

**[ $\mu$ -Bis(diphenylarsino)methane-1:2 $\kappa^2$ As:-As']nonacarbonyl-1 $\kappa^3$ C,2 $\kappa^3$ C,3 $\kappa^3$ C-[triphenylstibine-3 $\kappa$ Sb]-triangulo-triruthenium(0)**

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

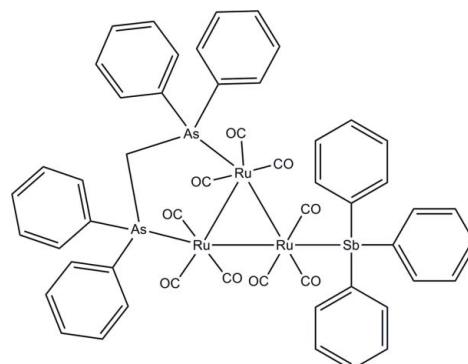
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Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(C-C) = 0.009$  Å;  
 $R$  factor = 0.037;  $wR$  factor = 0.096; data-to-parameter ratio = 18.8.

In the title *triangulo*-triruthenium compound,  $[\text{Ru}_3(\text{C}_{25}\text{H}_{22}\text{As}_2)(\text{C}_{18}\text{H}_{15}\text{Sb})(\text{CO})_9]$ , the bis(diphenylarsino)-methane ligand bridges an Ru–Ru bond and the monodentate stibine ligand bonds to the third Ru atom. Both the stibine and arsine ligands are equatorial with respect to the  $\text{Ru}_3$  triangle. Additionally, each Ru atom carries one equatorial and two axial terminal carbonyl ligands. The three stibine-substituted phenyl rings make dihedral angles of 84.3 (3), 80.4 (3) and 70.5 (3)° with each other. The dihedral angles between the two phenyl rings are 85.9 (3) and 75.2 (3)° for the two diphenylarsine groups. In the crystal packing, molecules are linked into chains down the  $c$  axis via intermolecular C–H···O hydrogen bonds. Weak intermolecular C–H···π interactions further stabilize the crystal structure.

## Related literature

For general background to *triangulo*-triruthenium derivatives, see: Bruce *et al.* (1985, 1988a,b); Shawkataly *et al.* (1998, 2004, 2009). For related structures, see: Shawkataly *et al.* (2009). For the synthesis of  $\mu$ -bis(diphenylarsino)methanecacarbonyl-triruthenium(0), see: Bruce *et al.* (1983). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



## Experimental

### Crystal data

|  |                                   |
|--|-----------------------------------|
| $[\text{Ru}_3(\text{C}_{25}\text{H}_{22}\text{As}_2)(\text{C}_{18}\text{H}_{15}\text{Sb})(\text{CO})_9]$ | $V = 9898.5$ (3) Å <sup>3</sup>   |
| $M_r = 1380.62$  | $Z = 8$                           |
| Monoclinic, $C2/c$   | Mo $K\alpha$ radiation            |
| $a = 42.3464$ (6) Å  | $\mu = 2.82$ mm <sup>-1</sup>     |
| $b = 11.6246$ (2) Å  | $T = 100$ K                       |
| $c = 20.1185$ (3) Å  | $0.36 \times 0.15 \times 0.09$ mm |
| $\beta = 91.823$ (1)°  |                                   |

### Data collection

|   |  |
|---|--|
| Bruker SMART APEXII CCD area-detector diffractometer              | 55374 measured reflections             |
| Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2005) | 11349 independent reflections          |
| $T_{\min} = 0.428$ , $T_{\max} = 0.796$                           | 8669 reflections with $I > 2\sigma(I)$ |
|   | $R_{\text{int}} = 0.042$               |

### Refinement

|                                 |   |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.037$ | 605 parameters                                |
| $wR(F^2) = 0.096$               | H-atom parameters constrained                 |
| $S = 1.08$                      | $\Delta\rho_{\max} = 1.45$ e Å <sup>-3</sup>  |
| 11349 reflections               | $\Delta\rho_{\min} = -1.24$ e Å <sup>-3</sup> |

**Table 1**

Hydrogen-bond geometry (Å, °).

| $D-\text{H} \cdots A$         | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|-------------------------------|--------------|---------------------|--------------|-----------------------|
| C13–H13B···O8 <sup>i</sup>    | 0.97         | 2.59                | 3.290 (7)    | 129                   |
| C23–H23A···Cg1 <sup>ii</sup>  | 0.93         | 2.88                | 3.686 (6)    | 146                   |
| C34–H34A···Cg2 <sup>iii</sup> | 0.93         | 2.72                | 3.564 (6)    | 151                   |

Symmetry codes: (i)  $x, -y + 1, z - \frac{1}{2}$ ; (ii)  $x, -y, z - \frac{3}{2}$ ; (iii)  $-x, y, -z + \frac{1}{2}$ . Cg1 and Cg2 are the centroids of the C14–C19 and C26–C31phenyl rings, respectively.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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).

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<sup>#</sup> On secondment to: Multimedia University, Melaka Campus, Jalan Ayer Keroh Lama, 74750 Melaka, Malaysia.

<sup>§</sup> Thomson Reuters ResearcherID: A-5523-2009.

<sup>¶</sup> Thomson Reuters ResearcherID: A-3561-2009. Additional correspondence author, e-mail: hkfunk@usm.my.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2682).

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# supporting information

*Acta Cryst.* (2010). E66, m94–m95 [doi:10.1107/S1600536809049927]

## [ $\mu$ -Bis(diphenylarsino)methane-1:2 $\kappa^2$ As:As']nonacarbonyl-1 $\kappa^3$ C,2 $\kappa^3$ C,3 $\kappa^3$ C-[triphenylstibine-3 $\kappa$ Sb]-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<sub>3</sub>(CO)<sub>12-n</sub>L<sub>n</sub> (L= group 15 ligand) have been reported (Bruce *et al.*, 1985, 1988a,b). As part of our study on 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, 2009). Herein we report the synthesis and structure of Ru<sub>3</sub>(C<sub>18</sub>H<sub>15</sub>Sb)(C<sub>25</sub>H<sub>22</sub>As<sub>2</sub>)(CO)<sub>9</sub>.

The bond lengths and angles of title compound (Fig. 1) are comparable to those found in a related structure (Shawkataly *et al.*, 2009). The bis(diphenylarsino)methane ligand bridges the Ru1—Ru2 bond and the monodentate stibine ligand bonds to the Ru3 atom. Both the stibine and arsine ligands are equatorial with respect to the Ru<sub>3</sub> triangle. Additionally, each Ru atom carries one equatorial and two axial terminal carbonyl ligands. The three stibine substituted phenyl rings make dihedral angles (C26—C31/C32—C37, C26—C31/C38—C43 and C32—C37/C38—C43) of 84.3 (3), 80.4 (3) and 70.5 (3)° with each other respectively. The dihedral angles between the two phenyl rings (C1—C6/C7—C12 and C14—C19/C20—C25) are 85.9 (3) and 75.2 (3)° for the two diphenylarsino groups respectively.

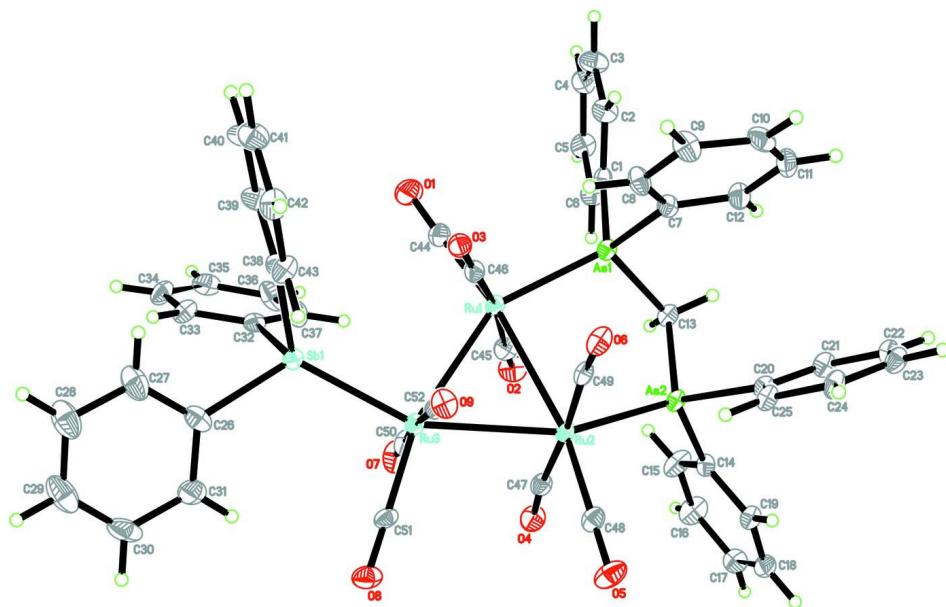
In the crystal packing (Fig. 2), the molecules are linked together into chains *via* intermolecular C13—H13B···O8 along *c* axis. Weak intermolecular C—H···π interactions further stabilize the crystal structure (Table 1).

### S2. Experimental

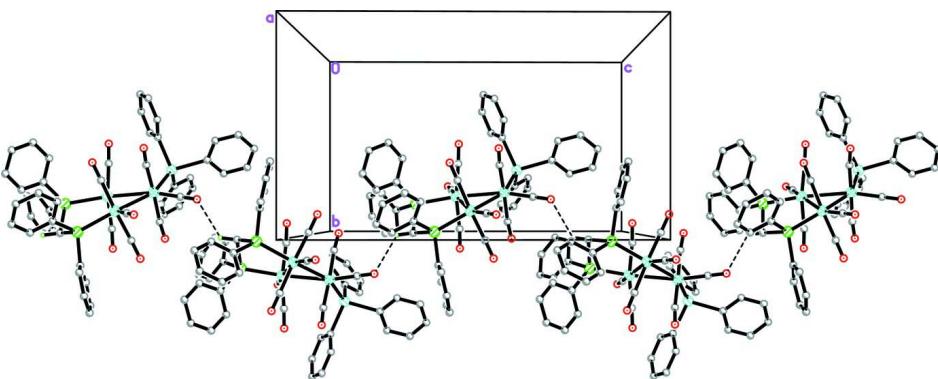
All manipulations were performed under a dry oxygen-free dinitrogen atmosphere using standard Schlenk techniques, all solvents were dried over sodium and distilled from sodium benzophenone ketyl under nitrogen. Triphenylstibine (Fluka) used as received and  $\mu$ -bis(diphenylarsino)methanecacarbonyltriruthenium(0) (Bruce *et al.*, 1983) was prepared by reported procedure. The title compound was obtained by refluxing equimolar quantities of Ru<sub>3</sub>(CO)<sub>10</sub>( $\mu$ -Ph<sub>2</sub>AsCH<sub>2</sub>AsPh<sub>2</sub>) (105.5 mg, 0.1 mmol) and triphenylstibine (35.3 mg, 0.1 mmol) in hexane under nitrogen atmosphere. Crystals suitable for X-ray diffraction were grown by slow solvent / solvent diffusion of CH<sub>3</sub>OH into CH<sub>2</sub>Cl<sub>2</sub>.

### S3. Refinement

All hydrogen atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.97 Å and  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ . The final difference Fourier map reveals high peaks, ~1.5 e Å<sup>-3</sup>, two of which are quite separate from the heavy atoms. These could be due to the presence of additional solvent, possibly methanol, and perhaps at partial occupancy. Attempts to produce a satisfactory model of this solvent were not successful.

**Figure 1**

The molecular structure of the title compound with 30% probability ellipsoids for non-H atoms.

**Figure 2**

The crystal packing of the title compound, viewed down the *a* axis, showing the molecules linked along the *c* axis. Hydrogen atoms that are not involved in the hydrogen-bonding (dashed lines) have been omitted for clarity.

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*Crystal data*



$M_r = 1380.62$

Monoclinic,  $C2/c$

Hall symbol: -C 2yc

$a = 42.3464 (6)$  Å

$b = 11.6246 (2)$  Å

$c = 20.1185 (3)$  Å

$\beta = 91.823 (1)^\circ$

$V = 9898.5 (3)$  Å<sup>3</sup>

$Z = 8$

$F(000) = 5360$

$D_x = 1.853 \text{ Mg m}^{-3}$

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

Cell parameters from 9674 reflections

$\theta = 2.3\text{--}30.6^\circ$

$\mu = 2.82 \text{ mm}^{-1}$

$T = 100$  K

Block, red

$0.36 \times 0.15 \times 0.09$  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, 2005)  
 $T_{\min} = 0.428$ ,  $T_{\max} = 0.796$

55374 measured reflections  
11349 independent reflections  
8669 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.042$   
 $\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 2.0^\circ$   
 $h = -54 \rightarrow 50$   
 $k = -14 \rightarrow 15$   
 $l = -25 \rightarrow 26$

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.096$   
 $S = 1.08$   
11349 reflections  
605 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  
 $w = 1/[\sigma^2(F_o^2) + (0.027P)^2 + 103.4772P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 1.45 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -1.24 \text{ e } \text{\AA}^{-3}$

*Special details*

**Experimental.** The crystal was placed in the cold stream of an Oxford Cyrosystems 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 ( $\text{\AA}^2$ )*

|     | $x$           | $y$         | $z$           | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|-------------|---------------|----------------------------------|
| Sb1 | 0.084142 (8)  | 0.82926 (3) | 0.122293 (17) | 0.02485 (8)                      |
| Ru1 | 0.111861 (9)  | 0.69580 (3) | -0.05368 (2)  | 0.02414 (10)                     |
| Ru2 | 0.173966 (9)  | 0.62369 (3) | -0.01095 (2)  | 0.02287 (9)                      |
| Ru3 | 0.132574 (9)  | 0.71467 (3) | 0.08382 (2)   | 0.02524 (10)                     |
| As1 | 0.124706 (12) | 0.65958 (4) | -0.16939 (3)  | 0.02403 (11)                     |
| As2 | 0.185533 (11) | 0.52317 (4) | -0.11339 (3)  | 0.02262 (11)                     |
| O1  | 0.04220 (10)  | 0.7484 (5)  | -0.0798 (2)   | 0.0569 (13)                      |
| O2  | 0.09819 (10)  | 0.4372 (3)  | -0.0433 (2)   | 0.0431 (10)                      |
| O3  | 0.12504 (9)   | 0.9554 (3)  | -0.04611 (18) | 0.0311 (8)                       |
| O4  | 0.15850 (10)  | 0.3916 (3)  | 0.0537 (2)    | 0.0409 (10)                      |
| O5  | 0.23787 (10)  | 0.6078 (4)  | 0.0599 (2)    | 0.0491 (11)                      |
| O6  | 0.19089 (9)   | 0.8586 (3)  | -0.0700 (2)   | 0.0355 (9)                       |
| O7  | 0.09752 (10)  | 0.4866 (3)  | 0.1062 (2)    | 0.0467 (11)                      |
| O8  | 0.16762 (9)   | 0.6817 (4)  | 0.2157 (2)    | 0.0432 (10)                      |

|      |              |            |              |             |
|------|--------------|------------|--------------|-------------|
| O9   | 0.17354 (9)  | 0.9301 (3) | 0.06805 (19) | 0.0338 (9)  |
| C1   | 0.08858 (12) | 0.6283 (4) | -0.2287 (3)  | 0.0268 (11) |
| C2   | 0.07734 (14) | 0.7137 (5) | -0.2713 (3)  | 0.0382 (13) |
| H2A  | 0.0887       | 0.7816     | -0.2753      | 0.046*      |
| C3   | 0.04930 (15) | 0.6994 (5) | -0.3082 (3)  | 0.0422 (15) |
| H3A  | 0.0416       | 0.7582     | -0.3356      | 0.051*      |
| C4   | 0.03303 (14) | 0.5975 (6) | -0.3038 (3)  | 0.0388 (14) |
| H4A  | 0.0143       | 0.5876     | -0.3284      | 0.047*      |
| C5   | 0.04410 (13) | 0.5110 (5) | -0.2639 (3)  | 0.0398 (14) |
| H5A  | 0.0332       | 0.4417     | -0.2622      | 0.048*      |
| C6   | 0.07193 (13) | 0.5261 (5) | -0.2253 (3)  | 0.0341 (13) |
| H6A  | 0.0792       | 0.4673     | -0.1975      | 0.041*      |
| C7   | 0.14865 (12) | 0.7655 (5) | -0.2226 (3)  | 0.0279 (11) |
| C8   | 0.14999 (14) | 0.8819 (5) | -0.2059 (3)  | 0.0351 (13) |
| H8A  | 0.1393       | 0.9089     | -0.1693      | 0.042*      |
| C9   | 0.16728 (15) | 0.9577 (5) | -0.2442 (3)  | 0.0400 (14) |
| H9A  | 0.1679       | 1.0354     | -0.2334      | 0.048*      |
| C10  | 0.18329 (14) | 0.9184 (5) | -0.2973 (3)  | 0.0374 (14) |
| H10A | 0.1957       | 0.9689     | -0.3212      | 0.045*      |
| C11  | 0.18129 (15) | 0.8051 (6) | -0.3158 (3)  | 0.0441 (15) |
| H11A | 0.1914       | 0.7796     | -0.3534      | 0.053*      |
| C12  | 0.16402 (14) | 0.7281 (5) | -0.2780 (3)  | 0.0367 (13) |
| H12A | 0.1629       | 0.6511     | -0.2903      | 0.044*      |
| C13  | 0.14903 (12) | 0.5166 (4) | -0.1756 (3)  | 0.0268 (11) |
| H13A | 0.1358       | 0.4515     | -0.1649      | 0.032*      |
| H13B | 0.1561       | 0.5068     | -0.2206      | 0.032*      |
| C14  | 0.19684 (12) | 0.3618 (4) | -0.1015 (3)  | 0.0259 (11) |
| C15  | 0.17403 (14) | 0.2789 (5) | -0.0939 (4)  | 0.0428 (15) |
| H15A | 0.1528       | 0.2983     | -0.0989      | 0.051*      |
| C16  | 0.18254 (15) | 0.1664 (5) | -0.0788 (4)  | 0.0462 (16) |
| H16A | 0.1670       | 0.1107     | -0.0747      | 0.055*      |
| C17  | 0.21371 (15) | 0.1370 (5) | -0.0699 (3)  | 0.0377 (13) |
| H17A | 0.2193       | 0.0617     | -0.0591      | 0.045*      |
| C18  | 0.23675 (14) | 0.2198 (5) | -0.0770 (3)  | 0.0353 (13) |
| H18A | 0.2579       | 0.2003     | -0.0711      | 0.042*      |
| C19  | 0.22837 (12) | 0.3321 (4) | -0.0930 (3)  | 0.0297 (11) |
| H19A | 0.2440       | 0.3874     | -0.0980      | 0.036*      |
| C20  | 0.21906 (11) | 0.5759 (4) | -0.1697 (3)  | 0.0238 (10) |
| C21  | 0.22437 (12) | 0.5219 (5) | -0.2302 (3)  | 0.0311 (12) |
| H21A | 0.2123       | 0.4584     | -0.2431      | 0.037*      |
| C22  | 0.24741 (12) | 0.5623 (5) | -0.2708 (3)  | 0.0317 (12) |
| H22A | 0.2509       | 0.5258     | -0.3110      | 0.038*      |
| C23  | 0.26547 (12) | 0.6576 (5) | -0.2520 (3)  | 0.0324 (12) |
| H23A | 0.2807       | 0.6860     | -0.2800      | 0.039*      |
| C24  | 0.26066 (12) | 0.7096 (5) | -0.1917 (3)  | 0.0327 (12) |
| H24A | 0.2730       | 0.7724     | -0.1786      | 0.039*      |
| C25  | 0.23753 (12) | 0.6687 (4) | -0.1502 (3)  | 0.0285 (11) |
| H25A | 0.2345       | 0.7039     | -0.1094      | 0.034*      |

|      |               |            |             |             |
|------|---------------|------------|-------------|-------------|
| C26  | 0.08319 (14)  | 0.8791 (5) | 0.2245 (3)  | 0.0362 (13) |
| C27  | 0.06664 (18)  | 0.9775 (6) | 0.2432 (3)  | 0.0527 (18) |
| H27A | 0.0580        | 1.0250     | 0.2101      | 0.063*      |
| C28  | 0.0626 (2)    | 1.0070 (6) | 0.3096 (4)  | 0.062 (2)   |
| H28A | 0.0513        | 1.0722     | 0.3209      | 0.074*      |
| C29  | 0.07591 (19)  | 0.9367 (8) | 0.3582 (4)  | 0.062 (2)   |
| H29A | 0.0732        | 0.9541     | 0.4027      | 0.074*      |
| C30  | 0.09304 (15)  | 0.8420 (8) | 0.3418 (3)  | 0.060 (2)   |
| H30A | 0.1025        | 0.7974     | 0.3752      | 0.072*      |
| C31  | 0.09648 (14)  | 0.8112 (7) | 0.2746 (3)  | 0.0491 (17) |
| H31A | 0.1077        | 0.7453     | 0.2639      | 0.059*      |
| C32  | 0.03824 (12)  | 0.7518 (4) | 0.1172 (3)  | 0.0266 (11) |
| C33  | 0.01478 (13)  | 0.7924 (5) | 0.1571 (3)  | 0.0355 (13) |
| H33A | 0.0188        | 0.8555     | 0.1845      | 0.043*      |
| C34  | -0.01436 (13) | 0.7407 (5) | 0.1569 (3)  | 0.0391 (14) |
| H34A | -0.0299       | 0.7678     | 0.1846      | 0.047*      |
| C35  | -0.02059 (13) | 0.6480 (6) | 0.1154 (3)  | 0.0424 (15) |
| H35A | -0.0406       | 0.6146     | 0.1139      | 0.051*      |
| C36  | 0.00261 (16)  | 0.6057 (6) | 0.0767 (3)  | 0.0480 (17) |
| H36A | -0.0014       | 0.5413     | 0.0503      | 0.058*      |
| C37  | 0.03201 (13)  | 0.6578 (5) | 0.0764 (3)  | 0.0350 (13) |
| H37A | 0.0475        | 0.6299     | 0.0489      | 0.042*      |
| C38  | 0.07462 (13)  | 0.9943 (4) | 0.0789 (3)  | 0.0278 (11) |
| C39  | 0.04575 (14)  | 1.0187 (5) | 0.0475 (3)  | 0.0376 (14) |
| H39A | 0.0301        | 0.9624     | 0.0443      | 0.045*      |
| C40  | 0.04024 (16)  | 1.1274 (5) | 0.0207 (3)  | 0.0445 (15) |
| H40A | 0.0208        | 1.1443     | 0.0001      | 0.053*      |
| C41  | 0.06361 (15)  | 1.2100 (5) | 0.0246 (3)  | 0.0416 (14) |
| H41A | 0.0601        | 1.2821     | 0.0058      | 0.050*      |
| C42  | 0.09210 (14)  | 1.1861 (5) | 0.0562 (3)  | 0.0377 (14) |
| H42A | 0.1077        | 1.2423     | 0.0591      | 0.045*      |
| C43  | 0.09760 (13)  | 1.0786 (5) | 0.0837 (3)  | 0.0328 (12) |
| H43A | 0.1168        | 1.0629     | 0.1055      | 0.039*      |
| C44  | 0.06855 (14)  | 0.7302 (5) | -0.0681 (3) | 0.0366 (13) |
| C45  | 0.10430 (13)  | 0.5344 (5) | -0.0440 (3) | 0.0335 (12) |
| C46  | 0.12143 (12)  | 0.8580 (5) | -0.0476 (3) | 0.0281 (11) |
| C47  | 0.16233 (13)  | 0.4801 (5) | 0.0298 (3)  | 0.0313 (12) |
| C48  | 0.21364 (13)  | 0.6139 (5) | 0.0330 (3)  | 0.0320 (12) |
| C49  | 0.18295 (12)  | 0.7728 (4) | -0.0483 (3) | 0.0274 (11) |
| C50  | 0.11020 (13)  | 0.5703 (5) | 0.0947 (3)  | 0.0360 (13) |
| C51  | 0.15435 (12)  | 0.6939 (5) | 0.1651 (3)  | 0.0312 (12) |
| C52  | 0.15780 (13)  | 0.8488 (5) | 0.0705 (3)  | 0.0290 (11) |

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

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$      | $U^{13}$     | $U^{23}$     |
|-----|--------------|--------------|--------------|---------------|--------------|--------------|
| Sb1 | 0.02101 (17) | 0.02523 (17) | 0.02838 (18) | -0.00263 (13) | 0.00167 (13) | 0.00197 (14) |
| Ru1 | 0.0184 (2)   | 0.0245 (2)   | 0.0297 (2)   | -0.00163 (15) | 0.00413 (16) | 0.00320 (16) |

|     |              |              |            |               |              |               |
|-----|--------------|--------------|------------|---------------|--------------|---------------|
| Ru2 | 0.01783 (19) | 0.02012 (19) | 0.0308 (2) | -0.00182 (15) | 0.00339 (16) | -0.00040 (16) |
| Ru3 | 0.0209 (2)   | 0.0246 (2)   | 0.0304 (2) | -0.00150 (16) | 0.00461 (16) | 0.00228 (17)  |
| As1 | 0.0213 (3)   | 0.0211 (2)   | 0.0299 (3) | -0.00367 (19) | 0.0037 (2)   | 0.0000 (2)    |
| As2 | 0.0189 (2)   | 0.0165 (2)   | 0.0326 (3) | -0.00326 (18) | 0.0048 (2)   | -0.0012 (2)   |
| O1  | 0.027 (2)    | 0.087 (4)    | 0.057 (3)  | 0.008 (2)     | 0.003 (2)    | 0.015 (3)     |
| O2  | 0.043 (2)    | 0.032 (2)    | 0.054 (3)  | -0.0134 (18)  | -0.001 (2)   | 0.0059 (19)   |
| O3  | 0.038 (2)    | 0.0244 (19)  | 0.031 (2)  | 0.0034 (16)   | 0.0047 (17)  | 0.0020 (15)   |
| O4  | 0.042 (2)    | 0.030 (2)    | 0.052 (3)  | -0.0002 (18)  | 0.011 (2)    | 0.0113 (19)   |
| O5  | 0.033 (2)    | 0.046 (3)    | 0.068 (3)  | 0.0054 (19)   | -0.014 (2)   | -0.013 (2)    |
| O6  | 0.028 (2)    | 0.0215 (19)  | 0.057 (3)  | -0.0020 (15)  | 0.0103 (18)  | 0.0024 (17)   |
| O7  | 0.051 (3)    | 0.027 (2)    | 0.064 (3)  | -0.0077 (19)  | 0.024 (2)    | 0.002 (2)     |
| O8  | 0.031 (2)    | 0.053 (3)    | 0.046 (3)  | -0.0016 (19)  | -0.0013 (19) | 0.020 (2)     |
| O9  | 0.039 (2)    | 0.0269 (19)  | 0.035 (2)  | -0.0100 (17)  | 0.0042 (17)  | -0.0029 (16)  |
| C1  | 0.023 (3)    | 0.027 (3)    | 0.031 (3)  | -0.003 (2)    | 0.006 (2)    | -0.004 (2)    |
| C2  | 0.041 (3)    | 0.032 (3)    | 0.041 (3)  | -0.008 (3)    | 0.000 (3)    | 0.001 (3)     |
| C3  | 0.041 (3)    | 0.042 (3)    | 0.043 (4)  | -0.010 (3)    | -0.010 (3)   | 0.009 (3)     |
| C4  | 0.029 (3)    | 0.054 (4)    | 0.033 (3)  | -0.008 (3)    | -0.004 (2)   | -0.002 (3)    |
| C5  | 0.031 (3)    | 0.037 (3)    | 0.051 (4)  | -0.012 (2)    | 0.000 (3)    | 0.001 (3)     |
| C6  | 0.030 (3)    | 0.032 (3)    | 0.041 (3)  | -0.009 (2)    | 0.002 (2)    | 0.005 (2)     |
| C7  | 0.024 (3)    | 0.030 (3)    | 0.030 (3)  | -0.005 (2)    | 0.003 (2)    | 0.002 (2)     |
| C8  | 0.046 (3)    | 0.030 (3)    | 0.031 (3)  | -0.009 (2)    | 0.011 (3)    | -0.004 (2)    |
| C9  | 0.049 (4)    | 0.031 (3)    | 0.041 (3)  | -0.016 (3)    | 0.006 (3)    | -0.001 (3)    |
| C10 | 0.037 (3)    | 0.042 (3)    | 0.033 (3)  | -0.014 (3)    | 0.000 (3)    | 0.012 (3)     |
| C11 | 0.044 (4)    | 0.047 (4)    | 0.042 (4)  | 0.006 (3)     | 0.019 (3)    | 0.006 (3)     |
| C12 | 0.041 (3)    | 0.032 (3)    | 0.038 (3)  | 0.000 (2)     | 0.010 (3)    | -0.001 (2)    |
| C13 | 0.024 (3)    | 0.020 (2)    | 0.036 (3)  | -0.0026 (19)  | 0.000 (2)    | -0.005 (2)    |
| C14 | 0.028 (3)    | 0.020 (2)    | 0.030 (3)  | -0.002 (2)    | 0.006 (2)    | -0.002 (2)    |
| C15 | 0.029 (3)    | 0.024 (3)    | 0.076 (5)  | -0.002 (2)    | 0.002 (3)    | 0.002 (3)     |
| C16 | 0.041 (4)    | 0.023 (3)    | 0.075 (5)  | -0.012 (3)    | 0.002 (3)    | 0.003 (3)     |
| C17 | 0.051 (4)    | 0.021 (3)    | 0.041 (3)  | 0.001 (2)     | 0.002 (3)    | -0.002 (2)    |
| C18 | 0.036 (3)    | 0.032 (3)    | 0.037 (3)  | 0.006 (2)     | 0.003 (3)    | 0.001 (2)     |
| C19 | 0.028 (3)    | 0.023 (2)    | 0.039 (3)  | -0.002 (2)    | 0.006 (2)    | 0.000 (2)     |
| C20 | 0.019 (2)    | 0.016 (2)    | 0.036 (3)  | -0.0029 (18)  | 0.003 (2)    | 0.002 (2)     |
| C21 | 0.027 (3)    | 0.026 (3)    | 0.040 (3)  | -0.005 (2)    | 0.003 (2)    | -0.003 (2)    |
| C22 | 0.027 (3)    | 0.035 (3)    | 0.034 (3)  | 0.001 (2)     | 0.005 (2)    | -0.001 (2)    |
| C23 | 0.024 (3)    | 0.027 (3)    | 0.046 (3)  | -0.001 (2)    | 0.008 (2)    | 0.005 (2)     |
| C24 | 0.024 (3)    | 0.027 (3)    | 0.048 (3)  | -0.004 (2)    | 0.010 (2)    | -0.001 (2)    |
| C25 | 0.023 (3)    | 0.023 (2)    | 0.040 (3)  | -0.001 (2)    | 0.005 (2)    | -0.004 (2)    |
| C26 | 0.036 (3)    | 0.045 (3)    | 0.028 (3)  | -0.017 (3)    | 0.000 (2)    | 0.004 (3)     |
| C27 | 0.081 (5)    | 0.040 (4)    | 0.038 (4)  | -0.012 (3)    | 0.011 (3)    | -0.005 (3)    |
| C28 | 0.100 (6)    | 0.042 (4)    | 0.044 (4)  | -0.016 (4)    | 0.014 (4)    | -0.009 (3)    |
| C29 | 0.061 (5)    | 0.086 (6)    | 0.038 (4)  | -0.034 (5)    | 0.001 (3)    | -0.013 (4)    |
| C30 | 0.025 (3)    | 0.116 (7)    | 0.037 (4)  | -0.010 (4)    | -0.004 (3)   | 0.026 (4)     |
| C31 | 0.022 (3)    | 0.081 (5)    | 0.044 (4)  | 0.002 (3)     | 0.001 (3)    | 0.010 (3)     |
| C32 | 0.027 (3)    | 0.024 (2)    | 0.030 (3)  | -0.003 (2)    | 0.001 (2)    | 0.010 (2)     |
| C33 | 0.027 (3)    | 0.032 (3)    | 0.048 (4)  | 0.004 (2)     | 0.001 (3)    | 0.001 (3)     |
| C34 | 0.025 (3)    | 0.041 (3)    | 0.052 (4)  | 0.006 (2)     | 0.008 (3)    | 0.005 (3)     |
| C35 | 0.021 (3)    | 0.061 (4)    | 0.044 (4)  | -0.013 (3)    | -0.005 (3)   | 0.017 (3)     |

|     |           |           |           |            |            |            |
|-----|-----------|-----------|-----------|------------|------------|------------|
| C36 | 0.049 (4) | 0.062 (4) | 0.033 (3) | -0.026 (3) | 0.003 (3)  | -0.008 (3) |
| C37 | 0.032 (3) | 0.041 (3) | 0.033 (3) | -0.007 (2) | 0.010 (2)  | -0.004 (2) |
| C38 | 0.032 (3) | 0.025 (3) | 0.027 (3) | -0.002 (2) | 0.005 (2)  | 0.002 (2)  |
| C39 | 0.042 (3) | 0.034 (3) | 0.037 (3) | -0.015 (3) | -0.008 (3) | 0.010 (2)  |
| C40 | 0.047 (4) | 0.041 (3) | 0.044 (4) | -0.008 (3) | -0.015 (3) | 0.014 (3)  |
| C41 | 0.053 (4) | 0.031 (3) | 0.041 (3) | -0.007 (3) | 0.000 (3)  | 0.007 (3)  |
| C42 | 0.039 (3) | 0.029 (3) | 0.046 (4) | -0.012 (2) | 0.009 (3)  | -0.002 (3) |
| C43 | 0.025 (3) | 0.026 (3) | 0.047 (3) | -0.002 (2) | 0.003 (2)  | -0.003 (2) |
| C44 | 0.029 (3) | 0.045 (3) | 0.037 (3) | 0.003 (3)  | 0.007 (2)  | 0.006 (3)  |
| C45 | 0.025 (3) | 0.039 (3) | 0.036 (3) | -0.009 (2) | 0.000 (2)  | 0.002 (2)  |
| C46 | 0.023 (3) | 0.035 (3) | 0.026 (3) | 0.001 (2)  | 0.003 (2)  | 0.000 (2)  |
| C47 | 0.030 (3) | 0.027 (3) | 0.037 (3) | 0.002 (2)  | 0.004 (2)  | 0.001 (2)  |
| C48 | 0.030 (3) | 0.027 (3) | 0.039 (3) | 0.001 (2)  | 0.000 (2)  | -0.008 (2) |
| C49 | 0.018 (2) | 0.028 (3) | 0.036 (3) | 0.000 (2)  | 0.006 (2)  | -0.003 (2) |
| C50 | 0.031 (3) | 0.030 (3) | 0.048 (4) | 0.003 (2)  | 0.014 (3)  | 0.000 (3)  |
| C51 | 0.020 (3) | 0.036 (3) | 0.038 (3) | 0.003 (2)  | 0.003 (2)  | 0.013 (2)  |
| C52 | 0.032 (3) | 0.030 (3) | 0.025 (3) | 0.010 (2)  | -0.001 (2) | -0.003 (2) |

*Geometric parameters ( $\text{\AA}$ ,  $^{\circ}$ )*

|         |            |          |            |
|---------|------------|----------|------------|
| Sb1—C26 | 2.138 (6)  | C13—H13B | 0.9700     |
| Sb1—C38 | 2.141 (5)  | C14—C15  | 1.377 (7)  |
| Sb1—C32 | 2.142 (5)  | C14—C19  | 1.385 (7)  |
| Sb1—Ru3 | 2.5847 (5) | C15—C16  | 1.387 (8)  |
| Ru1—C44 | 1.891 (6)  | C15—H15A | 0.9300     |
| Ru1—C45 | 1.914 (6)  | C16—C17  | 1.370 (9)  |
| Ru1—C46 | 1.932 (6)  | C16—H16A | 0.9300     |
| Ru1—As1 | 2.4439 (7) | C17—C18  | 1.382 (8)  |
| Ru1—Ru2 | 2.8661 (6) | C17—H17A | 0.9300     |
| Ru1—Ru3 | 2.8838 (6) | C18—C19  | 1.387 (7)  |
| Ru2—C48 | 1.876 (6)  | C18—H18A | 0.9300     |
| Ru2—C47 | 1.930 (5)  | C19—H19A | 0.9300     |
| Ru2—C49 | 1.932 (5)  | C20—C25  | 1.382 (7)  |
| Ru2—As2 | 2.4325 (6) | C20—C21  | 1.394 (7)  |
| Ru2—Ru3 | 2.8354 (6) | C21—C22  | 1.375 (7)  |
| Ru3—C51 | 1.866 (6)  | C21—H21A | 0.9300     |
| Ru3—C52 | 1.914 (6)  | C22—C23  | 1.392 (7)  |
| Ru3—C50 | 1.942 (6)  | C22—H22A | 0.9300     |
| As1—C7  | 1.939 (5)  | C23—C24  | 1.377 (8)  |
| As1—C1  | 1.944 (5)  | C23—H23A | 0.9300     |
| As1—C13 | 1.961 (5)  | C24—C25  | 1.390 (7)  |
| As2—C20 | 1.943 (5)  | C24—H24A | 0.9300     |
| As2—C14 | 1.948 (5)  | C25—H25A | 0.9300     |
| As2—C13 | 1.959 (5)  | C26—C31  | 1.385 (9)  |
| O1—C44  | 1.153 (7)  | C26—C27  | 1.399 (9)  |
| O2—C45  | 1.160 (7)  | C27—C28  | 1.396 (9)  |
| O3—C46  | 1.143 (6)  | C27—H27A | 0.9300     |
| O4—C47  | 1.150 (6)  | C28—C29  | 1.380 (11) |

|             |             |               |            |
|-------------|-------------|---------------|------------|
| O5—C48      | 1.148 (6)   | C28—H28A      | 0.9300     |
| O6—C49      | 1.143 (6)   | C29—C30       | 1.364 (11) |
| O7—C50      | 1.139 (7)   | C29—H29A      | 0.9300     |
| O8—C51      | 1.156 (7)   | C30—C31       | 1.411 (10) |
| O9—C52      | 1.158 (6)   | C30—H30A      | 0.9300     |
| C1—C6       | 1.385 (7)   | C31—H31A      | 0.9300     |
| C1—C2       | 1.386 (8)   | C32—C33       | 1.380 (8)  |
| C2—C3       | 1.391 (8)   | C32—C37       | 1.387 (7)  |
| C2—H2A      | 0.9300      | C33—C34       | 1.373 (8)  |
| C3—C4       | 1.374 (8)   | C33—H33A      | 0.9300     |
| C3—H3A      | 0.9300      | C34—C35       | 1.382 (9)  |
| C4—C5       | 1.361 (8)   | C34—H34A      | 0.9300     |
| C4—H4A      | 0.9300      | C35—C36       | 1.364 (9)  |
| C5—C6       | 1.401 (8)   | C35—H35A      | 0.9300     |
| C5—H5A      | 0.9300      | C36—C37       | 1.385 (8)  |
| C6—H6A      | 0.9300      | C36—H36A      | 0.9300     |
| C7—C12      | 1.379 (8)   | C37—H37A      | 0.9300     |
| C7—C8       | 1.395 (7)   | C38—C43       | 1.382 (7)  |
| C8—C9       | 1.393 (7)   | C38—C39       | 1.388 (8)  |
| C8—H8A      | 0.9300      | C39—C40       | 1.391 (8)  |
| C9—C10      | 1.362 (8)   | C39—H39A      | 0.9300     |
| C9—H9A      | 0.9300      | C40—C41       | 1.380 (8)  |
| C10—C11     | 1.371 (9)   | C40—H40A      | 0.9300     |
| C10—H10A    | 0.9300      | C41—C42       | 1.374 (9)  |
| C11—C12     | 1.396 (8)   | C41—H41A      | 0.9300     |
| C11—H11A    | 0.9300      | C42—C43       | 1.384 (8)  |
| C12—H12A    | 0.9300      | C42—H42A      | 0.9300     |
| C13—H13A    | 0.9700      | C43—H43A      | 0.9300     |
| <br>        |             |               |            |
| C26—Sb1—C38 | 98.0 (2)    | As2—C13—H13B  | 109.8      |
| C26—Sb1—C32 | 96.6 (2)    | As1—C13—H13B  | 109.8      |
| C38—Sb1—C32 | 101.44 (19) | H13A—C13—H13B | 108.2      |
| C26—Sb1—Ru3 | 117.84 (17) | C15—C14—C19   | 119.2 (5)  |
| C38—Sb1—Ru3 | 118.75 (14) | C15—C14—As2   | 121.2 (4)  |
| C32—Sb1—Ru3 | 119.78 (14) | C19—C14—As2   | 119.2 (4)  |
| C44—Ru1—C45 | 93.4 (2)    | C14—C15—C16   | 120.4 (6)  |
| C44—Ru1—C46 | 90.2 (2)    | C14—C15—H15A  | 119.8      |
| C45—Ru1—C46 | 170.3 (2)   | C16—C15—H15A  | 119.8      |
| C44—Ru1—As1 | 97.71 (18)  | C17—C16—C15   | 120.5 (5)  |
| C45—Ru1—As1 | 88.34 (17)  | C17—C16—H16A  | 119.8      |
| C46—Ru1—As1 | 100.15 (15) | C15—C16—H16A  | 119.8      |
| C44—Ru1—Ru2 | 169.88 (17) | C16—C17—C18   | 119.5 (5)  |
| C45—Ru1—Ru2 | 80.65 (16)  | C16—C17—H17A  | 120.3      |
| C46—Ru1—Ru2 | 94.46 (15)  | C18—C17—H17A  | 120.3      |
| As1—Ru1—Ru2 | 90.310 (19) | C17—C18—C19   | 120.2 (5)  |
| C44—Ru1—Ru3 | 113.30 (18) | C17—C18—H18A  | 119.9      |
| C45—Ru1—Ru3 | 91.36 (17)  | C19—C18—H18A  | 119.9      |
| C46—Ru1—Ru3 | 78.92 (16)  | C14—C19—C18   | 120.1 (5)  |

|             |             |              |           |
|-------------|-------------|--------------|-----------|
| As1—Ru1—Ru3 | 148.95 (2)  | C14—C19—H19A | 119.9     |
| Ru2—Ru1—Ru3 | 59.090 (14) | C18—C19—H19A | 119.9     |
| C48—Ru2—C47 | 89.1 (2)    | C25—C20—C21  | 119.6 (5) |
| C48—Ru2—C49 | 93.0 (2)    | C25—C20—As2  | 119.9 (4) |
| C47—Ru2—C49 | 175.6 (2)   | C21—C20—As2  | 120.5 (4) |
| C48—Ru2—As2 | 99.70 (16)  | C22—C21—C20  | 120.2 (5) |
| C47—Ru2—As2 | 90.30 (17)  | C22—C21—H21A | 119.9     |
| C49—Ru2—As2 | 93.09 (16)  | C20—C21—H21A | 119.9     |
| C48—Ru2—Ru3 | 105.62 (17) | C21—C22—C23  | 120.3 (5) |
| C47—Ru2—Ru3 | 82.27 (16)  | C21—C22—H22A | 119.8     |
| C49—Ru2—Ru3 | 93.47 (15)  | C23—C22—H22A | 119.9     |
| As2—Ru2—Ru3 | 153.43 (2)  | C24—C23—C22  | 119.5 (5) |
| C48—Ru2—Ru1 | 163.36 (16) | C24—C23—H23A | 120.2     |
| C47—Ru2—Ru1 | 97.82 (16)  | C22—C23—H23A | 120.2     |
| C49—Ru2—Ru1 | 79.10 (15)  | C23—C24—C25  | 120.4 (5) |
| As2—Ru2—Ru1 | 95.39 (2)   | C23—C24—H24A | 119.8     |
| Ru3—Ru2—Ru1 | 60.766 (14) | C25—C24—H24A | 119.8     |
| C51—Ru3—C52 | 88.0 (2)    | C20—C25—C24  | 120.0 (5) |
| C51—Ru3—C50 | 91.1 (2)    | C20—C25—H25A | 120.0     |
| C52—Ru3—C50 | 174.8 (2)   | C24—C25—H25A | 120.0     |
| C51—Ru3—Sb1 | 100.32 (17) | C31—C26—C27  | 117.8 (6) |
| C52—Ru3—Sb1 | 94.24 (15)  | C31—C26—Sb1  | 121.7 (5) |
| C50—Ru3—Sb1 | 90.98 (16)  | C27—C26—Sb1  | 120.3 (5) |
| C51—Ru3—Ru2 | 103.99 (17) | C28—C27—C26  | 122.3 (7) |
| C52—Ru3—Ru2 | 81.37 (15)  | C28—C27—H27A | 118.8     |
| C50—Ru3—Ru2 | 93.86 (16)  | C26—C27—H27A | 118.8     |
| Sb1—Ru3—Ru2 | 155.09 (2)  | C29—C28—C27  | 118.3 (8) |
| C51—Ru3—Ru1 | 163.12 (17) | C29—C28—H28A | 120.9     |
| C52—Ru3—Ru1 | 94.69 (16)  | C27—C28—H28A | 120.9     |
| C50—Ru3—Ru1 | 84.69 (19)  | C30—C29—C28  | 121.0 (7) |
| Sb1—Ru3—Ru1 | 96.108 (17) | C30—C29—H29A | 119.5     |
| Ru2—Ru3—Ru1 | 60.144 (14) | C28—C29—H29A | 119.5     |
| C7—As1—C1   | 101.2 (2)   | C29—C30—C31  | 120.6 (7) |
| C7—As1—C13  | 102.6 (2)   | C29—C30—H30A | 119.7     |
| C1—As1—C13  | 102.0 (2)   | C31—C30—H30A | 119.7     |
| C7—As1—Ru1  | 123.55 (16) | C26—C31—C30  | 120.0 (7) |
| C1—As1—Ru1  | 114.97 (15) | C26—C31—H31A | 120.0     |
| C13—As1—Ru1 | 109.85 (16) | C30—C31—H31A | 120.0     |
| C20—As2—C14 | 101.2 (2)   | C33—C32—C37  | 119.1 (5) |
| C20—As2—C13 | 102.5 (2)   | C33—C32—Sb1  | 119.8 (4) |
| C14—As2—C13 | 103.1 (2)   | C37—C32—Sb1  | 121.0 (4) |
| C20—As2—Ru2 | 120.83 (15) | C34—C33—C32  | 120.8 (6) |
| C14—As2—Ru2 | 114.44 (15) | C34—C33—H33A | 119.6     |
| C13—As2—Ru2 | 112.55 (15) | C32—C33—H33A | 119.6     |
| C6—C1—C2    | 118.7 (5)   | C33—C34—C35  | 119.8 (6) |
| C6—C1—As1   | 121.5 (4)   | C33—C34—H34A | 120.1     |
| C2—C1—As1   | 119.6 (4)   | C35—C34—H34A | 120.1     |
| C1—C2—C3    | 121.0 (5)   | C36—C35—C34  | 119.9 (5) |

|                 |              |                 |              |
|-----------------|--------------|-----------------|--------------|
| C1—C2—H2A       | 119.5        | C36—C35—H35A    | 120.1        |
| C3—C2—H2A       | 119.5        | C34—C35—H35A    | 120.1        |
| C4—C3—C2        | 119.3 (6)    | C35—C36—C37     | 120.6 (6)    |
| C4—C3—H3A       | 120.3        | C35—C36—H36A    | 119.7        |
| C2—C3—H3A       | 120.3        | C37—C36—H36A    | 119.7        |
| C5—C4—C3        | 120.7 (5)    | C36—C37—C32     | 119.7 (5)    |
| C5—C4—H4A       | 119.6        | C36—C37—H37A    | 120.1        |
| C3—C4—H4A       | 119.6        | C32—C37—H37A    | 120.1        |
| C4—C5—C6        | 120.1 (5)    | C43—C38—C39     | 119.7 (5)    |
| C4—C5—H5A       | 119.9        | C43—C38—Sb1     | 118.9 (4)    |
| C6—C5—H5A       | 119.9        | C39—C38—Sb1     | 121.3 (4)    |
| C1—C6—C5        | 120.1 (5)    | C38—C39—C40     | 119.8 (5)    |
| C1—C6—H6A       | 120.0        | C38—C39—H39A    | 120.1        |
| C5—C6—H6A       | 120.0        | C40—C39—H39A    | 120.1        |
| C12—C7—C8       | 118.9 (5)    | C41—C40—C39     | 119.9 (6)    |
| C12—C7—As1      | 121.0 (4)    | C41—C40—H40A    | 120.0        |
| C8—C7—As1       | 120.1 (4)    | C39—C40—H40A    | 120.0        |
| C9—C8—C7        | 119.9 (5)    | C42—C41—C40     | 120.3 (6)    |
| C9—C8—H8A       | 120.0        | C42—C41—H41A    | 119.9        |
| C7—C8—H8A       | 120.0        | C40—C41—H41A    | 119.9        |
| C10—C9—C8       | 120.4 (5)    | C41—C42—C43     | 120.1 (5)    |
| C10—C9—H9A      | 119.8        | C41—C42—H42A    | 120.0        |
| C8—C9—H9A       | 119.8        | C43—C42—H42A    | 120.0        |
| C9—C10—C11      | 120.5 (5)    | C38—C43—C42     | 120.2 (5)    |
| C9—C10—H10A     | 119.8        | C38—C43—H43A    | 119.9        |
| C11—C10—H10A    | 119.8        | C42—C43—H43A    | 119.9        |
| C10—C11—C12     | 119.8 (6)    | O1—C44—Ru1      | 176.7 (6)    |
| C10—C11—H11A    | 120.1        | O2—C45—Ru1      | 174.0 (5)    |
| C12—C11—H11A    | 120.1        | O3—C46—Ru1      | 175.1 (5)    |
| C7—C12—C11      | 120.5 (5)    | O4—C47—Ru2      | 173.2 (5)    |
| C7—C12—H12A     | 119.8        | O5—C48—Ru2      | 179.8 (6)    |
| C11—C12—H12A    | 119.8        | O6—C49—Ru2      | 174.2 (4)    |
| As2—C13—As1     | 109.4 (2)    | O7—C50—Ru3      | 174.7 (6)    |
| As2—C13—H13A    | 109.8        | O8—C51—Ru3      | 179.3 (5)    |
| As1—C13—H13A    | 109.8        | O9—C52—Ru3      | 174.4 (5)    |
| <br>            |              |                 |              |
| C44—Ru1—Ru2—C48 | -80.4 (13)   | Ru1—Ru2—As2—C14 | -123.40 (17) |
| C45—Ru1—Ru2—C48 | -134.6 (6)   | C48—Ru2—As2—C13 | -179.1 (2)   |
| C46—Ru1—Ru2—C48 | 36.9 (6)     | C47—Ru2—As2—C13 | 91.8 (2)     |
| As1—Ru1—Ru2—C48 | 137.1 (6)    | C49—Ru2—As2—C13 | -85.4 (2)    |
| Ru3—Ru1—Ru2—C48 | -37.4 (6)    | Ru3—Ru2—As2—C13 | 18.65 (17)   |
| C44—Ru1—Ru2—C47 | 33.5 (11)    | Ru1—Ru2—As2—C13 | -6.11 (16)   |
| C45—Ru1—Ru2—C47 | -20.7 (2)    | C7—As1—C1—C6    | 153.1 (4)    |
| C46—Ru1—Ru2—C47 | 150.8 (2)    | C13—As1—C1—C6   | 47.5 (5)     |
| As1—Ru1—Ru2—C47 | -108.97 (17) | Ru1—As1—C1—C6   | -71.3 (5)    |
| Ru3—Ru1—Ru2—C47 | 76.56 (17)   | C7—As1—C1—C2    | -32.7 (5)    |
| C44—Ru1—Ru2—C49 | -143.3 (11)  | C13—As1—C1—C2   | -138.4 (4)   |
| C45—Ru1—Ru2—C49 | 162.5 (2)    | Ru1—As1—C1—C2   | 102.8 (4)    |

|                 |              |                 |            |
|-----------------|--------------|-----------------|------------|
| C46—Ru1—Ru2—C49 | −26.0 (2)    | C6—C1—C2—C3     | 2.4 (9)    |
| As1—Ru1—Ru2—C49 | 74.19 (16)   | As1—C1—C2—C3    | −171.9 (5) |
| Ru3—Ru1—Ru2—C49 | −100.27 (16) | C1—C2—C3—C4     | −2.0 (10)  |
| C44—Ru1—Ru2—As2 | 124.6 (11)   | C2—C3—C4—C5     | −0.1 (10)  |
| C45—Ru1—Ru2—As2 | 70.34 (17)   | C3—C4—C5—C6     | 1.7 (10)   |
| C46—Ru1—Ru2—As2 | −118.13 (15) | C2—C1—C6—C5     | −0.8 (8)   |
| As1—Ru1—Ru2—As2 | −17.93 (2)   | As1—C1—C6—C5    | 173.3 (4)  |
| Ru3—Ru1—Ru2—As2 | 167.61 (2)   | C4—C5—C6—C1     | −1.2 (9)   |
| C44—Ru1—Ru2—Ru3 | −43.0 (11)   | C1—As1—C7—C12   | −71.1 (5)  |
| C45—Ru1—Ru2—Ru3 | −97.27 (17)  | C13—As1—C7—C12  | 34.1 (5)   |
| C46—Ru1—Ru2—Ru3 | 74.26 (15)   | Ru1—As1—C7—C12  | 158.5 (4)  |
| As1—Ru1—Ru2—Ru3 | 174.47 (2)   | C1—As1—C7—C8    | 107.6 (5)  |
| C26—Sb1—Ru3—C51 | 4.8 (2)      | C13—As1—C7—C8   | −147.3 (5) |
| C38—Sb1—Ru3—C51 | 122.8 (2)    | Ru1—As1—C7—C8   | −22.8 (5)  |
| C32—Sb1—Ru3—C51 | −112.1 (2)   | C12—C7—C8—C9    | −1.5 (9)   |
| C26—Sb1—Ru3—C52 | −84.0 (2)    | As1—C7—C8—C9    | 179.8 (5)  |
| C38—Sb1—Ru3—C52 | 34.1 (2)     | C7—C8—C9—C10    | −0.9 (9)   |
| C32—Sb1—Ru3—C52 | 159.2 (2)    | C8—C9—C10—C11   | 3.3 (10)   |
| C26—Sb1—Ru3—C50 | 96.1 (3)     | C9—C10—C11—C12  | −3.2 (10)  |
| C38—Sb1—Ru3—C50 | −145.9 (2)   | C8—C7—C12—C11   | 1.6 (9)    |
| C32—Sb1—Ru3—C50 | −20.8 (2)    | As1—C7—C12—C11  | −179.8 (5) |
| C26—Sb1—Ru3—Ru2 | −162.55 (17) | C10—C11—C12—C7  | 0.7 (10)   |
| C38—Sb1—Ru3—Ru2 | −44.51 (17)  | C20—As2—C13—As1 | −95.8 (3)  |
| C32—Sb1—Ru3—Ru2 | 80.56 (16)   | C14—As2—C13—As1 | 159.4 (2)  |
| C26—Sb1—Ru3—Ru1 | −179.14 (17) | Ru2—As2—C13—As1 | 35.6 (3)   |
| C38—Sb1—Ru3—Ru1 | −61.10 (16)  | C7—As1—C13—As2  | 80.0 (3)   |
| C32—Sb1—Ru3—Ru1 | 63.97 (15)   | C1—As1—C13—As2  | −175.5 (2) |
| C48—Ru2—Ru3—C51 | −16.7 (2)    | Ru1—As1—C13—As2 | −53.1 (3)  |
| C47—Ru2—Ru3—C51 | 70.2 (2)     | C20—As2—C14—C15 | −148.2 (5) |
| C49—Ru2—Ru3—C51 | −110.8 (2)   | C13—As2—C14—C15 | −42.4 (5)  |
| As2—Ru2—Ru3—C51 | 145.19 (18)  | Ru2—As2—C14—C15 | 80.2 (5)   |
| Ru1—Ru2—Ru3—C51 | 173.73 (17)  | C20—As2—C14—C19 | 39.2 (5)   |
| C48—Ru2—Ru3—C52 | 69.1 (2)     | C13—As2—C14—C19 | 145.1 (4)  |
| C47—Ru2—Ru3—C52 | 156.0 (2)    | Ru2—As2—C14—C19 | −92.3 (4)  |
| C49—Ru2—Ru3—C52 | −25.0 (2)    | C19—C14—C15—C16 | −0.9 (9)   |
| As2—Ru2—Ru3—C52 | −129.05 (16) | As2—C14—C15—C16 | −173.5 (5) |
| Ru1—Ru2—Ru3—C52 | −100.51 (16) | C14—C15—C16—C17 | 1.4 (11)   |
| C48—Ru2—Ru3—C50 | −108.8 (3)   | C15—C16—C17—C18 | −1.0 (10)  |
| C47—Ru2—Ru3—C50 | −21.9 (3)    | C16—C17—C18—C19 | 0.1 (9)    |
| C49—Ru2—Ru3—C50 | 157.1 (2)    | C15—C14—C19—C18 | 0.0 (8)    |
| As2—Ru2—Ru3—C50 | 53.08 (19)   | As2—C14—C19—C18 | 172.7 (4)  |
| Ru1—Ru2—Ru3—C50 | 81.62 (19)   | C17—C18—C19—C14 | 0.4 (9)    |
| C48—Ru2—Ru3—Sb1 | 150.50 (18)  | C14—As2—C20—C25 | −124.8 (4) |
| C47—Ru2—Ru3—Sb1 | −122.60 (18) | C13—As2—C20—C25 | 128.9 (4)  |
| C49—Ru2—Ru3—Sb1 | 56.36 (16)   | Ru2—As2—C20—C25 | 2.7 (5)    |
| As2—Ru2—Ru3—Sb1 | −47.65 (8)   | C14—As2—C20—C21 | 56.2 (5)   |
| Ru1—Ru2—Ru3—Sb1 | −19.11 (4)   | C13—As2—C20—C21 | −50.2 (5)  |
| C48—Ru2—Ru3—Ru1 | 169.61 (18)  | Ru2—As2—C20—C21 | −176.3 (4) |

|                 |              |                 |            |
|-----------------|--------------|-----------------|------------|
| C47—Ru2—Ru3—Ru1 | −103.49 (17) | C25—C20—C21—C22 | −1.3 (8)   |
| C49—Ru2—Ru3—Ru1 | 75.47 (16)   | As2—C20—C21—C22 | 177.7 (4)  |
| As2—Ru2—Ru3—Ru1 | −28.54 (5)   | C20—C21—C22—C23 | −0.3 (8)   |
| C44—Ru1—Ru3—C51 | 151.1 (6)    | C21—C22—C23—C24 | 1.6 (8)    |
| C45—Ru1—Ru3—C51 | 56.9 (6)     | C22—C23—C24—C25 | −1.2 (8)   |
| C46—Ru1—Ru3—C51 | −123.5 (6)   | C21—C20—C25—C24 | 1.7 (8)    |
| As1—Ru1—Ru3—C51 | −32.2 (6)    | As2—C20—C25—C24 | −177.3 (4) |
| Ru2—Ru1—Ru3—C51 | −21.4 (6)    | C23—C24—C25—C20 | −0.4 (8)   |
| C44—Ru1—Ru3—C52 | −110.3 (3)   | C38—Sb1—C26—C31 | −161.8 (5) |
| C45—Ru1—Ru3—C52 | 155.5 (2)    | C32—Sb1—C26—C31 | 95.6 (5)   |
| C46—Ru1—Ru3—C52 | −24.8 (2)    | Ru3—Sb1—C26—C31 | −33.2 (5)  |
| As1—Ru1—Ru3—C52 | 66.47 (16)   | C38—Sb1—C26—C27 | 23.6 (5)   |
| Ru2—Ru1—Ru3—C52 | 77.25 (15)   | C32—Sb1—C26—C27 | −79.0 (5)  |
| C44—Ru1—Ru3—C50 | 74.9 (3)     | Ru3—Sb1—C26—C27 | 152.2 (4)  |
| C45—Ru1—Ru3—C50 | −19.3 (2)    | C31—C26—C27—C28 | −1.6 (10)  |
| C46—Ru1—Ru3—C50 | 160.4 (2)    | Sb1—C26—C27—C28 | 173.3 (5)  |
| As1—Ru1—Ru3—C50 | −108.33 (17) | C26—C27—C28—C29 | 0.9 (11)   |
| Ru2—Ru1—Ru3—C50 | −97.55 (16)  | C27—C28—C29—C30 | 1.2 (11)   |
| C44—Ru1—Ru3—Sb1 | −15.5 (2)    | C28—C29—C30—C31 | −2.6 (11)  |
| C45—Ru1—Ru3—Sb1 | −109.71 (17) | C27—C26—C31—C30 | 0.1 (9)    |
| C46—Ru1—Ru3—Sb1 | 69.94 (15)   | Sb1—C26—C31—C30 | −174.6 (5) |
| As1—Ru1—Ru3—Sb1 | 161.25 (4)   | C29—C30—C31—C26 | 1.9 (10)   |
| Ru2—Ru1—Ru3—Sb1 | 172.030 (19) | C26—Sb1—C32—C33 | 30.1 (5)   |
| C44—Ru1—Ru3—Ru2 | 172.5 (2)    | C38—Sb1—C32—C33 | −69.5 (4)  |
| C45—Ru1—Ru3—Ru2 | 78.26 (17)   | Ru3—Sb1—C32—C33 | 157.6 (4)  |
| C46—Ru1—Ru3—Ru2 | −102.09 (15) | C26—Sb1—C32—C37 | −147.0 (4) |
| As1—Ru1—Ru3—Ru2 | −10.78 (4)   | C38—Sb1—C32—C37 | 113.4 (4)  |
| C44—Ru1—As1—C7  | 106.0 (3)    | Ru3—Sb1—C32—C37 | −19.6 (5)  |
| C45—Ru1—As1—C7  | −160.8 (3)   | C37—C32—C33—C34 | 0.2 (8)    |
| C46—Ru1—As1—C7  | 14.4 (2)     | Sb1—C32—C33—C34 | −177.0 (4) |
| Ru2—Ru1—As1—C7  | −80.15 (19)  | C32—C33—C34—C35 | −1.1 (9)   |
| Ru3—Ru1—As1—C7  | −70.92 (19)  | C33—C34—C35—C36 | 2.5 (9)    |
| C44—Ru1—As1—C1  | −18.5 (3)    | C34—C35—C36—C37 | −2.8 (10)  |
| C45—Ru1—As1—C1  | 74.7 (2)     | C35—C36—C37—C32 | 1.9 (10)   |
| C46—Ru1—As1—C1  | −110.1 (2)   | C33—C32—C37—C36 | −0.5 (8)   |
| Ru2—Ru1—As1—C1  | 155.33 (17)  | Sb1—C32—C37—C36 | 176.6 (5)  |
| Ru3—Ru1—As1—C1  | 164.56 (17)  | C26—Sb1—C38—C43 | 70.3 (4)   |
| C44—Ru1—As1—C13 | −132.8 (2)   | C32—Sb1—C38—C43 | 168.8 (4)  |
| C45—Ru1—As1—C13 | −39.6 (2)    | Ru3—Sb1—C38—C43 | −57.6 (5)  |
| C46—Ru1—As1—C13 | 135.6 (2)    | C26—Sb1—C38—C39 | −108.5 (5) |
| Ru2—Ru1—As1—C13 | 41.03 (15)   | C32—Sb1—C38—C39 | −10.0 (5)  |
| Ru3—Ru1—As1—C13 | 50.27 (16)   | Ru3—Sb1—C38—C39 | 123.6 (4)  |
| C48—Ru2—As2—C20 | −57.7 (2)    | C43—C38—C39—C40 | 0.3 (9)    |
| C47—Ru2—As2—C20 | −146.8 (2)   | Sb1—C38—C39—C40 | 179.1 (5)  |
| C49—Ru2—As2—C20 | 36.0 (2)     | C38—C39—C40—C41 | 1.0 (10)   |
| Ru3—Ru2—As2—C20 | 140.05 (17)  | C39—C40—C41—C42 | −1.5 (10)  |
| Ru1—Ru2—As2—C20 | 115.29 (17)  | C40—C41—C42—C43 | 0.6 (10)   |
| C48—Ru2—As2—C14 | 63.6 (2)     | C39—C38—C43—C42 | −1.2 (8)   |

|                 |             |                 |            |
|-----------------|-------------|-----------------|------------|
| C47—Ru2—As2—C14 | −25.5 (2)   | Sb1—C38—C43—C42 | −180.0 (4) |
| C49—Ru2—As2—C14 | 157.3 (2)   | C41—C42—C43—C38 | 0.7 (9)    |
| Ru3—Ru2—As2—C14 | −98.65 (17) |                 |            |

*Hydrogen-bond geometry (Å, °)*

| D—H···A  | D—H  | H···A | D···A     | D—H···A |
|--|------|-------|-----------|---------|
| C13—H13 <i>B</i> ···O8 <sup>i</sup>            | 0.97 | 2.59  | 3.290 (7) | 129     |
| C23—H23 <i>A</i> ··· <i>Cg1</i> <sup>ii</sup>  | 0.93 | 2.88  | 3.686 (6) | 146     |
| C34—H34 <i>A</i> ··· <i>Cg2</i> <sup>iii</sup> | 0.93 | 2.72  | 3.564 (6) | 151     |

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