

[μ -Bis(diphenylarsino)methane- $1:2\kappa^2\text{As}:\text{As}'$]nonacarbonyl- $1\kappa^3\text{C},2\kappa^3\text{C},3\kappa^3\text{C}$ -[tris(4-fluorophenyl)-phosphine- $3\kappa\text{P}$]-triangulo-triruthenium(0)

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Key indicators: single-crystal X-ray study; $T = 296\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$; R factor = 0.032; wR factor = 0.067; data-to-parameter ratio = 32.7.

In the title *triangulo*-triruthenium compound, $[\text{Ru}_3(\text{C}_{25}\text{H}_{22}(\text{As}_2)(\text{C}_{18}\text{H}_{12}\text{F}_3\text{P})(\text{CO})_9)]$, the bis(diphenylarsino)methane ligand bridges an Ru–Ru bond and the monodentate phosphine ligand bonds to the third Ru atom. Both the phosphine and arsine ligands are equatorial with respect to the Ru_3 triangle. Additionally, each Ru atom carries one equatorial and two axial terminal carbonyl ligands. The three phosphine-substituted rings make dihedral angles of $87.76(13)$, $57.43(13)$ and $73.81(12)^\circ$ with each other. The dihedral angles between the pairs of rings are $69.78(14)$ and $83.38(16)^\circ$ for the two diphenylarsino groups. In the crystal packing, molecules are linked by intermolecular C–H \cdots F and C–H \cdots O hydrogen bonds, forming two-dimensional planes parallel to the *ab* plane. These planes are also linked by intermolecular C–H \cdots O hydrogen bonds into a three-dimensional framework. Intermolecular C–H \cdots π interactions further stabilize the crystal structure.

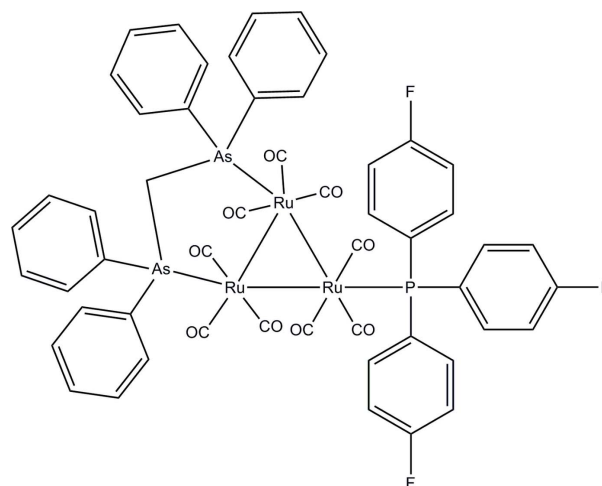
Related literature

For general background to *triangulo*-triruthenium derivatives, see: Bruce (1985, 1988*a,b*); Shawkataly *et al.* (1998). For related structures, see: Shawkataly *et al.* (2006, 2009*a,b*). For the synthesis of bis(diphenylarsino)methane, see: Bruce *et al.* (1983). For details of the Cambridge Structural Database, see: Allen (2002).

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Experimental

Crystal data

$[\text{Ru}_3(\text{C}_{25}\text{H}_{22}\text{As}_2)(\text{C}_{18}\text{H}_{12}\text{F}_3\text{P})(\text{CO})_9]$
 $M_r = 1343.81$
Monoclinic, $P2_1/c$
 $a = 16.3071(2)\text{ \AA}$
 $b = 16.8142(2)\text{ \AA}$
 $c = 18.8085(2)\text{ \AA}$

$\beta = 98.105(1)^\circ$
 $V = 5105.6(1)\text{ \AA}^3$
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 2.26\text{ mm}^{-1}$
 $T = 296\text{ K}$
 $0.38 \times 0.25 \times 0.14\text{ mm}$

Data collection

Bruker SMART APEXII CCD
area-detector diffractometer
Absorption correction: multi-scan
(*SADABS*; Bruker, 2005)
 $T_{\min} = 0.478$, $T_{\max} = 0.740$

89126 measured reflections
20637 independent reflections
13049 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.067$
 $S = 1.00$
20637 reflections

631 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.44\text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.54\text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

| $D\cdots H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|-------|-------------|-------------|---------------|
| $\text{C23}-\text{H23A}\cdots\text{F3}^{\text{i}}$ | 0.93 | 2.46 | 3.337 (5) | 157 |
| $\text{C34}-\text{H34A}\cdots\text{O3}^{\text{ii}}$ | 0.93 | 2.58 | 3.405 (3) | 148 |
| $\text{C42}-\text{H42A}\cdots\text{O2}^{\text{iii}}$ | 0.93 | 2.52 | 3.438 (3) | 167 |
| $\text{C11}-\text{H11A}\cdots\text{Cg1}^{\text{iv}}$ | 0.93 | 2.94 | 3.767 (3) | 149 |
| $\text{C28}-\text{H28A}\cdots\text{Cg2}^{\text{ii}}$ | 0.93 | 2.89 | 3.807 (3) | 168 |

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, -y, -z$; (iv) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$. Cg1 and Cg2 are the centroids of the C38–C43 and C1–C6 phenyl 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2667).

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supporting information

Acta Cryst. (2009). E65, m1620–m1621 [doi:10.1107/S1600536809047229]

[μ -Bis(diphenylarsino)methane-1:2 κ^2 As:As']nonacarbonyl-1 κ^3 C,2 κ^3 C,3 κ^3 C-[tris-(4-fluorophenyl)phosphine-3 κ P]-triangulo-triruthenium(0)

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S1. Comment

Tri-angulotruthenium clusters are known for their interesting structural variations and related catalytic activity. A large number of substituted derivatives, Ru₃(CO)_{12-n}L_n (L=15 group Ligand) have been reported (Bruce *et al.*, 1988a,b; 1985). In continuation of our interest in the substituted clusters (Shawkataly *et al.*, 1998) we report the synthesis and structure of Ru₃(CO)₉(μ -Ph₂AsCH₂AsPh₂)(P(4-FC₆H₄)₃). The Cambridge Structural Database (Allen, 2002) revealed no structure of the above cluster.

The bond lengths and angles of title compound (Fig. 1) are comparable to its related structures (Shawkataly *et al.*, 2006; Shawkataly *et al.*, 2009a,b). The bis(diphenylarsino)methane ligand bridges the Ru1—Ru2 bond and the monodentate phosphine ligand bonds to the Ru3 atom. Both the phosphine and arsine ligands are equatorial with respect to the Ru₃ triangle. Additionally, each Ru atom carries one equatorial and two axial terminal carbonyl ligands. The three phosphine substituted phenyl rings (C26–C31, C32–C37 and C38–C43) make dihedral angles (C26–C31/C32–C37, C26–C31/C38–C43 and C32–C37/C38–C43) of 87.76 (13), 57.43 (13) and 73.81 (12)° with each other respectively. The dihedral angles between the two phenyl rings (C1–C6/C7–C12 and C14–C19/C20–C25) are 69.78 (14) and 83.38 (16)° for the two diphenylarsino groups respectively.

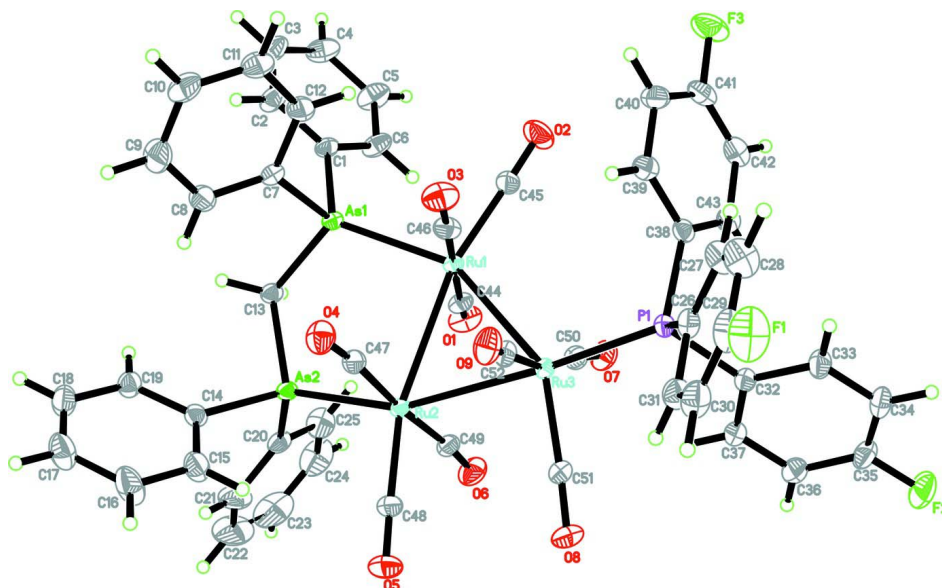
In the crystal packing (Fig. 2), the molecules are linked by intermolecular C23—H23A...F3 and C34—H34A...O3 hydrogen bonds to form two-dimensional planes parallel to *ab* plane. These planes are further linked by intermolecular C42—H42A...O2 hydrogen bonds into a three-dimensional framework. Intermolecular C—H... π interactions further stabilize the crystal structure (Table 1).

S2. Experimental

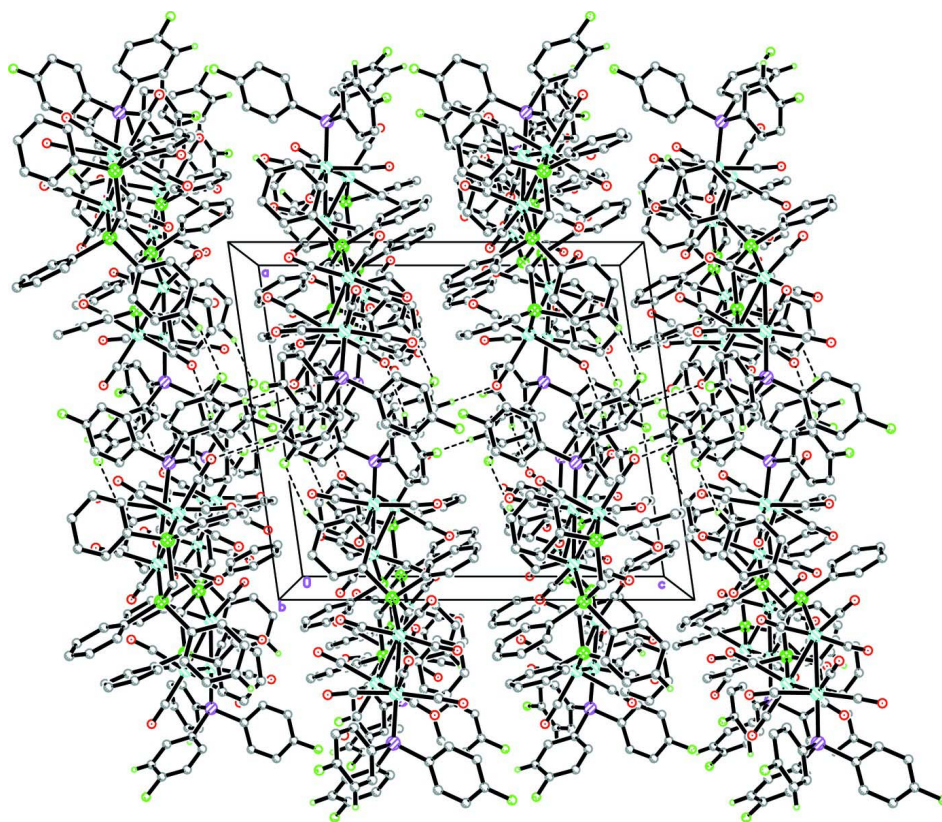
Tris(4-fluorophenyl)phosphine (Strem chemicals) is used as received and bis(diphenylarsino)methane (Bruce *et al.*, 1983) was prepared by reported procedure. Ru₃(CO)₁₀(μ -Ph₂AsCH₂AsPh₂) (105.5 mg, 0.1 mmol) and tris(4-fluorophenyl)-phosphine (31.62 mg, 0.1 mmol) were refluxed for 15 minutes in hexane (25 ml) under a current of nitrogen. The reaction mixture turned intense red. The solvent was removed under vacuum. The reaction mixture was separated by TLC (dichloromethane:hexane, 30:70). Two bands appeared. The major band (red) *R*_f = 0.56 yielded the title compound which was crystallized from CH₂Cl₂—CH₃OH, yield = 58 mg, 42.29%, m.p. 190 °C. IR(cyclohexane). ν (CO) 2054 s, 1993 s, 1976 s cm⁻¹. ¹H NMR (CDCl₃), δ 7.32–7.50 (m, 26H, Ph), δ 7.08–7.13 (t, 6H, Ph), δ 4.01 (s, 2H, —CH₂—).

S3. Refinement

All hydrogen atoms were positioned geometrically and refined using a riding model with C—H = 0.93–0.97 Å and *U*_{iso}(H) = 1.2 *U*_{eq}(C).

**Figure 1**

The molecular structure of the title compound with 20% probability ellipsoids for non-H atoms.

**Figure 2**

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

[μ -Bis(diphenylarsino)methane-1:2 κ^2 As:As']nonacarbonyl- 1 κ^3 C,2 κ^3 C,3 κ^3 C-[tris(4-fluorophenyl)phosphine- 3 κ P]-triangulo-triruthenium(0)*Crystal data*[Ru₃(C₂₅H₂₂As₂)(C₁₈H₁₂F₃P)(CO)₉] $M_r = 1343.81$ Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

 $a = 16.3071$ (2) Å $b = 16.8142$ (2) Å $c = 18.8085$ (2) Å $\beta = 98.105$ (1)° $V = 5105.6$ (1) Å³ $Z = 4$ $F(000) = 2632$ $D_x = 1.748$ Mg m⁻³Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9910 reflections

 $\theta = 2.5\text{--}31.1^\circ$ $\mu = 2.26$ mm⁻¹ $T = 296$ K

Plate, red

 $0.38 \times 0.25 \times 0.14$ mm*Data collection*Bruker SMART APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scansAbsorption correction: multi-scan
(*SADABS*; Bruker, 2005) $T_{\min} = 0.478$, $T_{\max} = 0.740$

89126 measured reflections

20637 independent reflections

13049 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.032$ $\theta_{\max} = 34.0^\circ$, $\theta_{\min} = 1.6^\circ$ $h = -25 \rightarrow 25$ $k = -23 \rightarrow 26$ $l = -29 \rightarrow 22$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.032$ $wR(F^2) = 0.067$ $S = 1.00$

20637 reflections

631 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0231P)^2 + 1.7596P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.002$ $\Delta\rho_{\max} = 0.44$ e Å⁻³ $\Delta\rho_{\min} = -0.54$ e Å⁻³*Special details*

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 (Å²)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|---------------|--------------|----------------------------------|
| Ru1 | 0.758329 (9) | -0.076419 (9) | 0.204485 (9) | 0.03449 (4) |
| Ru2 | 0.901268 (9) | 0.000219 (9) | 0.278744 (9) | 0.03474 (4) |
| Ru3 | 0.749043 (9) | 0.084526 (9) | 0.254257 (9) | 0.03606 (4) |

| | | | | |
|------|---------------|----------------|---------------|--------------|
| As1 | 0.822101 (12) | -0.206958 (11) | 0.223901 (11) | 0.03432 (5) |
| As2 | 0.996032 (11) | -0.110301 (12) | 0.269926 (12) | 0.03624 (5) |
| P1 | 0.61915 (3) | 0.14500 (3) | 0.23231 (3) | 0.03820 (12) |
| F1 | 0.47921 (13) | 0.24586 (13) | 0.49280 (9) | 0.1049 (7) |
| F2 | 0.58974 (12) | 0.44950 (10) | 0.07022 (12) | 0.1059 (7) |
| F3 | 0.38045 (10) | -0.06529 (11) | 0.05565 (11) | 0.0960 (6) |
| O1 | 0.84836 (12) | -0.05511 (11) | 0.07344 (10) | 0.0695 (5) |
| O2 | 0.60490 (12) | -0.12226 (13) | 0.10357 (11) | 0.0806 (6) |
| O3 | 0.66519 (12) | -0.10095 (12) | 0.33318 (11) | 0.0714 (5) |
| O4 | 0.85047 (11) | -0.08172 (11) | 0.41116 (10) | 0.0681 (5) |
| O5 | 1.00783 (13) | 0.11974 (12) | 0.36958 (12) | 0.0836 (6) |
| O6 | 0.95116 (12) | 0.08300 (11) | 0.14619 (11) | 0.0703 (5) |
| O7 | 0.74552 (12) | 0.09629 (11) | 0.09135 (10) | 0.0662 (5) |
| O8 | 0.85238 (12) | 0.22948 (10) | 0.29874 (11) | 0.0750 (6) |
| O9 | 0.71744 (12) | 0.05435 (11) | 0.40925 (10) | 0.0693 (5) |
| C1 | 0.79099 (13) | -0.28842 (12) | 0.15128 (12) | 0.0415 (5) |
| C2 | 0.79025 (18) | -0.36784 (14) | 0.16849 (15) | 0.0647 (7) |
| H2A | 0.8061 | -0.3839 | 0.2157 | 0.078* |
| C3 | 0.7660 (2) | -0.42404 (16) | 0.11581 (18) | 0.0807 (9) |
| H3A | 0.7646 | -0.4776 | 0.1280 | 0.097* |
| C4 | 0.74428 (19) | -0.40124 (17) | 0.04610 (17) | 0.0736 (8) |
| H4A | 0.7286 | -0.4392 | 0.0108 | 0.088* |
| C5 | 0.7455 (2) | -0.32306 (17) | 0.02835 (15) | 0.0733 (8) |
| H5A | 0.7308 | -0.3074 | -0.0192 | 0.088* |
| C6 | 0.76868 (17) | -0.26642 (15) | 0.08092 (13) | 0.0589 (6) |
| H6A | 0.7691 | -0.2129 | 0.0684 | 0.071* |
| C7 | 0.80087 (12) | -0.26512 (12) | 0.30795 (11) | 0.0397 (4) |
| C8 | 0.86048 (15) | -0.29136 (15) | 0.36136 (13) | 0.0580 (6) |
| H8A | 0.9156 | -0.2775 | 0.3608 | 0.070* |
| C9 | 0.8391 (2) | -0.33831 (19) | 0.41617 (15) | 0.0769 (8) |
| H9A | 0.8799 | -0.3560 | 0.4522 | 0.092* |
| C10 | 0.7580 (2) | -0.35891 (17) | 0.41770 (15) | 0.0720 (8) |
| H10A | 0.7441 | -0.3915 | 0.4541 | 0.086* |
| C11 | 0.69801 (18) | -0.33164 (18) | 0.36595 (17) | 0.0733 (8) |
| H11A | 0.6429 | -0.3446 | 0.3675 | 0.088* |
| C12 | 0.71888 (15) | -0.28477 (16) | 0.31108 (15) | 0.0626 (7) |
| H12A | 0.6776 | -0.2662 | 0.2758 | 0.075* |
| C13 | 0.94271 (12) | -0.20738 (12) | 0.22724 (12) | 0.0398 (4) |
| H13A | 0.9559 | -0.2133 | 0.1788 | 0.048* |
| H13B | 0.9653 | -0.2530 | 0.2549 | 0.048* |
| C14 | 1.05731 (12) | -0.14627 (13) | 0.36072 (12) | 0.0435 (5) |
| C15 | 1.06977 (17) | -0.09360 (17) | 0.41720 (16) | 0.0715 (8) |
| H15A | 1.0507 | -0.0416 | 0.4108 | 0.086* |
| C16 | 1.1103 (2) | -0.1172 (2) | 0.48308 (17) | 0.0928 (11) |
| H16A | 1.1191 | -0.0808 | 0.5206 | 0.111* |
| C17 | 1.13761 (19) | -0.1938 (2) | 0.49360 (16) | 0.0802 (9) |
| H17A | 1.1637 | -0.2100 | 0.5385 | 0.096* |
| C18 | 1.12629 (17) | -0.24650 (17) | 0.43766 (15) | 0.0682 (7) |

| | | | | |
|------|--------------|---------------|--------------|-------------|
| H18A | 1.1451 | -0.2985 | 0.4444 | 0.082* |
| C19 | 1.08719 (14) | -0.22290 (14) | 0.37142 (13) | 0.0516 (6) |
| H19A | 1.0808 | -0.2588 | 0.3335 | 0.062* |
| C20 | 1.08183 (13) | -0.09446 (13) | 0.20931 (15) | 0.0499 (6) |
| C21 | 1.16319 (16) | -0.08505 (17) | 0.2382 (2) | 0.0799 (9) |
| H21A | 1.1784 | -0.0872 | 0.2877 | 0.096* |
| C22 | 1.2224 (2) | -0.0724 (3) | 0.1941 (3) | 0.1253 (17) |
| H22A | 1.2776 | -0.0664 | 0.2140 | 0.150* |
| C23 | 1.2010 (3) | -0.0686 (3) | 0.1217 (3) | 0.130 (2) |
| H23A | 1.2417 | -0.0599 | 0.0925 | 0.157* |
| C24 | 1.1203 (3) | -0.0775 (2) | 0.0913 (2) | 0.1048 (13) |
| H24A | 1.1057 | -0.0752 | 0.0417 | 0.126* |
| C25 | 1.06032 (19) | -0.09009 (18) | 0.13602 (18) | 0.0756 (9) |
| H25A | 1.0051 | -0.0956 | 0.1161 | 0.091* |
| C26 | 0.57217 (14) | 0.17311 (13) | 0.31183 (12) | 0.0466 (5) |
| C27 | 0.49231 (16) | 0.15401 (17) | 0.32221 (14) | 0.0632 (7) |
| H27A | 0.4591 | 0.1246 | 0.2875 | 0.076* |
| C28 | 0.46076 (19) | 0.1780 (2) | 0.38355 (16) | 0.0776 (9) |
| H28A | 0.4073 | 0.1642 | 0.3907 | 0.093* |
| C29 | 0.5098 (2) | 0.22193 (18) | 0.43266 (14) | 0.0721 (8) |
| C30 | 0.5882 (2) | 0.24341 (17) | 0.42481 (15) | 0.0709 (8) |
| H30A | 0.6200 | 0.2740 | 0.4596 | 0.085* |
| C31 | 0.61979 (17) | 0.21875 (15) | 0.36371 (14) | 0.0597 (6) |
| H31A | 0.6734 | 0.2329 | 0.3574 | 0.072* |
| C32 | 0.61221 (12) | 0.24017 (12) | 0.18371 (12) | 0.0426 (5) |
| C33 | 0.53927 (15) | 0.28460 (14) | 0.17773 (14) | 0.0552 (6) |
| H33A | 0.4951 | 0.2664 | 0.1995 | 0.066* |
| C34 | 0.53190 (17) | 0.35528 (15) | 0.13977 (15) | 0.0649 (7) |
| H34A | 0.4834 | 0.3850 | 0.1361 | 0.078* |
| C35 | 0.59754 (18) | 0.38056 (15) | 0.10780 (16) | 0.0664 (7) |
| C36 | 0.66977 (16) | 0.33947 (15) | 0.11234 (15) | 0.0636 (7) |
| H36A | 0.7135 | 0.3583 | 0.0903 | 0.076* |
| C37 | 0.67676 (14) | 0.26870 (14) | 0.15073 (13) | 0.0526 (6) |
| H37A | 0.7259 | 0.2399 | 0.1543 | 0.063* |
| C38 | 0.54110 (12) | 0.08408 (13) | 0.17909 (12) | 0.0406 (5) |
| C39 | 0.51251 (14) | 0.01470 (15) | 0.20801 (14) | 0.0541 (6) |
| H39A | 0.5307 | 0.0019 | 0.2557 | 0.065* |
| C40 | 0.45758 (15) | -0.03552 (16) | 0.16702 (17) | 0.0644 (7) |
| H40A | 0.4379 | -0.0813 | 0.1866 | 0.077* |
| C41 | 0.43315 (14) | -0.01542 (17) | 0.09671 (16) | 0.0621 (7) |
| C42 | 0.46057 (15) | 0.05001 (17) | 0.06592 (14) | 0.0579 (6) |
| H42A | 0.4432 | 0.0610 | 0.0177 | 0.069* |
| C43 | 0.51485 (13) | 0.10050 (14) | 0.10721 (12) | 0.0472 (5) |
| H43A | 0.5339 | 0.1459 | 0.0866 | 0.057* |
| C44 | 0.81765 (14) | -0.05964 (13) | 0.12443 (13) | 0.0472 (5) |
| C45 | 0.66118 (14) | -0.10384 (14) | 0.14291 (13) | 0.0491 (5) |
| C46 | 0.70225 (14) | -0.08582 (14) | 0.28761 (14) | 0.0497 (5) |
| C47 | 0.86518 (12) | -0.05113 (13) | 0.36024 (13) | 0.0444 (5) |

| | | | | |
|-----|--------------|--------------|--------------|------------|
| C48 | 0.96867 (14) | 0.07385 (14) | 0.33563 (14) | 0.0523 (6) |
| C49 | 0.92893 (13) | 0.05136 (13) | 0.19364 (14) | 0.0479 (5) |
| C50 | 0.75062 (14) | 0.08463 (13) | 0.15216 (14) | 0.0479 (5) |
| C51 | 0.81181 (14) | 0.17562 (13) | 0.28089 (13) | 0.0471 (5) |
| C52 | 0.73155 (14) | 0.06203 (13) | 0.35212 (14) | 0.0476 (5) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|--------------|--------------|--------------|--------------|--------------|
| Ru1 | 0.03469 (7) | 0.02893 (8) | 0.03910 (9) | -0.00302 (6) | 0.00266 (6) | -0.00330 (7) |
| Ru2 | 0.03017 (7) | 0.02739 (8) | 0.04667 (10) | -0.00148 (5) | 0.00549 (6) | -0.00464 (7) |
| Ru3 | 0.03345 (7) | 0.02839 (8) | 0.04538 (10) | 0.00152 (6) | 0.00223 (7) | -0.00243 (7) |
| As1 | 0.03681 (9) | 0.02778 (10) | 0.03869 (11) | -0.00436 (7) | 0.00647 (8) | -0.00183 (8) |
| As2 | 0.03112 (9) | 0.02945 (10) | 0.04899 (13) | -0.00058 (7) | 0.00856 (9) | -0.00339 (9) |
| P1 | 0.0356 (2) | 0.0364 (3) | 0.0421 (3) | 0.0036 (2) | 0.0036 (2) | -0.0004 (2) |
| F1 | 0.1420 (17) | 0.1256 (16) | 0.0524 (10) | 0.0436 (14) | 0.0324 (11) | -0.0097 (10) |
| F2 | 0.1104 (14) | 0.0618 (11) | 0.1438 (18) | 0.0148 (10) | 0.0117 (13) | 0.0494 (11) |
| F3 | 0.0637 (10) | 0.1025 (14) | 0.1172 (15) | -0.0194 (9) | -0.0035 (10) | -0.0525 (12) |
| O1 | 0.0940 (14) | 0.0663 (12) | 0.0538 (11) | -0.0166 (10) | 0.0300 (10) | -0.0113 (9) |
| O2 | 0.0611 (11) | 0.0898 (15) | 0.0816 (14) | -0.0028 (10) | -0.0220 (10) | -0.0238 (12) |
| O3 | 0.0743 (12) | 0.0746 (13) | 0.0734 (13) | -0.0144 (10) | 0.0382 (11) | -0.0073 (10) |
| O4 | 0.0722 (12) | 0.0739 (13) | 0.0611 (12) | 0.0065 (9) | 0.0192 (10) | 0.0154 (10) |
| O5 | 0.0797 (13) | 0.0609 (12) | 0.1027 (16) | -0.0200 (10) | -0.0135 (12) | -0.0250 (11) |
| O6 | 0.0775 (12) | 0.0568 (11) | 0.0818 (14) | -0.0046 (9) | 0.0287 (11) | 0.0182 (10) |
| O7 | 0.0889 (13) | 0.0570 (11) | 0.0523 (11) | 0.0062 (9) | 0.0091 (10) | 0.0036 (9) |
| O8 | 0.0824 (13) | 0.0430 (10) | 0.0953 (15) | -0.0199 (9) | -0.0021 (11) | -0.0059 (10) |
| O9 | 0.0901 (14) | 0.0657 (12) | 0.0529 (11) | 0.0191 (10) | 0.0123 (10) | 0.0093 (9) |
| C1 | 0.0460 (11) | 0.0319 (11) | 0.0477 (13) | -0.0054 (8) | 0.0105 (9) | -0.0093 (9) |
| C2 | 0.095 (2) | 0.0357 (13) | 0.0606 (16) | -0.0064 (12) | -0.0008 (14) | -0.0063 (12) |
| C3 | 0.120 (3) | 0.0358 (15) | 0.085 (2) | -0.0107 (15) | 0.008 (2) | -0.0127 (14) |
| C4 | 0.096 (2) | 0.0546 (17) | 0.073 (2) | -0.0207 (15) | 0.0233 (17) | -0.0319 (15) |
| C5 | 0.115 (2) | 0.0596 (18) | 0.0469 (15) | -0.0188 (16) | 0.0186 (16) | -0.0166 (13) |
| C6 | 0.0906 (18) | 0.0412 (13) | 0.0475 (14) | -0.0137 (12) | 0.0185 (13) | -0.0087 (11) |
| C7 | 0.0465 (11) | 0.0316 (10) | 0.0421 (12) | -0.0043 (8) | 0.0104 (9) | 0.0004 (9) |
| C8 | 0.0531 (13) | 0.0669 (17) | 0.0532 (15) | -0.0070 (12) | 0.0051 (12) | 0.0111 (13) |
| C9 | 0.084 (2) | 0.089 (2) | 0.0557 (17) | 0.0009 (17) | 0.0038 (15) | 0.0246 (16) |
| C10 | 0.098 (2) | 0.0651 (19) | 0.0574 (17) | -0.0151 (16) | 0.0267 (16) | 0.0148 (14) |
| C11 | 0.0660 (16) | 0.076 (2) | 0.081 (2) | -0.0195 (14) | 0.0237 (15) | 0.0220 (17) |
| C12 | 0.0501 (13) | 0.0680 (17) | 0.0704 (17) | -0.0111 (12) | 0.0108 (12) | 0.0202 (14) |
| C13 | 0.0379 (9) | 0.0331 (11) | 0.0496 (12) | -0.0014 (8) | 0.0105 (9) | -0.0053 (9) |
| C14 | 0.0369 (10) | 0.0432 (12) | 0.0496 (13) | 0.0025 (8) | 0.0032 (9) | -0.0054 (10) |
| C15 | 0.0713 (17) | 0.0582 (17) | 0.076 (2) | 0.0199 (13) | -0.0196 (15) | -0.0224 (14) |
| C16 | 0.096 (2) | 0.097 (2) | 0.073 (2) | 0.0368 (19) | -0.0300 (18) | -0.0384 (19) |
| C17 | 0.083 (2) | 0.095 (2) | 0.0556 (17) | 0.0251 (17) | -0.0122 (15) | -0.0056 (17) |
| C18 | 0.0735 (17) | 0.0595 (17) | 0.0684 (19) | 0.0149 (13) | -0.0006 (14) | 0.0081 (14) |
| C19 | 0.0577 (13) | 0.0448 (13) | 0.0512 (14) | 0.0078 (10) | 0.0036 (11) | -0.0050 (11) |
| C20 | 0.0449 (11) | 0.0327 (11) | 0.0769 (18) | 0.0009 (9) | 0.0252 (12) | 0.0005 (11) |
| C21 | 0.0491 (14) | 0.077 (2) | 0.118 (3) | -0.0181 (13) | 0.0283 (16) | -0.0133 (18) |

| | | | | | | |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C22 | 0.065 (2) | 0.124 (4) | 0.200 (5) | -0.026 (2) | 0.065 (3) | -0.012 (4) |
| C23 | 0.108 (3) | 0.101 (3) | 0.209 (6) | -0.006 (2) | 0.115 (4) | 0.019 (4) |
| C24 | 0.123 (3) | 0.096 (3) | 0.113 (3) | 0.016 (2) | 0.080 (3) | 0.024 (2) |
| C25 | 0.0691 (17) | 0.082 (2) | 0.084 (2) | 0.0072 (15) | 0.0394 (16) | 0.0145 (17) |
| C26 | 0.0513 (12) | 0.0468 (13) | 0.0409 (12) | 0.0136 (10) | 0.0040 (10) | 0.0005 (10) |
| C27 | 0.0565 (14) | 0.085 (2) | 0.0494 (15) | 0.0059 (13) | 0.0112 (12) | -0.0099 (14) |
| C28 | 0.0731 (18) | 0.103 (2) | 0.0617 (18) | 0.0115 (17) | 0.0265 (15) | -0.0069 (17) |
| C29 | 0.097 (2) | 0.079 (2) | 0.0426 (15) | 0.0362 (17) | 0.0181 (15) | 0.0000 (14) |
| C30 | 0.093 (2) | 0.0637 (18) | 0.0516 (16) | 0.0205 (16) | -0.0037 (15) | -0.0136 (13) |
| C31 | 0.0664 (15) | 0.0543 (15) | 0.0569 (16) | 0.0101 (12) | 0.0030 (13) | -0.0108 (12) |
| C32 | 0.0415 (10) | 0.0367 (11) | 0.0485 (13) | 0.0046 (8) | 0.0028 (9) | -0.0018 (9) |
| C33 | 0.0530 (13) | 0.0498 (14) | 0.0636 (16) | 0.0129 (10) | 0.0104 (12) | 0.0042 (12) |
| C34 | 0.0661 (16) | 0.0476 (15) | 0.0799 (19) | 0.0211 (12) | 0.0066 (14) | 0.0075 (13) |
| C35 | 0.0801 (18) | 0.0388 (14) | 0.0773 (19) | 0.0054 (12) | 0.0007 (15) | 0.0135 (13) |
| C36 | 0.0589 (14) | 0.0495 (15) | 0.082 (2) | -0.0036 (12) | 0.0088 (14) | 0.0159 (14) |
| C37 | 0.0479 (12) | 0.0418 (13) | 0.0668 (16) | 0.0022 (10) | 0.0035 (11) | 0.0058 (11) |
| C38 | 0.0324 (9) | 0.0442 (12) | 0.0457 (12) | 0.0041 (8) | 0.0067 (8) | -0.0028 (10) |
| C39 | 0.0470 (12) | 0.0560 (15) | 0.0589 (15) | -0.0035 (10) | 0.0054 (11) | 0.0036 (12) |
| C40 | 0.0485 (13) | 0.0524 (15) | 0.094 (2) | -0.0106 (11) | 0.0154 (14) | -0.0067 (15) |
| C41 | 0.0369 (11) | 0.0715 (18) | 0.0768 (19) | -0.0007 (11) | 0.0044 (12) | -0.0318 (15) |
| C42 | 0.0509 (13) | 0.0739 (18) | 0.0474 (14) | 0.0114 (12) | 0.0018 (11) | -0.0185 (13) |
| C43 | 0.0460 (11) | 0.0516 (14) | 0.0446 (13) | 0.0057 (10) | 0.0090 (10) | -0.0065 (10) |
| C44 | 0.0578 (13) | 0.0340 (12) | 0.0498 (14) | -0.0071 (9) | 0.0075 (11) | -0.0050 (10) |
| C45 | 0.0475 (12) | 0.0447 (13) | 0.0523 (14) | -0.0011 (10) | -0.0024 (11) | -0.0052 (11) |
| C46 | 0.0439 (11) | 0.0491 (14) | 0.0567 (15) | -0.0063 (10) | 0.0090 (11) | -0.0108 (11) |
| C47 | 0.0388 (10) | 0.0403 (12) | 0.0544 (14) | 0.0031 (8) | 0.0076 (10) | -0.0033 (11) |
| C48 | 0.0455 (12) | 0.0411 (13) | 0.0684 (16) | -0.0056 (9) | 0.0015 (11) | -0.0060 (11) |
| C49 | 0.0447 (11) | 0.0347 (12) | 0.0652 (16) | -0.0002 (9) | 0.0104 (11) | -0.0002 (11) |
| C50 | 0.0488 (12) | 0.0423 (13) | 0.0521 (14) | 0.0028 (9) | 0.0057 (11) | -0.0063 (11) |
| C51 | 0.0497 (12) | 0.0349 (12) | 0.0554 (14) | -0.0004 (9) | 0.0029 (10) | -0.0004 (10) |
| C52 | 0.0491 (12) | 0.0371 (12) | 0.0548 (15) | 0.0075 (9) | 0.0013 (11) | 0.0018 (10) |

Geometric parameters (Å, °)

| | | | |
|---------|------------|----------|-----------|
| Ru1—C45 | 1.883 (2) | C11—H11A | 0.9300 |
| Ru1—C44 | 1.922 (2) | C12—H12A | 0.9300 |
| Ru1—C46 | 1.926 (3) | C13—H13A | 0.9700 |
| Ru1—As1 | 2.4342 (3) | C13—H13B | 0.9700 |
| Ru1—Ru2 | 2.8507 (2) | C14—C15 | 1.376 (3) |
| Ru1—Ru3 | 2.8745 (2) | C14—C19 | 1.382 (3) |
| Ru2—C48 | 1.885 (2) | C15—C16 | 1.378 (4) |
| Ru2—C47 | 1.922 (2) | C15—H15A | 0.9300 |
| Ru2—C49 | 1.926 (3) | C16—C17 | 1.369 (4) |
| Ru2—As2 | 2.4374 (2) | C16—H16A | 0.9300 |
| Ru2—Ru3 | 2.8392 (2) | C17—C18 | 1.368 (4) |
| Ru3—C51 | 1.871 (2) | C17—H17A | 0.9300 |
| Ru3—C50 | 1.924 (3) | C18—C19 | 1.376 (3) |
| Ru3—C52 | 1.939 (3) | C18—H18A | 0.9300 |

| | | | |
|-------------|-------------|---------------|-------------|
| Ru3—P1 | 2.3334 (5) | C19—H19A | 0.9300 |
| As1—C7 | 1.931 (2) | C20—C21 | 1.370 (3) |
| As1—C1 | 1.950 (2) | C20—C25 | 1.376 (4) |
| As1—C13 | 1.9589 (19) | C21—C22 | 1.376 (5) |
| As2—C20 | 1.944 (2) | C21—H21A | 0.9300 |
| As2—C14 | 1.949 (2) | C22—C23 | 1.359 (7) |
| As2—C13 | 1.9668 (19) | C22—H22A | 0.9300 |
| P1—C38 | 1.820 (2) | C23—C24 | 1.367 (6) |
| P1—C26 | 1.836 (2) | C23—H23A | 0.9300 |
| P1—C32 | 1.838 (2) | C24—C25 | 1.393 (4) |
| F1—C29 | 1.360 (3) | C24—H24A | 0.9300 |
| F2—C35 | 1.354 (3) | C25—H25A | 0.9300 |
| F3—C41 | 1.360 (3) | C26—C27 | 1.382 (3) |
| O1—C44 | 1.145 (3) | C26—C31 | 1.389 (3) |
| O2—C45 | 1.138 (3) | C27—C28 | 1.388 (4) |
| O3—C46 | 1.145 (3) | C27—H27A | 0.9300 |
| O4—C47 | 1.142 (3) | C28—C29 | 1.353 (4) |
| O5—C48 | 1.138 (3) | C28—H28A | 0.9300 |
| O6—C49 | 1.141 (3) | C29—C30 | 1.356 (4) |
| O7—C50 | 1.152 (3) | C30—C31 | 1.388 (4) |
| O8—C51 | 1.144 (3) | C30—H30A | 0.9300 |
| O9—C52 | 1.138 (3) | C31—H31A | 0.9300 |
| C1—C6 | 1.373 (3) | C32—C37 | 1.381 (3) |
| C1—C2 | 1.374 (3) | C32—C33 | 1.396 (3) |
| C2—C3 | 1.386 (4) | C33—C34 | 1.383 (3) |
| C2—H2A | 0.9300 | C33—H33A | 0.9300 |
| C3—C4 | 1.364 (4) | C34—C35 | 1.367 (4) |
| C3—H3A | 0.9300 | C34—H34A | 0.9300 |
| C4—C5 | 1.357 (4) | C35—C36 | 1.358 (4) |
| C4—H4A | 0.9300 | C36—C37 | 1.388 (3) |
| C5—C6 | 1.386 (3) | C36—H36A | 0.9300 |
| C5—H5A | 0.9300 | C37—H37A | 0.9300 |
| C6—H6A | 0.9300 | C38—C43 | 1.387 (3) |
| C7—C8 | 1.369 (3) | C38—C39 | 1.395 (3) |
| C7—C12 | 1.387 (3) | C39—C40 | 1.384 (3) |
| C8—C9 | 1.382 (4) | C39—H39A | 0.9300 |
| C8—H8A | 0.9300 | C40—C41 | 1.369 (4) |
| C9—C10 | 1.371 (4) | C40—H40A | 0.9300 |
| C9—H9A | 0.9300 | C41—C42 | 1.349 (4) |
| C10—C11 | 1.358 (4) | C42—C43 | 1.383 (3) |
| C10—H10A | 0.9300 | C42—H42A | 0.9300 |
| C11—C12 | 1.379 (3) | C43—H43A | 0.9300 |
| C45—Ru1—C44 | 91.54 (10) | As1—C13—H13B | 108.9 |
| C45—Ru1—C46 | 91.41 (10) | As2—C13—H13B | 108.9 |
| C44—Ru1—C46 | 175.72 (9) | H13A—C13—H13B | 107.7 |
| C45—Ru1—As1 | 100.14 (7) | C15—C14—C19 | 118.5 (2) |
| C44—Ru1—As1 | 89.90 (7) | C15—C14—As2 | 118.58 (17) |

| | | | |
|-------------|--------------|--------------|-------------|
| C46—Ru1—As1 | 92.63 (7) | C19—C14—As2 | 122.92 (17) |
| C45—Ru1—Ru2 | 166.13 (7) | C14—C15—C16 | 120.6 (3) |
| C44—Ru1—Ru2 | 81.39 (7) | C14—C15—H15A | 119.7 |
| C46—Ru1—Ru2 | 95.07 (7) | C16—C15—H15A | 119.7 |
| As1—Ru1—Ru2 | 91.810 (7) | C17—C16—C15 | 120.4 (3) |
| C45—Ru1—Ru3 | 110.63 (7) | C17—C16—H16A | 119.8 |
| C44—Ru1—Ru3 | 99.93 (6) | C15—C16—H16A | 119.8 |
| C46—Ru1—Ru3 | 76.12 (7) | C18—C17—C16 | 119.5 (3) |
| As1—Ru1—Ru3 | 147.251 (9) | C18—C17—H17A | 120.3 |
| Ru2—Ru1—Ru3 | 59.460 (5) | C16—C17—H17A | 120.3 |
| C48—Ru2—C47 | 93.55 (10) | C17—C18—C19 | 120.3 (3) |
| C48—Ru2—C49 | 89.56 (10) | C17—C18—H18A | 119.8 |
| C47—Ru2—C49 | 175.70 (9) | C19—C18—H18A | 119.8 |
| C48—Ru2—As2 | 102.41 (7) | C18—C19—C14 | 120.6 (2) |
| C47—Ru2—As2 | 88.86 (6) | C18—C19—H19A | 119.7 |
| C49—Ru2—As2 | 93.37 (6) | C14—C19—H19A | 119.7 |
| C48—Ru2—Ru3 | 100.99 (7) | C21—C20—C25 | 119.2 (2) |
| C47—Ru2—Ru3 | 89.69 (6) | C21—C20—As2 | 121.3 (2) |
| C49—Ru2—Ru3 | 86.80 (6) | C25—C20—As2 | 119.48 (19) |
| As2—Ru2—Ru3 | 156.606 (9) | C20—C21—C22 | 120.0 (4) |
| C48—Ru2—Ru1 | 161.07 (7) | C20—C21—H21A | 120.0 |
| C47—Ru2—Ru1 | 82.33 (6) | C22—C21—H21A | 120.0 |
| C49—Ru2—Ru1 | 93.77 (7) | C23—C22—C21 | 120.6 (4) |
| As2—Ru2—Ru1 | 95.997 (7) | C23—C22—H22A | 119.7 |
| Ru3—Ru2—Ru1 | 60.687 (6) | C21—C22—H22A | 119.7 |
| C51—Ru3—C50 | 100.53 (10) | C22—C23—C24 | 120.6 (3) |
| C51—Ru3—C52 | 93.07 (10) | C22—C23—H23A | 119.7 |
| C50—Ru3—C52 | 166.40 (10) | C24—C23—H23A | 119.7 |
| C51—Ru3—P1 | 98.01 (7) | C23—C24—C25 | 118.7 (4) |
| C50—Ru3—P1 | 87.86 (7) | C23—C24—H24A | 120.6 |
| C52—Ru3—P1 | 90.09 (6) | C25—C24—H24A | 120.6 |
| C51—Ru3—Ru2 | 86.13 (7) | C20—C25—C24 | 120.8 (3) |
| C50—Ru3—Ru2 | 91.60 (7) | C20—C25—H25A | 119.6 |
| C52—Ru3—Ru2 | 89.48 (6) | C24—C25—H25A | 119.6 |
| P1—Ru3—Ru2 | 175.856 (15) | C27—C26—C31 | 118.3 (2) |
| C51—Ru3—Ru1 | 143.71 (7) | C27—C26—P1 | 124.42 (19) |
| C50—Ru3—Ru1 | 70.56 (7) | C31—C26—P1 | 117.28 (18) |
| C52—Ru3—Ru1 | 98.46 (6) | C26—C27—C28 | 121.2 (3) |
| P1—Ru3—Ru1 | 116.158 (15) | C26—C27—H27A | 119.4 |
| Ru2—Ru3—Ru1 | 59.854 (5) | C28—C27—H27A | 119.4 |
| C7—As1—C1 | 99.13 (9) | C29—C28—C27 | 118.3 (3) |
| C7—As1—C13 | 105.49 (9) | C29—C28—H28A | 120.9 |
| C1—As1—C13 | 100.42 (8) | C27—C28—H28A | 120.9 |
| C7—As1—Ru1 | 117.21 (6) | C28—C29—C30 | 123.1 (3) |
| C1—As1—Ru1 | 117.69 (7) | C28—C29—F1 | 118.6 (3) |
| C13—As1—Ru1 | 114.45 (6) | C30—C29—F1 | 118.3 (3) |
| C20—As2—C14 | 103.52 (10) | C29—C30—C31 | 118.5 (3) |
| C20—As2—C13 | 100.82 (9) | C29—C30—H30A | 120.8 |

| | | | |
|--------------|-------------|--------------|-------------|
| C14—As2—C13 | 104.04 (9) | C31—C30—H30A | 120.8 |
| C20—As2—Ru2 | 116.82 (6) | C30—C31—C26 | 120.7 (3) |
| C14—As2—Ru2 | 115.38 (6) | C30—C31—H31A | 119.6 |
| C13—As2—Ru2 | 114.36 (6) | C26—C31—H31A | 119.6 |
| C38—P1—C26 | 104.67 (10) | C37—C32—C33 | 118.2 (2) |
| C38—P1—C32 | 103.13 (10) | C37—C32—P1 | 121.90 (16) |
| C26—P1—C32 | 100.23 (10) | C33—C32—P1 | 119.87 (17) |
| C38—P1—Ru3 | 113.52 (7) | C34—C33—C32 | 120.8 (2) |
| C26—P1—Ru3 | 116.15 (7) | C34—C33—H33A | 119.6 |
| C32—P1—Ru3 | 117.26 (7) | C32—C33—H33A | 119.6 |
| C6—C1—C2 | 118.6 (2) | C35—C34—C33 | 118.5 (2) |
| C6—C1—As1 | 119.56 (16) | C35—C34—H34A | 120.7 |
| C2—C1—As1 | 121.83 (18) | C33—C34—H34A | 120.7 |
| C1—C2—C3 | 120.3 (3) | F2—C35—C36 | 119.0 (3) |
| C1—C2—H2A | 119.8 | F2—C35—C34 | 118.3 (2) |
| C3—C2—H2A | 119.8 | C36—C35—C34 | 122.7 (2) |
| C4—C3—C2 | 120.3 (3) | C35—C36—C37 | 118.4 (2) |
| C4—C3—H3A | 119.8 | C35—C36—H36A | 120.8 |
| C2—C3—H3A | 119.8 | C37—C36—H36A | 120.8 |
| C5—C4—C3 | 119.9 (3) | C32—C37—C36 | 121.3 (2) |
| C5—C4—H4A | 120.1 | C32—C37—H37A | 119.4 |
| C3—C4—H4A | 120.1 | C36—C37—H37A | 119.4 |
| C4—C5—C6 | 120.1 (3) | C43—C38—C39 | 118.2 (2) |
| C4—C5—H5A | 119.9 | C43—C38—P1 | 121.32 (17) |
| C6—C5—H5A | 119.9 | C39—C38—P1 | 120.17 (17) |
| C1—C6—C5 | 120.7 (2) | C40—C39—C38 | 121.2 (2) |
| C1—C6—H6A | 119.6 | C40—C39—H39A | 119.4 |
| C5—C6—H6A | 119.6 | C38—C39—H39A | 119.4 |
| C8—C7—C12 | 118.8 (2) | C41—C40—C39 | 117.7 (2) |
| C8—C7—As1 | 124.98 (16) | C41—C40—H40A | 121.1 |
| C12—C7—As1 | 116.15 (17) | C39—C40—H40A | 121.1 |
| C7—C8—C9 | 120.2 (2) | C42—C41—F3 | 118.7 (3) |
| C7—C8—H8A | 119.9 | C42—C41—C40 | 123.2 (2) |
| C9—C8—H8A | 119.9 | F3—C41—C40 | 118.1 (3) |
| C10—C9—C8 | 120.4 (3) | C41—C42—C43 | 119.0 (2) |
| C10—C9—H9A | 119.8 | C41—C42—H42A | 120.5 |
| C8—C9—H9A | 119.8 | C43—C42—H42A | 120.5 |
| C11—C10—C9 | 119.9 (3) | C42—C43—C38 | 120.7 (2) |
| C11—C10—H10A | 120.0 | C42—C43—H43A | 119.7 |
| C9—C10—H10A | 120.0 | C38—C43—H43A | 119.7 |
| C10—C11—C12 | 120.0 (3) | O1—C44—Ru1 | 173.5 (2) |
| C10—C11—H11A | 120.0 | O2—C45—Ru1 | 176.6 (2) |
| C12—C11—H11A | 120.0 | O3—C46—Ru1 | 170.8 (2) |
| C11—C12—C7 | 120.6 (2) | O4—C47—Ru2 | 174.32 (19) |
| C11—C12—H12A | 119.7 | O5—C48—Ru2 | 178.3 (2) |
| C7—C12—H12A | 119.7 | O6—C49—Ru2 | 174.7 (2) |
| As1—C13—As2 | 113.22 (9) | O7—C50—Ru3 | 169.1 (2) |
| As1—C13—H13A | 108.9 | O8—C51—Ru3 | 177.4 (2) |

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|-----------------|--------------|-----------------|--------------|
| As2—C13—H13A | 108.9 | O9—C52—Ru3 | 174.4 (2) |
| C45—Ru1—Ru2—C48 | 62.5 (4) | C7—As1—C1—C2 | -22.1 (2) |
| C44—Ru1—Ru2—C48 | 122.5 (3) | C13—As1—C1—C2 | 85.6 (2) |
| C46—Ru1—Ru2—C48 | -55.1 (3) | Ru1—As1—C1—C2 | -149.55 (18) |
| As1—Ru1—Ru2—C48 | -147.9 (2) | C6—C1—C2—C3 | -1.1 (4) |
| Ru3—Ru1—Ru2—C48 | 15.5 (2) | As1—C1—C2—C3 | 178.6 (2) |
| C45—Ru1—Ru2—C47 | 140.9 (3) | C1—C2—C3—C4 | 1.3 (5) |
| C44—Ru1—Ru2—C47 | -159.06 (9) | C2—C3—C4—C5 | -0.7 (5) |
| C46—Ru1—Ru2—C47 | 23.38 (10) | C3—C4—C5—C6 | -0.1 (5) |
| As1—Ru1—Ru2—C47 | -69.43 (6) | C2—C1—C6—C5 | 0.3 (4) |
| Ru3—Ru1—Ru2—C47 | 93.98 (6) | As1—C1—C6—C5 | -179.4 (2) |
| C45—Ru1—Ru2—C49 | -37.3 (3) | C4—C5—C6—C1 | 0.3 (4) |
| C44—Ru1—Ru2—C49 | 22.77 (9) | C1—As1—C7—C8 | 110.6 (2) |
| C46—Ru1—Ru2—C49 | -154.80 (10) | C13—As1—C7—C8 | 7.0 (2) |
| As1—Ru1—Ru2—C49 | 112.40 (6) | Ru1—As1—C7—C8 | -121.69 (19) |
| Ru3—Ru1—Ru2—C49 | -84.19 (6) | C1—As1—C7—C12 | -65.70 (19) |
| C45—Ru1—Ru2—As2 | -131.0 (3) | C13—As1—C7—C12 | -169.26 (18) |
| C44—Ru1—Ru2—As2 | -71.02 (7) | Ru1—As1—C7—C12 | 62.03 (19) |
| C46—Ru1—Ru2—As2 | 111.41 (7) | C12—C7—C8—C9 | 1.7 (4) |
| As1—Ru1—Ru2—As2 | 18.605 (9) | As1—C7—C8—C9 | -174.5 (2) |
| Ru3—Ru1—Ru2—As2 | -177.986 (9) | C7—C8—C9—C10 | -0.2 (5) |
| C45—Ru1—Ru2—Ru3 | 46.9 (3) | C8—C9—C10—C11 | -1.4 (5) |
| C44—Ru1—Ru2—Ru3 | 106.96 (7) | C9—C10—C11—C12 | 1.4 (5) |
| C46—Ru1—Ru2—Ru3 | -70.61 (7) | C10—C11—C12—C7 | 0.1 (5) |
| As1—Ru1—Ru2—Ru3 | -163.409 (9) | C8—C7—C12—C11 | -1.7 (4) |
| C48—Ru2—Ru3—C51 | 18.29 (11) | As1—C7—C12—C11 | 174.8 (2) |
| C47—Ru2—Ru3—C51 | 111.85 (10) | C7—As1—C13—As2 | -96.54 (12) |
| C49—Ru2—Ru3—C51 | -70.64 (10) | C1—As1—C13—As2 | 160.85 (11) |
| As2—Ru2—Ru3—C51 | -161.73 (8) | Ru1—As1—C13—As2 | 33.79 (13) |
| Ru1—Ru2—Ru3—C51 | -166.78 (7) | C20—As2—C13—As1 | -141.78 (12) |
| C48—Ru2—Ru3—C50 | 118.73 (11) | C14—As2—C13—As1 | 111.17 (11) |
| C47—Ru2—Ru3—C50 | -147.71 (9) | Ru2—As2—C13—As1 | -15.57 (13) |
| C49—Ru2—Ru3—C50 | 29.80 (10) | C20—As2—C14—C15 | 104.4 (2) |
| As2—Ru2—Ru3—C50 | -61.29 (7) | C13—As2—C14—C15 | -150.6 (2) |
| Ru1—Ru2—Ru3—C50 | -66.34 (7) | Ru2—As2—C14—C15 | -24.5 (2) |
| C48—Ru2—Ru3—C52 | -74.83 (11) | C20—As2—C14—C19 | -77.1 (2) |
| C47—Ru2—Ru3—C52 | 18.73 (9) | C13—As2—C14—C19 | 27.9 (2) |
| C49—Ru2—Ru3—C52 | -163.76 (10) | Ru2—As2—C14—C19 | 154.01 (16) |
| As2—Ru2—Ru3—C52 | 105.15 (7) | C19—C14—C15—C16 | -0.8 (4) |
| Ru1—Ru2—Ru3—C52 | 100.10 (7) | As2—C14—C15—C16 | 177.8 (3) |
| C48—Ru2—Ru3—Ru1 | -174.93 (8) | C14—C15—C16—C17 | -1.0 (5) |
| C47—Ru2—Ru3—Ru1 | -81.37 (7) | C15—C16—C17—C18 | 1.6 (5) |
| C49—Ru2—Ru3—Ru1 | 96.14 (7) | C16—C17—C18—C19 | -0.5 (5) |
| As2—Ru2—Ru3—Ru1 | 5.05 (2) | C17—C18—C19—C14 | -1.3 (4) |
| C45—Ru1—Ru3—C51 | -146.55 (15) | C15—C14—C19—C18 | 1.9 (4) |
| C44—Ru1—Ru3—C51 | -51.09 (14) | As2—C14—C19—C18 | -176.55 (19) |
| C46—Ru1—Ru3—C51 | 127.24 (14) | C14—As2—C20—C21 | -19.8 (2) |

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|-----------------|---------------|-----------------|--------------|
| As1—Ru1—Ru3—C51 | 54.51 (12) | C13—As2—C20—C21 | -127.3 (2) |
| Ru2—Ru1—Ru3—C51 | 22.67 (12) | Ru2—As2—C20—C21 | 108.2 (2) |
| C45—Ru1—Ru3—C50 | -65.37 (11) | C14—As2—C20—C25 | 162.3 (2) |
| C44—Ru1—Ru3—C50 | 30.08 (10) | C13—As2—C20—C25 | 54.8 (2) |
| C46—Ru1—Ru3—C50 | -151.59 (10) | Ru2—As2—C20—C25 | -69.7 (2) |
| As1—Ru1—Ru3—C50 | 135.69 (7) | C25—C20—C21—C22 | -0.8 (4) |
| Ru2—Ru1—Ru3—C50 | 103.84 (7) | As2—C20—C21—C22 | -178.7 (3) |
| C45—Ru1—Ru3—C52 | 106.35 (10) | C20—C21—C22—C23 | 0.4 (6) |
| C44—Ru1—Ru3—C52 | -158.19 (10) | C21—C22—C23—C24 | -0.2 (7) |
| C46—Ru1—Ru3—C52 | 20.14 (10) | C22—C23—C24—C25 | 0.4 (7) |
| As1—Ru1—Ru3—C52 | -52.59 (7) | C21—C20—C25—C24 | 1.0 (4) |
| Ru2—Ru1—Ru3—C52 | -84.43 (7) | As2—C20—C25—C24 | 179.0 (2) |
| C45—Ru1—Ru3—P1 | 12.06 (8) | C23—C24—C25—C20 | -0.8 (5) |
| C44—Ru1—Ru3—P1 | 107.52 (7) | C38—P1—C26—C27 | -3.9 (2) |
| C46—Ru1—Ru3—P1 | -74.15 (7) | C32—P1—C26—C27 | 102.7 (2) |
| As1—Ru1—Ru3—P1 | -146.88 (2) | Ru3—P1—C26—C27 | -129.9 (2) |
| Ru2—Ru1—Ru3—P1 | -178.723 (18) | C38—P1—C26—C31 | 178.21 (18) |
| C45—Ru1—Ru3—Ru2 | -169.22 (8) | C32—P1—C26—C31 | -75.17 (19) |
| C44—Ru1—Ru3—Ru2 | -73.76 (7) | Ru3—P1—C26—C31 | 52.2 (2) |
| C46—Ru1—Ru3—Ru2 | 104.57 (7) | C31—C26—C27—C28 | -1.5 (4) |
| As1—Ru1—Ru3—Ru2 | 31.841 (15) | P1—C26—C27—C28 | -179.4 (2) |
| C45—Ru1—As1—C7 | -94.36 (10) | C26—C27—C28—C29 | 1.1 (5) |
| C44—Ru1—As1—C7 | 174.09 (9) | C27—C28—C29—C30 | -0.1 (5) |
| C46—Ru1—As1—C7 | -2.46 (9) | C27—C28—C29—F1 | 179.8 (3) |
| Ru2—Ru1—As1—C7 | 92.71 (7) | C28—C29—C30—C31 | -0.4 (5) |
| Ru3—Ru1—As1—C7 | 65.67 (7) | F1—C29—C30—C31 | 179.6 (2) |
| C45—Ru1—As1—C1 | 23.77 (10) | C29—C30—C31—C26 | 0.0 (4) |
| C44—Ru1—As1—C1 | -67.78 (9) | C27—C26—C31—C30 | 0.9 (4) |
| C46—Ru1—As1—C1 | 115.67 (9) | P1—C26—C31—C30 | 179.0 (2) |
| Ru2—Ru1—As1—C1 | -149.17 (7) | C38—P1—C32—C37 | -114.8 (2) |
| Ru3—Ru1—As1—C1 | -176.21 (7) | C26—P1—C32—C37 | 137.4 (2) |
| C45—Ru1—As1—C13 | 141.34 (10) | Ru3—P1—C32—C37 | 10.7 (2) |
| C44—Ru1—As1—C13 | 49.79 (10) | C38—P1—C32—C33 | 63.4 (2) |
| C46—Ru1—As1—C13 | -126.76 (10) | C26—P1—C32—C33 | -44.4 (2) |
| Ru2—Ru1—As1—C13 | -31.59 (7) | Ru3—P1—C32—C33 | -171.08 (16) |
| Ru3—Ru1—As1—C13 | -58.63 (7) | C37—C32—C33—C34 | 0.0 (4) |
| C48—Ru2—As2—C20 | -72.35 (12) | P1—C32—C33—C34 | -178.2 (2) |
| C47—Ru2—As2—C20 | -165.73 (11) | C32—C33—C34—C35 | 0.4 (4) |
| C49—Ru2—As2—C20 | 17.94 (11) | C33—C34—C35—F2 | 179.5 (3) |
| Ru3—Ru2—As2—C20 | 107.67 (9) | C33—C34—C35—C36 | -0.6 (5) |
| Ru1—Ru2—As2—C20 | 112.10 (9) | F2—C35—C36—C37 | -179.7 (3) |
| C48—Ru2—As2—C14 | 49.64 (11) | C34—C35—C36—C37 | 0.4 (4) |
| C47—Ru2—As2—C14 | -43.74 (9) | C33—C32—C37—C36 | -0.2 (4) |
| C49—Ru2—As2—C14 | 139.93 (10) | P1—C32—C37—C36 | 178.0 (2) |
| Ru3—Ru2—As2—C14 | -130.34 (7) | C35—C36—C37—C32 | 0.0 (4) |
| Ru1—Ru2—As2—C14 | -125.91 (7) | C26—P1—C38—C43 | 127.61 (17) |
| C48—Ru2—As2—C13 | 170.28 (11) | C32—P1—C38—C43 | 23.16 (19) |
| C47—Ru2—As2—C13 | 76.90 (10) | Ru3—P1—C38—C43 | -104.75 (16) |

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| C49—Ru2—As2—C13 | -99.43 (10) | C26—P1—C38—C39 | -59.03 (19) |
| Ru3—Ru2—As2—C13 | -9.70 (8) | C32—P1—C38—C39 | -163.47 (17) |
| Ru1—Ru2—As2—C13 | -5.27 (7) | Ru3—P1—C38—C39 | 68.62 (18) |
| C51—Ru3—P1—C38 | 162.57 (11) | C43—C38—C39—C40 | -1.8 (3) |
| C50—Ru3—P1—C38 | 62.24 (10) | P1—C38—C39—C40 | -175.41 (18) |
| C52—Ru3—P1—C38 | -104.31 (10) | C38—C39—C40—C41 | 1.0 (4) |
| Ru1—Ru3—P1—C38 | -4.83 (8) | C39—C40—C41—C42 | 0.6 (4) |
| C51—Ru3—P1—C26 | -76.00 (11) | C39—C40—C41—F3 | 178.7 (2) |
| C50—Ru3—P1—C26 | -176.34 (11) | F3—C41—C42—C43 | -179.3 (2) |
| C52—Ru3—P1—C26 | 17.11 (11) | C40—C41—C42—C43 | -1.2 (4) |
| Ru1—Ru3—P1—C26 | 116.59 (9) | C41—C42—C43—C38 | 0.3 (3) |
| C51—Ru3—P1—C32 | 42.38 (11) | C39—C38—C43—C42 | 1.2 (3) |
| C50—Ru3—P1—C32 | -57.95 (10) | P1—C38—C43—C42 | 174.69 (16) |
| C52—Ru3—P1—C32 | 135.50 (10) | C51—Ru3—C50—O7 | -60.1 (11) |
| Ru1—Ru3—P1—C32 | -125.03 (8) | C52—Ru3—C50—O7 | 119.1 (11) |
| C7—As1—C1—C6 | 157.51 (19) | P1—Ru3—C50—O7 | 37.6 (11) |
| C13—As1—C1—C6 | -94.8 (2) | Ru2—Ru3—C50—O7 | -146.5 (11) |
| Ru1—As1—C1—C6 | 30.1 (2) | Ru1—Ru3—C50—O7 | 156.4 (11) |

Hydrogen-bond geometry (\AA , $^\circ$)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|---|-------------|---------------------|----------------------------|-------------------------------|
| C23—H23 <i>A</i> \cdots F3 ⁱ | 0.93 | 2.46 | 3.337 (5) | 157 |
| C34—H34 <i>A</i> \cdots O3 ⁱⁱ | 0.93 | 2.58 | 3.405 (3) | 148 |
| C42—H42 <i>A</i> \cdots O2 ⁱⁱⁱ | 0.93 | 2.52 | 3.438 (3) | 167 |
| C11—H11 <i>A</i> \cdots Cg1 ^{iv} | 0.93 | 2.94 | 3.767 (3) | 149 |
| C28—H28 <i>A</i> \cdots Cg2 ⁱⁱ | 0.93 | 2.89 | 3.807 (3) | 168 |

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