

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

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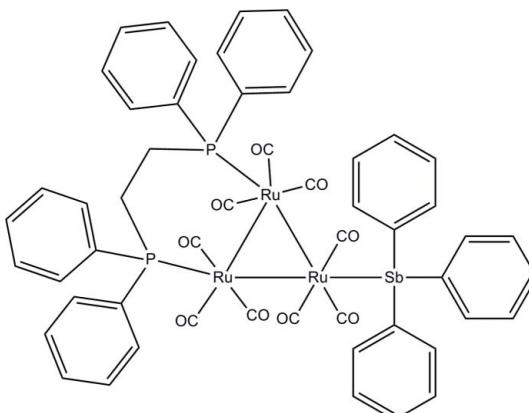
Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(C-C) = 0.009$  Å;  
 $R$  factor = 0.045;  $wR$  factor = 0.121; data-to-parameter ratio = 23.6.

The asymmetric unit of the title *triangulo-triruthenium* compound,  $[Ru_3(C_{26}H_{24}P_2)(C_{18}H_{15}Sb)(CO)_9]$ , consists of two crystallographically independent molecules, *A* and *B*. The bis(diphenylphosphanyl)ethane ligand bridges an Ru–Ru bond and the monodentate stibine ligand bonds to the third Ru atom. Both the stibine and phosphine ligands are equatorial with respect to the  $Ru_3$  triangle. Additionally, each Ru atom carries one equatorial and two axial terminal carbonyl ligands. The three stibine-substituted benzene rings make dihedral angles of 38.7 (3), 71.5 (3) and 70.0 (3)° with each other in molecule *A* whereas these angles are 83.9 (3), 88.2 (3) and 56.8 (3)° in molecule *B*. Similarly, the dihedral angles between the two benzene rings are 80.7 (3) and 87.6 (3)° for the two diphenylphosphanyl groups in molecule *A* and 84.0 (3) and 72.6 (4)° in molecule *B*. In the crystal, molecules are linked into tetramers 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, 1988*a,b*). For related structures, see: Shawkataly *et al.* (1998, 2004, 2010, 2011). For the synthesis of

$Ru_3(CO)_{10}(\mu\text{-Ph}_2PCH_2CH_2PPh_2)$ , see: Bruce *et al.* (1983). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



## Experimental

### Crystal data

|   |                                   |
|---|-----------------------------------|
| $[Ru_3(C_{26}H_{24}P_2)(C_{18}H_{15}Sb)(CO)_9]$ | $\gamma = 97.339$ (1)°            |
| $M_r = 1306.74$                                 | $V = 5041.5$ (5) Å <sup>3</sup>   |
| Triclinic, $P\bar{1}$                           | $Z = 4$                           |
| $a = 15.1589$ (8) Å                             | Mo $K\alpha$ radiation            |
| $b = 18.6156$ (10) Å                            | $\mu = 1.53$ mm <sup>-1</sup>     |
| $c = 20.0398$ (11) Å                            | $T = 100$ K                       |
| $\alpha = 113.233$ (1)°                         | $0.51 \times 0.15 \times 0.08$ mm |
| $\beta = 97.986$ (1)°                           |                                   |

### Data collection

|   |   |
|---|---|
| Bruker APEXII DUO CCD area-detector diffractometer                | 82542 measured reflections              |
| Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2009) | 28970 independent reflections           |
| $T_{min} = 0.506$ , $T_{max} = 0.885$                             | 21778 reflections with $I > 2\sigma(I)$ |
|   | $R_{int} = 0.033$                       |
|   |   |

### Refinement

|                                 |   |
|---------------------------------|---|
| $R[F^2 > 2\sigma(F^2)] = 0.045$ | 1225 parameters                               |
| $wR(F^2) = 0.121$               | H-atom parameters constrained                 |
| $S = 1.11$                      | $\Delta\rho_{\max} = 3.47$ e Å <sup>-3</sup>  |
| 28970 reflections               | $\Delta\rho_{\min} = -2.34$ e Å <sup>-3</sup> |

**Table 1**

Hydrogen-bond geometry (Å, °).

$Cg1$ ,  $Cg2$  and  $Cg3$  are the centroids of the  $C21B$ – $C26B$ ,  $C39B$ – $C44B$  and  $C15A$ – $C20A$  benzene rings, respectively.

| $D-H\cdots A$               | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-----------------------------|-------|-------------|-------------|---------------|
| $C18A-H18A\cdots O7B^i$     | 0.93  | 2.55        | 3.337 (7)   | 142           |
| $C34A-H34A\cdots O2A$       | 0.93  | 2.56        | 3.375 (7)   | 147           |
| $C34B-H34B\cdots O8B^i$     | 0.93  | 2.57        | 3.414 (7)   | 151           |
| $C5B-H5BA\cdots Cg1^{ii}$   | 0.93  | 3.00        | 3.723 (9)   | 136           |
| $C25B-H25B\cdots Cg2^{iii}$ | 0.93  | 2.95        | 3.856 (8)   | 166           |
| $C43A-H43A\cdots Cg3^{iii}$ | 0.93  | 2.91        | 3.624 (6)   | 135           |

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

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).

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# metal-organic compounds

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5087).

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# supporting information

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## [ $\mu$ -Bis(diphenylphosphanyl)ethane-1:2 $\kappa^2$ P:P']nonacarbonyl-1 $\kappa^3$ C,2 $\kappa^3$ C,3 $\kappa^3$ C-(tri-phenylstibine-3 $\kappa$ Sb)-triangulo-triruthenium(0)

**Omar bin Shawkataly, Imthyaz Ahmed Khan, Siti Syaida Sirat, Chin Sing Yeap and Hoong-Kun Fun**

### S1. Comment

A large number of substituted derivatives,  $\text{Ru}_3(\text{CO})_{12-n}L_n$  ( $L$  = group 15 ligand) have been reported (Bruce *et al.*, 1985, 1988*a,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, 2010, 2011). Herein we report the synthesis and structure of the title compound.

The asymmetric unit of title compound consists of two crystallographically independent molecules, *A* and *B* (Fig. 1). The bis(diphenylphosphanyl)ethane ligand bridges the Ru1–Ru2 bond and the monodentate stibine ligand bonds to the Ru3 atom. Both the stibine and phosphine 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 benzene rings make dihedral angles (C27–C32/C33–C38, C27–C32/C39–C44 and C33–C38/C39–C44) of 38.7 (3), 71.5 (3) and 70.0 (3) (19)° with each other respectively for molecule *A* whereas these angles are 83.9 (3), 88.2 (3) and 56.8 (3)° for molecule *B*. Similarly, the dihedral angles between the two benzene rings (C1–C6/C7–C12 and C15–C20/C21–C26) are 80.7 (3) and 87.6 (3)° in molecule *A* and 84.0 (3) and 72.6 (4)° in molecule *B* for the two diphenylphosphanyl groups respectively.

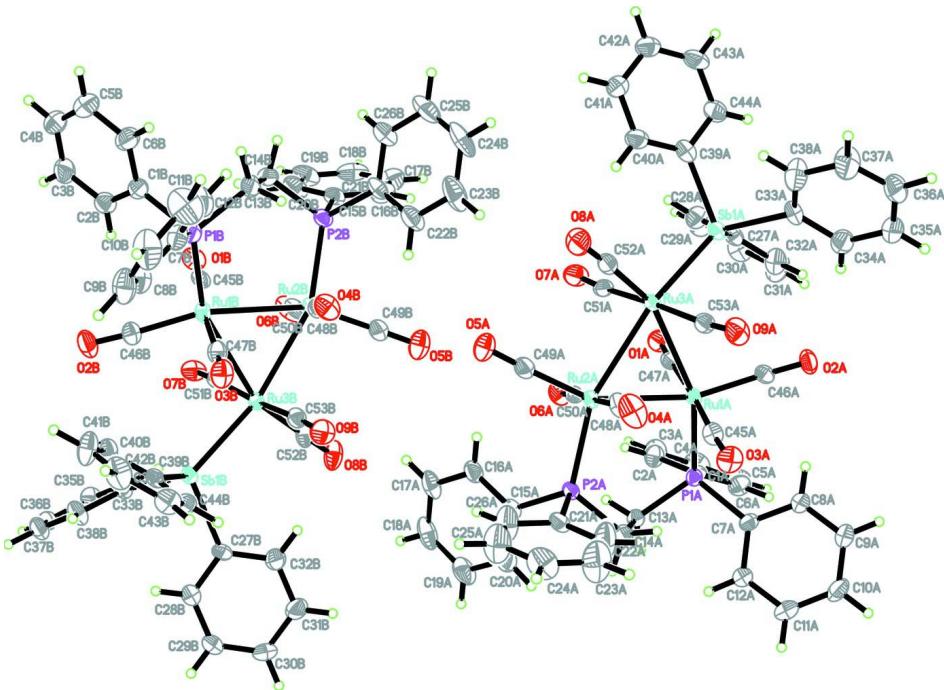
In the crystal packing, the molecules are linked together *via* intermolecular C18—H18A···O7B, C34A—H34A···O2A and C34B—H34B···O8B hydrogen bonds into tetramers (Fig. 2, Table 1). Weak intermolecular C—H··· $\pi$  interactions (Table 1) further stabilize the crystal structure.

### S2. Experimental

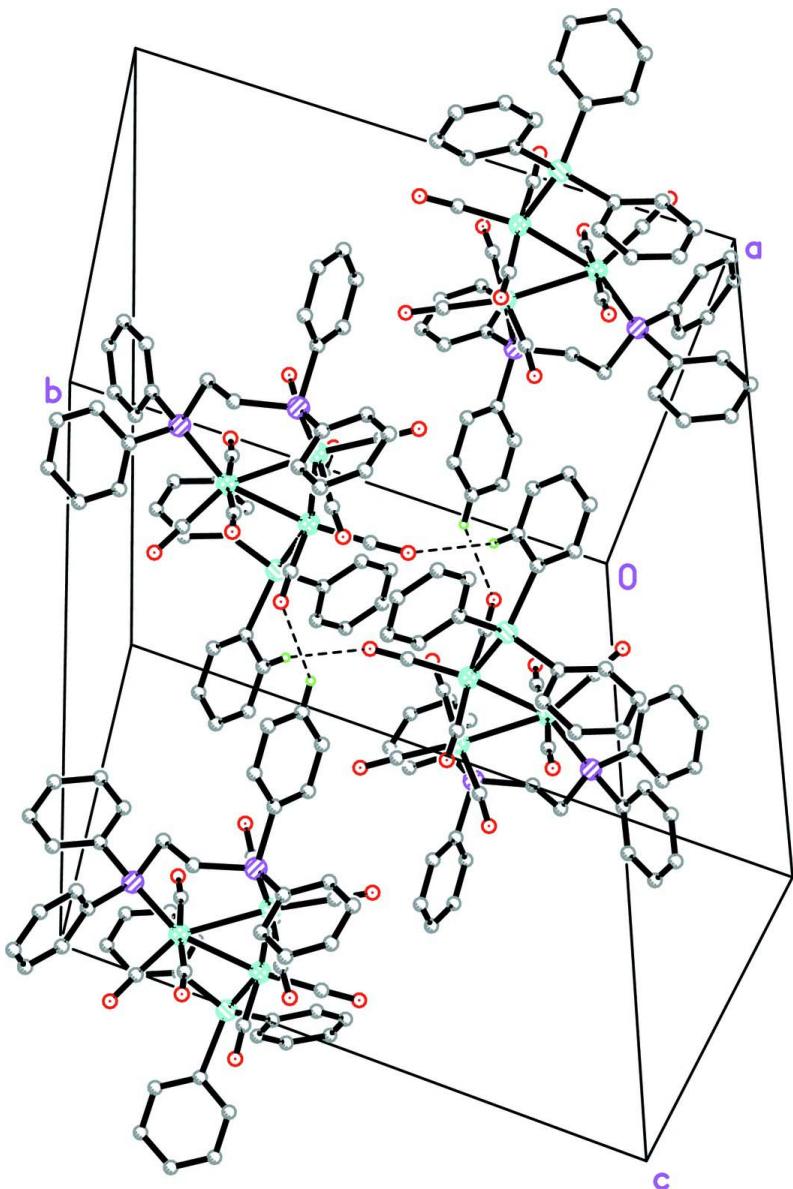
All manipulations were performed under a dry, oxygen-free nitrogen atmosphere using standard Schlenk techniques. All solvents were dried over sodium and distilled from sodium benzophenone ketyl under dry oxygen free nitrogen. Tri-phenylstibine (Fluka) is used as received and  $\text{Ru}_3(\text{CO})_{10}(\mu\text{-Ph}_2\text{PCH}_2\text{CH}_2\text{PPh}_2)$  (Bruce *et al.*, 1983) was prepared by a reported procedure. The title compound was obtained by refluxing equimolar quantities of  $\text{Ru}_3(\text{CO})_{10}(\mu\text{-Ph}_2\text{PCH}_2\text{CH}_2\text{PPh}_2)$  and triphenylstibine in hexane under a 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>3</sub>.

### S3. Refinement

All hydrogen atoms were positioned geometrically and refined using a riding model with C—H = 0.93 or 0.97 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The maximum and minimum residual electron density peaks of 2.13 and -1.16 e Å<sup>-3</sup> were located 0.85 Å and 1.41 Å, respectively from the Ru3 atom.

**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, showing the molecules linked into a tetramer. Hydrogen atoms that are not involved in the hydrogen-bonding (dashed lines) have been omitted for clarity.

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

*Crystal data*



$M_r = 1306.74$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 15.1589 (8) \text{ \AA}$

$b = 18.6156 (10) \text{ \AA}$

$c = 20.0398 (11) \text{ \AA}$

$\alpha = 113.233 (1)^\circ$

$\beta = 97.986 (1)^\circ$

$\gamma = 97.339 (1)^\circ$

$V = 5041.5 (5) \text{ \AA}^3$

$Z = 4$

$F(000) = 2568$

$D_x = 1.722 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 9952 reflections  
 $\theta = 2.6\text{--}32.6^\circ$   
 $\mu = 1.53 \text{ mm}^{-1}$

$T = 100 \text{ K}$   
 Plate, brown  
 $0.51 \times 0.15 \times 0.08 \text{ mm}$

#### Data collection

Bruker APEXII DUO CCD area-detector  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan  
 (*SADABS*; Bruker, 2009)  
 $T_{\min} = 0.506$ ,  $T_{\max} = 0.885$

82542 measured reflections  
 28970 independent reflections  
 21778 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.033$   
 $\theta_{\max} = 30.0^\circ$ ,  $\theta_{\min} = 1.9^\circ$   
 $h = -21 \rightarrow 21$   
 $k = -26 \rightarrow 26$   
 $l = -28 \rightarrow 28$

#### Refinement

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.121$   
 $S = 1.11$   
 28970 reflections  
 1225 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0352P)^2 + 25.152P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 3.47 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -2.34 \text{ e \AA}^{-3}$

#### 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 ( $\text{\AA}^2$ )

|      | $x$            | $y$           | $z$           | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|----------------|---------------|---------------|----------------------------------|
| Sb1A | -0.061486 (19) | 0.701152 (17) | 0.978302 (16) | 0.02093 (6)                      |
| Ru1A | 0.21003 (2)    | 0.819388 (19) | 1.014099 (18) | 0.01705 (7)                      |
| Ru2A | 0.27903 (2)    | 0.67570 (2)   | 0.955200 (18) | 0.01778 (7)                      |
| Ru3A | 0.09780 (2)    | 0.66624 (2)   | 0.973168 (18) | 0.01816 (7)                      |
| P1A  | 0.32886 (8)    | 0.91401 (6)   | 1.01639 (6)   | 0.0191 (2)                       |
| P2A  | 0.43433 (7)    | 0.72287 (7)   | 0.97737 (6)   | 0.0196 (2)                       |
| O1A  | 0.1010 (2)     | 0.8075 (2)    | 0.8671 (2)    | 0.0351 (8)                       |
| O2A  | 0.0940 (2)     | 0.9232 (2)    | 1.1051 (2)    | 0.0333 (8)                       |
| O3A  | 0.3215 (3)     | 0.8307 (2)    | 1.15895 (19)  | 0.0348 (8)                       |
| O4A  | 0.3109 (3)     | 0.6504 (3)    | 1.0984 (2)    | 0.0448 (10)                      |
| O5A  | 0.2593 (3)     | 0.4989 (2)    | 0.8596 (3)    | 0.0493 (11)                      |

|      |            |            |              |             |
|------|------------|------------|--------------|-------------|
| O6A  | 0.2524 (2) | 0.7124 (2) | 0.81825 (19) | 0.0318 (8)  |
| O7A  | 0.0570 (3) | 0.6188 (2) | 0.8050 (2)   | 0.0382 (9)  |
| O8A  | 0.0677 (3) | 0.4919 (2) | 0.9450 (2)   | 0.0409 (9)  |
| O9A  | 0.1349 (3) | 0.7158 (2) | 1.1413 (2)   | 0.0375 (8)  |
| C1A  | 0.3020 (3) | 0.9671 (3) | 0.9585 (2)   | 0.0224 (8)  |
| C2A  | 0.2874 (4) | 0.9255 (3) | 0.8817 (3)   | 0.0299 (10) |
| H2AA | 0.2923     | 0.8722     | 0.8610       | 0.036*      |
| C3A  | 0.2655 (4) | 0.9632 (4) | 0.8352 (3)   | 0.0402 (13) |
| H3AA | 0.2558     | 0.9350     | 0.7840       | 0.048*      |
| C4A  | 0.2585 (4) | 1.0422 (4) | 0.8656 (3)   | 0.0421 (13) |
| H4AA | 0.2449     | 1.0675     | 0.8348       | 0.051*      |
| C5A  | 0.2714 (4) | 1.0842 (3) | 0.9420 (3)   | 0.0377 (12) |
| H5AA | 0.2655     | 1.1372     | 0.9624       | 0.045*      |
| C6A  | 0.2934 (3) | 1.0465 (3) | 0.9879 (3)   | 0.0314 (10) |
| H6AA | 0.3024     | 1.0748     | 1.0391       | 0.038*      |
| C7A  | 0.3792 (3) | 0.9948 (3) | 1.1076 (2)   | 0.0229 (8)  |
| C8A  | 0.3235 (4) | 1.0310 (3) | 1.1547 (3)   | 0.0338 (11) |
| H8AA | 0.2610     | 1.0119     | 1.1399       | 0.041*      |
| C9A  | 0.3581 (4) | 1.0945 (3) | 1.2230 (3)   | 0.0397 (13) |
| H9AA | 0.3189     | 1.1181     | 1.2529       | 0.048*      |
| C10A | 0.4501 (4) | 1.1227 (3) | 1.2466 (3)   | 0.0388 (12) |
| H10A | 0.4735     | 1.1657     | 1.2923       | 0.047*      |
| C11A | 0.5076 (4) | 1.0868 (3) | 1.2017 (3)   | 0.0376 (12) |
| H11A | 0.5701     | 1.1050     | 1.2180       | 0.045*      |
| C12A | 0.4734 (3) | 1.0240 (3) | 1.1330 (3)   | 0.0299 (10) |
| H12A | 0.5131     | 1.0009     | 1.1033       | 0.036*      |
| C13A | 0.4276 (3) | 0.8756 (3) | 0.9828 (2)   | 0.0227 (8)  |
| H13A | 0.4087     | 0.8390     | 0.9308       | 0.027*      |
| H13B | 0.4729     | 0.9197     | 0.9869       | 0.027*      |
| C14A | 0.4710 (3) | 0.8320 (3) | 1.0261 (2)   | 0.0237 (9)  |
| H14A | 0.4548     | 0.8500     | 1.0745       | 0.028*      |
| H14B | 0.5367     | 0.8459     | 1.0339       | 0.028*      |
| C15A | 0.4848 (3) | 0.6985 (3) | 0.8949 (2)   | 0.0229 (8)  |
| C16A | 0.4413 (3) | 0.6350 (3) | 0.8281 (3)   | 0.0305 (10) |
| H16A | 0.3863     | 0.6044     | 0.8255       | 0.037*      |
| C17A | 0.4782 (4) | 0.6165 (4) | 0.7650 (3)   | 0.0387 (13) |
| H17A | 0.4489     | 0.5729     | 0.7212       | 0.046*      |
| C18A | 0.5570 (4) | 0.6619 (4) | 0.7672 (3)   | 0.0425 (14) |
| H18A | 0.5808     | 0.6501     | 0.7246       | 0.051*      |
| C19A | 0.6022 (4) | 0.7259 (4) | 0.8329 (4)   | 0.0453 (15) |
| H19A | 0.6562     | 0.7569     | 0.8344       | 0.054*      |
| C20A | 0.5664 (4) | 0.7436 (3) | 0.8968 (3)   | 0.0377 (12) |
| H20A | 0.5975     | 0.7858     | 0.9411       | 0.045*      |
| C21A | 0.5025 (3) | 0.6893 (3) | 1.0373 (3)   | 0.0254 (9)  |
| C22A | 0.5174 (5) | 0.7281 (4) | 1.1142 (3)   | 0.057 (2)   |
| H22A | 0.4983     | 0.7760     | 1.1361       | 0.069*      |
| C23A | 0.5599 (6) | 0.6968 (5) | 1.1585 (4)   | 0.065 (2)   |
| H23A | 0.5673     | 0.7232     | 1.2098       | 0.078*      |

|      |             |            |            |             |
|------|-------------|------------|------------|-------------|
| C24A | 0.5911 (4)  | 0.6284 (4) | 1.1292 (4) | 0.0468 (15) |
| H24A | 0.6210      | 0.6082     | 1.1597     | 0.056*      |
| C25A | 0.5776 (5)  | 0.5894 (4) | 1.0532 (4) | 0.0549 (18) |
| H25A | 0.5980      | 0.5420     | 1.0320     | 0.066*      |
| C26A | 0.5344 (5)  | 0.6194 (4) | 1.0083 (3) | 0.0478 (16) |
| H26A | 0.5264      | 0.5921     | 0.9570     | 0.057*      |
| C27A | -0.0963 (3) | 0.7794 (3) | 0.9286 (3) | 0.0244 (9)  |
| C28A | -0.1235 (4) | 0.7446 (3) | 0.8524 (3) | 0.0325 (10) |
| H28A | -0.1323     | 0.6894     | 0.8272     | 0.039*      |
| C29A | -0.1381 (4) | 0.7898 (4) | 0.8122 (3) | 0.0385 (12) |
| H29A | -0.1561     | 0.7650     | 0.7607     | 0.046*      |
| C30A | -0.1256 (4) | 0.8714 (4) | 0.8493 (3) | 0.0399 (13) |
| H30A | -0.1354     | 0.9022     | 0.8231     | 0.048*      |
| C31A | -0.0984 (5) | 0.9073 (4) | 0.9262 (4) | 0.0467 (15) |
| H31A | -0.0896     | 0.9624     | 0.9513     | 0.056*      |
| C32A | -0.0842 (4) | 0.8617 (3) | 0.9658 (3) | 0.0348 (11) |
| H32A | -0.0665     | 0.8863     | 1.0173     | 0.042*      |
| C33A | -0.1068 (3) | 0.7415 (3) | 1.0806 (3) | 0.0264 (9)  |
| C34A | -0.0888 (4) | 0.8221 (3) | 1.1319 (3) | 0.0374 (12) |
| H34A | -0.0580     | 0.8611     | 1.1208     | 0.045*      |
| C35A | -0.1168 (4) | 0.8437 (3) | 1.1990 (3) | 0.0396 (12) |
| H35A | -0.1057     | 0.8971     | 1.2323     | 0.048*      |
| C36A | -0.1614 (4) | 0.7854 (4) | 1.2163 (3) | 0.0440 (14) |
| H36A | -0.1833     | 0.7997     | 1.2599     | 0.053*      |
| C37A | -0.1725 (5) | 0.7078 (4) | 1.1692 (3) | 0.0508 (17) |
| H37A | -0.1978     | 0.6684     | 1.1826     | 0.061*      |
| C38A | -0.1467 (5) | 0.6859 (3) | 1.1008 (3) | 0.0467 (15) |
| H38A | -0.1571     | 0.6322     | 1.0685     | 0.056*      |
| C39A | -0.1726 (3) | 0.6039 (3) | 0.9140 (3) | 0.0265 (9)  |
| C40A | -0.1574 (3) | 0.5277 (3) | 0.8797 (3) | 0.0324 (11) |
| H40A | -0.0982     | 0.5189     | 0.8828     | 0.039*      |
| C41A | -0.2300 (4) | 0.4641 (3) | 0.8404 (3) | 0.0388 (12) |
| H41A | -0.2197     | 0.4126     | 0.8178     | 0.047*      |
| C42A | -0.3179 (4) | 0.4777 (3) | 0.8351 (3) | 0.0349 (11) |
| H42A | -0.3668     | 0.4351     | 0.8094     | 0.042*      |
| C43A | -0.3330 (3) | 0.5543 (3) | 0.8678 (3) | 0.0368 (12) |
| H43A | -0.3919     | 0.5634     | 0.8629     | 0.044*      |
| C44A | -0.2608 (3) | 0.6175 (3) | 0.9078 (3) | 0.0349 (11) |
| H44A | -0.2712     | 0.6690     | 0.9305     | 0.042*      |
| C45A | 0.2793 (3)  | 0.8205 (3) | 1.1024 (3) | 0.0259 (9)  |
| C46A | 0.1361 (3)  | 0.8842 (3) | 1.0680 (2) | 0.0226 (8)  |
| C47A | 0.1414 (3)  | 0.8080 (3) | 0.9201 (3) | 0.0248 (9)  |
| C48A | 0.2959 (3)  | 0.6618 (3) | 1.0469 (3) | 0.0290 (10) |
| C49A | 0.2688 (3)  | 0.5651 (3) | 0.8966 (3) | 0.0300 (10) |
| C50A | 0.2583 (3)  | 0.7017 (3) | 0.8714 (2) | 0.0224 (8)  |
| C51A | 0.0762 (3)  | 0.6387 (3) | 0.8677 (2) | 0.0249 (9)  |
| C52A | 0.0763 (3)  | 0.5579 (3) | 0.9553 (3) | 0.0267 (9)  |
| C53A | 0.1248 (3)  | 0.6998 (3) | 1.0792 (3) | 0.0248 (9)  |

|      |               |               |               |             |
|------|---------------|---------------|---------------|-------------|
| Sb1B | 0.591162 (19) | 0.322816 (17) | 0.539002 (15) | 0.01948 (6) |
| Ru1B | 0.32201 (2)   | 0.19935 (2)   | 0.497165 (19) | 0.02039 (7) |
| Ru2B | 0.24537 (2)   | 0.33890 (2)   | 0.55496 (2)   | 0.02058 (7) |
| Ru3B | 0.42965 (2)   | 0.35418 (2)   | 0.542128 (18) | 0.01812 (7) |
| P1B  | 0.21368 (9)   | 0.10411 (7)   | 0.50293 (7)   | 0.0261 (2)  |
| P2B  | 0.09114 (8)   | 0.28330 (7)   | 0.52371 (7)   | 0.0242 (2)  |
| O1B  | 0.2092 (2)    | 0.1901 (2)    | 0.3535 (2)    | 0.0332 (8)  |
| O2B  | 0.4344 (3)    | 0.0905 (2)    | 0.4061 (2)    | 0.0417 (9)  |
| O3B  | 0.4351 (3)    | 0.2219 (2)    | 0.6473 (2)    | 0.0361 (8)  |
| O4B  | 0.2727 (3)    | 0.2988 (2)    | 0.6902 (2)    | 0.0365 (8)  |
| O5B  | 0.2437 (3)    | 0.5110 (3)    | 0.6536 (3)    | 0.0613 (14) |
| O6B  | 0.2258 (3)    | 0.3753 (3)    | 0.4175 (3)    | 0.0490 (11) |
| O7B  | 0.3918 (2)    | 0.2976 (2)    | 0.37254 (19)  | 0.0339 (8)  |
| O8B  | 0.4642 (3)    | 0.5285 (2)    | 0.5714 (2)    | 0.0411 (9)  |
| O9B  | 0.4645 (3)    | 0.4055 (2)    | 0.7112 (2)    | 0.0364 (8)  |
| C1B  | 0.1669 (3)    | 0.0142 (3)    | 0.4166 (3)    | 0.0310 (10) |
| C2B  | 0.1947 (3)    | 0.0015 (3)    | 0.3512 (3)    | 0.0315 (10) |
| H2BA | 0.2379        | 0.0408        | 0.3497        | 0.038*      |
| C3B  | 0.1604 (4)    | -0.0680 (3)   | 0.2873 (3)    | 0.0397 (12) |
| H3BA | 0.1809        | -0.0752       | 0.2439        | 0.048*      |
| C4B  | 0.0965 (4)    | -0.1258 (4)   | 0.2885 (3)    | 0.0475 (15) |
| H4BA | 0.0719        | -0.1719       | 0.2454        | 0.057*      |
| C5B  | 0.0682 (4)    | -0.1159 (4)   | 0.3538 (4)    | 0.0485 (15) |
| H5BA | 0.0253        | -0.1558       | 0.3548        | 0.058*      |
| C6B  | 0.1035 (4)    | -0.0470 (3)   | 0.4175 (3)    | 0.0403 (13) |
| H6BA | 0.0851        | -0.0411       | 0.4614        | 0.048*      |
| C7B  | 0.2515 (4)    | 0.0621 (3)    | 0.5682 (3)    | 0.0304 (10) |
| C8B  | 0.3394 (4)    | 0.0449 (3)    | 0.5725 (3)    | 0.0384 (12) |
| H8BA | 0.3764        | 0.0556        | 0.5428        | 0.046*      |
| C9B  | 0.3718 (5)    | 0.0124 (4)    | 0.6201 (3)    | 0.0467 (15) |
| H9BA | 0.4302        | 0.0018        | 0.6226        | 0.056*      |
| C10B | 0.3171 (6)    | -0.0041 (4)   | 0.6639 (4)    | 0.0557 (18) |
| H10B | 0.3389        | -0.0256       | 0.6962        | 0.067*      |
| C11B | 0.2304 (5)    | 0.0109 (5)    | 0.6599 (4)    | 0.0569 (18) |
| H11B | 0.1933        | -0.0019       | 0.6885        | 0.068*      |
| C12B | 0.1974 (5)    | 0.0454 (4)    | 0.6130 (3)    | 0.0447 (14) |
| H12B | 0.1395        | 0.0570        | 0.6119        | 0.054*      |
| C13B | 0.1080 (4)    | 0.1364 (3)    | 0.5292 (3)    | 0.0325 (11) |
| H13C | 0.0655        | 0.0907        | 0.5255        | 0.039*      |
| H13D | 0.1222        | 0.1753        | 0.5805        | 0.039*      |
| C14B | 0.0626 (3)    | 0.1730 (3)    | 0.4805 (3)    | 0.0318 (10) |
| H14C | -0.0028       | 0.1556        | 0.4707        | 0.038*      |
| H14D | 0.0816        | 0.1534        | 0.4332        | 0.038*      |
| C15B | 0.0242 (3)    | 0.3097 (3)    | 0.4569 (3)    | 0.0284 (10) |
| C16B | -0.0167 (4)   | 0.3756 (3)    | 0.4824 (3)    | 0.0365 (11) |
| H16B | -0.0133       | 0.4030        | 0.5331        | 0.044*      |
| C17B | -0.0626 (4)   | 0.4012 (4)    | 0.4335 (3)    | 0.0442 (14) |
| H17B | -0.0895       | 0.4454        | 0.4515        | 0.053*      |

|      |             |            |            |             |
|------|-------------|------------|------------|-------------|
| C18B | -0.0681 (4) | 0.3604 (4) | 0.3581 (3) | 0.0451 (15) |
| H18B | -0.0993     | 0.3768     | 0.3250     | 0.054*      |
| C19B | -0.0273 (4) | 0.2955 (4) | 0.3321 (3) | 0.0454 (15) |
| H19B | -0.0301     | 0.2687     | 0.2814     | 0.054*      |
| C20B | 0.0180 (4)  | 0.2699 (4) | 0.3809 (3) | 0.0406 (13) |
| H20B | 0.0445      | 0.2255     | 0.3625     | 0.049*      |
| C21B | 0.0274 (3)  | 0.3058 (3) | 0.5985 (3) | 0.0269 (9)  |
| C22B | 0.0680 (4)  | 0.3562 (4) | 0.6709 (3) | 0.0430 (14) |
| H22B | 0.1290      | 0.3806     | 0.6827     | 0.052*      |
| C23B | 0.0178 (5)  | 0.3708 (5) | 0.7267 (4) | 0.059 (2)   |
| H23B | 0.0457      | 0.4051     | 0.7755     | 0.071*      |
| C24B | -0.0712 (5) | 0.3355 (5) | 0.7106 (4) | 0.0568 (19) |
| H24B | -0.1037     | 0.3446     | 0.7483     | 0.068*      |
| C25B | -0.1140 (5) | 0.2854 (5) | 0.6371 (4) | 0.0548 (18) |
| H25B | -0.1753     | 0.2620     | 0.6256     | 0.066*      |
| C26B | -0.0646 (4) | 0.2708 (4) | 0.5815 (3) | 0.0400 (13) |
| H26B | -0.0930     | 0.2375     | 0.5326     | 0.048*      |
| C27B | 0.6993 (3)  | 0.4228 (3) | 0.6026 (2) | 0.0227 (8)  |
| C28B | 0.7858 (4)  | 0.4236 (3) | 0.5888 (4) | 0.0427 (14) |
| H28B | 0.7972      | 0.3809     | 0.5494     | 0.051*      |
| C29B | 0.8555 (4)  | 0.4873 (3) | 0.6331 (4) | 0.0478 (16) |
| H29B | 0.9138      | 0.4867     | 0.6236     | 0.057*      |
| C30B | 0.8404 (3)  | 0.5514 (3) | 0.6907 (3) | 0.0318 (10) |
| H30B | 0.8879      | 0.5940     | 0.7203     | 0.038*      |
| C31B | 0.7536 (4)  | 0.5520 (3) | 0.7043 (3) | 0.0375 (12) |
| H31B | 0.7424      | 0.5954     | 0.7432     | 0.045*      |
| C32B | 0.6835 (4)  | 0.4885 (3) | 0.6605 (3) | 0.0349 (11) |
| H32B | 0.6251      | 0.4896     | 0.6697     | 0.042*      |
| C33B | 0.6441 (3)  | 0.2765 (3) | 0.4407 (2) | 0.0217 (8)  |
| C34B | 0.6234 (3)  | 0.3025 (3) | 0.3861 (3) | 0.0263 (9)  |
| H34B | 0.5800      | 0.3342     | 0.3894     | 0.032*      |
| C35B | 0.6664 (4)  | 0.2822 (3) | 0.3259 (3) | 0.0313 (10) |
| H35B | 0.6512      | 0.2995     | 0.2889     | 0.038*      |
| C36B | 0.7323 (3)  | 0.2358 (3) | 0.3216 (3) | 0.0289 (10) |
| H36B | 0.7621      | 0.2228     | 0.2821     | 0.035*      |
| C37B | 0.7536 (3)  | 0.2093 (3) | 0.3758 (3) | 0.0327 (11) |
| H37B | 0.7972      | 0.1778     | 0.3724     | 0.039*      |
| C38B | 0.7100 (3)  | 0.2292 (3) | 0.4359 (3) | 0.0320 (11) |
| H38B | 0.7247      | 0.2112     | 0.4724     | 0.038*      |
| C39B | 0.6245 (3)  | 0.2472 (3) | 0.5910 (2) | 0.0224 (8)  |
| C40B | 0.6090 (4)  | 0.1649 (3) | 0.5533 (3) | 0.0318 (10) |
| H40B | 0.5897      | 0.1410     | 0.5019     | 0.038*      |
| C41B | 0.6220 (5)  | 0.1176 (3) | 0.5918 (3) | 0.0429 (14) |
| H41B | 0.6121      | 0.0624     | 0.5661     | 0.052*      |
| C42B | 0.6495 (4)  | 0.1528 (4) | 0.6680 (3) | 0.0420 (13) |
| H42B | 0.6568      | 0.1211     | 0.6937     | 0.050*      |
| C43B | 0.6664 (4)  | 0.2347 (3) | 0.7063 (3) | 0.0345 (11) |
| H43B | 0.6859      | 0.2582     | 0.7577     | 0.041*      |

|      |            |            |            |             |
|------|------------|------------|------------|-------------|
| C44B | 0.6541 (3) | 0.2822 (3) | 0.6682 (3) | 0.0272 (9)  |
| H44B | 0.6656     | 0.3375     | 0.6941     | 0.033*      |
| C45B | 0.2505 (3) | 0.1991 (3) | 0.4099 (3) | 0.0248 (9)  |
| C46B | 0.3946 (3) | 0.1328 (3) | 0.4428 (2) | 0.0265 (9)  |
| C47B | 0.3945 (3) | 0.2181 (3) | 0.5931 (3) | 0.0265 (9)  |
| C48B | 0.2661 (3) | 0.3111 (3) | 0.6383 (3) | 0.0269 (9)  |
| C49B | 0.2434 (4) | 0.4467 (3) | 0.6153 (3) | 0.0353 (11) |
| C50B | 0.2353 (3) | 0.3600 (3) | 0.4666 (3) | 0.0323 (11) |
| C51B | 0.4029 (3) | 0.3167 (3) | 0.4355 (3) | 0.0246 (9)  |
| C52B | 0.4522 (3) | 0.4623 (3) | 0.5594 (3) | 0.0262 (9)  |
| C53B | 0.4480 (3) | 0.3832 (3) | 0.6477 (3) | 0.0251 (9)  |

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

|      | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|------|--------------|--------------|--------------|--------------|--------------|--------------|
| Sb1A | 0.01861 (13) | 0.02543 (14) | 0.02117 (13) | 0.00765 (11) | 0.00624 (10) | 0.01061 (11) |
| Ru1A | 0.01765 (15) | 0.01983 (15) | 0.01511 (14) | 0.00562 (12) | 0.00476 (12) | 0.00779 (12) |
| Ru2A | 0.01684 (15) | 0.02065 (15) | 0.01764 (15) | 0.00657 (12) | 0.00564 (12) | 0.00836 (12) |
| Ru3A | 0.01704 (15) | 0.02083 (15) | 0.01852 (15) | 0.00543 (12) | 0.00573 (12) | 0.00904 (12) |
| P1A  | 0.0210 (5)   | 0.0193 (5)   | 0.0165 (5)   | 0.0035 (4)   | 0.0053 (4)   | 0.0067 (4)   |
| P2A  | 0.0170 (5)   | 0.0247 (5)   | 0.0172 (5)   | 0.0063 (4)   | 0.0044 (4)   | 0.0080 (4)   |
| O1A  | 0.0322 (19)  | 0.047 (2)    | 0.0255 (17)  | 0.0062 (16)  | 0.0008 (14)  | 0.0161 (16)  |
| O2A  | 0.0356 (19)  | 0.0302 (17)  | 0.0361 (19)  | 0.0141 (15)  | 0.0184 (16)  | 0.0101 (15)  |
| O3A  | 0.041 (2)    | 0.043 (2)    | 0.0249 (17)  | 0.0106 (17)  | 0.0008 (15)  | 0.0198 (16)  |
| O4A  | 0.055 (3)    | 0.063 (3)    | 0.039 (2)    | 0.028 (2)    | 0.0200 (19)  | 0.037 (2)    |
| O5A  | 0.052 (3)    | 0.0236 (18)  | 0.061 (3)    | 0.0103 (18)  | 0.016 (2)    | 0.0041 (18)  |
| O6A  | 0.0326 (19)  | 0.046 (2)    | 0.0236 (16)  | 0.0126 (16)  | 0.0102 (14)  | 0.0181 (15)  |
| O7A  | 0.0311 (19)  | 0.054 (2)    | 0.0235 (17)  | -0.0002 (17) | 0.0037 (15)  | 0.0135 (17)  |
| O8A  | 0.045 (2)    | 0.0284 (18)  | 0.056 (3)    | 0.0123 (17)  | 0.0181 (19)  | 0.0205 (18)  |
| O9A  | 0.041 (2)    | 0.051 (2)    | 0.0263 (18)  | 0.0113 (18)  | 0.0122 (16)  | 0.0196 (17)  |
| C1A  | 0.020 (2)    | 0.026 (2)    | 0.024 (2)    | 0.0015 (16)  | 0.0035 (16)  | 0.0140 (17)  |
| C2A  | 0.037 (3)    | 0.032 (2)    | 0.023 (2)    | 0.008 (2)    | 0.0072 (19)  | 0.0124 (19)  |
| C3A  | 0.049 (3)    | 0.052 (3)    | 0.024 (2)    | 0.016 (3)    | 0.007 (2)    | 0.020 (2)    |
| C4A  | 0.044 (3)    | 0.054 (3)    | 0.044 (3)    | 0.017 (3)    | 0.008 (3)    | 0.035 (3)    |
| C5A  | 0.039 (3)    | 0.034 (3)    | 0.044 (3)    | 0.008 (2)    | 0.002 (2)    | 0.022 (2)    |
| C6A  | 0.033 (3)    | 0.033 (2)    | 0.028 (2)    | 0.005 (2)    | 0.001 (2)    | 0.014 (2)    |
| C7A  | 0.023 (2)    | 0.023 (2)    | 0.0193 (19)  | -0.0009 (16) | 0.0017 (16)  | 0.0076 (16)  |
| C8A  | 0.029 (2)    | 0.033 (3)    | 0.027 (2)    | 0.001 (2)    | 0.007 (2)    | 0.001 (2)    |
| C9A  | 0.038 (3)    | 0.037 (3)    | 0.030 (3)    | 0.004 (2)    | 0.009 (2)    | -0.001 (2)   |
| C10A | 0.042 (3)    | 0.031 (3)    | 0.026 (2)    | -0.003 (2)   | 0.001 (2)    | 0.000 (2)    |
| C11A | 0.031 (3)    | 0.033 (3)    | 0.034 (3)    | -0.004 (2)   | -0.001 (2)   | 0.006 (2)    |
| C12A | 0.026 (2)    | 0.028 (2)    | 0.029 (2)    | 0.0025 (19)  | 0.0050 (19)  | 0.0064 (19)  |
| C13A | 0.023 (2)    | 0.023 (2)    | 0.021 (2)    | 0.0033 (16)  | 0.0059 (16)  | 0.0076 (16)  |
| C14A | 0.021 (2)    | 0.028 (2)    | 0.0194 (19)  | 0.0053 (17)  | 0.0022 (16)  | 0.0078 (17)  |
| C15A | 0.022 (2)    | 0.028 (2)    | 0.024 (2)    | 0.0109 (17)  | 0.0079 (17)  | 0.0135 (18)  |
| C16A | 0.027 (2)    | 0.041 (3)    | 0.023 (2)    | 0.012 (2)    | 0.0096 (18)  | 0.010 (2)    |
| C17A | 0.042 (3)    | 0.057 (3)    | 0.025 (2)    | 0.030 (3)    | 0.015 (2)    | 0.017 (2)    |
| C18A | 0.061 (4)    | 0.053 (3)    | 0.042 (3)    | 0.036 (3)    | 0.036 (3)    | 0.033 (3)    |

|      |              |              |              |              |              |              |
|------|--------------|--------------|--------------|--------------|--------------|--------------|
| C19A | 0.046 (3)    | 0.043 (3)    | 0.063 (4)    | 0.014 (3)    | 0.037 (3)    | 0.029 (3)    |
| C20A | 0.040 (3)    | 0.031 (3)    | 0.045 (3)    | 0.007 (2)    | 0.022 (2)    | 0.014 (2)    |
| C21A | 0.019 (2)    | 0.036 (2)    | 0.025 (2)    | 0.0095 (18)  | 0.0063 (17)  | 0.0139 (19)  |
| C22A | 0.084 (5)    | 0.064 (4)    | 0.023 (3)    | 0.047 (4)    | 0.002 (3)    | 0.010 (3)    |
| C23A | 0.087 (6)    | 0.084 (5)    | 0.026 (3)    | 0.047 (5)    | 0.001 (3)    | 0.021 (3)    |
| C24A | 0.048 (4)    | 0.063 (4)    | 0.045 (3)    | 0.024 (3)    | 0.007 (3)    | 0.036 (3)    |
| C25A | 0.079 (5)    | 0.056 (4)    | 0.041 (3)    | 0.039 (4)    | 0.009 (3)    | 0.026 (3)    |
| C26A | 0.071 (4)    | 0.050 (3)    | 0.031 (3)    | 0.036 (3)    | 0.010 (3)    | 0.018 (3)    |
| C27A | 0.019 (2)    | 0.033 (2)    | 0.025 (2)    | 0.0105 (18)  | 0.0057 (17)  | 0.0157 (19)  |
| C28A | 0.038 (3)    | 0.032 (2)    | 0.027 (2)    | 0.006 (2)    | 0.006 (2)    | 0.013 (2)    |
| C29A | 0.043 (3)    | 0.050 (3)    | 0.028 (3)    | 0.012 (3)    | 0.008 (2)    | 0.021 (2)    |
| C30A | 0.045 (3)    | 0.048 (3)    | 0.041 (3)    | 0.021 (3)    | 0.008 (2)    | 0.030 (3)    |
| C31A | 0.064 (4)    | 0.034 (3)    | 0.045 (3)    | 0.020 (3)    | 0.006 (3)    | 0.018 (3)    |
| C32A | 0.044 (3)    | 0.036 (3)    | 0.029 (2)    | 0.018 (2)    | 0.005 (2)    | 0.015 (2)    |
| C33A | 0.028 (2)    | 0.034 (2)    | 0.025 (2)    | 0.0155 (19)  | 0.0118 (18)  | 0.0158 (19)  |
| C34A | 0.041 (3)    | 0.032 (3)    | 0.036 (3)    | 0.004 (2)    | 0.012 (2)    | 0.011 (2)    |
| C35A | 0.043 (3)    | 0.038 (3)    | 0.032 (3)    | 0.007 (2)    | 0.010 (2)    | 0.009 (2)    |
| C36A | 0.051 (4)    | 0.052 (3)    | 0.033 (3)    | 0.010 (3)    | 0.021 (3)    | 0.017 (3)    |
| C37A | 0.083 (5)    | 0.038 (3)    | 0.043 (3)    | 0.008 (3)    | 0.033 (3)    | 0.024 (3)    |
| C38A | 0.078 (5)    | 0.031 (3)    | 0.039 (3)    | 0.014 (3)    | 0.027 (3)    | 0.016 (2)    |
| C39A | 0.026 (2)    | 0.035 (2)    | 0.026 (2)    | 0.0124 (19)  | 0.0092 (18)  | 0.0179 (19)  |
| C40A | 0.022 (2)    | 0.034 (3)    | 0.039 (3)    | 0.0036 (19)  | 0.003 (2)    | 0.014 (2)    |
| C41A | 0.031 (3)    | 0.030 (3)    | 0.044 (3)    | 0.004 (2)    | 0.007 (2)    | 0.006 (2)    |
| C42A | 0.027 (2)    | 0.040 (3)    | 0.032 (3)    | -0.002 (2)   | 0.001 (2)    | 0.015 (2)    |
| C43A | 0.019 (2)    | 0.050 (3)    | 0.042 (3)    | 0.005 (2)    | 0.004 (2)    | 0.021 (3)    |
| C44A | 0.023 (2)    | 0.041 (3)    | 0.040 (3)    | 0.011 (2)    | 0.004 (2)    | 0.015 (2)    |
| C45A | 0.030 (2)    | 0.028 (2)    | 0.026 (2)    | 0.0105 (19)  | 0.0085 (18)  | 0.0158 (19)  |
| C46A | 0.022 (2)    | 0.026 (2)    | 0.024 (2)    | 0.0044 (17)  | 0.0086 (17)  | 0.0143 (17)  |
| C47A | 0.022 (2)    | 0.029 (2)    | 0.023 (2)    | 0.0057 (17)  | 0.0050 (17)  | 0.0096 (18)  |
| C48A | 0.033 (3)    | 0.033 (2)    | 0.030 (2)    | 0.015 (2)    | 0.014 (2)    | 0.018 (2)    |
| C49A | 0.025 (2)    | 0.029 (2)    | 0.036 (3)    | 0.0091 (19)  | 0.009 (2)    | 0.013 (2)    |
| C50A | 0.018 (2)    | 0.026 (2)    | 0.022 (2)    | 0.0044 (16)  | 0.0044 (16)  | 0.0094 (17)  |
| C51A | 0.022 (2)    | 0.027 (2)    | 0.022 (2)    | -0.0015 (17) | 0.0039 (17)  | 0.0084 (17)  |
| C52A | 0.024 (2)    | 0.029 (2)    | 0.028 (2)    | 0.0078 (18)  | 0.0090 (18)  | 0.0116 (19)  |
| C53A | 0.023 (2)    | 0.028 (2)    | 0.024 (2)    | 0.0048 (17)  | 0.0056 (17)  | 0.0113 (18)  |
| Sb1B | 0.01926 (13) | 0.02293 (13) | 0.01749 (12) | 0.00678 (10) | 0.00551 (10) | 0.00843 (10) |
| Ru1B | 0.02591 (17) | 0.02054 (15) | 0.01923 (15) | 0.00768 (13) | 0.00992 (13) | 0.01034 (13) |
| Ru2B | 0.02011 (16) | 0.02150 (16) | 0.02397 (17) | 0.00693 (13) | 0.01028 (13) | 0.01081 (13) |
| Ru3B | 0.01884 (16) | 0.02118 (15) | 0.01860 (15) | 0.00665 (12) | 0.00762 (12) | 0.01070 (12) |
| P1B  | 0.0347 (6)   | 0.0212 (5)   | 0.0257 (6)   | 0.0054 (5)   | 0.0161 (5)   | 0.0101 (5)   |
| P2B  | 0.0210 (5)   | 0.0293 (6)   | 0.0229 (5)   | 0.0038 (4)   | 0.0088 (4)   | 0.0106 (5)   |
| O1B  | 0.0322 (19)  | 0.045 (2)    | 0.0300 (18)  | 0.0109 (16)  | 0.0067 (15)  | 0.0222 (16)  |
| O2B  | 0.038 (2)    | 0.051 (2)    | 0.033 (2)    | 0.0233 (18)  | 0.0120 (17)  | 0.0094 (18)  |
| O3B  | 0.047 (2)    | 0.0373 (19)  | 0.0271 (18)  | 0.0160 (17)  | 0.0082 (16)  | 0.0141 (16)  |
| O4B  | 0.039 (2)    | 0.050 (2)    | 0.0294 (18)  | 0.0110 (17)  | 0.0159 (16)  | 0.0224 (17)  |
| O5B  | 0.064 (3)    | 0.030 (2)    | 0.077 (4)    | 0.016 (2)    | 0.020 (3)    | 0.005 (2)    |
| O6B  | 0.037 (2)    | 0.079 (3)    | 0.062 (3)    | 0.024 (2)    | 0.018 (2)    | 0.056 (3)    |
| O7B  | 0.0318 (19)  | 0.047 (2)    | 0.0248 (17)  | 0.0002 (16)  | 0.0077 (14)  | 0.0189 (16)  |

|      |             |             |             |              |              |             |
|------|-------------|-------------|-------------|--------------|--------------|-------------|
| O8B  | 0.068 (3)   | 0.0246 (17) | 0.040 (2)   | 0.0158 (18)  | 0.027 (2)    | 0.0158 (16) |
| O9B  | 0.039 (2)   | 0.046 (2)   | 0.0244 (17) | 0.0063 (17)  | 0.0077 (15)  | 0.0146 (16) |
| C1B  | 0.030 (2)   | 0.027 (2)   | 0.032 (3)   | 0.0026 (19)  | 0.012 (2)    | 0.008 (2)   |
| C2B  | 0.030 (2)   | 0.035 (3)   | 0.030 (2)   | 0.007 (2)    | 0.008 (2)    | 0.013 (2)   |
| C3B  | 0.041 (3)   | 0.041 (3)   | 0.030 (3)   | 0.011 (2)    | 0.011 (2)    | 0.006 (2)   |
| C4B  | 0.037 (3)   | 0.039 (3)   | 0.042 (3)   | 0.001 (2)    | 0.003 (2)    | -0.005 (3)  |
| C5B  | 0.044 (3)   | 0.036 (3)   | 0.048 (4)   | -0.002 (3)   | 0.006 (3)    | 0.004 (3)   |
| C6B  | 0.043 (3)   | 0.033 (3)   | 0.038 (3)   | -0.001 (2)   | 0.014 (2)    | 0.009 (2)   |
| C7B  | 0.044 (3)   | 0.024 (2)   | 0.026 (2)   | 0.007 (2)    | 0.013 (2)    | 0.0115 (19) |
| C8B  | 0.047 (3)   | 0.034 (3)   | 0.038 (3)   | 0.014 (2)    | 0.013 (2)    | 0.016 (2)   |
| C9B  | 0.067 (4)   | 0.041 (3)   | 0.039 (3)   | 0.028 (3)    | 0.010 (3)    | 0.019 (3)   |
| C10B | 0.086 (5)   | 0.054 (4)   | 0.050 (4)   | 0.033 (4)    | 0.026 (4)    | 0.035 (3)   |
| C11B | 0.069 (5)   | 0.081 (5)   | 0.047 (4)   | 0.023 (4)    | 0.026 (3)    | 0.047 (4)   |
| C12B | 0.054 (4)   | 0.049 (3)   | 0.043 (3)   | 0.018 (3)    | 0.026 (3)    | 0.024 (3)   |
| C13B | 0.038 (3)   | 0.025 (2)   | 0.037 (3)   | 0.004 (2)    | 0.022 (2)    | 0.012 (2)   |
| C14B | 0.026 (2)   | 0.031 (2)   | 0.031 (2)   | -0.0012 (19) | 0.0082 (19)  | 0.006 (2)   |
| C15B | 0.022 (2)   | 0.038 (3)   | 0.024 (2)   | 0.0003 (19)  | 0.0054 (17)  | 0.013 (2)   |
| C16B | 0.038 (3)   | 0.037 (3)   | 0.031 (3)   | 0.001 (2)    | 0.000 (2)    | 0.015 (2)   |
| C17B | 0.050 (4)   | 0.038 (3)   | 0.046 (3)   | 0.004 (3)    | 0.001 (3)    | 0.024 (3)   |
| C18B | 0.033 (3)   | 0.063 (4)   | 0.040 (3)   | -0.013 (3)   | -0.006 (2)   | 0.033 (3)   |
| C19B | 0.029 (3)   | 0.076 (4)   | 0.028 (3)   | 0.001 (3)    | 0.002 (2)    | 0.022 (3)   |
| C20B | 0.027 (3)   | 0.065 (4)   | 0.028 (3)   | 0.011 (3)    | 0.008 (2)    | 0.018 (3)   |
| C21B | 0.025 (2)   | 0.039 (3)   | 0.028 (2)   | 0.0136 (19)  | 0.0134 (18)  | 0.021 (2)   |
| C22B | 0.030 (3)   | 0.066 (4)   | 0.031 (3)   | 0.016 (3)    | 0.013 (2)    | 0.014 (3)   |
| C23B | 0.056 (4)   | 0.096 (6)   | 0.032 (3)   | 0.040 (4)    | 0.022 (3)    | 0.022 (3)   |
| C24B | 0.056 (4)   | 0.089 (5)   | 0.060 (4)   | 0.044 (4)    | 0.045 (4)    | 0.047 (4)   |
| C25B | 0.040 (3)   | 0.073 (5)   | 0.069 (5)   | 0.021 (3)    | 0.036 (3)    | 0.037 (4)   |
| C26B | 0.031 (3)   | 0.052 (3)   | 0.044 (3)   | 0.013 (2)    | 0.017 (2)    | 0.022 (3)   |
| C27B | 0.0159 (19) | 0.030 (2)   | 0.023 (2)   | 0.0048 (16)  | 0.0004 (16)  | 0.0130 (18) |
| C28B | 0.027 (3)   | 0.033 (3)   | 0.054 (4)   | 0.008 (2)    | 0.010 (2)    | 0.003 (2)   |
| C29B | 0.023 (3)   | 0.037 (3)   | 0.067 (4)   | 0.007 (2)    | 0.012 (3)    | 0.005 (3)   |
| C30B | 0.024 (2)   | 0.034 (3)   | 0.031 (2)   | -0.0051 (19) | -0.0015 (19) | 0.012 (2)   |
| C31B | 0.036 (3)   | 0.037 (3)   | 0.027 (2)   | -0.002 (2)   | 0.008 (2)    | 0.002 (2)   |
| C32B | 0.032 (3)   | 0.036 (3)   | 0.029 (2)   | 0.002 (2)    | 0.012 (2)    | 0.005 (2)   |
| C33B | 0.021 (2)   | 0.025 (2)   | 0.0202 (19) | 0.0062 (16)  | 0.0057 (16)  | 0.0090 (16) |
| C34B | 0.027 (2)   | 0.025 (2)   | 0.028 (2)   | 0.0061 (18)  | 0.0092 (18)  | 0.0113 (18) |
| C35B | 0.034 (3)   | 0.039 (3)   | 0.024 (2)   | 0.007 (2)    | 0.012 (2)    | 0.016 (2)   |
| C36B | 0.028 (2)   | 0.033 (2)   | 0.021 (2)   | 0.0016 (19)  | 0.0107 (18)  | 0.0058 (18) |
| C37B | 0.028 (2)   | 0.040 (3)   | 0.031 (2)   | 0.016 (2)    | 0.011 (2)    | 0.012 (2)   |
| C38B | 0.031 (3)   | 0.046 (3)   | 0.027 (2)   | 0.019 (2)    | 0.012 (2)    | 0.018 (2)   |
| C39B | 0.019 (2)   | 0.030 (2)   | 0.021 (2)   | 0.0092 (17)  | 0.0039 (16)  | 0.0125 (17) |
| C40B | 0.038 (3)   | 0.034 (2)   | 0.023 (2)   | 0.013 (2)    | 0.006 (2)    | 0.0096 (19) |
| C41B | 0.070 (4)   | 0.027 (2)   | 0.037 (3)   | 0.022 (3)    | 0.016 (3)    | 0.014 (2)   |
| C42B | 0.054 (4)   | 0.050 (3)   | 0.042 (3)   | 0.026 (3)    | 0.013 (3)    | 0.034 (3)   |
| C43B | 0.036 (3)   | 0.045 (3)   | 0.027 (2)   | 0.009 (2)    | 0.004 (2)    | 0.020 (2)   |
| C44B | 0.025 (2)   | 0.030 (2)   | 0.023 (2)   | 0.0042 (18)  | 0.0038 (17)  | 0.0078 (18) |
| C45B | 0.021 (2)   | 0.027 (2)   | 0.033 (2)   | 0.0066 (17)  | 0.0129 (18)  | 0.0172 (19) |
| C46B | 0.032 (2)   | 0.031 (2)   | 0.020 (2)   | 0.0111 (19)  | 0.0082 (18)  | 0.0121 (18) |

|      |           |           |           |             |             |             |
|------|-----------|-----------|-----------|-------------|-------------|-------------|
| C47B | 0.033 (2) | 0.027 (2) | 0.023 (2) | 0.0099 (19) | 0.0088 (18) | 0.0110 (18) |
| C48B | 0.027 (2) | 0.028 (2) | 0.025 (2) | 0.0034 (18) | 0.0106 (18) | 0.0097 (18) |
| C49B | 0.027 (2) | 0.031 (3) | 0.046 (3) | 0.011 (2)   | 0.011 (2)   | 0.012 (2)   |
| C50B | 0.024 (2) | 0.042 (3) | 0.046 (3) | 0.014 (2)   | 0.015 (2)   | 0.029 (2)   |
| C51B | 0.021 (2) | 0.034 (2) | 0.026 (2) | 0.0069 (18) | 0.0094 (17) | 0.0168 (19) |
| C52B | 0.036 (3) | 0.028 (2) | 0.022 (2) | 0.0137 (19) | 0.0150 (19) | 0.0130 (18) |
| C53B | 0.025 (2) | 0.026 (2) | 0.027 (2) | 0.0069 (18) | 0.0097 (18) | 0.0125 (18) |

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

|           |             |           |             |
|-----------|-------------|-----------|-------------|
| Sb1A—C33A | 2.133 (4)   | Sb1B—C39B | 2.125 (4)   |
| Sb1A—C39A | 2.133 (5)   | Sb1B—C27B | 2.132 (4)   |
| Sb1A—C27A | 2.142 (5)   | Sb1B—C33B | 2.132 (4)   |
| Sb1A—Ru3A | 2.5846 (4)  | Sb1B—Ru3B | 2.5919 (4)  |
| Ru1A—C46A | 1.879 (4)   | Ru1B—C46B | 1.884 (4)   |
| Ru1A—C45A | 1.919 (5)   | Ru1B—C45B | 1.923 (5)   |
| Ru1A—C47A | 1.939 (5)   | Ru1B—C47B | 1.953 (5)   |
| Ru1A—P1A  | 2.3350 (12) | Ru1B—P1B  | 2.3073 (12) |
| Ru1A—Ru2A | 2.8651 (5)  | Ru1B—Ru3B | 2.8500 (5)  |
| Ru1A—Ru3A | 2.8676 (5)  | Ru1B—Ru2B | 2.8655 (5)  |
| Ru2A—C49A | 1.898 (5)   | Ru2B—C49B | 1.898 (5)   |
| Ru2A—C50A | 1.919 (5)   | Ru2B—C48B | 1.932 (5)   |
| Ru2A—C48A | 1.942 (5)   | Ru2B—C50B | 1.950 (5)   |
| Ru2A—P2A  | 2.3202 (12) | Ru2B—P2B  | 2.3224 (12) |
| Ru2A—Ru3A | 2.8124 (5)  | Ru2B—Ru3B | 2.8292 (5)  |
| Ru3A—C52A | 1.880 (5)   | Ru3B—C52B | 1.879 (5)   |
| Ru3A—C53A | 1.929 (5)   | Ru3B—C51B | 1.930 (5)   |
| Ru3A—C51A | 1.936 (5)   | Ru3B—C53B | 1.935 (5)   |
| P1A—C7A   | 1.826 (4)   | P1B—C7B   | 1.834 (5)   |
| P1A—C1A   | 1.835 (5)   | P1B—C1B   | 1.836 (5)   |
| P1A—C13A  | 1.838 (4)   | P1B—C13B  | 1.853 (5)   |
| P2A—C21A  | 1.820 (5)   | P2B—C15B  | 1.826 (5)   |
| P2A—C15A  | 1.836 (4)   | P2B—C21B  | 1.834 (4)   |
| P2A—C14A  | 1.839 (5)   | P2B—C14B  | 1.850 (5)   |
| O1A—C47A  | 1.146 (6)   | O1B—C45B  | 1.151 (6)   |
| O2A—C46A  | 1.145 (5)   | O2B—C46B  | 1.146 (6)   |
| O3A—C45A  | 1.152 (6)   | O3B—C47B  | 1.143 (6)   |
| O4A—C48A  | 1.131 (6)   | O4B—C48B  | 1.145 (6)   |
| O5A—C49A  | 1.137 (6)   | O5B—C49B  | 1.137 (6)   |
| O6A—C50A  | 1.153 (5)   | O6B—C50B  | 1.125 (6)   |
| O7A—C51A  | 1.142 (6)   | O7B—C51B  | 1.149 (5)   |
| O8A—C52A  | 1.148 (6)   | O8B—C52B  | 1.143 (6)   |
| O9A—C53A  | 1.142 (6)   | O9B—C53B  | 1.149 (6)   |
| C1A—C6A   | 1.389 (7)   | C1B—C2B   | 1.374 (7)   |
| C1A—C2A   | 1.393 (6)   | C1B—C6B   | 1.401 (7)   |
| C2A—C3A   | 1.399 (7)   | C2B—C3B   | 1.385 (7)   |
| C2A—H2AA  | 0.9300      | C2B—H2BA  | 0.9300      |
| C3A—C4A   | 1.376 (8)   | C3B—C4B   | 1.363 (9)   |

|           |           |           |            |
|-----------|-----------|-----------|------------|
| C3A—H3AA  | 0.9300    | C3B—H3BA  | 0.9300     |
| C4A—C5A   | 1.388 (8) | C4B—C5B   | 1.386 (9)  |
| C4A—H4AA  | 0.9300    | C4B—H4BA  | 0.9300     |
| C5A—C6A   | 1.391 (7) | C5B—C6B   | 1.380 (8)  |
| C5A—H5AA  | 0.9300    | C5B—H5BA  | 0.9300     |
| C6A—H6AA  | 0.9300    | C6B—H6BA  | 0.9300     |
| C7A—C8A   | 1.386 (6) | C7B—C12B  | 1.390 (7)  |
| C7A—C12A  | 1.406 (6) | C7B—C8B   | 1.409 (8)  |
| C8A—C9A   | 1.383 (7) | C8B—C9B   | 1.386 (8)  |
| C8A—H8AA  | 0.9300    | C8B—H8BA  | 0.9300     |
| C9A—C10A  | 1.370 (8) | C9B—C10B  | 1.379 (9)  |
| C9A—H9AA  | 0.9300    | C9B—H9BA  | 0.9300     |
| C10A—C11A | 1.381 (8) | C10B—C11B | 1.377 (10) |
| C10A—H10A | 0.9300    | C10B—H10B | 0.9300     |
| C11A—C12A | 1.381 (7) | C11B—C12B | 1.405 (9)  |
| C11A—H11A | 0.9300    | C11B—H11B | 0.9300     |
| C12A—H12A | 0.9300    | C12B—H12B | 0.9300     |
| C13A—C14A | 1.542 (6) | C13B—C14B | 1.532 (8)  |
| C13A—H13A | 0.9700    | C13B—H13C | 0.9700     |
| C13A—H13B | 0.9700    | C13B—H13D | 0.9700     |
| C14A—H14A | 0.9700    | C14B—H14C | 0.9700     |
| C14A—H14B | 0.9700    | C14B—H14D | 0.9700     |
| C15A—C20A | 1.390 (7) | C15B—C20B | 1.390 (7)  |
| C15A—C16A | 1.390 (7) | C15B—C16B | 1.391 (8)  |
| C16A—C17A | 1.390 (6) | C16B—C17B | 1.390 (8)  |
| C16A—H16A | 0.9300    | C16B—H16B | 0.9300     |
| C17A—C18A | 1.357 (9) | C17B—C18B | 1.383 (9)  |
| C17A—H17A | 0.9300    | C17B—H17B | 0.9300     |
| C18A—C19A | 1.387 (9) | C18B—C19B | 1.378 (10) |
| C18A—H18A | 0.9300    | C18B—H18B | 0.9300     |
| C19A—C20A | 1.396 (7) | C19B—C20B | 1.385 (8)  |
| C19A—H19A | 0.9300    | C19B—H19B | 0.9300     |
| C20A—H20A | 0.9300    | C20B—H20B | 0.9300     |
| C21A—C26A | 1.381 (7) | C21B—C22B | 1.376 (7)  |
| C21A—C22A | 1.390 (7) | C21B—C26B | 1.395 (7)  |
| C22A—C23A | 1.373 (8) | C22B—C23B | 1.398 (8)  |
| C22A—H22A | 0.9300    | C22B—H22B | 0.9300     |
| C23A—C24A | 1.355 (9) | C23B—C24B | 1.357 (10) |
| C23A—H23A | 0.9300    | C23B—H23B | 0.9300     |
| C24A—C25A | 1.376 (9) | C24B—C25B | 1.398 (11) |
| C24A—H24A | 0.9300    | C24B—H24B | 0.9300     |
| C25A—C26A | 1.370 (8) | C25B—C26B | 1.386 (8)  |
| C25A—H25A | 0.9300    | C25B—H25B | 0.9300     |
| C26A—H26A | 0.9300    | C26B—H26B | 0.9300     |
| C27A—C28A | 1.376 (7) | C27B—C28B | 1.376 (7)  |
| C27A—C32A | 1.388 (7) | C27B—C32B | 1.389 (6)  |
| C28A—C29A | 1.393 (7) | C28B—C29B | 1.379 (8)  |
| C28A—H28A | 0.9300    | C28B—H28B | 0.9300     |

|                |             |                |             |
|----------------|-------------|----------------|-------------|
| C29A—C30A      | 1.376 (8)   | C29B—C30B      | 1.364 (8)   |
| C29A—H29A      | 0.9300      | C29B—H29B      | 0.9300      |
| C30A—C31A      | 1.389 (8)   | C30B—C31B      | 1.382 (7)   |
| C30A—H30A      | 0.9300      | C30B—H30B      | 0.9300      |
| C31A—C32A      | 1.389 (8)   | C31B—C32B      | 1.377 (7)   |
| C31A—H31A      | 0.9300      | C31B—H31B      | 0.9300      |
| C32A—H32A      | 0.9300      | C32B—H32B      | 0.9300      |
| C33A—C38A      | 1.357 (7)   | C33B—C34B      | 1.374 (6)   |
| C33A—C34A      | 1.408 (7)   | C33B—C38B      | 1.403 (6)   |
| C34A—C35A      | 1.387 (7)   | C34B—C35B      | 1.395 (6)   |
| C34A—H34A      | 0.9300      | C34B—H34B      | 0.9300      |
| C35A—C36A      | 1.390 (8)   | C35B—C36B      | 1.391 (7)   |
| C35A—H35A      | 0.9300      | C35B—H35B      | 0.9300      |
| C36A—C37A      | 1.350 (8)   | C36B—C37B      | 1.377 (7)   |
| C36A—H36A      | 0.9300      | C36B—H36B      | 0.9300      |
| C37A—C38A      | 1.396 (8)   | C37B—C38B      | 1.398 (6)   |
| C37A—H37A      | 0.9300      | C37B—H37B      | 0.9300      |
| C38A—H38A      | 0.9300      | C38B—H38B      | 0.9300      |
| C39A—C40A      | 1.376 (7)   | C39B—C40B      | 1.385 (7)   |
| C39A—C44A      | 1.390 (6)   | C39B—C44B      | 1.398 (6)   |
| C40A—C41A      | 1.387 (7)   | C40B—C41B      | 1.396 (7)   |
| C40A—H40A      | 0.9300      | C40B—H40B      | 0.9300      |
| C41A—C42A      | 1.384 (7)   | C41B—C42B      | 1.378 (8)   |
| C41A—H41A      | 0.9300      | C41B—H41B      | 0.9300      |
| C42A—C43A      | 1.379 (8)   | C42B—C43B      | 1.379 (8)   |
| C42A—H42A      | 0.9300      | C42B—H42B      | 0.9300      |
| C43A—C44A      | 1.381 (8)   | C43B—C44B      | 1.392 (7)   |
| C43A—H43A      | 0.9300      | C43B—H43B      | 0.9300      |
| C44A—H44A      | 0.9300      | C44B—H44B      | 0.9300      |
| <br>           |             |                |             |
| C33A—Sb1A—C39A | 98.08 (19)  | C39B—Sb1B—C27B | 98.51 (17)  |
| C33A—Sb1A—C27A | 105.68 (17) | C39B—Sb1B—C33B | 102.13 (16) |
| C39A—Sb1A—C27A | 97.20 (18)  | C27B—Sb1B—C33B | 97.89 (17)  |
| C33A—Sb1A—Ru3A | 120.39 (13) | C39B—Sb1B—Ru3B | 115.01 (12) |
| C39A—Sb1A—Ru3A | 115.03 (12) | C27B—Sb1B—Ru3B | 114.69 (12) |
| C27A—Sb1A—Ru3A | 116.63 (12) | C33B—Sb1B—Ru3B | 124.42 (12) |
| C46A—Ru1A—C45A | 92.10 (19)  | C46B—Ru1B—C45B | 93.28 (19)  |
| C46A—Ru1A—C47A | 92.31 (19)  | C46B—Ru1B—C47B | 93.58 (19)  |
| C45A—Ru1A—C47A | 174.59 (19) | C45B—Ru1B—C47B | 170.68 (19) |
| C46A—Ru1A—P1A  | 101.91 (14) | C46B—Ru1B—P1B  | 99.49 (15)  |
| C45A—Ru1A—P1A  | 88.87 (15)  | C45B—Ru1B—P1B  | 93.42 (14)  |
| C47A—Ru1A—P1A  | 93.28 (14)  | C47B—Ru1B—P1B  | 91.67 (15)  |
| C46A—Ru1A—Ru2A | 154.44 (13) | C46B—Ru1B—Ru3B | 102.02 (15) |
| C45A—Ru1A—Ru2A | 78.44 (14)  | C45B—Ru1B—Ru3B | 94.56 (14)  |
| C47A—Ru1A—Ru2A | 96.26 (13)  | C47B—Ru1B—Ru3B | 77.83 (14)  |
| P1A—Ru1A—Ru2A  | 101.59 (3)  | P1B—Ru1B—Ru3B  | 156.56 (3)  |
| C46A—Ru1A—Ru3A | 98.87 (14)  | C46B—Ru1B—Ru2B | 157.28 (15) |
| C45A—Ru1A—Ru3A | 93.91 (15)  | C45B—Ru1B—Ru2B | 76.72 (13)  |

|                |              |                |              |
|----------------|--------------|----------------|--------------|
| C47A—Ru1A—Ru3A | 82.31 (14)   | C47B—Ru1B—Ru2B | 94.62 (13)   |
| P1A—Ru1A—Ru3A  | 158.92 (3)   | P1B—Ru1B—Ru2B  | 101.41 (3)   |
| Ru2A—Ru1A—Ru3A | 58.759 (12)  | Ru3B—Ru1B—Ru2B | 59.339 (12)  |
| C49A—Ru2A—C50A | 94.3 (2)     | C49B—Ru2B—C48B | 93.7 (2)     |
| C49A—Ru2A—C48A | 92.3 (2)     | C49B—Ru2B—C50B | 91.1 (2)     |
| C50A—Ru2A—C48A | 172.99 (19)  | C48B—Ru2B—C50B | 173.32 (19)  |
| C49A—Ru2A—P2A  | 101.77 (15)  | C49B—Ru2B—P2B  | 100.33 (16)  |
| C50A—Ru2A—P2A  | 91.35 (13)   | C48B—Ru2B—P2B  | 92.98 (14)   |
| C48A—Ru2A—P2A  | 89.58 (15)   | C50B—Ru2B—P2B  | 90.74 (15)   |
| C49A—Ru2A—Ru3A | 96.33 (15)   | C49B—Ru2B—Ru3B | 100.09 (16)  |
| C50A—Ru2A—Ru3A | 95.05 (13)   | C48B—Ru2B—Ru3B | 94.22 (14)   |
| C48A—Ru2A—Ru3A | 81.88 (15)   | C50B—Ru2B—Ru3B | 80.34 (14)   |
| P2A—Ru2A—Ru3A  | 160.28 (3)   | P2B—Ru2B—Ru3B  | 157.84 (3)   |
| C49A—Ru2A—Ru1A | 154.29 (15)  | C49B—Ru2B—Ru1B | 156.86 (16)  |
| C50A—Ru2A—Ru1A | 77.77 (13)   | C48B—Ru2B—Ru1B | 77.34 (14)   |
| C48A—Ru2A—Ru1A | 95.24 (14)   | C50B—Ru2B—Ru1B | 96.49 (15)   |
| P2A—Ru2A—Ru1A  | 102.82 (3)   | P2B—Ru2B—Ru1B  | 101.39 (3)   |
| Ru3A—Ru2A—Ru1A | 60.664 (11)  | Ru3B—Ru2B—Ru1B | 60.057 (12)  |
| C52A—Ru3A—C53A | 92.0 (2)     | C52B—Ru3B—C51B | 93.8 (2)     |
| C52A—Ru3A—C51A | 91.2 (2)     | C52B—Ru3B—C53B | 90.71 (19)   |
| C53A—Ru3A—C51A | 176.3 (2)    | C51B—Ru3B—C53B | 174.62 (19)  |
| C52A—Ru3A—Sb1A | 103.07 (14)  | C52B—Ru3B—Sb1B | 101.26 (15)  |
| C53A—Ru3A—Sb1A | 90.78 (13)   | C51B—Ru3B—Sb1B | 90.55 (13)   |
| C51A—Ru3A—Sb1A | 90.36 (14)   | C53B—Ru3B—Sb1B | 91.52 (13)   |
| C52A—Ru3A—Ru2A | 95.94 (14)   | C52B—Ru3B—Ru2B | 98.10 (14)   |
| C53A—Ru3A—Ru2A | 96.45 (13)   | C51B—Ru3B—Ru2B | 94.91 (13)   |
| C51A—Ru3A—Ru2A | 81.31 (13)   | C53B—Ru3B—Ru2B | 81.48 (14)   |
| Sb1A—Ru3A—Ru2A | 159.415 (17) | Sb1B—Ru3B—Ru2B | 159.491 (17) |
| C52A—Ru3A—Ru1A | 154.47 (14)  | C52B—Ru3B—Ru1B | 156.09 (15)  |
| C53A—Ru3A—Ru1A | 81.75 (14)   | C51B—Ru3B—Ru1B | 78.56 (14)   |
| C51A—Ru3A—Ru1A | 94.55 (14)   | C53B—Ru3B—Ru1B | 96.16 (14)   |
| Sb1A—Ru3A—Ru1A | 101.740 (14) | Sb1B—Ru3B—Ru1B | 101.418 (15) |
| Ru2A—Ru3A—Ru1A | 60.576 (12)  | Ru2B—Ru3B—Ru1B | 60.604 (12)  |
| C7A—P1A—C1A    | 103.1 (2)    | C7B—P1B—C1B    | 102.2 (2)    |
| C7A—P1A—C13A   | 103.4 (2)    | C7B—P1B—C13B   | 103.6 (2)    |
| C1A—P1A—C13A   | 100.7 (2)    | C1B—P1B—C13B   | 100.9 (2)    |
| C7A—P1A—Ru1A   | 115.41 (15)  | C7B—P1B—Ru1B   | 115.21 (18)  |
| C1A—P1A—Ru1A   | 116.31 (15)  | C1B—P1B—Ru1B   | 116.72 (16)  |
| C13A—P1A—Ru1A  | 115.84 (15)  | C13B—P1B—Ru1B  | 116.02 (16)  |
| C21A—P2A—C15A  | 105.1 (2)    | C15B—P2B—C21B  | 102.8 (2)    |
| C21A—P2A—C14A  | 102.0 (2)    | C15B—P2B—C14B  | 103.2 (2)    |
| C15A—P2A—C14A  | 102.9 (2)    | C21B—P2B—C14B  | 100.9 (2)    |
| C21A—P2A—Ru2A  | 114.15 (16)  | C15B—P2B—Ru2B  | 114.64 (16)  |
| C15A—P2A—Ru2A  | 115.98 (16)  | C21B—P2B—Ru2B  | 118.02 (17)  |
| C14A—P2A—Ru2A  | 115.03 (15)  | C14B—P2B—Ru2B  | 115.19 (17)  |
| C6A—C1A—C2A    | 118.7 (4)    | C2B—C1B—C6B    | 117.6 (5)    |
| C6A—C1A—P1A    | 122.8 (4)    | C2B—C1B—P1B    | 123.1 (4)    |
| C2A—C1A—P1A    | 118.5 (4)    | C6B—C1B—P1B    | 119.2 (4)    |

|                |           |                |           |
|----------------|-----------|----------------|-----------|
| C1A—C2A—C3A    | 120.6 (5) | C1B—C2B—C3B    | 122.0 (5) |
| C1A—C2A—H2AA   | 119.7     | C1B—C2B—H2BA   | 119.0     |
| C3A—C2A—H2AA   | 119.7     | C3B—C2B—H2BA   | 119.0     |
| C4A—C3A—C2A    | 119.8 (5) | C4B—C3B—C2B    | 119.6 (5) |
| C4A—C3A—H3AA   | 120.1     | C4B—C3B—H3BA   | 120.2     |
| C2A—C3A—H3AA   | 120.1     | C2B—C3B—H3BA   | 120.2     |
| C3A—C4A—C5A    | 120.4 (5) | C3B—C4B—C5B    | 120.0 (5) |
| C3A—C4A—H4AA   | 119.8     | C3B—C4B—H4BA   | 120.0     |
| C5A—C4A—H4AA   | 119.8     | C5B—C4B—H4BA   | 120.0     |
| C4A—C5A—C6A    | 119.6 (5) | C6B—C5B—C4B    | 120.1 (6) |
| C4A—C5A—H5AA   | 120.2     | C6B—C5B—H5BA   | 120.0     |
| C6A—C5A—H5AA   | 120.2     | C4B—C5B—H5BA   | 120.0     |
| C1A—C6A—C5A    | 121.0 (5) | C5B—C6B—C1B    | 120.6 (5) |
| C1A—C6A—H6AA   | 119.5     | C5B—C6B—H6BA   | 119.7     |
| C5A—C6A—H6AA   | 119.5     | C1B—C6B—H6BA   | 119.7     |
| C8A—C7A—C12A   | 117.1 (4) | C12B—C7B—C8B   | 118.3 (5) |
| C8A—C7A—P1A    | 119.9 (4) | C12B—C7B—P1B   | 123.4 (5) |
| C12A—C7A—P1A   | 123.0 (3) | C8B—C7B—P1B    | 118.3 (4) |
| C9A—C8A—C7A    | 122.0 (5) | C9B—C8B—C7B    | 121.2 (5) |
| C9A—C8A—H8AA   | 119.0     | C9B—C8B—H8BA   | 119.4     |
| C7A—C8A—H8AA   | 119.0     | C7B—C8B—H8BA   | 119.4     |
| C10A—C9A—C8A   | 120.1 (5) | C10B—C9B—C8B   | 119.7 (6) |
| C10A—C9A—H9AA  | 119.9     | C10B—C9B—H9BA  | 120.1     |
| C8A—C9A—H9AA   | 119.9     | C8B—C9B—H9BA   | 120.1     |
| C9A—C10A—C11A  | 119.3 (5) | C11B—C10B—C9B  | 120.3 (6) |
| C9A—C10A—H10A  | 120.3     | C11B—C10B—H10B | 119.9     |
| C11A—C10A—H10A | 120.3     | C9B—C10B—H10B  | 119.9     |
| C12A—C11A—C10A | 120.8 (5) | C10B—C11B—C12B | 120.6 (6) |
| C12A—C11A—H11A | 119.6     | C10B—C11B—H11B | 119.7     |
| C10A—C11A—H11A | 119.6     | C12B—C11B—H11B | 119.7     |
| C11A—C12A—C7A  | 120.6 (5) | C7B—C12B—C11B  | 119.9 (6) |
| C11A—C12A—H12A | 119.7     | C7B—C12B—H12B  | 120.0     |
| C7A—C12A—H12A  | 119.7     | C11B—C12B—H12B | 120.0     |
| C14A—C13A—P1A  | 113.1 (3) | C14B—C13B—P1B  | 113.1 (3) |
| C14A—C13A—H13A | 109.0     | C14B—C13B—H13C | 109.0     |
| P1A—C13A—H13A  | 109.0     | P1B—C13B—H13C  | 109.0     |
| C14A—C13A—H13B | 109.0     | C14B—C13B—H13D | 109.0     |
| P1A—C13A—H13B  | 109.0     | P1B—C13B—H13D  | 109.0     |
| H13A—C13A—H13B | 107.8     | H13C—C13B—H13D | 107.8     |
| C13A—C14A—P2A  | 112.5 (3) | C13B—C14B—P2B  | 112.8 (4) |
| C13A—C14A—H14A | 109.1     | C13B—C14B—H14C | 109.0     |
| P2A—C14A—H14A  | 109.1     | P2B—C14B—H14C  | 109.0     |
| C13A—C14A—H14B | 109.1     | C13B—C14B—H14D | 109.0     |
| P2A—C14A—H14B  | 109.1     | P2B—C14B—H14D  | 109.0     |
| H14A—C14A—H14B | 107.8     | H14C—C14B—H14D | 107.8     |
| C20A—C15A—C16A | 118.0 (4) | C20B—C15B—C16B | 118.1 (5) |
| C20A—C15A—P2A  | 121.3 (4) | C20B—C15B—P2B  | 122.2 (4) |
| C16A—C15A—P2A  | 120.7 (4) | C16B—C15B—P2B  | 119.5 (4) |

|                |           |                |           |
|----------------|-----------|----------------|-----------|
| C17A—C16A—C15A | 121.3 (5) | C17B—C16B—C15B | 121.4 (5) |
| C17A—C16A—H16A | 119.4     | C17B—C16B—H16B | 119.3     |
| C15A—C16A—H16A | 119.4     | C15B—C16B—H16B | 119.3     |
| C18A—C17A—C16A | 120.2 (6) | C18B—C17B—C16B | 119.5 (6) |
| C18A—C17A—H17A | 119.9     | C18B—C17B—H17B | 120.3     |
| C16A—C17A—H17A | 119.9     | C16B—C17B—H17B | 120.3     |
| C17A—C18A—C19A | 120.1 (5) | C19B—C18B—C17B | 119.9 (6) |
| C17A—C18A—H18A | 120.0     | C19B—C18B—H18B | 120.1     |
| C19A—C18A—H18A | 120.0     | C17B—C18B—H18B | 120.1     |
| C18A—C19A—C20A | 119.9 (5) | C18B—C19B—C20B | 120.4 (6) |
| C18A—C19A—H19A | 120.0     | C18B—C19B—H19B | 119.8     |
| C20A—C19A—H19A | 120.0     | C20B—C19B—H19B | 119.8     |
| C15A—C20A—C19A | 120.5 (5) | C19B—C20B—C15B | 120.8 (6) |
| C15A—C20A—H20A | 119.7     | C19B—C20B—H20B | 119.6     |
| C19A—C20A—H20A | 119.7     | C15B—C20B—H20B | 119.6     |
| C26A—C21A—C22A | 116.7 (5) | C22B—C21B—C26B | 119.1 (5) |
| C26A—C21A—P2A  | 121.2 (4) | C22B—C21B—P2B  | 121.8 (4) |
| C22A—C21A—P2A  | 121.9 (4) | C26B—C21B—P2B  | 119.1 (4) |
| C23A—C22A—C21A | 121.1 (6) | C21B—C22B—C23B | 120.3 (6) |
| C23A—C22A—H22A | 119.4     | C21B—C22B—H22B | 119.9     |
| C21A—C22A—H22A | 119.4     | C23B—C22B—H22B | 119.9     |
| C24A—C23A—C22A | 121.5 (6) | C24B—C23B—C22B | 120.7 (6) |
| C24A—C23A—H23A | 119.3     | C24B—C23B—H23B | 119.6     |
| C22A—C23A—H23A | 119.3     | C22B—C23B—H23B | 119.6     |
| C23A—C24A—C25A | 118.2 (6) | C23B—C24B—C25B | 119.8 (5) |
| C23A—C24A—H24A | 120.9     | C23B—C24B—H24B | 120.1     |
| C25A—C24A—H24A | 120.9     | C25B—C24B—H24B | 120.1     |
| C26A—C25A—C24A | 120.9 (6) | C26B—C25B—C24B | 119.7 (6) |
| C26A—C25A—H25A | 119.5     | C26B—C25B—H25B | 120.1     |
| C24A—C25A—H25A | 119.5     | C24B—C25B—H25B | 120.1     |
| C25A—C26A—C21A | 121.5 (6) | C25B—C26B—C21B | 120.4 (6) |
| C25A—C26A—H26A | 119.2     | C25B—C26B—H26B | 119.8     |
| C21A—C26A—H26A | 119.2     | C21B—C26B—H26B | 119.8     |
| C28A—C27A—C32A | 118.7 (5) | C28B—C27B—C32B | 118.5 (5) |
| C28A—C27A—Sb1A | 115.7 (4) | C28B—C27B—Sb1B | 121.6 (4) |
| C32A—C27A—Sb1A | 125.2 (4) | C32B—C27B—Sb1B | 119.9 (3) |
| C27A—C28A—C29A | 121.8 (5) | C27B—C28B—C29B | 120.4 (5) |
| C27A—C28A—H28A | 119.1     | C27B—C28B—H28B | 119.8     |
| C29A—C28A—H28A | 119.1     | C29B—C28B—H28B | 119.8     |
| C30A—C29A—C28A | 119.3 (5) | C30B—C29B—C28B | 121.1 (5) |
| C30A—C29A—H29A | 120.3     | C30B—C29B—H29B | 119.5     |
| C28A—C29A—H29A | 120.3     | C28B—C29B—H29B | 119.5     |
| C29A—C30A—C31A | 119.5 (5) | C29B—C30B—C31B | 119.1 (5) |
| C29A—C30A—H30A | 120.3     | C29B—C30B—H30B | 120.5     |
| C31A—C30A—H30A | 120.3     | C31B—C30B—H30B | 120.5     |
| C32A—C31A—C30A | 120.8 (5) | C32B—C31B—C30B | 120.2 (5) |
| C32A—C31A—H31A | 119.6     | C32B—C31B—H31B | 119.9     |
| C30A—C31A—H31A | 119.6     | C30B—C31B—H31B | 119.9     |

|                |           |                |           |
|----------------|-----------|----------------|-----------|
| C27A—C32A—C31A | 119.9 (5) | C31B—C32B—C27B | 120.6 (5) |
| C27A—C32A—H32A | 120.0     | C31B—C32B—H32B | 119.7     |
| C31A—C32A—H32A | 120.0     | C27B—C32B—H32B | 119.7     |
| C38A—C33A—C34A | 118.1 (5) | C34B—C33B—C38B | 119.4 (4) |
| C38A—C33A—Sb1A | 118.1 (4) | C34B—C33B—Sb1B | 119.4 (3) |
| C34A—C33A—Sb1A | 123.4 (4) | C38B—C33B—Sb1B | 120.5 (3) |
| C35A—C34A—C33A | 120.3 (5) | C33B—C34B—C35B | 121.0 (4) |
| C35A—C34A—H34A | 119.8     | C33B—C34B—H34B | 119.5     |
| C33A—C34A—H34A | 119.8     | C35B—C34B—H34B | 119.5     |
| C34A—C35A—C36A | 119.9 (5) | C36B—C35B—C34B | 119.4 (5) |
| C34A—C35A—H35A | 120.0     | C36B—C35B—H35B | 120.3     |
| C36A—C35A—H35A | 120.0     | C34B—C35B—H35B | 120.3     |
| C37A—C36A—C35A | 119.4 (5) | C37B—C36B—C35B | 120.1 (4) |
| C37A—C36A—H36A | 120.3     | C37B—C36B—H36B | 120.0     |
| C35A—C36A—H36A | 120.3     | C35B—C36B—H36B | 120.0     |
| C36A—C37A—C38A | 120.8 (5) | C36B—C37B—C38B | 120.5 (5) |
| C36A—C37A—H37A | 119.6     | C36B—C37B—H37B | 119.8     |
| C38A—C37A—H37A | 119.6     | C38B—C37B—H37B | 119.8     |
| C33A—C38A—C37A | 121.2 (5) | C37B—C38B—C33B | 119.5 (5) |
| C33A—C38A—H38A | 119.4     | C37B—C38B—H38B | 120.2     |
| C37A—C38A—H38A | 119.4     | C33B—C38B—H38B | 120.2     |
| C40A—C39A—C44A | 120.0 (5) | C40B—C39B—C44B | 119.0 (4) |
| C40A—C39A—Sb1A | 120.3 (3) | C40B—C39B—Sb1B | 123.0 (3) |
| C44A—C39A—Sb1A | 119.7 (4) | C44B—C39B—Sb1B | 117.6 (3) |
| C39A—C40A—C41A | 120.2 (5) | C39B—C40B—C41B | 120.5 (5) |
| C39A—C40A—H40A | 119.9     | C39B—C40B—H40B | 119.7     |
| C41A—C40A—H40A | 119.9     | C41B—C40B—H40B | 119.7     |
| C42A—C41A—C40A | 119.8 (5) | C42B—C41B—C40B | 119.9 (5) |
| C42A—C41A—H41A | 120.1     | C42B—C41B—H41B | 120.1     |
| C40A—C41A—H41A | 120.1     | C40B—C41B—H41B | 120.1     |
| C43A—C42A—C41A | 120.1 (5) | C41B—C42B—C43B | 120.4 (5) |
| C43A—C42A—H42A | 120.0     | C41B—C42B—H42B | 119.8     |
| C41A—C42A—H42A | 120.0     | C43B—C42B—H42B | 119.8     |
| C42A—C43A—C44A | 120.2 (5) | C42B—C43B—C44B | 120.0 (5) |
| C42A—C43A—H43A | 119.9     | C42B—C43B—H43B | 120.0     |
| C44A—C43A—H43A | 119.9     | C44B—C43B—H43B | 120.0     |
| C43A—C44A—C39A | 119.8 (5) | C43B—C44B—C39B | 120.2 (5) |
| C43A—C44A—H44A | 120.1     | C43B—C44B—H44B | 119.9     |
| C39A—C44A—H44A | 120.1     | C39B—C44B—H44B | 119.9     |
| O3A—C45A—Ru1A  | 172.0 (4) | O1B—C45B—Ru1B  | 172.1 (4) |
| O2A—C46A—Ru1A  | 175.3 (4) | O2B—C46B—Ru1B  | 175.8 (4) |
| O1A—C47A—Ru1A  | 174.6 (4) | O3B—C47B—Ru1B  | 173.8 (4) |
| O4A—C48A—Ru2A  | 174.6 (4) | O4B—C48B—Ru2B  | 173.6 (4) |
| O5A—C49A—Ru2A  | 177.1 (5) | O5B—C49B—Ru2B  | 177.5 (6) |
| O6A—C50A—Ru2A  | 172.8 (4) | O6B—C50B—Ru2B  | 175.6 (5) |
| O7A—C51A—Ru3A  | 174.5 (4) | O7B—C51B—Ru3B  | 175.8 (4) |
| O8A—C52A—Ru3A  | 176.7 (4) | O8B—C52B—Ru3B  | 178.0 (4) |
| O9A—C53A—Ru3A  | 174.8 (4) | O9B—C53B—Ru3B  | 174.4 (4) |

|                     |              |                     |              |
|---------------------|--------------|---------------------|--------------|
| C46A—Ru1A—Ru2A—C49A | 60.7 (5)     | C46B—Ru1B—Ru2B—C49B | -71.4 (6)    |
| C45A—Ru1A—Ru2A—C49A | 130.7 (4)    | C45B—Ru1B—Ru2B—C49B | -137.1 (5)   |
| C47A—Ru1A—Ru2A—C49A | -48.2 (4)    | C47B—Ru1B—Ru2B—C49B | 39.4 (5)     |
| P1A—Ru1A—Ru2A—C49A  | -142.9 (4)   | P1B—Ru1B—Ru2B—C49B  | 132.0 (5)    |
| Ru3A—Ru1A—Ru2A—C49A | 28.9 (4)     | Ru3B—Ru1B—Ru2B—C49B | -33.5 (5)    |
| C46A—Ru1A—Ru2A—C50A | 134.8 (4)    | C46B—Ru1B—Ru2B—C48B | -140.4 (4)   |
| C45A—Ru1A—Ru2A—C50A | -155.1 (2)   | C45B—Ru1B—Ru2B—C48B | 153.9 (2)    |
| C47A—Ru1A—Ru2A—C50A | 25.95 (19)   | C47B—Ru1B—Ru2B—C48B | -29.6 (2)    |
| P1A—Ru1A—Ru2A—C50A  | -68.71 (14)  | P1B—Ru1B—Ru2B—C48B  | 63.06 (15)   |
| Ru3A—Ru1A—Ru2A—C50A | 103.01 (13)  | Ru3B—Ru1B—Ru2B—C48B | -102.50 (15) |
| C46A—Ru1A—Ru2A—C48A | -45.8 (4)    | C46B—Ru1B—Ru2B—C50B | 37.0 (4)     |
| C45A—Ru1A—Ru2A—C48A | 24.2 (2)     | C45B—Ru1B—Ru2B—C50B | -28.7 (2)    |
| C47A—Ru1A—Ru2A—C48A | -154.7 (2)   | C47B—Ru1B—Ru2B—C50B | 147.8 (2)    |
| P1A—Ru1A—Ru2A—C48A  | 110.64 (16)  | P1B—Ru1B—Ru2B—C50B  | -119.54 (16) |
| Ru3A—Ru1A—Ru2A—C48A | -77.63 (16)  | Ru3B—Ru1B—Ru2B—C50B | 74.90 (16)   |
| C46A—Ru1A—Ru2A—P2A  | -136.6 (3)   | C46B—Ru1B—Ru2B—P2B  | 129.1 (4)    |
| C45A—Ru1A—Ru2A—P2A  | -66.54 (15)  | C45B—Ru1B—Ru2B—P2B  | 63.38 (13)   |
| C47A—Ru1A—Ru2A—P2A  | 114.54 (14)  | C47B—Ru1B—Ru2B—P2B  | -120.11 (15) |
| P1A—Ru1A—Ru2A—P2A   | 19.88 (4)    | P1B—Ru1B—Ru2B—P2B   | -27.47 (5)   |
| Ru3A—Ru1A—Ru2A—P2A  | -168.40 (3)  | Ru3B—Ru1B—Ru2B—P2B  | 166.97 (3)   |
| C46A—Ru1A—Ru2A—Ru3A | 31.8 (3)     | C46B—Ru1B—Ru2B—Ru3B | -37.9 (4)    |
| C45A—Ru1A—Ru2A—Ru3A | 101.86 (15)  | C45B—Ru1B—Ru2B—Ru3B | -103.59 (13) |
| C47A—Ru1A—Ru2A—Ru3A | -77.06 (14)  | C47B—Ru1B—Ru2B—Ru3B | 72.91 (14)   |
| P1A—Ru1A—Ru2A—Ru3A  | -171.72 (3)  | P1B—Ru1B—Ru2B—Ru3B  | 165.56 (4)   |
| C33A—Sb1A—Ru3A—C52A | 88.6 (2)     | C39B—Sb1B—Ru3B—C52B | 140.72 (19)  |
| C39A—Sb1A—Ru3A—C52A | -28.4 (2)    | C27B—Sb1B—Ru3B—C52B | 27.51 (19)   |
| C27A—Sb1A—Ru3A—C52A | -141.3 (2)   | C33B—Sb1B—Ru3B—C52B | -92.4 (2)    |
| C33A—Sb1A—Ru3A—C53A | -3.6 (2)     | C39B—Sb1B—Ru3B—C51B | -125.34 (19) |
| C39A—Sb1A—Ru3A—C53A | -120.60 (19) | C27B—Sb1B—Ru3B—C51B | 121.45 (19)  |
| C27A—Sb1A—Ru3A—C53A | 126.5 (2)    | C33B—Sb1B—Ru3B—C51B | 1.6 (2)      |
| C33A—Sb1A—Ru3A—C51A | 179.9 (2)    | C39B—Sb1B—Ru3B—C53B | 49.70 (19)   |
| C39A—Sb1A—Ru3A—C51A | 62.94 (19)   | C27B—Sb1B—Ru3B—C53B | -63.52 (19)  |
| C27A—Sb1A—Ru3A—C51A | -50.0 (2)    | C33B—Sb1B—Ru3B—C53B | 176.6 (2)    |
| C33A—Sb1A—Ru3A—Ru2A | -114.47 (16) | C39B—Sb1B—Ru3B—Ru2B | -19.69 (14)  |
| C39A—Sb1A—Ru3A—Ru2A | 128.56 (14)  | C27B—Sb1B—Ru3B—Ru2B | -132.91 (14) |
| C27A—Sb1A—Ru3A—Ru2A | 15.66 (15)   | C33B—Sb1B—Ru3B—Ru2B | 107.22 (15)  |
| C33A—Sb1A—Ru3A—Ru1A | -85.37 (16)  | C39B—Sb1B—Ru3B—Ru1B | -46.90 (13)  |
| C39A—Sb1A—Ru3A—Ru1A | 157.66 (14)  | C27B—Sb1B—Ru3B—Ru1B | -160.11 (13) |
| C27A—Sb1A—Ru3A—Ru1A | 44.77 (14)   | C33B—Sb1B—Ru3B—Ru1B | 80.02 (15)   |
| C49A—Ru2A—Ru3A—C52A | 22.8 (2)     | C49B—Ru2B—Ru3B—C52B | -24.3 (2)    |
| C50A—Ru2A—Ru3A—C52A | 117.7 (2)    | C48B—Ru2B—Ru3B—C52B | -118.8 (2)   |
| C48A—Ru2A—Ru3A—C52A | -68.7 (2)    | C50B—Ru2B—Ru3B—C52B | 65.1 (2)     |
| P2A—Ru2A—Ru3A—C52A  | -133.87 (18) | P2B—Ru2B—Ru3B—C52B  | 132.58 (17)  |
| Ru1A—Ru2A—Ru3A—C52A | -169.41 (15) | Ru1B—Ru2B—Ru3B—C52B | 168.44 (14)  |
| C49A—Ru2A—Ru3A—C53A | 115.4 (2)    | C49B—Ru2B—Ru3B—C51B | -118.8 (2)   |
| C50A—Ru2A—Ru3A—C53A | -149.66 (19) | C48B—Ru2B—Ru3B—C51B | 146.7 (2)    |
| C48A—Ru2A—Ru3A—C53A | 24.0 (2)     | C50B—Ru2B—Ru3B—C51B | -29.4 (2)    |

|                     |               |                     |              |
|---------------------|---------------|---------------------|--------------|
| P2A—Ru2A—Ru3A—C53A  | −41.19 (17)   | P2B—Ru2B—Ru3B—C51B  | 38.07 (17)   |
| Ru1A—Ru2A—Ru3A—C53A | −76.73 (14)   | Ru1B—Ru2B—Ru3B—C51B | 73.93 (14)   |
| C49A—Ru2A—Ru3A—C51A | −67.6 (2)     | C49B—Ru2B—Ru3B—C53B | 65.2 (2)     |
| C50A—Ru2A—Ru3A—C51A | 27.35 (19)    | C48B—Ru2B—Ru3B—C53B | −29.3 (2)    |
| C48A—Ru2A—Ru3A—C51A | −159.0 (2)    | C50B—Ru2B—Ru3B—C53B | 154.6 (2)    |
| P2A—Ru2A—Ru3A—C51A  | 135.82 (17)   | P2B—Ru2B—Ru3B—C53B  | −137.92 (16) |
| Ru1A—Ru2A—Ru3A—C51A | 100.27 (14)   | Ru1B—Ru2B—Ru3B—C53B | −102.06 (14) |
| C49A—Ru2A—Ru3A—Sb1A | −134.69 (17)  | C49B—Ru2B—Ru3B—Sb1B | 136.30 (19)  |
| C50A—Ru2A—Ru3A—Sb1A | −39.78 (14)   | C48B—Ru2B—Ru3B—Sb1B | 41.82 (15)   |
| C48A—Ru2A—Ru3A—Sb1A | 133.86 (16)   | C50B—Ru2B—Ru3B—Sb1B | −134.28 (17) |
| P2A—Ru2A—Ru3A—Sb1A  | 68.69 (11)    | P2B—Ru2B—Ru3B—Sb1B  | −66.82 (11)  |
| Ru1A—Ru2A—Ru3A—Sb1A | 33.14 (5)     | Ru1B—Ru2B—Ru3B—Sb1B | −30.96 (5)   |
| C49A—Ru2A—Ru3A—Ru1A | −167.83 (16)  | C49B—Ru2B—Ru3B—Ru1B | 167.26 (19)  |
| C50A—Ru2A—Ru3A—Ru1A | −72.93 (13)   | C48B—Ru2B—Ru3B—Ru1B | 72.77 (14)   |
| C48A—Ru2A—Ru3A—Ru1A | 100.72 (15)   | C50B—Ru2B—Ru3B—Ru1B | −103.32 (16) |
| P2A—Ru2A—Ru3A—Ru1A  | 35.55 (9)     | P2B—Ru2B—Ru3B—Ru1B  | −35.86 (9)   |
| C46A—Ru1A—Ru3A—C52A | −141.6 (4)    | C46B—Ru1B—Ru3B—C52B | 136.6 (4)    |
| C45A—Ru1A—Ru3A—C52A | −48.9 (4)     | C45B—Ru1B—Ru3B—C52B | 42.3 (3)     |
| C47A—Ru1A—Ru3A—C52A | 127.2 (4)     | C47B—Ru1B—Ru3B—C52B | −132.2 (4)   |
| P1A—Ru1A—Ru3A—C52A  | 48.2 (3)      | P1B—Ru1B—Ru3B—C52B  | −67.2 (3)    |
| Ru2A—Ru1A—Ru3A—C52A | 25.1 (3)      | Ru2B—Ru1B—Ru3B—C52B | −29.3 (3)    |
| C46A—Ru1A—Ru3A—C53A | −64.46 (19)   | C46B—Ru1B—Ru3B—C51B | 63.6 (2)     |
| C45A—Ru1A—Ru3A—C53A | 28.29 (19)    | C45B—Ru1B—Ru3B—C51B | −30.74 (18)  |
| C47A—Ru1A—Ru3A—C53A | −155.60 (19)  | C47B—Ru1B—Ru3B—C51B | 154.71 (19)  |
| P1A—Ru1A—Ru3A—C53A  | 125.32 (16)   | P1B—Ru1B—Ru3B—C51B  | −140.27 (16) |
| Ru2A—Ru1A—Ru3A—C53A | 102.24 (14)   | Ru2B—Ru1B—Ru3B—C51B | −102.37 (13) |
| C46A—Ru1A—Ru3A—C51A | 115.9 (2)     | C46B—Ru1B—Ru3B—C53B | −117.4 (2)   |
| C45A—Ru1A—Ru3A—C51A | −151.31 (19)  | C45B—Ru1B—Ru3B—C53B | 148.22 (18)  |
| C47A—Ru1A—Ru3A—C51A | 24.80 (19)    | C47B—Ru1B—Ru3B—C53B | −26.33 (19)  |
| P1A—Ru1A—Ru3A—C51A  | −54.28 (17)   | P1B—Ru1B—Ru3B—C53B  | 38.69 (17)   |
| Ru2A—Ru1A—Ru3A—C51A | −77.36 (14)   | Ru2B—Ru1B—Ru3B—C53B | 76.60 (13)   |
| C46A—Ru1A—Ru3A—Sb1A | 24.62 (14)    | C46B—Ru1B—Ru3B—Sb1B | −24.63 (14)  |
| C45A—Ru1A—Ru3A—Sb1A | 117.37 (13)   | C45B—Ru1B—Ru3B—Sb1B | −118.97 (13) |
| C47A—Ru1A—Ru3A—Sb1A | −66.52 (13)   | C47B—Ru1B—Ru3B—Sb1B | 66.48 (14)   |
| P1A—Ru1A—Ru3A—Sb1A  | −145.60 (9)   | P1B—Ru1B—Ru3B—Sb1B  | 131.50 (9)   |
| Ru2A—Ru1A—Ru3A—Sb1A | −168.678 (17) | Ru2B—Ru1B—Ru3B—Sb1B | 169.406 (17) |
| C46A—Ru1A—Ru3A—Ru2A | −166.70 (14)  | C46B—Ru1B—Ru3B—Ru2B | 165.96 (14)  |
| C45A—Ru1A—Ru3A—Ru2A | −73.95 (13)   | C45B—Ru1B—Ru3B—Ru2B | 71.62 (13)   |
| C47A—Ru1A—Ru3A—Ru2A | 102.15 (13)   | C47B—Ru1B—Ru3B—Ru2B | −102.93 (14) |
| P1A—Ru1A—Ru3A—Ru2A  | 23.07 (9)     | P1B—Ru1B—Ru3B—Ru2B  | −37.91 (9)   |
| C46A—Ru1A—P1A—C7A   | 48.9 (2)      | C46B—Ru1B—P1B—C7B   | 74.8 (2)     |
| C45A—Ru1A—P1A—C7A   | −43.0 (2)     | C45B—Ru1B—P1B—C7B   | 168.7 (2)    |
| C47A—Ru1A—P1A—C7A   | 141.9 (2)     | C47B—Ru1B—P1B—C7B   | −19.1 (2)    |
| Ru2A—Ru1A—P1A—C7A   | −121.00 (17)  | Ru3B—Ru1B—P1B—C7B   | −81.6 (2)    |
| Ru3A—Ru1A—P1A—C7A   | −141.00 (17)  | Ru2B—Ru1B—P1B—C7B   | −114.18 (17) |
| C46A—Ru1A—P1A—C1A   | −72.1 (2)     | C46B—Ru1B—P1B—C1B   | −45.1 (2)    |
| C45A—Ru1A—P1A—C1A   | −164.1 (2)    | C45B—Ru1B—P1B—C1B   | 48.8 (2)     |
| C47A—Ru1A—P1A—C1A   | 20.9 (2)      | C47B—Ru1B—P1B—C1B   | −139.0 (2)   |

|                    |              |                    |              |
|--------------------|--------------|--------------------|--------------|
| Ru2A—Ru1A—P1A—C1A  | 117.99 (16)  | Ru3B—Ru1B—P1B—C1B  | 158.53 (19)  |
| Ru3A—Ru1A—P1A—C1A  | 97.98 (18)   | Ru2B—Ru1B—P1B—C1B  | 125.9 (2)    |
| C46A—Ru1A—P1A—C13A | 169.8 (2)    | C46B—Ru1B—P1B—C13B | -163.9 (2)   |
| C45A—Ru1A—P1A—C13A | 77.9 (2)     | C45B—Ru1B—P1B—C13B | -70.0 (2)    |
| C47A—Ru1A—P1A—C13A | -97.1 (2)    | C47B—Ru1B—P1B—C13B | 102.2 (2)    |
| Ru2A—Ru1A—P1A—C13A | -0.03 (17)   | Ru3B—Ru1B—P1B—C13B | 39.8 (2)     |
| Ru3A—Ru1A—P1A—C13A | -20.0 (2)    | Ru2B—Ru1B—P1B—C13B | 7.1 (2)      |
| C49A—Ru2A—P2A—C21A | -68.3 (2)    | C49B—Ru2B—P2B—C15B | 72.9 (3)     |
| C50A—Ru2A—P2A—C21A | -163.0 (2)   | C48B—Ru2B—P2B—C15B | 167.2 (2)    |
| C48A—Ru2A—P2A—C21A | 24.0 (2)     | C50B—Ru2B—P2B—C15B | -18.4 (2)    |
| Ru3A—Ru2A—P2A—C21A | 87.96 (19)   | Ru3B—Ru2B—P2B—C15B | -84.0 (2)    |
| Ru1A—Ru2A—P2A—C21A | 119.28 (17)  | Ru1B—Ru2B—P2B—C15B | -115.14 (18) |
| C49A—Ru2A—P2A—C15A | 54.1 (2)     | C49B—Ru2B—P2B—C21B | -48.4 (3)    |
| C50A—Ru2A—P2A—C15A | -40.5 (2)    | C48B—Ru2B—P2B—C21B | 45.8 (2)     |
| C48A—Ru2A—P2A—C15A | 146.4 (2)    | C50B—Ru2B—P2B—C21B | -139.7 (2)   |
| Ru3A—Ru2A—P2A—C15A | -149.62 (16) | Ru3B—Ru2B—P2B—C21B | 154.70 (17)  |
| Ru1A—Ru2A—P2A—C15A | -118.30 (16) | Ru1B—Ru2B—P2B—C21B | 123.51 (18)  |
| C49A—Ru2A—P2A—C14A | 174.2 (2)    | C49B—Ru2B—P2B—C14B | -167.6 (3)   |
| C50A—Ru2A—P2A—C14A | 79.6 (2)     | C48B—Ru2B—P2B—C14B | -73.3 (2)    |
| C48A—Ru2A—P2A—C14A | -93.5 (2)    | C50B—Ru2B—P2B—C14B | 101.1 (2)    |
| Ru3A—Ru2A—P2A—C14A | -29.5 (2)    | Ru3B—Ru2B—P2B—C14B | 35.6 (2)     |
| Ru1A—Ru2A—P2A—C14A | 1.80 (16)    | Ru1B—Ru2B—P2B—C14B | 4.38 (19)    |
| C7A—P1A—C1A—C6A    | -20.2 (4)    | C7B—P1B—C1B—C2B    | -125.4 (5)   |
| C13A—P1A—C1A—C6A   | -126.8 (4)   | C13B—P1B—C1B—C2B   | 127.9 (5)    |
| Ru1A—P1A—C1A—C6A   | 107.2 (4)    | Ru1B—P1B—C1B—C2B   | 1.3 (5)      |
| C7A—P1A—C1A—C2A    | 161.4 (4)    | C7B—P1B—C1B—C6B    | 50.9 (5)     |
| C13A—P1A—C1A—C2A   | 54.8 (4)     | C13B—P1B—C1B—C6B   | -55.8 (5)    |
| Ru1A—P1A—C1A—C2A   | -71.2 (4)    | Ru1B—P1B—C1B—C6B   | 177.5 (4)    |
| C6A—C1A—C2A—C3A    | 0.7 (7)      | C6B—C1B—C2B—C3B    | 1.6 (8)      |
| P1A—C1A—C2A—C3A    | 179.1 (4)    | P1B—C1B—C2B—C3B    | 177.9 (4)    |
| C1A—C2A—C3A—C4A    | 0.1 (9)      | C1B—C2B—C3B—C4B    | 0.6 (9)      |
| C2A—C3A—C4A—C5A    | -1.1 (9)     | C2B—C3B—C4B—C5B    | -2.0 (10)    |
| C3A—C4A—C5A—C6A    | 1.2 (9)      | C3B—C4B—C5B—C6B    | 1.1 (10)     |
| C2A—C1A—C6A—C5A    | -0.5 (7)     | C4B—C5B—C6B—C1B    | 1.2 (10)     |
| P1A—C1A—C6A—C5A    | -178.9 (4)   | C2B—C1B—C6B—C5B    | -2.5 (9)     |
| C4A—C5A—C6A—C1A    | -0.4 (8)     | P1B—C1B—C6B—C5B    | -178.9 (5)   |
| C1A—P1A—C7A—C8A    | 84.7 (4)     | C1B—P1B—C7B—C12B   | -92.3 (5)    |
| C13A—P1A—C7A—C8A   | -170.8 (4)   | C13B—P1B—C7B—C12B  | 12.2 (5)     |
| Ru1A—P1A—C7A—C8A   | -43.3 (5)    | Ru1B—P1B—C7B—C12B  | 140.1 (4)    |
| C1A—P1A—C7A—C12A   | -94.4 (4)    | C1B—P1B—C7B—C8B    | 86.8 (4)     |
| C13A—P1A—C7A—C12A  | 10.2 (5)     | C13B—P1B—C7B—C8B   | -168.6 (4)   |
| Ru1A—P1A—C7A—C12A  | 137.7 (4)    | Ru1B—P1B—C7B—C8B   | -40.8 (4)    |
| C12A—C7A—C8A—C9A   | 1.8 (8)      | C12B—C7B—C8B—C9B   | -0.2 (8)     |
| P1A—C7A—C8A—C9A    | -177.3 (5)   | P1B—C7B—C8B—C9B    | -179.4 (4)   |
| C7A—C8A—C9A—C10A   | -1.2 (9)     | C7B—C8B—C9B—C10B   | 0.5 (9)      |
| C8A—C9A—C10A—C11A  | -0.5 (9)     | C8B—C9B—C10B—C11B  | 0.5 (11)     |
| C9A—C10A—C11A—C12A | 1.4 (9)      | C9B—C10B—C11B—C12B | -1.9 (11)    |
| C10A—C11A—C12A—C7A | -0.8 (9)     | C8B—C7B—C12B—C11B  | -1.2 (9)     |

|                     |            |                     |            |
|---------------------|------------|---------------------|------------|
| C8A—C7A—C12A—C11A   | −0.8 (8)   | P1B—C7B—C12B—C11B   | 178.0 (5)  |
| P1A—C7A—C12A—C11A   | 178.2 (4)  | C10B—C11B—C12B—C7B  | 2.2 (11)   |
| C7A—P1A—C13A—C14A   | 69.4 (3)   | C7B—P1B—C13B—C14B   | −179.1 (4) |
| C1A—P1A—C13A—C14A   | 175.8 (3)  | C1B—P1B—C13B—C14B   | −73.6 (4)  |
| Ru1A—P1A—C13A—C14A  | −57.8 (3)  | Ru1B—P1B—C13B—C14B  | 53.5 (4)   |
| P1A—C13A—C14A—P2A   | 98.9 (3)   | P1B—C13B—C14B—P2B   | −97.8 (4)  |
| C21A—P2A—C14A—C13A  | 175.7 (3)  | C15B—P2B—C14B—C13B  | −177.1 (3) |
| C15A—P2A—C14A—C13A  | 66.9 (3)   | C21B—P2B—C14B—C13B  | −71.0 (4)  |
| Ru2A—P2A—C14A—C13A  | −60.2 (3)  | Ru2B—P2B—C14B—C13B  | 57.2 (4)   |
| C21A—P2A—C15A—C20A  | −75.2 (5)  | C21B—P2B—C15B—C20B  | −148.0 (4) |
| C14A—P2A—C15A—C20A  | 31.2 (5)   | C14B—P2B—C15B—C20B  | −43.4 (5)  |
| Ru2A—P2A—C15A—C20A  | 157.7 (4)  | Ru2B—P2B—C15B—C20B  | 82.6 (5)   |
| C21A—P2A—C15A—C16A  | 106.1 (4)  | C21B—P2B—C15B—C16B  | 37.0 (5)   |
| C14A—P2A—C15A—C16A  | −147.5 (4) | C14B—P2B—C15B—C16B  | 141.6 (4)  |
| Ru2A—P2A—C15A—C16A  | −21.0 (4)  | Ru2B—P2B—C15B—C16B  | −92.3 (4)  |
| C20A—C15A—C16A—C17A | 0.5 (7)    | C20B—C15B—C16B—C17B | 0.0 (8)    |
| P2A—C15A—C16A—C17A  | 179.3 (4)  | P2B—C15B—C16B—C17B  | 175.2 (4)  |
| C15A—C16A—C17A—C18A | −1.8 (8)   | C15B—C16B—C17B—C18B | 0.2 (9)    |
| C16A—C17A—C18A—C19A | 1.6 (8)    | C16B—C17B—C18B—C19B | −0.7 (9)   |
| C17A—C18A—C19A—C20A | −0.1 (9)   | C17B—C18B—C19B—C20B | 1.1 (9)    |
| C16A—C15A—C20A—C19A | 1.0 (8)    | C18B—C19B—C20B—C15B | −0.9 (9)   |
| P2A—C15A—C20A—C19A  | −177.7 (4) | C16B—C15B—C20B—C19B | 0.3 (8)    |
| C18A—C19A—C20A—C15A | −1.2 (9)   | P2B—C15B—C20B—C19B  | −174.7 (4) |
| C15A—P2A—C21A—C26A  | −38.5 (5)  | C15B—P2B—C21B—C22B  | −125.0 (5) |
| C14A—P2A—C21A—C26A  | −145.6 (5) | C14B—P2B—C21B—C22B  | 128.6 (5)  |
| Ru2A—P2A—C21A—C26A  | 89.7 (5)   | Ru2B—P2B—C21B—C22B  | 2.2 (5)    |
| C15A—P2A—C21A—C22A  | 147.9 (5)  | C15B—P2B—C21B—C26B  | 55.0 (5)   |
| C14A—P2A—C21A—C22A  | 40.8 (6)   | C14B—P2B—C21B—C26B  | −51.3 (5)  |
| Ru2A—P2A—C21A—C22A  | −83.9 (6)  | Ru2B—P2B—C21B—C26B  | −177.7 (4) |
| C26A—C21A—C22A—C23A | −1.6 (11)  | C26B—C21B—C22B—C23B | 1.2 (9)    |
| P2A—C21A—C22A—C23A  | 172.3 (7)  | P2B—C21B—C22B—C23B  | −178.7 (5) |
| C21A—C22A—C23A—C24A | 1.9 (14)   | C21B—C22B—C23B—C24B | 0.2 (11)   |
| C22A—C23A—C24A—C25A | −1.4 (13)  | C22B—C23B—C24B—C25B | −1.5 (11)  |
| C23A—C24A—C25A—C26A | 0.6 (12)   | C23B—C24B—C25B—C26B | 1.4 (11)   |
| C24A—C25A—C26A—C21A | −0.3 (12)  | C24B—C25B—C26B—C21B | 0.0 (10)   |
| C22A—C21A—C26A—C25A | 0.8 (10)   | C22B—C21B—C26B—C25B | −1.3 (9)   |
| P2A—C21A—C26A—C25A  | −173.1 (6) | P2B—C21B—C26B—C25B  | 178.6 (5)  |
| C33A—Sb1A—C27A—C28A | −143.9 (4) | C39B—Sb1B—C27B—C28B | 78.7 (5)   |
| C39A—Sb1A—C27A—C28A | −43.4 (4)  | C33B—Sb1B—C27B—C28B | −24.9 (5)  |
| Ru3A—Sb1A—C27A—C28A | 79.3 (4)   | Ru3B—Sb1B—C27B—C28B | −158.7 (4) |
| C33A—Sb1A—C27A—C32A | 43.4 (5)   | C39B—Sb1B—C27B—C32B | −100.1 (4) |
| C39A—Sb1A—C27A—C32A | 143.9 (4)  | C33B—Sb1B—C27B—C32B | 156.3 (4)  |
| Ru3A—Sb1A—C27A—C32A | −93.3 (4)  | Ru3B—Sb1B—C27B—C32B | 22.5 (4)   |
| C32A—C27A—C28A—C29A | 0.6 (8)    | C32B—C27B—C28B—C29B | 2.1 (9)    |
| Sb1A—C27A—C28A—C29A | −172.5 (4) | Sb1B—C27B—C28B—C29B | −176.8 (5) |
| C27A—C28A—C29A—C30A | −0.4 (8)   | C27B—C28B—C29B—C30B | −1.1 (11)  |
| C28A—C29A—C30A—C31A | 0.3 (9)    | C28B—C29B—C30B—C31B | −0.1 (10)  |
| C29A—C30A—C31A—C32A | −0.4 (10)  | C29B—C30B—C31B—C32B | 0.3 (9)    |

|                     |            |                     |            |
|---------------------|------------|---------------------|------------|
| C28A—C27A—C32A—C31A | −0.7 (8)   | C30B—C31B—C32B—C27B | 0.7 (9)    |
| Sb1A—C27A—C32A—C31A | 171.8 (4)  | C28B—C27B—C32B—C31B | −1.9 (8)   |
| C30A—C31A—C32A—C27A | 0.6 (9)    | Sb1B—C27B—C32B—C31B | 177.0 (4)  |
| C39A—Sb1A—C33A—C38A | 39.5 (5)   | C39B—Sb1B—C33B—C34B | 170.1 (4)  |
| C27A—Sb1A—C33A—C38A | 139.3 (5)  | C27B—Sb1B—C33B—C34B | −89.4 (4)  |
| Ru3A—Sb1A—C33A—C38A | −85.9 (5)  | Ru3B—Sb1B—C33B—C34B | 37.9 (4)   |
| C39A—Sb1A—C33A—C34A | −147.6 (4) | C39B—Sb1B—C33B—C38B | −19.3 (4)  |
| C27A—Sb1A—C33A—C34A | −47.7 (5)  | C27B—Sb1B—C33B—C38B | 81.2 (4)   |
| Ru3A—Sb1A—C33A—C34A | 87.0 (4)   | Ru3B—Sb1B—C33B—C38B | −151.5 (3) |
| C38A—C33A—C34A—C35A | −4.1 (9)   | C38B—C33B—C34B—C35B | 0.4 (7)    |
| Sb1A—C33A—C34A—C35A | −177.0 (4) | Sb1B—C33B—C34B—C35B | 171.1 (4)  |
| C33A—C34A—C35A—C36A | 1.2 (9)    | C33B—C34B—C35B—C36B | −1.0 (8)   |
| C34A—C35A—C36A—C37A | 3.6 (10)   | C34B—C35B—C36B—C37B | 1.1 (8)    |
| C35A—C36A—C37A—C38A | −5.3 (11)  | C35B—C36B—C37B—C38B | −0.7 (8)   |
| C34A—C33A—C38A—C37A | 2.4 (10)   | C36B—C37B—C38B—C33B | 0.1 (8)    |
| Sb1A—C33A—C38A—C37A | 175.7 (5)  | C34B—C33B—C38B—C37B | 0.0 (8)    |
| C36A—C37A—C38A—C33A | 2.4 (11)   | Sb1B—C33B—C38B—C37B | −170.6 (4) |
| C33A—Sb1A—C39A—C40A | −122.7 (4) | C27B—Sb1B—C39B—C40B | −146.7 (4) |
| C27A—Sb1A—C39A—C40A | 130.3 (4)  | C33B—Sb1B—C39B—C40B | −46.7 (4)  |
| Ru3A—Sb1A—C39A—C40A | 6.4 (4)    | Ru3B—Sb1B—C39B—C40B | 90.9 (4)   |
| C33A—Sb1A—C39A—C44A | 56.4 (4)   | C27B—Sb1B—C39B—C44B | 40.5 (4)   |
| C27A—Sb1A—C39A—C44A | −50.6 (4)  | C33B—Sb1B—C39B—C44B | 140.5 (3)  |
| Ru3A—Sb1A—C39A—C44A | −174.5 (4) | Ru3B—Sb1B—C39B—C44B | −81.9 (4)  |
| C44A—C39A—C40A—C41A | −1.7 (8)   | C44B—C39B—C40B—C41B | 0.4 (7)    |
| Sb1A—C39A—C40A—C41A | 177.4 (4)  | Sb1B—C39B—C40B—C41B | −172.2 (4) |
| C39A—C40A—C41A—C42A | 0.9 (9)    | C39B—C40B—C41B—C42B | 0.7 (9)    |
| C40A—C41A—C42A—C43A | 0.9 (9)    | C40B—C41B—C42B—C43B | −1.5 (9)   |
| C41A—C42A—C43A—C44A | −1.9 (9)   | C41B—C42B—C43B—C44B | 1.1 (9)    |
| C42A—C43A—C44A—C39A | 1.1 (8)    | C42B—C43B—C44B—C39B | 0.1 (8)    |
| C40A—C39A—C44A—C43A | 0.7 (8)    | C40B—C39B—C44B—C43B | −0.9 (7)   |
| Sb1A—C39A—C44A—C43A | −178.4 (4) | Sb1B—C39B—C44B—C43B | 172.2 (4)  |

*Hydrogen-bond geometry (Å, °)*

Cg1, Cg2 and Cg3 are the centroids of the C21B—C26B, C39B—C44B and C15A—C20A benzene rings, respectively.

| D—H···A                        | D—H  | H···A | D···A     | D—H···A |
|--------------------------------|------|-------|-----------|---------|
| C18A—H18A···O7B <sup>i</sup>   | 0.93 | 2.55  | 3.337 (7) | 142     |
| C34A—H34A···O2A                | 0.93 | 2.56  | 3.375 (7) | 147     |
| C34B—H34B···O8B <sup>i</sup>   | 0.93 | 2.57  | 3.414 (7) | 151     |
| C5B—H5BA···Cg1 <sup>ii</sup>   | 0.93 | 3.00  | 3.723 (9) | 136     |
| C25B—H25B···Cg2 <sup>iii</sup> | 0.93 | 2.95  | 3.856 (8) | 166     |
| C43A—H43A···Cg3 <sup>iii</sup> | 0.93 | 2.91  | 3.624 (6) | 135     |

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