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Crystal structure of tris(2-dicyclohexylphosphino-2',6'-dimethoxy-1,1'-biphenyl- κP)- μ -oxoethenylidene-*triangulo*-trigold(I) bis(trifluoromethanesulfonyl)imide

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The title ketenylidene, $[\text{Au}_3(\text{C}_2\text{O})(\text{C}_{26}\text{H}_{35}\text{O}_2\text{P})_3](\text{C}_2\text{F}_6\text{NO}_4\text{S}_2)$, was obtained upon exposure of [2-(dicyclohexylphosphino)-2',6'-dimethoxy-1,1'-biphenyl]-gold(I) bis(trifluoromethanesulfonyl)imide to acetic anhydride at elevated temperature. The ketenylidene bridge caps the tri-gold cluster. The title compound has provided crystals that upon analysis represent the first tri-gold ketenylidene with atomic distances indicative of bonding interaction between the gold atoms.

1. Chemical context

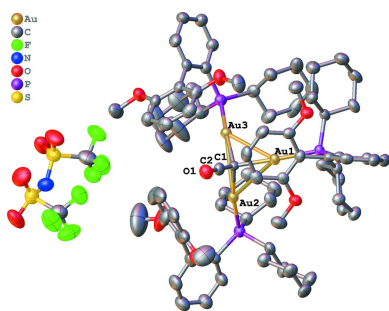
Metal clusters containing ketenylidenes are of interest for their wide range of applications. For instance, ketenylidenes are useful for facilitating C–C bond formation and cleavage (Went *et al.*, 1987), metal cluster building (Sailor & Shriver, 1985), and as potential intermediates for carbon monoxide chemistry (Jensen & Shriver, 1992). One of the first transition-metal ketenylidene complexes described was a tricobalt cluster reported by Seyferth *et al.* in 1974 (Seyferth *et al.*, 1974). Since then, the scope of ketenylidene clusters has been expanded to include metals such as osmium (Went *et al.*, 1987), ruthenium (Sailor & Shriver, 1985), molybdenum (Ramalakshmi *et al.*, 2015), and manganese (Crespi & Shriver, 1986) to name a few.

However, relatively few ketenylidenes involving gold have been reported. Work by Green and co-workers uncovered a surface-bound gold ketenylidene $[\text{Au}_2\text{CCO}]$, which serves as a reactive intermediate in the aerobic oxidation of acetic acid on Au/TiO₂ surfaces (Green *et al.*, 2012). More recently, Daugherty and co-workers reported the first instance of a tri-gold ketenylidene (Daugherty *et al.*, 2017). In that case, the Au···Au distances suggest that there is no bonding interaction between the metal atoms.

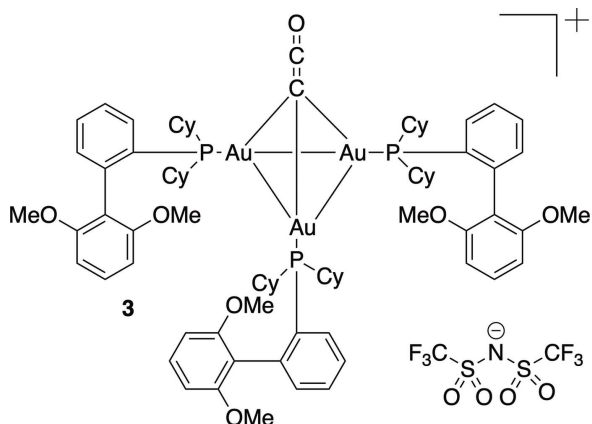
Herein, we describe the first crystal structure analysis of a tri-gold ketenylidene in which the atomic distances suggest a bonding interaction between the gold atoms

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. Four molecules are present in the unit cell ($Z = 4$) and there is one component in the asymmetric unit. The title



compound consists of three molecules of (2-dicyclohexylphosphino-2',6'-dimethoxy-1,1'-biphenyl)gold(I) bis(trifluoromethanesulfonyl)imide capped by a ketylidene unit (C=C=O) to form a tri-gold cluster. The tri-gold cluster has an overall charge of +1, with trifluoromethanesulfonylimide serving as the counter-ion. As shown in Fig. 1, the ketylidene atoms (C=C=O) form an angle of 88.1 (5)° with the mean Au1–Au2–Au3 gold plane.



The Au–Au bond distances suggest auriphilic interaction (Schmidbaur & Schier, 2012). The shortest Au–Au bond length is 3.1910 (5) Å (Au1–Au3), which is significantly shorter than the sum of two van der Waals radii (Bondi, 1964). The Au2–Au3 bond length of 3.2101 (5) Å also indicates a

significant Au–Au interaction, although the complex is not entirely symmetrical, with the Au1–Au2 bond length measuring 3.3005 (5) Å. Other bond lengths within the cluster are more highly conserved within each subunit of the trimeric structure [e.g. Au–C1 distances: 2.090 (7) to 2.098 (7) Å; Au–P distances: 2.273 (2) to 2.281 (2) Å].

3. Supramolecular features

In the crystal structure of the title compound, the discrete complexes are arranged into columns along the *b* axis (Fig. 2). Within these columns, the ketylidene atoms alternate between the +*a* and –*a*-axis directions. The only other similar cluster with Au was reported by Daugherty and co-workers (Daugherty *et al.*, 2017), and it does not show this alternating arrangement. However, in this earlier case, the Au atoms are all bonded to the carbon of *N*-heterocyclic carbene ligands, rather than to phosphines. As such, the title compound is the first trimetallic ketylidene cluster of any metal that involves the metal bound to only phosphine and the ketylidene bridge, rather than the more common C=O ligand found in most trimetallic metal complexes in the CSD.

4. Database survey

The Cambridge Structural Database (CSD, Version 5.42, February 2021; Groom *et al.*, 2016) contains 12 unique struc-

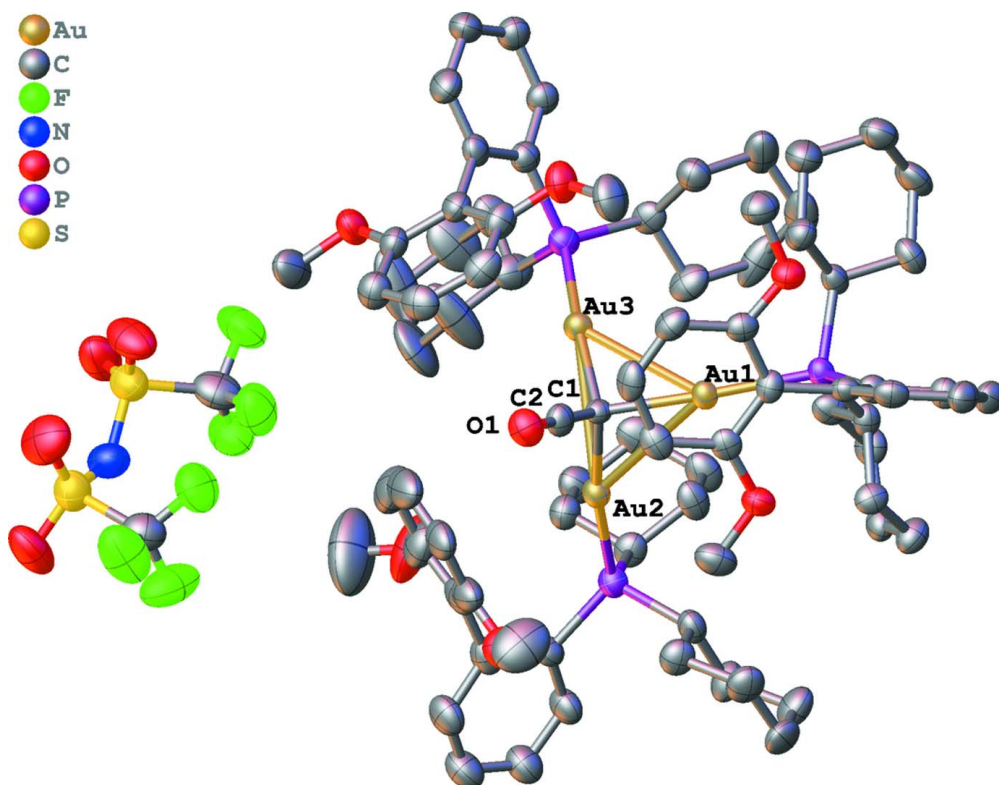


Figure 1

The molecular structure of the title compound with select atom labeling. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are omitted for clarity reasons.

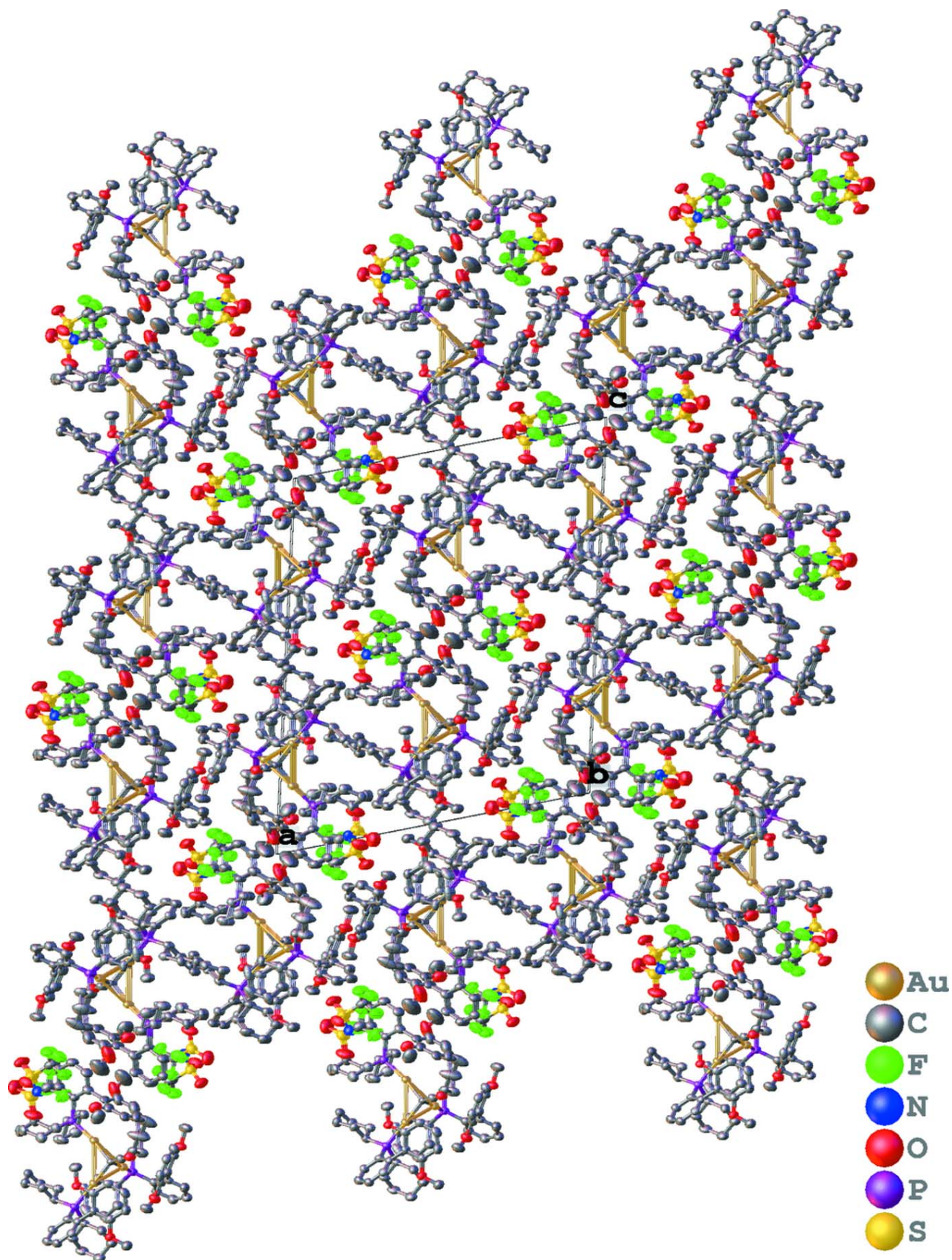


Figure 2
Packing diagram of the title compound along the *b* axis.

tures of ketylidene-bridged metal clusters. Of these, ten contain clusters of three metal atoms, including: all iron (CAXVAY, Kolis *et al.*, 1983; GEFPIQ, Bogdan *et al.*, 1988), all ruthenium (DELSAO, Sailor & Shriver, 1985; FONWAG, Sailor *et al.*, 1987), all osmium (FONYEM, Went *et al.*, 1987), and all gold(I) (LEBFOQ, Daugherty *et al.*, 2017) and various combinations of iron, cobalt, manganese, molybdenum, and ruthenium (DUHDIT, Crespi & Shriver, 1986 and Crespi *et al.*, 1988; GAHBIA, Ching *et al.*, 1988; HUQBIG, Ramalakshmi *et al.*, 2015; KALVAU, Ching *et al.*, 1989). Two additional structures of this type with central clusters of four metal atoms, either three ruthenium and one copper (PAJWOM, Gunale *et al.*, 1992) or three iron and one copper (KINFOC10, Gunale *et al.*, 1992) have also been reported. Within this group, only one 2Fe/1Co cluster bears a phosphine ligand (KALVAU, Ching *et al.*, 1989) similar to the reported title compound; however, even in this case, the reported cluster is much simpler than the title compound, as all of the remaining positions are occupied by CO.

The only other known all gold(I) cluster (LEBFOQ, Daugherty *et al.*, 2017) differs from both the reported title compound as well as the other structures in the CSD, as it bears *N*-heterocyclic carbene ligands attached to gold, rather than either phosphines or carbon monoxide ligands. Additionally, the gold(I) atoms in this previously reported cluster were too far apart from each other to have any metal–metal bonding interaction.

Thus, the reported ketylidene cluster differs from similar compounds in the CSD in both the title cluster's unique phosphine ligands and the short Au–Au bonding interactions.

5. Synthesis and crystallization

The title compound was observed during scope studies related to the gold(I)-catalyzed synthesis of trisubstituted indolizine **2**

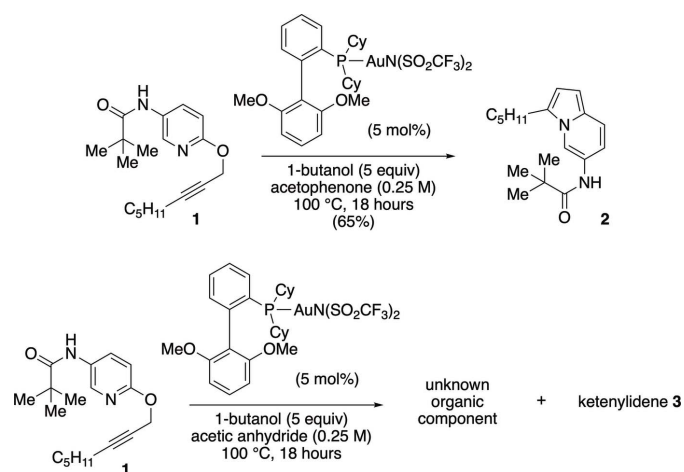


Figure 3

Reaction scheme. The title ketenylidene **3** was discovered as an unexpected by-product of a reaction exploring the gold(I)-catalyzed rearrangement of 2-propargyloxypyridine **1**.

Table 1

Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | [Au ₃ (C ₂ O)(C ₂₆ H ₃₅ O ₂ P) ₃] ⁻ (C ₂ F ₆ NO ₄ S ₂) |
| <i>M_r</i> | 2142.59 |
| Crystal system, space group | Monoclinic, <i>P</i> 2 ₁ / <i>n</i> |
| Temperature (K) | 173 |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 24.0018 (3), 12.4867 (1), 28.4299 (3) |
| β (°) | 103.7669 (8) |
| <i>V</i> (Å ³) | 8275.75 (15) |
| <i>Z</i> | 4 |
| Radiation type | Cu <i>K</i> α |
| μ (mm ⁻¹) | 11.42 |
| Crystal size (mm) | 0.2 × 0.05 × 0.03 |
| Data collection | |
| Diffractionmeter | Bruker APEXII CCD |
| Absorption correction | Multi-scan (SADABS; Bruker, 2013) |
| <i>T_{min}</i> , <i>T_{max}</i> | 0.321, 0.735 |
| No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections | 73587, 15716, 11064 |
| <i>R_{int}</i> | 0.110 |
| (<i>sin</i> θ / λ) _{max} (Å ⁻¹) | 0.610 |
| Refinement | |
| <i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i> | 0.048, 0.120, 1.01 |
| No. of reflections | 15716 |
| No. of parameters | 979 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³) | 1.77, -0.95 |

Computer programs: COSMO and SAINT (Bruker, 2013), SHELXT (Sheldrick, 2015a), SHELXL2018/3 (Sheldrick, 2015b) and OLEX2 (Dolomanov *et al.*, 2009).

from 2-propargyloxypyridine **1** (Rossler *et al.*, 2019). While initial studies had shown that treatment of pyridine **1** with methyl ketones in the presence of alcohols and (2-dicyclohexylphosphino-2',6'-dimethoxy-1,1'-biphenyl)gold(I) bis(trifluoromethane-sulfonyl)imide could provide trisubstituted indolizines **2** in moderate to good yields, when the methyl ketone was replaced with acetic anhydride, an unknown organic product and the title ketylidene cluster **3** were observed (Fig. 3). In an attempt to determine the organic product of the reaction, crystals were grown by the slow evaporation of a concentrated ethanol solution over several weeks at room temperature. Using this method, a few tiny yellow needle-shaped crystals, suitable for X-ray diffraction, were obtained and analyzed. However, rather than revealing the structure of the organic product as expected, the X-ray structure revealed the title ketylidene-bridged tri-gold cluster **3**. Subsequent studies aimed at the independent synthesis of cluster **3** and related species stoichiometrically were unsuccessful.

6. Refinement

Crystal data, data collection, and refinement details are collected in Table 1. All non-hydrogen atoms were refined anisotropically. Hydrogen-atom positions were calculated geometrically (C–H = 0.95–1.00 Å) and refined using a riding model with *U*_{iso}(H) = 1.2*U*_{eq}(C) or 1.5*U*_{eq}(C-methyl).

Acknowledgements

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supporting information

Acta Cryst. (2021). E77, 537-541 [https://doi.org/10.1107/S2056989021003844]

Crystal structure of tris(2-dicyclohexylphosphino-2',6'-dimethoxy-1,1'-biphenyl- κ P)- μ -oxoethenyldene-triangulo-trigold(I) bis(trifluoromethanesulfonyl)imide

Colin T. Hartgerink, Richard J. Staples and Carolyn E. Anderson

Computing details

Data collection: *COSMO* (Bruker, 2013); cell refinement: *SAINTE* (Bruker, 2013); data reduction: *SAINTE* (Bruker, 2013); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *Olex2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *Olex2* (Dolomanov *et al.*, 2009).

Tris(2-dicyclohexylphosphino-2',6'-dimethoxy-1,1'-biphenyl- κ P)- μ -oxoethenyldene-triangulo-trigold(I) bis(trifluoromethanesulfonyl)imide

Crystal data

[Au₃(C₂O)(C₂₆H₃₅O₂P)₃](C₂F₆NO₄S₂)
 $M_r = 2142.59$
 Monoclinic, $P2_1/n$
 $a = 24.0018$ (3) Å
 $b = 12.4867$ (1) Å
 $c = 28.4299$ (3) Å
 $\beta = 103.7669$ (8)°
 $V = 8275.75$ (15) Å³
 $Z = 4$

$F(000) = 4240$
 $D_x = 1.720$ Mg m⁻³
 Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
 Cell parameters from 9988 reflections
 $\theta = 2.2\text{--}70.1^\circ$
 $\mu = 11.42$ mm⁻¹
 $T = 173$ K
 Needle, yellow
 0.2 × 0.05 × 0.03 mm

Data collection

Bruker APEXII CCD
 diffractometer
 Radiation source: sealed tube
 Graphite monochromator
 Detector resolution: 8.36 pixels mm⁻¹
 ω and φ scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2013)
 $T_{\min} = 0.321$, $T_{\max} = 0.735$

73587 measured reflections
 15716 independent reflections
 11064 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.110$
 $\theta_{\max} = 70.1^\circ$, $\theta_{\min} = 2.2^\circ$
 $h = -29\text{--}28$
 $k = -15\text{--}15$
 $l = -34\text{--}34$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.120$
 $S = 1.01$
 15716 reflections

979 parameters
 0 restraints
 Primary atom site location: dual
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2 + 20.5744P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 1.77 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.95 \text{ e } \text{\AA}^{-3}$$

Special details

Experimental. Data was collected using a BRUKER CCD (charge coupled device) based diffractometer equipped with an Oxford low-temperature apparatus operating at 173 K. A suitable crystal was chosen and mounted on a nylon loop using Paratone oil. Data were measured using omega scans of 0.5° per frame for 30 s. The total number of images were based on results from the program COSMO where redundancy was expected to be 4 and completeness to 0.83Å to 100%. Cell parameters were retrieved using APEX II software and refined using SAINT on all observed reflections. Data reduction was performed using the SAINT software which corrects for Lp. Scaling and absorption corrections were applied using SADABS6 multi-scan technique, supplied by George Sheldrick. The structure was solved by the direct method using the SHELXT program and refined by least squares method on F2, SHELXL, incorporated in OLEX2.

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

Refinement. The structure was refined by Least Squares using version 2014/6 of XL (Sheldrick, 2008) incorporated in Olex2 (Dolomanov *et al.*, 2009). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model.'

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

| | <i>x</i> | <i>y</i> | <i>z</i> | <i>U</i> _{iso} */ <i>U</i> _{eq} |
|-----|--------------|--------------|-------------|---|
| Au1 | 0.53937 (2) | 0.36171 (3) | 0.21151 (2) | 0.03027 (9) |
| Au2 | 0.54502 (2) | 0.30927 (3) | 0.32634 (2) | 0.03393 (9) |
| Au3 | 0.44934 (2) | 0.20237 (3) | 0.24086 (2) | 0.03374 (9) |
| P1 | 0.59759 (9) | 0.34972 (16) | 0.15898 (8) | 0.0314 (4) |
| P2 | 0.61858 (10) | 0.26651 (18) | 0.39059 (8) | 0.0368 (5) |
| P3 | 0.41808 (10) | 0.03219 (17) | 0.22248 (8) | 0.0364 (5) |
| O1 | 0.4258 (3) | 0.5067 (5) | 0.2643 (2) | 0.0507 (16) |
| O2 | 0.5926 (3) | 0.6146 (5) | 0.2136 (2) | 0.0412 (14) |
| O3 | 0.4780 (3) | 0.5587 (5) | 0.0590 (2) | 0.0425 (14) |
| O4 | 0.4879 (4) | 0.2011 (9) | 0.4500 (5) | 0.118 (4) |
| O5 | 0.5453 (4) | 0.5423 (6) | 0.4146 (3) | 0.071 (2) |
| O6 | 0.2659 (3) | 0.1195 (5) | 0.2662 (2) | 0.0518 (17) |
| O7 | 0.3411 (3) | 0.2431 (6) | 0.1389 (3) | 0.0555 (18) |
| C1 | 0.4875 (3) | 0.3511 (6) | 0.2611 (3) | 0.0274 (16) |
| C2 | 0.4552 (4) | 0.4319 (7) | 0.2631 (3) | 0.038 (2) |
| C3 | 0.6180 (4) | 0.4679 (6) | 0.1282 (3) | 0.0336 (18) |
| C4 | 0.6653 (4) | 0.4587 (7) | 0.1086 (3) | 0.0367 (19) |
| H4 | 0.688034 | 0.395750 | 0.115090 | 0.044* |
| C5 | 0.6808 (4) | 0.5367 (7) | 0.0801 (3) | 0.043 (2) |
| H5 | 0.713897 | 0.527777 | 0.067595 | 0.052* |
| C6 | 0.6482 (4) | 0.6270 (8) | 0.0698 (3) | 0.043 (2) |
| H6 | 0.657838 | 0.680655 | 0.049466 | 0.052* |
| C7 | 0.6006 (4) | 0.6402 (7) | 0.0894 (3) | 0.040 (2) |
| H7 | 0.578703 | 0.704180 | 0.082893 | 0.048* |
| C8 | 0.5845 (3) | 0.5616 (6) | 0.1184 (3) | 0.0330 (18) |
| C9 | 0.5331 (3) | 0.5833 (6) | 0.1374 (3) | 0.0340 (18) |

| | | | | |
|------|------------|------------|------------|-------------|
| C10 | 0.5377 (4) | 0.6131 (6) | 0.1857 (3) | 0.0339 (18) |
| C11 | 0.4892 (4) | 0.6375 (7) | 0.2022 (3) | 0.043 (2) |
| H11 | 0.492373 | 0.655634 | 0.235195 | 0.052* |
| C12 | 0.4365 (4) | 0.6351 (7) | 0.1700 (4) | 0.046 (2) |
| H12 | 0.403331 | 0.652251 | 0.181156 | 0.055* |
| C13 | 0.4304 (4) | 0.6090 (7) | 0.1224 (4) | 0.044 (2) |
| H13 | 0.393527 | 0.607929 | 0.100791 | 0.053* |
| C14 | 0.4790 (4) | 0.5838 (6) | 0.1060 (3) | 0.0366 (19) |
| C15 | 0.6001 (5) | 0.6310 (8) | 0.2644 (4) | 0.058 (3) |
| H15A | 0.584512 | 0.701133 | 0.270078 | 0.087* |
| H15B | 0.641006 | 0.628363 | 0.280373 | 0.087* |
| H15C | 0.579768 | 0.574788 | 0.277735 | 0.087* |
| C16 | 0.4226 (4) | 0.5417 (9) | 0.0267 (4) | 0.056 (3) |
| H16A | 0.427567 | 0.514674 | -0.004380 | 0.083* |
| H16B | 0.401483 | 0.609579 | 0.021584 | 0.083* |
| H16C | 0.400999 | 0.489350 | 0.040980 | 0.083* |
| C17 | 0.5643 (4) | 0.2573 (7) | 0.1096 (3) | 0.0347 (18) |
| H17 | 0.554779 | 0.190324 | 0.125365 | 0.042* |
| C18 | 0.6013 (4) | 0.2237 (7) | 0.0751 (3) | 0.044 (2) |
| H18A | 0.611749 | 0.287751 | 0.058530 | 0.053* |
| H18B | 0.637162 | 0.190220 | 0.093769 | 0.053* |
| C19 | 0.5692 (5) | 0.1446 (8) | 0.0374 (4) | 0.057 (3) |
| H19A | 0.593181 | 0.126978 | 0.014542 | 0.068* |
| H19B | 0.562425 | 0.077565 | 0.053808 | 0.068* |
| C20 | 0.5121 (5) | 0.1897 (9) | 0.0094 (4) | 0.057 (3) |
| H20A | 0.519205 | 0.251229 | -0.010338 | 0.068* |
| H20B | 0.491462 | 0.134176 | -0.013001 | 0.068* |
| C21 | 0.4745 (5) | 0.2260 (9) | 0.0425 (4) | 0.057 (3) |
| H21A | 0.462137 | 0.162899 | 0.058536 | 0.069* |
| H21B | 0.439727 | 0.261723 | 0.023096 | 0.069* |
| C22 | 0.5074 (4) | 0.3038 (7) | 0.0810 (4) | 0.044 (2) |
| H22A | 0.514978 | 0.370838 | 0.065036 | 0.053* |
| H22B | 0.483260 | 0.321855 | 0.103709 | 0.053* |
| C23 | 0.6663 (4) | 0.2883 (6) | 0.1892 (3) | 0.0347 (18) |
| H23 | 0.687237 | 0.268777 | 0.163914 | 0.042* |
| C24 | 0.6562 (4) | 0.1845 (6) | 0.2160 (3) | 0.041 (2) |
| H24A | 0.636134 | 0.202298 | 0.241689 | 0.049* |
| H24B | 0.631552 | 0.134861 | 0.192923 | 0.049* |
| C25 | 0.7139 (4) | 0.1300 (7) | 0.2387 (4) | 0.046 (2) |
| H25A | 0.706969 | 0.065621 | 0.256844 | 0.056* |
| H25B | 0.732180 | 0.106649 | 0.212692 | 0.056* |
| C26 | 0.7544 (4) | 0.2061 (8) | 0.2731 (3) | 0.043 (2) |
| H26A | 0.738786 | 0.220874 | 0.301645 | 0.052* |
| H26B | 0.792276 | 0.171329 | 0.284525 | 0.052* |
| C27 | 0.7619 (4) | 0.3117 (8) | 0.2480 (4) | 0.048 (2) |
| H27A | 0.785333 | 0.361275 | 0.271920 | 0.058* |
| H27B | 0.782679 | 0.298093 | 0.222420 | 0.058* |
| C28 | 0.7043 (4) | 0.3639 (7) | 0.2255 (3) | 0.0383 (19) |

| | | | | |
|------|------------|-------------|------------|------------|
| H28A | 0.710730 | 0.430873 | 0.208902 | 0.046* |
| H28B | 0.684717 | 0.382670 | 0.251365 | 0.046* |
| C29 | 0.6169 (4) | 0.3013 (7) | 0.4529 (3) | 0.040 (2) |
| C30 | 0.6664 (4) | 0.2764 (8) | 0.4899 (4) | 0.051 (2) |
| H30 | 0.696362 | 0.235542 | 0.482178 | 0.061* |
| C31 | 0.6715 (5) | 0.3106 (9) | 0.5367 (4) | 0.058 (3) |
| H31 | 0.704642 | 0.293109 | 0.561268 | 0.069* |
| C32 | 0.6277 (5) | 0.3712 (9) | 0.5478 (4) | 0.060 (3) |
| H32 | 0.631325 | 0.397685 | 0.579737 | 0.072* |
| C33 | 0.5792 (5) | 0.3923 (8) | 0.5125 (4) | 0.058 (3) |
| H33 | 0.549451 | 0.433181 | 0.520603 | 0.069* |
| C34 | 0.5723 (4) | 0.3561 (8) | 0.4655 (4) | 0.049 (2) |
| C35 | 0.5158 (4) | 0.3740 (9) | 0.4305 (4) | 0.052 (3) |
| C36 | 0.4742 (5) | 0.2971 (11) | 0.4246 (5) | 0.071 (3) |
| C37 | 0.4210 (6) | 0.3079 (13) | 0.3935 (6) | 0.090 (5) |
| H37 | 0.393316 | 0.252199 | 0.389193 | 0.108* |
| C38 | 0.4098 (5) | 0.4049 (13) | 0.3686 (5) | 0.082 (4) |
| H38 | 0.373598 | 0.414986 | 0.346543 | 0.098* |
| C39 | 0.4489 (5) | 0.4852 (10) | 0.3748 (4) | 0.061 (3) |
| H39 | 0.440122 | 0.551058 | 0.357920 | 0.073* |
| C40 | 0.5020 (4) | 0.4694 (10) | 0.4064 (4) | 0.058 (3) |
| C41 | 0.4611 (9) | 0.1637 (19) | 0.4802 (8) | 0.178 (11) |
| H41A | 0.454369 | 0.086915 | 0.474341 | 0.268* |
| H41B | 0.424264 | 0.200710 | 0.476118 | 0.268* |
| H41C | 0.484121 | 0.174786 | 0.513242 | 0.268* |
| C42 | 0.5349 (7) | 0.6405 (12) | 0.3875 (6) | 0.106 (5) |
| H42A | 0.531818 | 0.625531 | 0.353136 | 0.160* |
| H42B | 0.566778 | 0.690217 | 0.399398 | 0.160* |
| H42C | 0.499126 | 0.672768 | 0.391507 | 0.160* |
| C43 | 0.6354 (4) | 0.1216 (7) | 0.3930 (4) | 0.043 (2) |
| H43 | 0.669434 | 0.108234 | 0.420426 | 0.052* |
| C44 | 0.5838 (4) | 0.0590 (7) | 0.4024 (4) | 0.045 (2) |
| H44A | 0.575897 | 0.082988 | 0.433312 | 0.054* |
| H44B | 0.549456 | 0.074185 | 0.376123 | 0.054* |
| C45 | 0.5956 (5) | -0.0607 (8) | 0.4046 (4) | 0.053 (3) |
| H45A | 0.628158 | -0.076379 | 0.432397 | 0.064* |
| H45B | 0.561465 | -0.099116 | 0.409858 | 0.064* |
| C46 | 0.6095 (5) | -0.1007 (7) | 0.3584 (4) | 0.059 (3) |
| H46A | 0.575521 | -0.092007 | 0.331002 | 0.070* |
| H46B | 0.619145 | -0.177892 | 0.361620 | 0.070* |
| C47 | 0.6599 (5) | -0.0383 (7) | 0.3481 (4) | 0.055 (3) |
| H47A | 0.667039 | -0.062736 | 0.316940 | 0.066* |
| H47B | 0.694749 | -0.053823 | 0.373861 | 0.066* |
| C48 | 0.6493 (5) | 0.0829 (7) | 0.3458 (4) | 0.048 (2) |
| H48A | 0.616908 | 0.099917 | 0.318028 | 0.057* |
| H48B | 0.683828 | 0.120460 | 0.340921 | 0.057* |
| C49 | 0.6807 (4) | 0.3412 (7) | 0.3790 (3) | 0.042 (2) |
| H49 | 0.681878 | 0.324040 | 0.344894 | 0.051* |

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|------|------------|-------------|------------|-------------|
| C50 | 0.7410 (4) | 0.3146 (8) | 0.4104 (4) | 0.052 (2) |
| H50A | 0.743247 | 0.334052 | 0.444534 | 0.062* |
| H50B | 0.748318 | 0.236771 | 0.408944 | 0.062* |
| C51 | 0.7866 (4) | 0.3773 (9) | 0.3916 (5) | 0.061 (3) |
| H51A | 0.825119 | 0.361399 | 0.412326 | 0.073* |
| H51B | 0.786035 | 0.353851 | 0.358255 | 0.073* |
| C52 | 0.7760 (4) | 0.4959 (8) | 0.3918 (4) | 0.055 (3) |
| H52A | 0.804607 | 0.533685 | 0.377895 | 0.066* |
| H52B | 0.780626 | 0.520844 | 0.425589 | 0.066* |
| C53 | 0.7158 (4) | 0.5233 (8) | 0.3625 (4) | 0.056 (3) |
| H53A | 0.712916 | 0.506597 | 0.327995 | 0.067* |
| H53B | 0.709109 | 0.601050 | 0.365162 | 0.067* |
| C54 | 0.6692 (4) | 0.4610 (7) | 0.3799 (4) | 0.049 (2) |
| H54A | 0.668976 | 0.483412 | 0.413288 | 0.059* |
| H54B | 0.631127 | 0.477376 | 0.358665 | 0.059* |
| C55 | 0.3468 (4) | 0.0062 (7) | 0.1833 (3) | 0.0379 (19) |
| C56 | 0.3376 (4) | -0.0890 (7) | 0.1569 (3) | 0.043 (2) |
| H56 | 0.368843 | -0.136941 | 0.158874 | 0.051* |
| C57 | 0.2845 (4) | -0.1157 (8) | 0.1280 (4) | 0.048 (2) |
| H57 | 0.279522 | -0.180323 | 0.109843 | 0.058* |
| C58 | 0.2396 (4) | -0.0482 (8) | 0.1260 (4) | 0.052 (3) |
| H58 | 0.202989 | -0.065319 | 0.106163 | 0.062* |
| C59 | 0.2471 (4) | 0.0462 (9) | 0.1531 (4) | 0.051 (2) |
| H59 | 0.214942 | 0.090974 | 0.152273 | 0.061* |
| C60 | 0.2999 (4) | 0.0761 (7) | 0.1808 (3) | 0.038 (2) |
| C61 | 0.3043 (4) | 0.1850 (7) | 0.2036 (3) | 0.040 (2) |
| C62 | 0.2853 (4) | 0.2068 (7) | 0.2452 (3) | 0.041 (2) |
| C63 | 0.2845 (4) | 0.3103 (8) | 0.2625 (4) | 0.052 (2) |
| H63 | 0.270172 | 0.324800 | 0.290286 | 0.063* |
| C64 | 0.3049 (4) | 0.3914 (8) | 0.2387 (4) | 0.050 (2) |
| H64 | 0.305709 | 0.462204 | 0.251004 | 0.060* |
| C65 | 0.3242 (4) | 0.3736 (7) | 0.1976 (4) | 0.051 (2) |
| H65 | 0.337491 | 0.431394 | 0.181520 | 0.061* |
| C66 | 0.3239 (4) | 0.2710 (7) | 0.1802 (4) | 0.044 (2) |
| C67 | 0.2525 (6) | 0.1374 (10) | 0.3121 (4) | 0.070 (3) |
| H67A | 0.218638 | 0.183715 | 0.307596 | 0.105* |
| H67B | 0.285073 | 0.172065 | 0.334161 | 0.105* |
| H67C | 0.244473 | 0.068721 | 0.325783 | 0.105* |
| C68 | 0.3657 (5) | 0.3256 (9) | 0.1159 (4) | 0.068 (3) |
| H68A | 0.376332 | 0.296503 | 0.087230 | 0.102* |
| H68B | 0.399909 | 0.353722 | 0.138478 | 0.102* |
| H68C | 0.337692 | 0.383396 | 0.106079 | 0.102* |
| C69 | 0.4678 (4) | -0.0396 (7) | 0.1926 (3) | 0.041 (2) |
| H69 | 0.458485 | -0.117645 | 0.192114 | 0.049* |
| C70 | 0.5302 (4) | -0.0252 (8) | 0.2206 (4) | 0.056 (3) |
| H70A | 0.534730 | -0.049412 | 0.254429 | 0.067* |
| H70B | 0.540854 | 0.051437 | 0.221069 | 0.067* |
| C71 | 0.5697 (4) | -0.0910 (8) | 0.1962 (5) | 0.071 (4) |

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|------|--------------|--------------|--------------|------------|
| H71A | 0.610169 | -0.077509 | 0.213111 | 0.085* |
| H71B | 0.561906 | -0.168218 | 0.199365 | 0.085* |
| C72 | 0.5613 (5) | -0.0634 (8) | 0.1429 (5) | 0.071 (4) |
| H72A | 0.576272 | 0.009536 | 0.140059 | 0.085* |
| H72B | 0.583877 | -0.113960 | 0.128011 | 0.085* |
| C73 | 0.4995 (5) | -0.0681 (9) | 0.1153 (5) | 0.069 (4) |
| H73A | 0.486483 | -0.143518 | 0.112594 | 0.083* |
| H73B | 0.496094 | -0.040098 | 0.082154 | 0.083* |
| C74 | 0.4611 (4) | -0.0027 (7) | 0.1402 (3) | 0.048 (2) |
| H74A | 0.420620 | -0.010943 | 0.122242 | 0.057* |
| H74B | 0.471363 | 0.074001 | 0.139774 | 0.057* |
| C75 | 0.4208 (5) | -0.0479 (9) | 0.2776 (4) | 0.057 (3) |
| H75 | 0.462643 | -0.061847 | 0.290921 | 0.069* |
| C76 | 0.3946 (6) | -0.1572 (8) | 0.2695 (4) | 0.061 (3) |
| H76A | 0.413062 | -0.196718 | 0.247087 | 0.073* |
| H76B | 0.353463 | -0.149391 | 0.253436 | 0.073* |
| C77 | 0.3998 (8) | -0.2226 (10) | 0.3145 (5) | 0.100 (5) |
| H77A | 0.375486 | -0.287293 | 0.306663 | 0.120* |
| H77B | 0.440066 | -0.246404 | 0.326290 | 0.120* |
| C78 | 0.3830 (9) | -0.1643 (11) | 0.3516 (6) | 0.131 (8) |
| H78A | 0.391791 | -0.208200 | 0.381419 | 0.157* |
| H78B | 0.340910 | -0.154361 | 0.342031 | 0.157* |
| C79 | 0.4115 (8) | -0.0526 (13) | 0.3637 (5) | 0.105 (6) |
| H79A | 0.393233 | -0.013570 | 0.386334 | 0.126* |
| H79B | 0.452864 | -0.060859 | 0.379026 | 0.126* |
| C80 | 0.4034 (10) | 0.0097 (10) | 0.3158 (5) | 0.127 (8) |
| H80A | 0.362459 | 0.029214 | 0.304421 | 0.152* |
| H80B | 0.425722 | 0.077068 | 0.322131 | 0.152* |
| S1A | 0.24408 (13) | 0.2219 (2) | 0.52100 (11) | 0.0607 (7) |
| S2A | 0.24474 (12) | 0.0341 (3) | 0.46694 (11) | 0.0639 (7) |
| F1A | 0.3480 (4) | 0.2976 (7) | 0.5371 (3) | 0.112 (3) |
| F2A | 0.2805 (5) | 0.4110 (6) | 0.5073 (3) | 0.110 (3) |
| F3A | 0.3042 (3) | 0.2920 (6) | 0.4621 (3) | 0.086 (2) |
| F4A | 0.3499 (3) | -0.0314 (6) | 0.4807 (3) | 0.081 (2) |
| F5A | 0.2957 (4) | -0.0660 (7) | 0.4113 (3) | 0.092 (2) |
| F6A | 0.3264 (4) | 0.0971 (6) | 0.4288 (3) | 0.095 (3) |
| O1A | 0.1904 (4) | 0.2535 (8) | 0.4885 (4) | 0.096 (3) |
| O2A | 0.2535 (5) | 0.2361 (7) | 0.5724 (3) | 0.092 (3) |
| O3A | 0.2090 (4) | 0.0861 (8) | 0.4249 (3) | 0.086 (3) |
| O4A | 0.2313 (4) | -0.0722 (7) | 0.4819 (3) | 0.085 (3) |
| N1A | 0.2676 (4) | 0.1084 (7) | 0.5117 (4) | 0.065 (3) |
| C1A | 0.2971 (6) | 0.3084 (10) | 0.5070 (5) | 0.068 (3) |
| C2A | 0.3075 (6) | 0.0072 (11) | 0.4477 (4) | 0.073 (4) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|---------------|
| Au1 | 0.03350 (16) | 0.02516 (16) | 0.03426 (18) | 0.00089 (14) | 0.01226 (13) | -0.00147 (14) |

| | | | | | | |
|-----|--------------|--------------|-------------|--------------|--------------|---------------|
| Au2 | 0.03692 (18) | 0.03095 (17) | 0.0360 (2) | 0.00151 (15) | 0.01285 (14) | -0.00129 (14) |
| Au3 | 0.03603 (18) | 0.02896 (17) | 0.0372 (2) | 0.00002 (14) | 0.01056 (14) | -0.00228 (14) |
| P1 | 0.0365 (10) | 0.0263 (9) | 0.0337 (11) | 0.0014 (9) | 0.0129 (9) | -0.0010 (8) |
| P2 | 0.0391 (11) | 0.0341 (11) | 0.0385 (12) | 0.0042 (9) | 0.0117 (9) | 0.0010 (9) |
| P3 | 0.0416 (12) | 0.0316 (10) | 0.0361 (12) | -0.0012 (9) | 0.0095 (9) | 0.0005 (9) |
| O1 | 0.057 (4) | 0.045 (4) | 0.053 (4) | 0.007 (3) | 0.017 (3) | 0.001 (3) |
| O2 | 0.045 (3) | 0.041 (3) | 0.037 (3) | 0.000 (3) | 0.006 (3) | -0.005 (3) |
| O3 | 0.043 (3) | 0.045 (3) | 0.038 (4) | 0.001 (3) | 0.005 (3) | 0.001 (3) |
| O4 | 0.074 (7) | 0.098 (8) | 0.201 (13) | -0.002 (6) | 0.070 (8) | 0.033 (8) |
| O5 | 0.078 (6) | 0.059 (5) | 0.070 (5) | 0.008 (4) | 0.006 (4) | 0.012 (4) |
| O6 | 0.064 (4) | 0.052 (4) | 0.046 (4) | -0.008 (3) | 0.025 (3) | -0.006 (3) |
| O7 | 0.061 (4) | 0.056 (4) | 0.057 (4) | 0.002 (4) | 0.028 (4) | 0.008 (4) |
| C1 | 0.027 (4) | 0.028 (4) | 0.025 (4) | -0.002 (3) | 0.004 (3) | 0.000 (3) |
| C2 | 0.040 (5) | 0.035 (5) | 0.043 (5) | -0.003 (4) | 0.017 (4) | 0.001 (4) |
| C3 | 0.041 (5) | 0.027 (4) | 0.033 (5) | -0.003 (4) | 0.009 (4) | 0.000 (3) |
| C4 | 0.039 (5) | 0.031 (4) | 0.041 (5) | 0.002 (4) | 0.011 (4) | -0.001 (4) |
| C5 | 0.043 (5) | 0.045 (5) | 0.045 (5) | -0.011 (4) | 0.017 (4) | 0.000 (4) |
| C6 | 0.044 (5) | 0.048 (5) | 0.040 (5) | -0.010 (4) | 0.013 (4) | 0.003 (4) |
| C7 | 0.048 (5) | 0.028 (4) | 0.041 (5) | -0.003 (4) | 0.005 (4) | -0.006 (4) |
| C8 | 0.035 (4) | 0.030 (4) | 0.032 (4) | -0.004 (3) | 0.005 (3) | -0.007 (3) |
| C9 | 0.033 (4) | 0.028 (4) | 0.043 (5) | 0.005 (3) | 0.013 (4) | 0.005 (4) |
| C10 | 0.044 (5) | 0.018 (4) | 0.042 (5) | 0.002 (3) | 0.013 (4) | 0.002 (3) |
| C11 | 0.058 (6) | 0.029 (4) | 0.045 (5) | 0.008 (4) | 0.018 (4) | 0.005 (4) |
| C12 | 0.046 (5) | 0.032 (4) | 0.069 (7) | 0.009 (4) | 0.030 (5) | 0.000 (4) |
| C13 | 0.034 (5) | 0.038 (5) | 0.059 (6) | 0.003 (4) | 0.006 (4) | 0.001 (4) |
| C14 | 0.040 (5) | 0.028 (4) | 0.040 (5) | -0.002 (4) | 0.006 (4) | 0.001 (4) |
| C15 | 0.074 (7) | 0.050 (6) | 0.048 (6) | -0.006 (6) | 0.009 (5) | -0.009 (5) |
| C16 | 0.051 (6) | 0.062 (6) | 0.050 (6) | -0.004 (5) | 0.006 (5) | 0.001 (5) |
| C17 | 0.044 (5) | 0.029 (4) | 0.035 (5) | -0.005 (4) | 0.017 (4) | -0.003 (4) |
| C18 | 0.060 (6) | 0.040 (5) | 0.039 (5) | 0.004 (4) | 0.023 (4) | -0.002 (4) |
| C19 | 0.081 (8) | 0.047 (6) | 0.047 (6) | -0.005 (6) | 0.025 (5) | -0.018 (5) |
| C20 | 0.066 (7) | 0.055 (6) | 0.049 (6) | -0.009 (6) | 0.012 (5) | -0.013 (5) |
| C21 | 0.055 (6) | 0.068 (7) | 0.047 (6) | -0.004 (5) | 0.010 (5) | -0.008 (5) |
| C22 | 0.037 (5) | 0.044 (5) | 0.052 (6) | 0.000 (4) | 0.011 (4) | -0.006 (4) |
| C23 | 0.037 (4) | 0.027 (4) | 0.044 (5) | 0.000 (4) | 0.018 (4) | 0.002 (4) |
| C24 | 0.055 (5) | 0.026 (4) | 0.042 (5) | -0.006 (4) | 0.011 (4) | -0.002 (4) |
| C25 | 0.045 (5) | 0.041 (5) | 0.055 (6) | 0.011 (4) | 0.016 (4) | 0.004 (4) |
| C26 | 0.036 (5) | 0.054 (5) | 0.041 (5) | 0.006 (4) | 0.013 (4) | 0.001 (4) |
| C27 | 0.036 (5) | 0.054 (6) | 0.052 (6) | 0.001 (4) | 0.008 (4) | 0.009 (5) |
| C28 | 0.040 (5) | 0.033 (4) | 0.039 (5) | 0.001 (4) | 0.005 (4) | 0.007 (4) |
| C29 | 0.045 (5) | 0.046 (5) | 0.031 (5) | -0.001 (4) | 0.010 (4) | 0.000 (4) |
| C30 | 0.056 (6) | 0.053 (6) | 0.046 (6) | 0.010 (5) | 0.019 (5) | -0.007 (5) |
| C31 | 0.067 (7) | 0.060 (6) | 0.048 (6) | 0.007 (6) | 0.018 (5) | -0.001 (5) |
| C32 | 0.075 (8) | 0.063 (7) | 0.045 (6) | 0.009 (6) | 0.017 (5) | -0.002 (5) |
| C33 | 0.065 (7) | 0.057 (6) | 0.056 (7) | 0.016 (5) | 0.024 (5) | -0.007 (5) |
| C34 | 0.058 (6) | 0.039 (5) | 0.054 (6) | 0.006 (5) | 0.024 (5) | -0.004 (5) |
| C35 | 0.051 (6) | 0.068 (7) | 0.041 (6) | 0.018 (5) | 0.019 (4) | -0.011 (5) |
| C36 | 0.050 (6) | 0.074 (8) | 0.095 (10) | 0.003 (6) | 0.031 (6) | -0.007 (7) |

| | | | | | | |
|-----|-------------|-------------|-------------|-------------|-------------|--------------|
| C37 | 0.057 (8) | 0.099 (11) | 0.121 (13) | -0.007 (8) | 0.035 (8) | -0.021 (10) |
| C38 | 0.046 (7) | 0.124 (12) | 0.076 (9) | 0.019 (8) | 0.017 (6) | -0.031 (9) |
| C39 | 0.048 (6) | 0.084 (8) | 0.055 (7) | 0.019 (6) | 0.022 (5) | -0.011 (6) |
| C40 | 0.044 (6) | 0.082 (8) | 0.051 (6) | 0.011 (6) | 0.015 (5) | -0.018 (6) |
| C41 | 0.16 (2) | 0.23 (3) | 0.18 (2) | 0.042 (19) | 0.101 (19) | 0.11 (2) |
| C42 | 0.099 (11) | 0.094 (11) | 0.114 (13) | 0.007 (9) | 0.001 (10) | 0.042 (10) |
| C43 | 0.045 (5) | 0.029 (4) | 0.057 (6) | 0.002 (4) | 0.015 (4) | -0.001 (4) |
| C44 | 0.043 (5) | 0.046 (5) | 0.048 (6) | 0.000 (4) | 0.015 (4) | 0.002 (4) |
| C45 | 0.067 (7) | 0.046 (6) | 0.049 (6) | -0.006 (5) | 0.019 (5) | 0.004 (5) |
| C46 | 0.083 (8) | 0.030 (5) | 0.061 (7) | 0.000 (5) | 0.014 (6) | 0.003 (5) |
| C47 | 0.077 (7) | 0.035 (5) | 0.059 (7) | 0.004 (5) | 0.027 (6) | -0.003 (5) |
| C48 | 0.068 (7) | 0.032 (5) | 0.052 (6) | 0.000 (5) | 0.030 (5) | 0.004 (4) |
| C49 | 0.048 (5) | 0.040 (5) | 0.043 (5) | -0.001 (4) | 0.021 (4) | -0.007 (4) |
| C50 | 0.039 (5) | 0.051 (6) | 0.067 (7) | 0.006 (5) | 0.018 (5) | 0.008 (5) |
| C51 | 0.037 (5) | 0.064 (7) | 0.081 (8) | -0.001 (5) | 0.013 (5) | 0.003 (6) |
| C52 | 0.047 (6) | 0.055 (6) | 0.066 (7) | -0.023 (5) | 0.017 (5) | -0.005 (5) |
| C53 | 0.058 (6) | 0.040 (5) | 0.072 (7) | -0.011 (5) | 0.019 (5) | -0.007 (5) |
| C54 | 0.052 (6) | 0.036 (5) | 0.060 (7) | -0.003 (4) | 0.016 (5) | 0.000 (4) |
| C55 | 0.040 (5) | 0.036 (5) | 0.039 (5) | -0.002 (4) | 0.012 (4) | 0.001 (4) |
| C56 | 0.045 (5) | 0.036 (5) | 0.048 (6) | -0.004 (4) | 0.014 (4) | -0.001 (4) |
| C57 | 0.047 (5) | 0.045 (5) | 0.054 (6) | -0.006 (4) | 0.016 (5) | -0.007 (4) |
| C58 | 0.050 (6) | 0.062 (6) | 0.045 (6) | -0.011 (5) | 0.013 (5) | -0.015 (5) |
| C59 | 0.036 (5) | 0.063 (6) | 0.052 (6) | 0.004 (5) | 0.009 (4) | -0.001 (5) |
| C60 | 0.043 (5) | 0.039 (5) | 0.036 (5) | -0.003 (4) | 0.018 (4) | 0.001 (4) |
| C61 | 0.031 (4) | 0.047 (5) | 0.042 (5) | -0.002 (4) | 0.009 (4) | -0.003 (4) |
| C62 | 0.033 (4) | 0.045 (5) | 0.046 (5) | -0.002 (4) | 0.013 (4) | -0.001 (4) |
| C63 | 0.052 (6) | 0.046 (5) | 0.061 (7) | 0.000 (5) | 0.020 (5) | -0.002 (5) |
| C64 | 0.051 (6) | 0.041 (5) | 0.056 (6) | 0.013 (4) | 0.009 (5) | -0.005 (5) |
| C65 | 0.043 (5) | 0.035 (5) | 0.073 (7) | 0.004 (4) | 0.010 (5) | 0.009 (5) |
| C66 | 0.040 (5) | 0.041 (5) | 0.051 (6) | -0.002 (4) | 0.014 (4) | 0.012 (4) |
| C67 | 0.091 (9) | 0.073 (8) | 0.054 (7) | -0.031 (7) | 0.032 (6) | -0.002 (6) |
| C68 | 0.081 (8) | 0.070 (8) | 0.062 (7) | 0.005 (6) | 0.036 (6) | 0.016 (6) |
| C69 | 0.043 (5) | 0.025 (4) | 0.055 (6) | 0.005 (4) | 0.011 (4) | -0.006 (4) |
| C70 | 0.040 (5) | 0.047 (6) | 0.075 (8) | 0.008 (5) | 0.005 (5) | 0.000 (5) |
| C71 | 0.042 (6) | 0.028 (5) | 0.147 (13) | 0.004 (4) | 0.031 (7) | 0.015 (6) |
| C72 | 0.083 (9) | 0.036 (5) | 0.111 (11) | -0.010 (6) | 0.059 (8) | -0.026 (6) |
| C73 | 0.074 (8) | 0.048 (6) | 0.099 (10) | -0.021 (6) | 0.048 (7) | -0.026 (6) |
| C74 | 0.051 (6) | 0.043 (5) | 0.051 (6) | 0.000 (4) | 0.015 (5) | -0.006 (4) |
| C75 | 0.063 (7) | 0.057 (6) | 0.049 (6) | -0.012 (5) | 0.007 (5) | 0.011 (5) |
| C76 | 0.095 (9) | 0.035 (5) | 0.060 (7) | -0.001 (5) | 0.033 (6) | 0.011 (5) |
| C77 | 0.164 (17) | 0.055 (8) | 0.088 (11) | 0.003 (9) | 0.045 (11) | 0.026 (7) |
| C78 | 0.24 (2) | 0.061 (9) | 0.136 (15) | 0.039 (12) | 0.134 (17) | 0.041 (9) |
| C79 | 0.173 (17) | 0.110 (12) | 0.054 (8) | 0.010 (12) | 0.068 (10) | 0.011 (8) |
| C80 | 0.28 (3) | 0.047 (7) | 0.090 (11) | 0.004 (11) | 0.108 (14) | 0.000 (7) |
| S1A | 0.0655 (17) | 0.0536 (15) | 0.0668 (19) | 0.0006 (13) | 0.0234 (14) | -0.0011 (13) |
| S2A | 0.0580 (16) | 0.0746 (18) | 0.0583 (17) | 0.0027 (15) | 0.0125 (13) | -0.0114 (15) |
| F1A | 0.091 (6) | 0.132 (7) | 0.092 (6) | -0.038 (5) | -0.019 (5) | 0.025 (5) |
| F2A | 0.175 (9) | 0.061 (4) | 0.113 (7) | -0.006 (5) | 0.070 (7) | 0.000 (5) |

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|-----|-----------|-----------|-----------|------------|------------|------------|
| F3A | 0.100 (6) | 0.092 (5) | 0.071 (5) | 0.003 (5) | 0.032 (4) | 0.013 (4) |
| F4A | 0.075 (5) | 0.094 (5) | 0.070 (5) | 0.024 (4) | 0.008 (4) | -0.002 (4) |
| F5A | 0.108 (6) | 0.103 (6) | 0.063 (5) | 0.015 (5) | 0.018 (4) | -0.026 (4) |
| F6A | 0.114 (7) | 0.091 (6) | 0.095 (6) | -0.014 (5) | 0.055 (5) | 0.002 (5) |
| O1A | 0.068 (6) | 0.091 (7) | 0.125 (9) | 0.025 (5) | 0.014 (6) | -0.010 (6) |
| O2A | 0.144 (9) | 0.073 (6) | 0.073 (6) | -0.010 (6) | 0.055 (6) | -0.019 (5) |
| O3A | 0.082 (6) | 0.110 (7) | 0.056 (5) | 0.033 (5) | -0.005 (4) | -0.008 (5) |
| O4A | 0.115 (8) | 0.065 (5) | 0.086 (6) | -0.025 (5) | 0.049 (6) | -0.018 (5) |
| N1A | 0.060 (6) | 0.064 (6) | 0.068 (6) | -0.004 (5) | 0.007 (5) | -0.014 (5) |
| C1A | 0.075 (8) | 0.067 (7) | 0.060 (8) | -0.001 (7) | 0.008 (6) | -0.001 (6) |
| C2A | 0.089 (9) | 0.074 (8) | 0.048 (7) | 0.007 (7) | 0.000 (6) | 0.004 (6) |

Geometric parameters (Å, °)

| | | | |
|---------|------------|----------|------------|
| Au1—Au2 | 3.3005 (5) | C41—H41B | 0.9800 |
| Au1—Au3 | 3.1909 (5) | C41—H41C | 0.9800 |
| Au1—P1 | 2.280 (2) | C42—H42A | 0.9800 |
| Au1—C1 | 2.094 (8) | C42—H42B | 0.9800 |
| Au2—Au3 | 3.2101 (5) | C42—H42C | 0.9800 |
| Au2—P2 | 2.281 (2) | C43—H43 | 1.0000 |
| Au2—C1 | 2.098 (7) | C43—C44 | 1.539 (12) |
| Au3—P3 | 2.273 (2) | C43—C48 | 1.536 (13) |
| Au3—C1 | 2.090 (7) | C44—H44A | 0.9900 |
| P1—C3 | 1.840 (8) | C44—H44B | 0.9900 |
| P1—C17 | 1.846 (8) | C44—C45 | 1.520 (13) |
| P1—C23 | 1.837 (8) | C45—H45A | 0.9900 |
| P2—C29 | 1.833 (9) | C45—H45B | 0.9900 |
| P2—C43 | 1.852 (8) | C45—C46 | 1.516 (14) |
| P2—C49 | 1.853 (9) | C46—H46A | 0.9900 |
| P3—C55 | 1.835 (9) | C46—H46B | 0.9900 |
| P3—C69 | 1.854 (9) | C46—C47 | 1.526 (14) |
| P3—C75 | 1.847 (10) | C47—H47A | 0.9900 |
| O1—C2 | 1.176 (10) | C47—H47B | 0.9900 |
| O2—C10 | 1.366 (10) | C47—C48 | 1.534 (12) |
| O2—C15 | 1.427 (11) | C48—H48A | 0.9900 |
| O3—C14 | 1.368 (10) | C48—H48B | 0.9900 |
| O3—C16 | 1.441 (11) | C49—H49 | 1.0000 |
| O4—C36 | 1.397 (16) | C49—C50 | 1.546 (13) |
| O4—C41 | 1.278 (18) | C49—C54 | 1.523 (12) |
| O5—C40 | 1.360 (13) | C50—H50A | 0.9900 |
| O5—C42 | 1.438 (14) | C50—H50B | 0.9900 |
| O6—C62 | 1.376 (11) | C50—C51 | 1.541 (14) |
| O6—C67 | 1.432 (12) | C51—H51A | 0.9900 |
| O7—C66 | 1.378 (11) | C51—H51B | 0.9900 |
| O7—C68 | 1.422 (12) | C51—C52 | 1.503 (14) |
| C1—C2 | 1.282 (12) | C52—H52A | 0.9900 |
| C3—C4 | 1.385 (11) | C52—H52B | 0.9900 |
| C3—C8 | 1.409 (11) | C52—C53 | 1.524 (14) |

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|----------|------------|----------|------------|
| C4—H4 | 0.9500 | C53—H53A | 0.9900 |
| C4—C5 | 1.373 (12) | C53—H53B | 0.9900 |
| C5—H5 | 0.9500 | C53—C54 | 1.537 (13) |
| C5—C6 | 1.364 (13) | C54—H54A | 0.9900 |
| C6—H6 | 0.9500 | C54—H54B | 0.9900 |
| C6—C7 | 1.394 (12) | C55—C56 | 1.395 (12) |
| C7—H7 | 0.9500 | C55—C60 | 1.412 (12) |
| C7—C8 | 1.394 (12) | C56—H56 | 0.9500 |
| C8—C9 | 1.486 (11) | C56—C57 | 1.383 (13) |
| C9—C10 | 1.401 (12) | C57—H57 | 0.9500 |
| C9—C14 | 1.389 (11) | C57—C58 | 1.359 (14) |
| C10—C11 | 1.390 (12) | C58—H58 | 0.9500 |
| C11—H11 | 0.9500 | C58—C59 | 1.395 (14) |
| C11—C12 | 1.374 (13) | C59—H59 | 0.9500 |
| C12—H12 | 0.9500 | C59—C60 | 1.375 (12) |
| C12—C13 | 1.365 (13) | C60—C61 | 1.499 (12) |
| C13—H13 | 0.9500 | C61—C62 | 1.390 (12) |
| C13—C14 | 1.390 (12) | C61—C66 | 1.404 (12) |
| C15—H15A | 0.9800 | C62—C63 | 1.386 (13) |
| C15—H15B | 0.9800 | C63—H63 | 0.9500 |
| C15—H15C | 0.9800 | C63—C64 | 1.372 (14) |
| C16—H16A | 0.9800 | C64—H64 | 0.9500 |
| C16—H16B | 0.9800 | C64—C65 | 1.372 (14) |
| C16—H16C | 0.9800 | C65—H65 | 0.9500 |
| C17—H17 | 1.0000 | C65—C66 | 1.374 (13) |
| C17—C18 | 1.533 (11) | C67—H67A | 0.9800 |
| C17—C22 | 1.527 (12) | C67—H67B | 0.9800 |
| C18—H18A | 0.9900 | C67—H67C | 0.9800 |
| C18—H18B | 0.9900 | C68—H68A | 0.9800 |
| C18—C19 | 1.523 (13) | C68—H68B | 0.9800 |
| C19—H19A | 0.9900 | C68—H68C | 0.9800 |
| C19—H19B | 0.9900 | C69—H69 | 1.0000 |
| C19—C20 | 1.522 (15) | C69—C70 | 1.529 (12) |
| C20—H20A | 0.9900 | C69—C74 | 1.530 (13) |
| C20—H20B | 0.9900 | C70—H70A | 0.9900 |
| C20—C21 | 1.520 (14) | C70—H70B | 0.9900 |
| C21—H21A | 0.9900 | C70—C71 | 1.539 (14) |
| C21—H21B | 0.9900 | C71—H71A | 0.9900 |
| C21—C22 | 1.535 (13) | C71—H71B | 0.9900 |
| C22—H22A | 0.9900 | C71—C72 | 1.520 (17) |
| C22—H22B | 0.9900 | C72—H72A | 0.9900 |
| C23—H23 | 1.0000 | C72—H72B | 0.9900 |
| C23—C24 | 1.551 (11) | C72—C73 | 1.504 (17) |
| C23—C28 | 1.531 (11) | C73—H73A | 0.9900 |
| C24—H24A | 0.9900 | C73—H73B | 0.9900 |
| C24—H24B | 0.9900 | C73—C74 | 1.524 (13) |
| C24—C25 | 1.541 (12) | C74—H74A | 0.9900 |
| C25—H25A | 0.9900 | C74—H74B | 0.9900 |

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|-------------|-------------|---------------|------------|
| C25—H25B | 0.9900 | C75—H75 | 1.0000 |
| C25—C26 | 1.533 (13) | C75—C76 | 1.497 (14) |
| C26—H26A | 0.9900 | C75—C80 | 1.444 (16) |
| C26—H26B | 0.9900 | C76—H76A | 0.9900 |
| C26—C27 | 1.529 (13) | C76—H76B | 0.9900 |
| C27—H27A | 0.9900 | C76—C77 | 1.498 (15) |
| C27—H27B | 0.9900 | C77—H77A | 0.9900 |
| C27—C28 | 1.524 (11) | C77—H77B | 0.9900 |
| C28—H28A | 0.9900 | C77—C78 | 1.416 (19) |
| C28—H28B | 0.9900 | C78—H78A | 0.9900 |
| C29—C30 | 1.421 (13) | C78—H78B | 0.9900 |
| C29—C34 | 1.389 (13) | C78—C79 | 1.56 (2) |
| C30—H30 | 0.9500 | C79—H79A | 0.9900 |
| C30—C31 | 1.376 (14) | C79—H79B | 0.9900 |
| C31—H31 | 0.9500 | C79—C80 | 1.539 (18) |
| C31—C32 | 1.391 (14) | C80—H80A | 0.9900 |
| C32—H32 | 0.9500 | C80—H80B | 0.9900 |
| C32—C33 | 1.368 (15) | S1A—O1A | 1.450 (9) |
| C33—H33 | 0.9500 | S1A—O2A | 1.436 (9) |
| C33—C34 | 1.383 (14) | S1A—N1A | 1.570 (10) |
| C34—C35 | 1.496 (14) | S1A—C1A | 1.784 (13) |
| C35—C36 | 1.366 (16) | S2A—O3A | 1.448 (8) |
| C35—C40 | 1.376 (16) | S2A—O4A | 1.453 (9) |
| C36—C37 | 1.376 (18) | S2A—N1A | 1.566 (9) |
| C37—H37 | 0.9500 | S2A—C2A | 1.754 (14) |
| C37—C38 | 1.40 (2) | F1A—C1A | 1.321 (14) |
| C38—H38 | 0.9500 | F2A—C1A | 1.342 (14) |
| C38—C39 | 1.356 (17) | F3A—C1A | 1.346 (14) |
| C39—H39 | 0.9500 | F4A—C2A | 1.301 (13) |
| C39—C40 | 1.386 (14) | F5A—C2A | 1.360 (14) |
| C41—H41A | 0.9800 | F6A—C2A | 1.368 (14) |
| | | | |
| Au3—Au1—Au2 | 59.247 (11) | P2—C43—H43 | 108.8 |
| P1—Au1—Au2 | 138.37 (5) | C44—C43—P2 | 109.0 (6) |
| P1—Au1—Au3 | 133.55 (5) | C44—C43—H43 | 108.8 |
| C1—Au1—Au2 | 38.1 (2) | C48—C43—P2 | 111.4 (6) |
| C1—Au1—Au3 | 40.3 (2) | C48—C43—H43 | 108.8 |
| C1—Au1—P1 | 172.5 (2) | C48—C43—C44 | 110.0 (8) |
| Au3—Au2—Au1 | 58.675 (11) | C43—C44—H44A | 109.4 |
| P2—Au2—Au1 | 132.86 (6) | C43—C44—H44B | 109.4 |
| P2—Au2—Au3 | 141.89 (6) | H44A—C44—H44B | 108.0 |
| C1—Au2—Au1 | 38.0 (2) | C45—C44—C43 | 111.0 (8) |
| C1—Au2—Au3 | 39.9 (2) | C45—C44—H44A | 109.4 |
| C1—Au2—P2 | 170.9 (2) | C45—C44—H44B | 109.4 |
| Au1—Au3—Au2 | 62.077 (11) | C44—C45—H45A | 109.4 |
| P3—Au3—Au1 | 136.88 (6) | C44—C45—H45B | 109.4 |
| P3—Au3—Au2 | 134.46 (6) | H45A—C45—H45B | 108.0 |
| C1—Au3—Au1 | 40.3 (2) | C46—C45—C44 | 111.4 (8) |

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| C1—Au3—Au2 | 40.1 (2) | C46—C45—H45A | 109.4 |
| C1—Au3—P3 | 173.3 (2) | C46—C45—H45B | 109.4 |
| C3—P1—Au1 | 122.2 (3) | C45—C46—H46A | 109.6 |
| C3—P1—C17 | 104.8 (4) | C45—C46—H46B | 109.6 |
| C17—P1—Au1 | 108.5 (3) | C45—C46—C47 | 110.2 (9) |
| C23—P1—Au1 | 110.1 (3) | H46A—C46—H46B | 108.1 |
| C23—P1—C3 | 104.3 (4) | C47—C46—H46A | 109.6 |
| C23—P1—C17 | 105.8 (4) | C47—C46—H46B | 109.6 |
| C29—P2—Au2 | 121.8 (3) | C46—C47—H47A | 109.1 |
| C29—P2—C43 | 104.5 (4) | C46—C47—H47B | 109.1 |
| C29—P2—C49 | 104.8 (4) | C46—C47—C48 | 112.4 (9) |
| C43—P2—Au2 | 112.2 (3) | H47A—C47—H47B | 107.9 |
| C43—P2—C49 | 108.7 (4) | C48—C47—H47A | 109.1 |
| C49—P2—Au2 | 104.0 (3) | C48—C47—H47B | 109.1 |
| C55—P3—Au3 | 121.0 (3) | C43—C48—H48A | 109.7 |
| C55—P3—C69 | 104.2 (4) | C43—C48—H48B | 109.7 |
| C55—P3—C75 | 105.0 (4) | C47—C48—C43 | 109.9 (8) |
| C69—P3—Au3 | 110.1 (3) | C47—C48—H48A | 109.7 |
| C75—P3—Au3 | 111.6 (4) | C47—C48—H48B | 109.7 |
| C75—P3—C69 | 103.4 (5) | H48A—C48—H48B | 108.2 |
| C10—O2—C15 | 117.5 (7) | P2—C49—H49 | 105.9 |
| C14—O3—C16 | 117.1 (7) | C50—C49—P2 | 118.2 (7) |
| C41—O4—C36 | 124.5 (14) | C50—C49—H49 | 105.9 |
| C40—O5—C42 | 116.7 (10) | C54—C49—P2 | 109.6 (6) |
| C62—O6—C67 | 116.4 (8) | C54—C49—H49 | 105.9 |
| C66—O7—C68 | 116.7 (8) | C54—C49—C50 | 110.5 (8) |
| Au1—C1—Au2 | 103.9 (3) | C49—C50—H50A | 109.7 |
| Au3—C1—Au1 | 99.4 (3) | C49—C50—H50B | 109.7 |
| Au3—C1—Au2 | 100.1 (3) | H50A—C50—H50B | 108.2 |
| C2—C1—Au1 | 116.3 (6) | C51—C50—C49 | 109.7 (8) |
| C2—C1—Au2 | 115.6 (6) | C51—C50—H50A | 109.7 |
| C2—C1—Au3 | 118.8 (6) | C51—C50—H50B | 109.7 |
| O1—C2—C1 | 178.9 (10) | C50—C51—H51A | 109.4 |
| C4—C3—P1 | 117.5 (6) | C50—C51—H51B | 109.4 |
| C4—C3—C8 | 118.2 (8) | H51A—C51—H51B | 108.0 |
| C8—C3—P1 | 123.8 (6) | C52—C51—C50 | 111.4 (9) |
| C3—C4—H4 | 118.6 | C52—C51—H51A | 109.4 |
| C5—C4—C3 | 122.9 (8) | C52—C51—H51B | 109.4 |
| C5—C4—H4 | 118.6 | C51—C52—H52A | 109.4 |
| C4—C5—H5 | 120.4 | C51—C52—H52B | 109.4 |
| C6—C5—C4 | 119.3 (9) | C51—C52—C53 | 111.0 (8) |
| C6—C5—H5 | 120.4 | H52A—C52—H52B | 108.0 |
| C5—C6—H6 | 120.1 | C53—C52—H52A | 109.4 |
| C5—C6—C7 | 119.7 (9) | C53—C52—H52B | 109.4 |
| C7—C6—H6 | 120.1 | C52—C53—H53A | 109.2 |
| C6—C7—H7 | 119.3 | C52—C53—H53B | 109.2 |
| C8—C7—C6 | 121.4 (8) | C52—C53—C54 | 112.2 (9) |
| C8—C7—H7 | 119.3 | H53A—C53—H53B | 107.9 |

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| C3—C8—C9 | 124.3 (8) | C54—C53—H53A | 109.2 |
| C7—C8—C3 | 118.5 (8) | C54—C53—H53B | 109.2 |
| C7—C8—C9 | 117.2 (7) | C49—C54—C53 | 110.1 (8) |
| C10—C9—C8 | 121.7 (8) | C49—C54—H54A | 109.6 |
| C14—C9—C8 | 119.9 (8) | C49—C54—H54B | 109.6 |
| C14—C9—C10 | 118.2 (8) | C53—C54—H54A | 109.6 |
| O2—C10—C9 | 114.5 (7) | C53—C54—H54B | 109.6 |
| O2—C10—C11 | 124.8 (8) | H54A—C54—H54B | 108.2 |
| C11—C10—C9 | 120.7 (8) | C56—C55—P3 | 118.8 (7) |
| C10—C11—H11 | 120.6 | C56—C55—C60 | 118.6 (8) |
| C12—C11—C10 | 118.9 (9) | C60—C55—P3 | 122.5 (7) |
| C12—C11—H11 | 120.6 | C55—C56—H56 | 119.0 |
| C11—C12—H12 | 119.0 | C57—C56—C55 | 122.0 (9) |
| C13—C12—C11 | 122.1 (9) | C57—C56—H56 | 119.0 |
| C13—C12—H12 | 119.0 | C56—C57—H57 | 120.5 |
| C12—C13—H13 | 120.5 | C58—C57—C56 | 119.0 (9) |
| C12—C13—C14 | 119.0 (9) | C58—C57—H57 | 120.5 |
| C14—C13—H13 | 120.5 | C57—C58—H58 | 119.9 |
| O3—C14—C9 | 115.0 (8) | C57—C58—C59 | 120.3 (9) |
| O3—C14—C13 | 123.9 (8) | C59—C58—H58 | 119.9 |
| C9—C14—C13 | 121.1 (8) | C58—C59—H59 | 119.1 |
| O2—C15—H15A | 109.5 | C60—C59—C58 | 121.7 (9) |
| O2—C15—H15B | 109.5 | C60—C59—H59 | 119.1 |
| O2—C15—H15C | 109.5 | C55—C60—C61 | 124.5 (8) |
| H15A—C15—H15B | 109.5 | C59—C60—C55 | 118.3 (9) |
| H15A—C15—H15C | 109.5 | C59—C60—C61 | 117.0 (8) |
| H15B—C15—H15C | 109.5 | C62—C61—C60 | 122.8 (8) |
| O3—C16—H16A | 109.5 | C62—C61—C66 | 118.0 (9) |
| O3—C16—H16B | 109.5 | C66—C61—C60 | 119.0 (8) |
| O3—C16—H16C | 109.5 | O6—C62—C61 | 115.3 (8) |
| H16A—C16—H16B | 109.5 | O6—C62—C63 | 123.3 (8) |
| H16A—C16—H16C | 109.5 | C63—C62—C61 | 121.4 (9) |
| H16B—C16—H16C | 109.5 | C62—C63—H63 | 120.8 |
| P1—C17—H17 | 106.6 | C64—C63—C62 | 118.4 (10) |
| C18—C17—P1 | 116.5 (6) | C64—C63—H63 | 120.8 |
| C18—C17—H17 | 106.6 | C63—C64—H64 | 118.9 |
| C22—C17—P1 | 109.7 (6) | C65—C64—C63 | 122.2 (9) |
| C22—C17—H17 | 106.6 | C65—C64—H64 | 118.9 |
| C22—C17—C18 | 110.1 (7) | C64—C65—H65 | 120.5 |
| C17—C18—H18A | 109.5 | C64—C65—C66 | 119.0 (9) |
| C17—C18—H18B | 109.5 | C66—C65—H65 | 120.5 |
| H18A—C18—H18B | 108.1 | O7—C66—C61 | 114.4 (8) |
| C19—C18—C17 | 110.8 (8) | C65—C66—O7 | 124.5 (9) |
| C19—C18—H18A | 109.5 | C65—C66—C61 | 121.0 (9) |
| C19—C18—H18B | 109.5 | O6—C67—H67A | 109.5 |
| C18—C19—H19A | 109.3 | O6—C67—H67B | 109.5 |
| C18—C19—H19B | 109.3 | O6—C67—H67C | 109.5 |
| H19A—C19—H19B | 107.9 | H67A—C67—H67B | 109.5 |

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| C20—C19—C18 | 111.7 (8) | H67A—C67—H67C | 109.5 |
| C20—C19—H19A | 109.3 | H67B—C67—H67C | 109.5 |
| C20—C19—H19B | 109.3 | O7—C68—H68A | 109.5 |
| C19—C20—H20A | 109.1 | O7—C68—H68B | 109.5 |
| C19—C20—H20B | 109.1 | O7—C68—H68C | 109.5 |
| H20A—C20—H20B | 107.9 | H68A—C68—H68B | 109.5 |
| C21—C20—C19 | 112.3 (9) | H68A—C68—H68C | 109.5 |
| C21—C20—H20A | 109.1 | H68B—C68—H68C | 109.5 |
| C21—C20—H20B | 109.1 | P3—C69—H69 | 108.0 |
| C20—C21—H21A | 109.6 | C70—C69—P3 | 111.2 (7) |
| C20—C21—H21B | 109.6 | C70—C69—H69 | 108.0 |
| C20—C21—C22 | 110.5 (8) | C70—C69—C74 | 109.6 (8) |
| H21A—C21—H21B | 108.1 | C74—C69—P3 | 111.8 (6) |
| C22—C21—H21A | 109.6 | C74—C69—H69 | 108.0 |
| C22—C21—H21B | 109.6 | C69—C70—H70A | 109.8 |
| C17—C22—C21 | 112.5 (8) | C69—C70—H70B | 109.8 |
| C17—C22—H22A | 109.1 | C69—C70—C71 | 109.6 (9) |
| C17—C22—H22B | 109.1 | H70A—C70—H70B | 108.2 |
| C21—C22—H22A | 109.1 | C71—C70—H70A | 109.8 |
| C21—C22—H22B | 109.1 | C71—C70—H70B | 109.8 |
| H22A—C22—H22B | 107.8 | C70—C71—H71A | 109.2 |
| P1—C23—H23 | 108.3 | C70—C71—H71B | 109.2 |
| C24—C23—P1 | 110.5 (6) | H71A—C71—H71B | 107.9 |
| C24—C23—H23 | 108.3 | C72—C71—C70 | 112.2 (9) |
| C28—C23—P1 | 112.5 (5) | C72—C71—H71A | 109.2 |
| C28—C23—H23 | 108.3 | C72—C71—H71B | 109.2 |
| C28—C23—C24 | 108.8 (7) | C71—C72—H72A | 109.0 |
| C23—C24—H24A | 109.6 | C71—C72—H72B | 109.0 |
| C23—C24—H24B | 109.6 | H72A—C72—H72B | 107.8 |
| H24A—C24—H24B | 108.1 | C73—C72—C71 | 113.1 (10) |
| C25—C24—C23 | 110.1 (7) | C73—C72—H72A | 109.0 |
| C25—C24—H24A | 109.6 | C73—C72—H72B | 109.0 |
| C25—C24—H24B | 109.6 | C72—C73—H73A | 109.3 |
| C24—C25—H25A | 109.4 | C72—C73—H73B | 109.3 |
| C24—C25—H25B | 109.4 | C72—C73—C74 | 111.5 (9) |
| H25A—C25—H25B | 108.0 | H73A—C73—H73B | 108.0 |
| C26—C25—C24 | 111.3 (7) | C74—C73—H73A | 109.3 |
| C26—C25—H25A | 109.4 | C74—C73—H73B | 109.3 |
| C26—C25—H25B | 109.4 | C69—C74—H74A | 109.5 |
| C25—C26—H26A | 109.3 | C69—C74—H74B | 109.5 |
| C25—C26—H26B | 109.3 | C73—C74—C69 | 110.8 (9) |
| H26A—C26—H26B | 108.0 | C73—C74—H74A | 109.5 |
| C27—C26—C25 | 111.4 (8) | C73—C74—H74B | 109.5 |
| C27—C26—H26A | 109.3 | H74A—C74—H74B | 108.1 |
| C27—C26—H26B | 109.3 | P3—C75—H75 | 104.2 |
| C26—C27—H27A | 109.3 | C76—C75—P3 | 115.7 (8) |
| C26—C27—H27B | 109.3 | C76—C75—H75 | 104.2 |
| H27A—C27—H27B | 107.9 | C80—C75—P3 | 114.2 (9) |

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| C28—C27—C26 | 111.7 (7) | C80—C75—H75 | 104.2 |
| C28—C27—H27A | 109.3 | C80—C75—C76 | 112.5 (11) |
| C28—C27—H27B | 109.3 | C75—C76—H76A | 108.6 |
| C23—C28—H28A | 109.5 | C75—C76—H76B | 108.6 |
| C23—C28—H28B | 109.5 | C75—C76—C77 | 114.8 (11) |
| C27—C28—C23 | 110.7 (7) | H76A—C76—H76B | 107.5 |
| C27—C28—H28A | 109.5 | C77—C76—H76A | 108.6 |
| C27—C28—H28B | 109.5 | C77—C76—H76B | 108.6 |
| H28A—C28—H28B | 108.1 | C76—C77—H77A | 109.2 |
| C30—C29—P2 | 117.2 (7) | C76—C77—H77B | 109.2 |
| C34—C29—P2 | 124.2 (7) | H77A—C77—H77B | 107.9 |
| C34—C29—C30 | 118.4 (9) | C78—C77—C76 | 112.0 (12) |
| C29—C30—H30 | 119.5 | C78—C77—H77A | 109.2 |
| C31—C30—C29 | 121.1 (10) | C78—C77—H77B | 109.2 |
| C31—C30—H30 | 119.5 | C77—C78—H78A | 108.3 |
| C30—C31—H31 | 120.4 | C77—C78—H78B | 108.3 |
| C30—C31—C32 | 119.3 (11) | C77—C78—C79 | 115.9 (13) |
| C32—C31—H31 | 120.4 | H78A—C78—H78B | 107.4 |
| C31—C32—H32 | 120.2 | C79—C78—H78A | 108.3 |
| C33—C32—C31 | 119.7 (10) | C79—C78—H78B | 108.3 |
| C33—C32—H32 | 120.2 | C78—C79—H79A | 110.2 |
| C32—C33—H33 | 118.9 | C78—C79—H79B | 110.2 |
| C32—C33—C34 | 122.1 (10) | H79A—C79—H79B | 108.5 |
| C34—C33—H33 | 118.9 | C80—C79—C78 | 107.5 (13) |
| C29—C34—C35 | 122.3 (9) | C80—C79—H79A | 110.2 |
| C33—C34—C29 | 119.2 (10) | C80—C79—H79B | 110.2 |
| C33—C34—C35 | 118.5 (9) | C75—C80—C79 | 114.5 (12) |
| C36—C35—C34 | 119.7 (11) | C75—C80—H80A | 108.6 |
| C36—C35—C40 | 117.7 (11) | C75—C80—H80B | 108.6 |
| C40—C35—C34 | 122.3 (10) | C79—C80—H80A | 108.6 |
| C35—C36—O4 | 117.6 (12) | C79—C80—H80B | 108.6 |
| C35—C36—C37 | 123.3 (14) | H80A—C80—H80B | 107.6 |
| C37—C36—O4 | 119.0 (13) | O1A—S1A—N1A | 116.1 (6) |
| C36—C37—H37 | 121.7 | O1A—S1A—C1A | 105.4 (6) |
| C36—C37—C38 | 116.7 (14) | O2A—S1A—O1A | 121.1 (6) |
| C38—C37—H37 | 121.7 | O2A—S1A—N1A | 107.9 (6) |
| C37—C38—H38 | 119.0 | O2A—S1A—C1A | 101.7 (6) |
| C39—C38—C37 | 122.0 (13) | N1A—S1A—C1A | 101.8 (6) |
| C39—C38—H38 | 119.0 | O3A—S2A—O4A | 121.5 (6) |
| C38—C39—H39 | 120.6 | O3A—S2A—N1A | 115.4 (6) |
| C38—C39—C40 | 118.7 (13) | O3A—S2A—C2A | 102.3 (6) |
| C40—C39—H39 | 120.6 | O4A—S2A—N1A | 111.2 (5) |
| O5—C40—C35 | 114.2 (10) | O4A—S2A—C2A | 100.6 (6) |
| O5—C40—C39 | 124.3 (12) | N1A—S2A—C2A | 101.8 (6) |
| C35—C40—C39 | 121.4 (12) | S2A—N1A—S1A | 126.9 (7) |
| O4—C41—H41A | 109.5 | F1A—C1A—S1A | 113.1 (9) |
| O4—C41—H41B | 109.5 | F1A—C1A—F2A | 108.9 (11) |
| O4—C41—H41C | 109.5 | F1A—C1A—F3A | 106.9 (11) |

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| H41A—C41—H41B | 109.5 | F2A—C1A—S1A | 110.4 (9) |
| H41A—C41—H41C | 109.5 | F2A—C1A—F3A | 104.9 (10) |
| H41B—C41—H41C | 109.5 | F3A—C1A—S1A | 112.2 (9) |
| O5—C42—H42A | 109.5 | F4A—C2A—S2A | 115.4 (9) |
| O5—C42—H42B | 109.5 | F4A—C2A—F5A | 106.6 (11) |
| O5—C42—H42C | 109.5 | F4A—C2A—F6A | 108.2 (12) |
| H42A—C42—H42B | 109.5 | F5A—C2A—S2A | 109.1 (9) |
| H42A—C42—H42C | 109.5 | F5A—C2A—F6A | 106.3 (10) |
| H42B—C42—H42C | 109.5 | F6A—C2A—S2A | 110.8 (9) |
| | | | |
| Au1—P1—C3—C4 | 161.8 (5) | C34—C35—C40—O5 | 4.4 (14) |
| Au1—P1—C3—C8 | -26.2 (8) | C34—C35—C40—C39 | -178.6 (9) |
| Au1—P1—C17—C18 | -170.1 (6) | C35—C36—C37—C38 | -2 (2) |
| Au1—P1—C17—C22 | 63.9 (6) | C36—C35—C40—O5 | 179.2 (10) |
| Au1—P1—C23—C24 | 48.8 (6) | C36—C35—C40—C39 | -3.8 (16) |
| Au1—P1—C23—C28 | -73.0 (6) | C36—C37—C38—C39 | -1 (2) |
| Au2—P2—C29—C30 | -176.5 (6) | C37—C38—C39—C40 | 1.1 (18) |
| Au2—P2—C29—C34 | -0.7 (10) | C38—C39—C40—O5 | 177.9 (10) |
| Au2—P2—C43—C44 | -65.2 (7) | C38—C39—C40—C35 | 1.2 (16) |
| Au2—P2—C43—C48 | 56.4 (7) | C40—C35—C36—O4 | -178.5 (11) |
| Au2—P2—C49—C50 | -168.7 (7) | C40—C35—C36—C37 | 4.4 (18) |
| Au2—P2—C49—C54 | 63.7 (7) | C41—O4—C36—C35 | 122 (2) |
| Au3—P3—C55—C56 | 153.7 (6) | C41—O4—C36—C37 | -61 (3) |
| Au3—P3—C55—C60 | -29.8 (9) | C42—O5—C40—C35 | 175.4 (11) |
| Au3—P3—C69—C70 | 48.3 (7) | C42—O5—C40—C39 | -1.5 (17) |
| Au3—P3—C69—C74 | -74.5 (7) | C43—P2—C29—C30 | 55.1 (8) |
| Au3—P3—C75—C76 | 173.0 (8) | C43—P2—C29—C34 | -129.1 (8) |
| Au3—P3—C75—C80 | 39.9 (13) | C43—P2—C49—C50 | -48.9 (8) |
| P1—C3—C4—C5 | 172.4 (7) | C43—P2—C49—C54 | -176.6 (7) |
| P1—C3—C8—C7 | -171.8 (6) | C43—C44—C45—C46 | -57.7 (12) |
| P1—C3—C8—C9 | 8.8 (12) | C44—C43—C48—C47 | -56.1 (11) |
| P1—C17—C18—C19 | 178.0 (7) | C44—C45—C46—C47 | 55.9 (12) |
| P1—C17—C22—C21 | -174.4 (7) | C45—C46—C47—C48 | -55.7 (12) |
| P1—C23—C24—C25 | 176.7 (6) | C46—C47—C48—C43 | 56.2 (12) |
| P1—C23—C28—C27 | -177.4 (6) | C48—C43—C44—C45 | 57.5 (10) |
| P2—C29—C30—C31 | 172.5 (8) | C49—P2—C29—C30 | -59.2 (8) |
| P2—C29—C34—C33 | -170.3 (8) | C49—P2—C29—C34 | 116.6 (9) |
| P2—C29—C34—C35 | 12.0 (14) | C49—P2—C43—C44 | -179.7 (6) |
| P2—C43—C44—C45 | 180.0 (7) | C49—P2—C43—C48 | -58.1 (8) |
| P2—C43—C48—C47 | -177.1 (7) | C49—C50—C51—C52 | 57.7 (12) |
| P2—C49—C50—C51 | 174.5 (7) | C50—C49—C54—C53 | 57.0 (11) |
| P2—C49—C54—C53 | -171.1 (7) | C50—C51—C52—C53 | -55.9 (13) |
| P3—C55—C56—C57 | 177.7 (7) | C51—C52—C53—C54 | 55.0 (12) |
| P3—C55—C60—C59 | -175.4 (7) | C52—C53—C54—C49 | -55.5 (11) |
| P3—C55—C60—C61 | 9.0 (12) | C54—C49—C50—C51 | -58.2 (11) |
| P3—C69—C70—C71 | 176.8 (7) | C55—P3—C69—C70 | 179.4 (7) |
| P3—C69—C74—C73 | -176.1 (7) | C55—P3—C69—C74 | 56.6 (7) |
| P3—C75—C76—C77 | 177.2 (10) | C55—P3—C75—C76 | 40.3 (10) |

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| P3—C75—C80—C79 | -174.0 (12) | C55—P3—C75—C80 | -92.8 (12) |
| O2—C10—C11—C12 | 178.6 (8) | C55—C56—C57—C58 | -1.3 (15) |
| O4—C36—C37—C38 | -179.3 (12) | C55—C60—C61—C62 | -105.9 (11) |
| O6—C62—C63—C64 | 180.0 (9) | C55—C60—C61—C66 | 79.5 (12) |
| C3—P1—C17—C18 | 57.9 (7) | C56—C55—C60—C59 | 1.1 (13) |
| C3—P1—C17—C22 | -68.1 (7) | C56—C55—C60—C61 | -174.5 (8) |
| C3—P1—C23—C24 | -178.5 (6) | C56—C57—C58—C59 | -0.4 (15) |
| C3—P1—C23—C28 | 59.7 (7) | C57—C58—C59—C60 | 2.6 (16) |
| C3—C4—C5—C6 | -0.8 (14) | C58—C59—C60—C55 | -2.9 (15) |
| C3—C8—C9—C10 | 75.4 (11) | C58—C59—C60—C61 | 173.0 (9) |
| C3—C8—C9—C14 | -110.5 (10) | C59—C60—C61—C62 | 78.5 (12) |
| C4—C3—C8—C7 | 0.2 (12) | C59—C60—C61—C66 | -96.1 (10) |
| C4—C3—C8—C9 | -179.2 (8) | C60—C55—C56—C57 | 1.0 (14) |
| C4—C5—C6—C7 | 1.7 (14) | C60—C61—C62—O6 | 4.7 (13) |
| C5—C6—C7—C8 | -1.7 (13) | C60—C61—C62—C63 | -173.3 (9) |
| C6—C7—C8—C3 | 0.7 (12) | C60—C61—C66—O7 | -4.1 (12) |
| C6—C7—C8—C9 | -179.8 (8) | C60—C61—C66—C65 | 174.6 (9) |
| C7—C8—C9—C10 | -104.1 (9) | C61—C62—C63—C64 | -2.2 (15) |
| C7—C8—C9—C14 | 70.1 (10) | C62—C61—C66—O7 | -178.9 (8) |
| C8—C3—C4—C5 | -0.2 (13) | C62—C61—C66—C65 | -0.3 (14) |
| C8—C9—C10—O2 | -3.3 (11) | C62—C63—C64—C65 | 2.1 (15) |
| C8—C9—C10—C11 | 177.1 (7) | C63—C64—C65—C66 | -1.1 (15) |
| C8—C9—C14—O3 | 2.8 (11) | C64—C65—C66—O7 | 178.6 (9) |
| C8—C9—C14—C13 | -176.9 (8) | C64—C65—C66—C61 | 0.1 (14) |
| C9—C10—C11—C12 | -1.9 (12) | C66—C61—C62—O6 | 179.3 (8) |
| C10—C9—C14—O3 | 177.1 (7) | C66—C61—C62—C63 | 1.3 (14) |
| C10—C9—C14—C13 | -2.5 (12) | C67—O6—C62—C61 | 172.9 (9) |
| C10—C11—C12—C13 | 0.3 (14) | C67—O6—C62—C63 | -9.2 (14) |
| C11—C12—C13—C14 | 0.1 (14) | C68—O7—C66—C61 | -175.1 (9) |
| C12—C13—C14—O3 | -178.5 (8) | C68—O7—C66—C65 | 6.3 (14) |
| C12—C13—C14—C9 | 1.1 (13) | C69—P3—C55—C56 | 29.3 (8) |
| C14—C9—C10—O2 | -177.5 (7) | C69—P3—C55—C60 | -154.2 (7) |
| C14—C9—C10—C11 | 2.9 (12) | C69—P3—C75—C76 | -68.7 (10) |
| C15—O2—C10—C9 | -172.4 (7) | C69—P3—C75—C80 | 158.2 (12) |
| C15—O2—C10—C11 | 7.2 (12) | C69—C70—C71—C72 | 55.0 (12) |
| C16—O3—C14—C9 | 170.5 (8) | C70—C69—C74—C73 | 60.1 (10) |
| C16—O3—C14—C13 | -9.8 (12) | C70—C71—C72—C73 | -51.6 (12) |
| C17—P1—C3—C4 | -74.6 (7) | C71—C72—C73—C74 | 51.4 (12) |
| C17—P1—C3—C8 | 97.4 (7) | C72—C73—C74—C69 | -55.8 (12) |
| C17—P1—C23—C24 | -68.2 (7) | C74—C69—C70—C71 | -59.1 (10) |
| C17—P1—C23—C28 | 170.0 (6) | C75—P3—C55—C56 | -79.1 (8) |
| C17—C18—C19—C20 | 56.0 (11) | C75—P3—C55—C60 | 97.4 (8) |
| C18—C17—C22—C21 | 56.1 (10) | C75—P3—C69—C70 | -71.0 (8) |
| C18—C19—C20—C21 | -54.9 (12) | C75—P3—C69—C74 | 166.2 (7) |
| C19—C20—C21—C22 | 53.1 (12) | C75—C76—C77—C78 | 49 (2) |
| C20—C21—C22—C17 | -54.4 (12) | C76—C75—C80—C79 | 51 (2) |
| C22—C17—C18—C19 | -56.2 (10) | C76—C77—C78—C79 | -51 (2) |
| C23—P1—C3—C4 | 36.4 (8) | C77—C78—C79—C80 | 52 (2) |

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| C23—P1—C3—C8 | -151.5 (7) | C78—C79—C80—C75 | -51 (2) |
| C23—P1—C17—C18 | -52.0 (7) | C80—C75—C76—C77 | -48.9 (17) |
| C23—P1—C17—C22 | -178.0 (6) | O1A—S1A—N1A—S2A | 10.1 (11) |
| C23—C24—C25—C26 | 56.7 (10) | O1A—S1A—C1A—F1A | 173.3 (10) |
| C24—C23—C28—C27 | 59.8 (9) | O1A—S1A—C1A—F2A | 51.0 (10) |
| C24—C25—C26—C27 | -53.5 (10) | O1A—S1A—C1A—F3A | -65.6 (10) |
| C25—C26—C27—C28 | 53.8 (11) | O2A—S1A—N1A—S2A | 149.6 (8) |
| C26—C27—C28—C23 | -57.6 (10) | O2A—S1A—C1A—F1A | 46.2 (11) |
| C28—C23—C24—C25 | -59.4 (9) | O2A—S1A—C1A—F2A | -76.1 (10) |
| C29—P2—C43—C44 | 68.8 (7) | O2A—S1A—C1A—F3A | 167.3 (9) |
| C29—P2—C43—C48 | -169.6 (7) | O3A—S2A—N1A—S1A | 17.2 (10) |
| C29—P2—C49—C50 | 62.4 (8) | O3A—S2A—C2A—F4A | 173.8 (10) |
| C29—P2—C49—C54 | -65.3 (8) | O3A—S2A—C2A—F5A | -66.3 (10) |
| C29—C30—C31—C32 | -0.4 (16) | O3A—S2A—C2A—F6A | 50.4 (10) |
| C29—C34—C35—C36 | 85.6 (13) | O4A—S2A—N1A—S1A | -126.4 (8) |
| C29—C34—C35—C40 | -99.8 (12) | O4A—S2A—C2A—F4A | -60.4 (11) |
| C30—C29—C34—C33 | 5.4 (15) | O4A—S2A—C2A—F5A | 59.5 (9) |
| C30—C29—C34—C35 | -172.3 (10) | O4A—S2A—C2A—F6A | 176.2 (8) |
| C30—C31—C32—C33 | 2.5 (17) | N1A—S1A—C1A—F1A | -65.1 (11) |
| C31—C32—C33—C34 | -0.5 (18) | N1A—S1A—C1A—F2A | 172.6 (9) |
| C32—C33—C34—C29 | -3.5 (17) | N1A—S1A—C1A—F3A | 56.0 (10) |
| C32—C33—C34—C35 | 174.3 (11) | N1A—S2A—C2A—F4A | 54.2 (11) |
| C33—C34—C35—C36 | -92.2 (13) | N1A—S2A—C2A—F5A | 174.1 (8) |
| C33—C34—C35—C40 | 82.5 (13) | N1A—S2A—C2A—F6A | -69.2 (9) |
| C34—C29—C30—C31 | -3.5 (15) | C1A—S1A—N1A—S2A | -103.8 (9) |
| C34—C35—C36—O4 | -3.6 (16) | C2A—S2A—N1A—S1A | 127.1 (8) |
| C34—C35—C36—C37 | 179.3 (12) | | |
