | 0.035 (3) | -0.0042 (18) | 0.001 (2)  | -0.002 (2) |
| C8  | 0.023 (5) | 0.022 (5)  | 0.027 (5) | 0.000 (4)    | -0.001 (4) | -0.003 (4) |
| C9  | 0.016 (5) | 0.030 (6)  | 0.040 (6) | 0.000 (4)    | 0.001 (5)  | -0.009 (5) |
| C10 | 0.023 (5) | 0.032 (6)  | 0.033 (6) | 0.004 (5)    | -0.009 (4) | -0.008 (5) |
| C11 | 0.037 (6) | 0.024 (6)  | 0.029 (6) | 0.003 (5)    | -0.003 (5) | 0.006 (5)  |
| C12 | 0.025 (5) | 0.017 (5)  | 0.031 (5) | 0.001 (4)    | 0.002 (5)  | -0.003 (4) |
| C13 | 0.007 (4) | 0.006 (4)  | 0.034 (5) | 0.001 (3)    | 0.003 (4)  | -0.003 (4) |
| C14 | 0.018 (5) | 0.013 (5)  | 0.031 (5) | -0.005 (4)   | 0.001 (4)  | 0.001 (4)  |
| C15 | 0.028 (6) | 0.061 (9)  | 0.049 (8) | -0.024 (6)   | 0.012 (6)  | -0.026 (7) |
| C16 | 0.038 (7) | 0.081 (11) | 0.047 (8) | -0.029 (8)   | 0.012 (6)  | -0.038 (8) |
| C17 | 0.017 (2) | 0.011 (2)  | 0.035 (3) | -0.0042 (18) | 0.001 (2)  | -0.002 (2) |
| C18 | 0.020 (5) | 0.023 (5)  | 0.050 (7) | 0.005 (4)    | 0.002 (5)  | 0.007 (5)  |
| C19 | 0.023 (5) | 0.014 (5)  | 0.036 (6) | 0.005 (4)    | 0.000 (4)  | -0.004 (4) |
| C20 | 0.017 (2) | 0.011 (2)  | 0.035 (3) | -0.0042 (18) | 0.001 (2)  | -0.002 (2) |
| C21 | 0.009 (4) | 0.019 (5)  | 0.031 (5) | -0.002 (4)   | 0.002 (4)  | -0.001 (4) |
| C22 | 0.012 (4) | 0.029 (5)  | 0.024 (5) | 0.000 (4)    | 0.002 (4)  | -0.001 (4) |
| C23 | 0.022 (5) | 0.010 (4)  | 0.034 (6) | 0.005 (4)    | -0.003 (4) | 0.005 (4)  |
| C24 | 0.021 (5) | 0.012 (5)  | 0.035 (6) | 0.000 (4)    | 0.009 (4)  | 0.001 (4)  |
| C25 | 0.017 (5) | 0.029 (6)  | 0.036 (6) | 0.000 (4)    | 0.009 (4)  | 0.005 (5)  |
| C26 | 0.032 (6) | 0.033 (7)  | 0.037 (7) | -0.002 (5)   | -0.005 (5) | 0.003 (5)  |
| C27 | 0.027 (6) | 0.030 (6)  | 0.038 (6) | -0.003 (5)   | 0.001 (5)  | 0.002 (5)  |
| C28 | 0.044 (7) | 0.023 (6)  | 0.057 (8) | -0.011 (6)   | 0.003 (6)  | 0.017 (6)  |
| C29 | 0.054 (9) | 0.028 (7)  | 0.053 (8) | -0.005 (6)   | -0.005 (7) | 0.005 (6)  |
| C30 | 0.028 (6) | 0.030 (6)  | 0.039 (7) | 0.005 (5)    | 0.009 (5)  | -0.004 (5) |
| C31 | 0.052 (8) | 0.042 (7)  | 0.031 (6) | -0.010 (6)   | 0.016 (6)  | -0.004 (6) |
| C32 | 0.029 (6) | 0.008 (4)  | 0.026 (5) | -0.002 (4)   | 0.004 (4)  | -0.001 (4) |
| C33 | 0.021 (5) | 0.021 (5)  | 0.031 (6) | 0.001 (4)    | 0.002 (4)  | 0.010 (4)  |
| C34 | 0.032 (6) | 0.022 (5)  | 0.026 (5) | 0.003 (5)    | -0.003 (5) | -0.008 (4) |
| C35 | 0.016 (5) | 0.038 (6)  | 0.036 (6) | -0.018 (5)   | 0.003 (5)  | 0.000 (5)  |
| C36 | 0.024 (5) | 0.026 (6)  | 0.036 (6) | -0.008 (5)   | 0.007 (5)  | 0.000 (5)  |
| C37 | 0.019 (5) | 0.018 (5)  | 0.036 (6) | 0.002 (4)    | 0.007 (4)  | 0.007 (4)  |
| C38 | 0.027 (6) | 0.025 (6)  | 0.031 (6) | 0.000 (5)    | 0.013 (5)  | 0.000 (5)  |

|     |           |           |           |            |           |            |
|-----|-----------|-----------|-----------|------------|-----------|------------|
| C39 | 0.037 (6) | 0.018 (5) | 0.031 (6) | 0.007 (5)  | 0.010 (5) | -0.002 (5) |
| C40 | 0.026 (6) | 0.031 (6) | 0.029 (6) | -0.006 (5) | 0.000 (5) | 0.004 (5)  |

*Geometric parameters (Å, °)*

|         |             |          |            |
|---------|-------------|----------|------------|
| Ru1—C33 | 1.894 (11)  | C7—C12   | 1.381 (14) |
| Ru1—C34 | 1.924 (11)  | C7—C8    | 1.400 (14) |
| Ru1—C32 | 1.941 (11)  | C8—C9    | 1.397 (15) |
| Ru1—As1 | 2.4182 (12) | C8—H8A   | 0.9300     |
| Ru1—Ru3 | 2.8437 (11) | C9—C10   | 1.367 (17) |
| Ru1—Ru2 | 2.8621 (11) | C9—H9A   | 0.9300     |
| Ru2—C36 | 1.878 (12)  | C10—C11  | 1.383 (16) |
| Ru2—C37 | 1.917 (11)  | C10—H10A | 0.9300     |
| Ru2—C35 | 1.928 (12)  | C11—C12  | 1.392 (15) |
| Ru2—As2 | 2.4341 (12) | C11—H11A | 0.9300     |
| Ru2—Ru3 | 2.8382 (11) | C12—H12A | 0.9300     |
| Ru3—C39 | 1.904 (11)  | C13—H13A | 0.9700     |
| Ru3—C38 | 1.923 (12)  | C13—H13B | 0.9700     |
| Ru3—C40 | 1.942 (12)  | C14—C15  | 1.383 (16) |
| Ru3—P1  | 2.280 (3)   | C14—C19  | 1.401 (15) |
| As1—C7  | 1.938 (11)  | C15—C16  | 1.399 (17) |
| As1—C1  | 1.948 (10)  | C15—H15A | 0.9300     |
| As1—C13 | 1.969 (9)   | C16—C17  | 1.374 (16) |
| As2—C14 | 1.943 (10)  | C16—H16A | 0.9300     |
| As2—C20 | 1.949 (11)  | C17—C18  | 1.374 (16) |
| As2—C13 | 1.955 (9)   | C17—H17A | 0.9300     |
| Cl1—C27 | 1.779 (12)  | C18—C19  | 1.379 (15) |
| Cl2—C29 | 1.744 (15)  | C18—H18A | 0.9300     |
| Cl3—C31 | 1.784 (15)  | C19—H19A | 0.9300     |
| P1—O11  | 1.589 (8)   | C20—C25  | 1.383 (14) |
| P1—O10  | 1.605 (8)   | C20—C21  | 1.401 (14) |
| P1—O12  | 1.610 (8)   | C21—C22  | 1.394 (14) |
| O1—C32  | 1.130 (13)  | C21—H21A | 0.9300     |
| O2—C33  | 1.147 (13)  | C22—C23  | 1.378 (14) |
| O3—C34  | 1.151 (14)  | C22—H22A | 0.9300     |
| O4—C35  | 1.172 (14)  | C23—C24  | 1.385 (15) |
| O5—C36  | 1.157 (14)  | C23—H23A | 0.9300     |
| O6—C37  | 1.155 (13)  | C24—C25  | 1.398 (15) |
| O7—C38  | 1.153 (14)  | C24—H24A | 0.9300     |
| O8—C39  | 1.139 (14)  | C25—H25A | 0.9300     |
| O9—C40  | 1.131 (14)  | C26—C27  | 1.492 (16) |
| O10—C26 | 1.442 (14)  | C26—H26A | 0.9700     |
| O11—C28 | 1.427 (13)  | C26—H26B | 0.9700     |
| O12—C30 | 1.440 (14)  | C27—H27A | 0.9700     |
| C1—C2   | 1.378 (14)  | C27—H27B | 0.9700     |
| C1—C6   | 1.402 (14)  | C28—C29  | 1.487 (18) |
| C2—C3   | 1.420 (15)  | C28—H28A | 0.9700     |
| C2—H2A  | 0.9300      | C28—H28B | 0.9700     |

|             |            |               |            |
|-------------|------------|---------------|------------|
| C3—C4       | 1.382 (16) | C29—H29A      | 0.9700     |
| C3—H3A      | 0.9300     | C29—H29B      | 0.9700     |
| C4—C5       | 1.373 (15) | C30—C31       | 1.493 (18) |
| C4—H4A      | 0.9300     | C30—H30A      | 0.9700     |
| C5—C6       | 1.382 (14) | C30—H30B      | 0.9700     |
| C5—H5A      | 0.9300     | C31—H31A      | 0.9700     |
| C6—H6A      | 0.9300     | C31—H31B      | 0.9700     |
|             |            |               |            |
| C33—Ru1—C34 | 94.3 (5)   | C11—C10—H10A  | 119.2      |
| C33—Ru1—C32 | 89.8 (4)   | C10—C11—C12   | 119.8 (11) |
| C34—Ru1—C32 | 175.0 (4)  | C10—C11—H11A  | 120.1      |
| C33—Ru1—As1 | 101.7 (3)  | C12—C11—H11A  | 120.1      |
| C34—Ru1—As1 | 86.9 (3)   | C7—C12—C11    | 120.0 (10) |
| C32—Ru1—As1 | 94.8 (3)   | C7—C12—H12A   | 120.0      |
| C33—Ru1—Ru3 | 105.9 (3)  | C11—C12—H12A  | 120.0      |
| C34—Ru1—Ru3 | 94.3 (3)   | As2—C13—As1   | 112.7 (4)  |
| C32—Ru1—Ru3 | 81.9 (3)   | As2—C13—H13A  | 109.1      |
| As1—Ru1—Ru3 | 152.20 (4) | As1—C13—H13A  | 109.1      |
| C33—Ru1—Ru2 | 165.5 (3)  | As2—C13—H13B  | 109.1      |
| C34—Ru1—Ru2 | 85.6 (3)   | As1—C13—H13B  | 109.1      |
| C32—Ru1—Ru2 | 89.7 (3)   | H13A—C13—H13B | 107.8      |
| As1—Ru1—Ru2 | 92.85 (4)  | C15—C14—C19   | 119.9 (10) |
| Ru3—Ru1—Ru2 | 59.66 (3)  | C15—C14—As2   | 119.1 (8)  |
| C36—Ru2—C37 | 90.3 (5)   | C19—C14—As2   | 120.9 (8)  |
| C36—Ru2—C35 | 92.9 (5)   | C14—C15—C16   | 118.8 (11) |
| C37—Ru2—C35 | 174.6 (4)  | C14—C15—H15A  | 120.6      |
| C36—Ru2—As2 | 102.8 (3)  | C16—C15—H15A  | 120.6      |
| C37—Ru2—As2 | 89.7 (3)   | C17—C16—C15   | 121.5 (12) |
| C35—Ru2—As2 | 93.9 (3)   | C17—C16—H16A  | 119.3      |
| C36—Ru2—Ru3 | 102.3 (3)  | C15—C16—H16A  | 119.3      |
| C37—Ru2—Ru3 | 94.8 (3)   | C16—C17—C18   | 119.0 (10) |
| C35—Ru2—Ru3 | 80.3 (3)   | C16—C17—H17A  | 120.5      |
| As2—Ru2—Ru3 | 154.52 (4) | C18—C17—H17A  | 120.5      |
| C36—Ru2—Ru1 | 160.8 (3)  | C17—C18—C19   | 121.4 (11) |
| C37—Ru2—Ru1 | 84.8 (3)   | C17—C18—H18A  | 119.3      |
| C35—Ru2—Ru1 | 90.9 (4)   | C19—C18—H18A  | 119.3      |
| As2—Ru2—Ru1 | 95.74 (4)  | C18—C19—C14   | 119.4 (10) |
| Ru3—Ru2—Ru1 | 59.85 (3)  | C18—C19—H19A  | 120.3      |
| C39—Ru3—C38 | 91.8 (5)   | C14—C19—H19A  | 120.3      |
| C39—Ru3—C40 | 90.2 (5)   | C25—C20—C21   | 118.7 (10) |
| C38—Ru3—C40 | 177.2 (5)  | C25—C20—As2   | 118.0 (8)  |
| C39—Ru3—P1  | 108.7 (4)  | C21—C20—As2   | 122.9 (7)  |
| C38—Ru3—P1  | 91.7 (3)   | C22—C21—C20   | 120.0 (9)  |
| C40—Ru3—P1  | 89.5 (3)   | C22—C21—H21A  | 120.0      |
| C39—Ru3—Ru2 | 98.3 (3)   | C20—C21—H21A  | 120.0      |
| C38—Ru3—Ru2 | 81.2 (3)   | C23—C22—C21   | 121.4 (10) |
| C40—Ru3—Ru2 | 96.6 (3)   | C23—C22—H22A  | 119.3      |
| P1—Ru3—Ru2  | 152.34 (8) | C21—C22—H22A  | 119.3      |

|             |            |               |            |
|-------------|------------|---------------|------------|
| C39—Ru3—Ru1 | 155.6 (4)  | C22—C23—C24   | 118.3 (9)  |
| C38—Ru3—Ru1 | 96.1 (3)   | C22—C23—H23A  | 120.8      |
| C40—Ru3—Ru1 | 81.3 (3)   | C24—C23—H23A  | 120.8      |
| P1—Ru3—Ru1  | 94.11 (8)  | C23—C24—C25   | 121.2 (9)  |
| Ru2—Ru3—Ru1 | 60.49 (3)  | C23—C24—H24A  | 119.4      |
| C7—As1—C1   | 99.3 (4)   | C25—C24—H24A  | 119.4      |
| C7—As1—C13  | 107.8 (4)  | C20—C25—C24   | 120.3 (10) |
| C1—As1—C13  | 98.0 (4)   | C20—C25—H25A  | 119.8      |
| C7—As1—Ru1  | 116.8 (3)  | C24—C25—H25A  | 119.8      |
| C1—As1—Ru1  | 118.7 (3)  | O10—C26—C27   | 110.4 (10) |
| C13—As1—Ru1 | 113.7 (3)  | O10—C26—H26A  | 109.6      |
| C14—As2—C20 | 98.6 (4)   | C27—C26—H26A  | 109.6      |
| C14—As2—C13 | 102.5 (4)  | O10—C26—H26B  | 109.6      |
| C20—As2—C13 | 104.3 (4)  | C27—C26—H26B  | 109.6      |
| C14—As2—Ru2 | 116.0 (3)  | H26A—C26—H26B | 108.1      |
| C20—As2—Ru2 | 118.9 (3)  | C26—C27—C11   | 110.2 (9)  |
| C13—As2—Ru2 | 114.1 (3)  | C26—C27—H27A  | 109.6      |
| O11—P1—O10  | 99.7 (4)   | C11—C27—H27A  | 109.6      |
| O11—P1—O12  | 103.0 (4)  | C26—C27—H27B  | 109.6      |
| O10—P1—O12  | 98.6 (4)   | C11—C27—H27B  | 109.6      |
| O11—P1—Ru3  | 114.5 (3)  | H27A—C27—H27B | 108.1      |
| O10—P1—Ru3  | 115.4 (3)  | O11—C28—C29   | 111.0 (11) |
| O12—P1—Ru3  | 122.2 (3)  | O11—C28—H28A  | 109.4      |
| C26—O10—P1  | 122.8 (7)  | C29—C28—H28A  | 109.4      |
| C28—O11—P1  | 121.2 (8)  | O11—C28—H28B  | 109.4      |
| C30—O12—P1  | 126.5 (7)  | C29—C28—H28B  | 109.4      |
| C2—C1—C6    | 119.3 (10) | H28A—C28—H28B | 108.0      |
| C2—C1—As1   | 121.4 (8)  | C28—C29—C12   | 115.1 (10) |
| C6—C1—As1   | 119.3 (8)  | C28—C29—H29A  | 108.5      |
| C1—C2—C3    | 120.5 (10) | C12—C29—H29A  | 108.5      |
| C1—C2—H2A   | 119.7      | C28—C29—H29B  | 108.5      |
| C3—C2—H2A   | 119.7      | C12—C29—H29B  | 108.5      |
| C4—C3—C2    | 118.2 (10) | H29A—C29—H29B | 107.5      |
| C4—C3—H3A   | 120.9      | O12—C30—C31   | 110.2 (10) |
| C2—C3—H3A   | 120.9      | O12—C30—H30A  | 109.6      |
| C5—C4—C3    | 121.6 (10) | C31—C30—H30A  | 109.6      |
| C5—C4—H4A   | 119.2      | O12—C30—H30B  | 109.6      |
| C3—C4—H4A   | 119.2      | C31—C30—H30B  | 109.6      |
| C4—C5—C6    | 119.9 (10) | H30A—C30—H30B | 108.1      |
| C4—C5—H5A   | 120.1      | C30—C31—C13   | 112.0 (9)  |
| C6—C5—H5A   | 120.1      | C30—C31—H31A  | 109.2      |
| C5—C6—C1    | 120.3 (10) | C13—C31—H31A  | 109.2      |
| C5—C6—H6A   | 119.8      | C30—C31—H31B  | 109.2      |
| C1—C6—H6A   | 119.8      | C13—C31—H31B  | 109.2      |
| C12—C7—C8   | 119.3 (10) | H31A—C31—H31B | 107.9      |
| C12—C7—As1  | 125.5 (8)  | O1—C32—Ru1    | 173.4 (9)  |
| C8—C7—As1   | 115.1 (8)  | O2—C33—Ru1    | 176.6 (10) |
| C9—C8—C7    | 120.8 (10) | O3—C34—Ru1    | 174.5 (10) |

|                 |             |                 |            |
|-----------------|-------------|-----------------|------------|
| C9—C8—H8A       | 119.6       | O4—C35—Ru2      | 173.8 (10) |
| C7—C8—H8A       | 119.6       | O5—C36—Ru2      | 176.3 (11) |
| C10—C9—C8       | 118.6 (10)  | O6—C37—Ru2      | 172.6 (9)  |
| C10—C9—H9A      | 120.7       | O7—C38—Ru3      | 173.4 (10) |
| C8—C9—H9A       | 120.7       | O8—C39—Ru3      | 178.1 (12) |
| C9—C10—C11      | 121.6 (10)  | O9—C40—Ru3      | 172.9 (10) |
| C9—C10—H10A     | 119.2       |                 |            |
|                 |             |                 |            |
| C33—Ru1—Ru2—C36 | -30.3 (17)  | C36—Ru2—As2—C13 | 179.9 (5)  |
| C34—Ru1—Ru2—C36 | -120.6 (12) | C37—Ru2—As2—C13 | -89.9 (4)  |
| C32—Ru1—Ru2—C36 | 57.8 (12)   | C35—Ru2—As2—C13 | 86.1 (5)   |
| As1—Ru1—Ru2—C36 | 152.7 (11)  | Ru3—Ru2—As2—C13 | 10.5 (3)   |
| Ru3—Ru1—Ru2—C36 | -23.0 (11)  | Ru1—Ru2—As2—C13 | -5.2 (3)   |
| C33—Ru1—Ru2—C37 | -105.9 (13) | C39—Ru3—P1—O11  | -109.6 (5) |
| C34—Ru1—Ru2—C37 | 163.7 (5)   | C38—Ru3—P1—O11  | 157.9 (5)  |
| C32—Ru1—Ru2—C37 | -17.8 (4)   | C40—Ru3—P1—O11  | -19.6 (5)  |
| As1—Ru1—Ru2—C37 | 77.0 (3)    | Ru2—Ru3—P1—O11  | 83.8 (4)   |
| Ru3—Ru1—Ru2—C37 | -98.6 (3)   | Ru1—Ru3—P1—O11  | 61.7 (4)   |
| C33—Ru1—Ru2—C35 | 70.9 (13)   | C39—Ru3—P1—O10  | 135.5 (5)  |
| C34—Ru1—Ru2—C35 | -19.4 (5)   | C38—Ru3—P1—O10  | 43.0 (5)   |
| C32—Ru1—Ru2—C35 | 159.1 (4)   | C40—Ru3—P1—O10  | -134.5 (5) |
| As1—Ru1—Ru2—C35 | -106.1 (3)  | Ru2—Ru3—P1—O10  | -31.1 (4)  |
| Ru3—Ru1—Ru2—C35 | 78.2 (3)    | Ru1—Ru3—P1—O10  | -53.2 (3)  |
| C33—Ru1—Ru2—As2 | 164.9 (13)  | C39—Ru3—P1—O12  | 15.9 (5)   |
| C34—Ru1—Ru2—As2 | 74.6 (3)    | C38—Ru3—P1—O12  | -76.6 (5)  |
| C32—Ru1—Ru2—As2 | -106.9 (3)  | C40—Ru3—P1—O12  | 105.9 (5)  |
| As1—Ru1—Ru2—As2 | -12.09 (4)  | Ru2—Ru3—P1—O12  | -150.8 (4) |
| Ru3—Ru1—Ru2—As2 | 172.24 (4)  | Ru1—Ru3—P1—O12  | -172.9 (4) |
| C33—Ru1—Ru2—Ru3 | -7.3 (13)   | O11—P1—O10—C26  | 145.8 (8)  |
| C34—Ru1—Ru2—Ru3 | -97.6 (3)   | O12—P1—O10—C26  | 40.9 (9)   |
| C32—Ru1—Ru2—Ru3 | 80.8 (3)    | Ru3—P1—O10—C26  | -91.0 (8)  |
| As1—Ru1—Ru2—Ru3 | 175.68 (4)  | O10—P1—O11—C28  | -59.6 (10) |
| C36—Ru2—Ru3—C39 | -20.3 (5)   | O12—P1—O11—C28  | 41.7 (10)  |
| C37—Ru2—Ru3—C39 | -111.6 (5)  | Ru3—P1—O11—C28  | 176.6 (9)  |
| C35—Ru2—Ru3—C39 | 70.5 (5)    | O11—P1—O12—C30  | 120.5 (9)  |
| As2—Ru2—Ru3—C39 | 149.0 (4)   | O10—P1—O12—C30  | -137.4 (9) |
| Ru1—Ru2—Ru3—C39 | 167.2 (4)   | Ru3—P1—O12—C30  | -9.9 (11)  |
| C36—Ru2—Ru3—C38 | 70.2 (5)    | C7—As1—C1—C2    | -134.8 (8) |
| C37—Ru2—Ru3—C38 | -21.1 (5)   | C13—As1—C1—C2   | 115.6 (9)  |
| C35—Ru2—Ru3—C38 | 161.1 (5)   | Ru1—As1—C1—C2   | -7.1 (10)  |
| As2—Ru2—Ru3—C38 | -120.4 (4)  | C7—As1—C1—C6    | 44.8 (9)   |
| Ru1—Ru2—Ru3—C38 | -102.2 (3)  | C13—As1—C1—C6   | -64.8 (9)  |
| C36—Ru2—Ru3—C40 | -111.5 (5)  | Ru1—As1—C1—C6   | 172.5 (7)  |
| C37—Ru2—Ru3—C40 | 157.2 (5)   | C6—C1—C2—C3     | 1.1 (15)   |
| C35—Ru2—Ru3—C40 | -20.6 (5)   | As1—C1—C2—C3    | -179.3 (8) |
| As2—Ru2—Ru3—C40 | 57.9 (4)    | C1—C2—C3—C4     | -0.8 (15)  |
| Ru1—Ru2—Ru3—C40 | 76.1 (4)    | C2—C3—C4—C5     | 0.8 (16)   |
| C36—Ru2—Ru3—P1  | 146.9 (4)   | C3—C4—C5—C6     | -0.9 (16)  |

|                 |             |                 |             |
|-----------------|-------------|-----------------|-------------|
| C37—Ru2—Ru3—P1  | 55.6 (4)    | C4—C5—C6—C1     | 1.2 (16)    |
| C35—Ru2—Ru3—P1  | -122.3 (4)  | C2—C1—C6—C5     | -1.3 (15)   |
| As2—Ru2—Ru3—P1  | -43.8 (2)   | As1—C1—C6—C5    | 179.1 (8)   |
| Ru1—Ru2—Ru3—P1  | -25.54 (17) | C1—As1—C7—C12   | -99.4 (9)   |
| C36—Ru2—Ru3—Ru1 | 172.4 (4)   | C13—As1—C7—C12  | 2.1 (10)    |
| C37—Ru2—Ru3—Ru1 | 81.1 (3)    | Ru1—As1—C7—C12  | 131.7 (8)   |
| C35—Ru2—Ru3—Ru1 | -96.7 (4)   | C1—As1—C7—C8    | 75.7 (8)    |
| As2—Ru2—Ru3—Ru1 | -18.21 (10) | C13—As1—C7—C8   | 177.3 (7)   |
| C33—Ru1—Ru3—C39 | 146.1 (9)   | Ru1—As1—C7—C8   | -53.2 (8)   |
| C34—Ru1—Ru3—C39 | 50.3 (9)    | C12—C7—C8—C9    | -0.1 (16)   |
| C32—Ru1—Ru3—C39 | -126.4 (9)  | As1—C7—C8—C9    | -175.5 (8)  |
| As1—Ru1—Ru3—C39 | -41.3 (8)   | C7—C8—C9—C10    | -1.0 (16)   |
| Ru2—Ru1—Ru3—C39 | -32.0 (8)   | C8—C9—C10—C11   | 0.9 (17)    |
| C33—Ru1—Ru3—C38 | -105.7 (5)  | C9—C10—C11—C12  | 0.2 (18)    |
| C34—Ru1—Ru3—C38 | 158.6 (5)   | C8—C7—C12—C11   | 1.2 (16)    |
| C32—Ru1—Ru3—C38 | -18.2 (4)   | As1—C7—C12—C11  | 176.1 (8)   |
| As1—Ru1—Ru3—C38 | 66.9 (3)    | C10—C11—C12—C7  | -1.2 (17)   |
| Ru2—Ru1—Ru3—C38 | 76.2 (3)    | C14—As2—C13—As1 | 152.2 (5)   |
| C33—Ru1—Ru3—C40 | 75.4 (5)    | C20—As2—C13—As1 | -105.4 (5)  |
| C34—Ru1—Ru3—C40 | -20.4 (5)   | Ru2—As2—C13—As1 | 25.9 (6)    |
| C32—Ru1—Ru3—C40 | 162.9 (4)   | C7—As1—C13—As2  | 93.3 (6)    |
| As1—Ru1—Ru3—C40 | -112.0 (3)  | C1—As1—C13—As2  | -164.1 (5)  |
| Ru2—Ru1—Ru3—C40 | -102.7 (3)  | Ru1—As1—C13—As2 | -37.9 (6)   |
| C33—Ru1—Ru3—P1  | -13.5 (3)   | C20—As2—C14—C15 | 108.7 (11)  |
| C34—Ru1—Ru3—P1  | -109.2 (4)  | C13—As2—C14—C15 | -144.4 (10) |
| C32—Ru1—Ru3—P1  | 74.0 (3)    | Ru2—As2—C14—C15 | -19.4 (11)  |
| As1—Ru1—Ru3—P1  | 159.13 (11) | C20—As2—C14—C19 | -68.2 (9)   |
| Ru2—Ru1—Ru3—P1  | 168.42 (8)  | C13—As2—C14—C19 | 38.6 (9)    |
| C33—Ru1—Ru3—Ru2 | 178.1 (3)   | Ru2—As2—C14—C19 | 163.6 (7)   |
| C34—Ru1—Ru3—Ru2 | 82.3 (3)    | C19—C14—C15—C16 | 0 (2)       |
| C32—Ru1—Ru3—Ru2 | -94.4 (3)   | As2—C14—C15—C16 | -177.1 (12) |
| As1—Ru1—Ru3—Ru2 | -9.29 (9)   | C14—C15—C16—C17 | 0 (3)       |
| C33—Ru1—As1—C7  | 83.0 (5)    | C15—C16—C17—C18 | 1 (2)       |
| C34—Ru1—As1—C7  | 176.8 (5)   | C16—C17—C18—C19 | -1.9 (18)   |
| C32—Ru1—As1—C7  | -7.9 (4)    | C17—C18—C19—C14 | 2.0 (16)    |
| Ru3—Ru1—As1—C7  | -89.8 (3)   | C15—C14—C19—C18 | -1.0 (17)   |
| Ru2—Ru1—As1—C7  | -97.8 (3)   | As2—C14—C19—C18 | 176.0 (8)   |
| C33—Ru1—As1—C1  | -36.0 (5)   | C14—As2—C20—C25 | -94.4 (9)   |
| C34—Ru1—As1—C1  | 57.8 (5)    | C13—As2—C20—C25 | 160.3 (8)   |
| C32—Ru1—As1—C1  | -126.8 (4)  | Ru2—As2—C20—C25 | 31.8 (9)    |
| Ru3—Ru1—As1—C1  | 151.3 (3)   | C14—As2—C20—C21 | 79.0 (9)    |
| Ru2—Ru1—As1—C1  | 143.2 (3)   | C13—As2—C20—C21 | -26.3 (9)   |
| C33—Ru1—As1—C13 | -150.4 (4)  | Ru2—As2—C20—C21 | -154.8 (7)  |
| C34—Ru1—As1—C13 | -56.6 (4)   | C25—C20—C21—C22 | -1.4 (14)   |
| C32—Ru1—As1—C13 | 118.8 (4)   | As2—C20—C21—C22 | -174.7 (7)  |
| Ru3—Ru1—As1—C13 | 36.9 (3)    | C20—C21—C22—C23 | 3.0 (15)    |
| Ru2—Ru1—As1—C13 | 28.8 (3)    | C21—C22—C23—C24 | -3.2 (15)   |
| C36—Ru2—As2—C14 | 61.0 (5)    | C22—C23—C24—C25 | 1.8 (16)    |

|                 |            |                 |             |
|-----------------|------------|-----------------|-------------|
| C37—Ru2—As2—C14 | 151.2 (5)  | C21—C20—C25—C24 | 0.1 (15)    |
| C35—Ru2—As2—C14 | -32.8 (5)  | As2—C20—C25—C24 | 173.8 (8)   |
| Ru3—Ru2—As2—C14 | -108.3 (3) | C23—C24—C25—C20 | -0.3 (17)   |
| Ru1—Ru2—As2—C14 | -124.1 (3) | P1—O10—C26—C27  | -105.3 (10) |
| C36—Ru2—As2—C20 | -56.4 (5)  | O10—C26—C27—C11 | -62.3 (12)  |
| C37—Ru2—As2—C20 | 33.8 (5)   | P1—O11—C28—C29  | 158.8 (9)   |
| C35—Ru2—As2—C20 | -150.2 (5) | O11—C28—C29—C12 | 65.8 (15)   |
| Ru3—Ru2—As2—C20 | 134.3 (3)  | P1—O12—C30—C31  | -107.2 (11) |
| Ru1—Ru2—As2—C20 | 118.5 (3)  | O12—C30—C31—C13 | 65.1 (12)   |

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

Cg1 and Cg2 are the centroids of the C1–C6 and C20–C25 benzene rings, respectively.

| $D-H\cdots A$                        | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------------|-------|-------------|-------------|---------------|
| C19—H19A $\cdots$ O6 <sup>i</sup>    | 0.93  | 2.57        | 3.275 (14)  | 133           |
| C27—H27B $\cdots$ O9 <sup>ii</sup>   | 0.97  | 2.47        | 3.231 (15)  | 135           |
| C30—H30A $\cdots$ O5 <sup>iii</sup>  | 0.97  | 2.56        | 3.297 (15)  | 133           |
| C4—H4A $\cdots$ Cg1 <sup>iv</sup>    | 0.93  | 2.77        | 3.468 (11)  | 133           |
| C9—H9A $\cdots$ Cg2 <sup>v</sup>     | 0.93  | 2.89        | 3.684 (12)  | 144           |
| C18—H18A $\cdots$ Cg1 <sup>vi</sup>  | 0.93  | 2.71        | 3.505 (12)  | 145           |
| C24—H24A $\cdots$ Cg2 <sup>vii</sup> | 0.93  | 2.69        | 3.473 (11)  | 142           |

Symmetry codes: (i)  $x+1/2, y, -z+1/2$ ; (ii)  $x-1/2, -y+1/2, -z+1$ ; (iii)  $-x, -y+1, -z+1$ ; (iv)  $-x+1, y-1/2, -z+1/2$ ; (v)  $x-3/2, y, -z-1/2$ ; (vi)  $x-1/2, y, -z-1/2$ ; (vii)  $-x-1/2, y-1/2, z$ .