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Acetatotris(triphenylarsine)silver(I) acetonitrile solvate monohydrate

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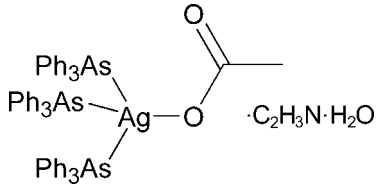
Key indicators: single-crystal X-ray study; T = 101 K; mean σ(C–C) = 0.003 Å; R factor = 0.022; wR factor = 0.075; data-to-parameter ratio = 20.4.

In the title compound, $[Ag(C_2H_3O_2)(C_{18}H_{15}As)_3]\cdot C_2H_3N\cdot H_2O$, the Ag atom is coordinated by three arsine ligands and one O atom, forming a distorted tetrahedral configuration. The Ag—As bond distances are 2.5921 (6), 2.6190 (8) and 2.6373 (9) Å, and the Ag—O bond distance is 2.3269 (18) Å. The Ag atom is displaced 0.7781 (3) Å out of the plane defined by the three As atoms.

Related literature

The crystal structure of the highly related complex $[Ag(4\text{-}MeC_6H_4SO_3)(AsPh_3)_3]$ has already been published (Meijboom, Janse van Rensburg, Senekal & Venter, 2006).

For related literature, see: Allen (2002); Mann *et al.* (1937); Meijboom, Janse van Rensburg, Kirsten & Viljoen (2006); Nardelli *et al.* (1985).



Experimental

Crystal data

$[Ag(C_2H_3O_2)(C_{18}H_{15}As)_3]\cdot C_2H_3N\cdot H_2O$
M_r = 1144.64
Triclinic, $P\overline{1}$
a = 13.121 (5) Å
b = 13.739 (5) Å
c = 14.051 (5) Å
α = 83.625 (5)°
β = 86.621 (5)°
γ = 79.662 (5)°
V = 2475 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.44 mm^{-1}
T = 101 (2) K
0.39 × 0.32 × 0.29 mm

Data collection

Bruker X8 APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.432, T_{max} = 0.495
66588 measured reflections
12287 independent reflections
11117 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.075
S = 1.20
12287 reflections
603 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.70 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O2	0.887 (17)	1.879 (18)	2.765 (3)	177 (3)
C54—H54···N	0.95	2.56	3.307 (3)	135
O3—H3B···O3^{i}	0.865 (17)	2.17 (2)	2.973 (4)	154 (3)

Symmetry code: (i) $-x+2, -y+1, -z+1$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2035).

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supplementary materials

Acta Cryst. (2007). E**63**, m2572 [**doi:10.1107/S1600536807044595**]

Acetatotris(triphenylarsine)silver(I) acetonitrile solvate monohydrate

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Comment

Silver(I) complexes of the type $[AgL_nX]$ (*L* is a tertiary phosphine or arsine, n = 1–4 and *X* is a coordinating or noncoordinating anion) were first prepared by Mann *et al.* (1937) and are the first crystallographically investigated examples of metal phosphine complexes. These compounds display a rich diversity of structural types due to the interplay of parameters such as the geometric flexibility of Ag(I), the bite angle, the electronic properties of the group 15 donor ligand, the coordination of the supporting ligand, *etc*. We present here the title compound, (I), a silver(I) tris(triphenylarsine) complex, of which only relatively few (11) examples can be found in the literature [Cambridge Structural Database (CSD), Version 5.28, November 2006 update; Allen, 2002].

Comparison of the title compound, (I), to the analogous $[Ag(4\text{-}MeC_6H_4SO_3)(AsPh_3)_3]$ complex (Meijboom, Janse van Rensburg, Senekal & Venter, 2006) indicate the expected tetrahedral environment around Ag. Coordination bond angles show a good correlation and all other bond distances and angles are unremarkable. The Ag atom in compound (I) is surrounded by three arsine ligands and an O atom of the acetate, forming a distorted tetrahedral configuration. The Ag—As bond distances are within the expected range (2.5921 (6), 2.6190 (8) and 2.6373 (9) Å). Also noted is the displacement of the Ag atom out of the plane defined by the three As atoms. In the title compound, (I) the Ag is displaced 0.7781 (3) Å, In addition, some weak inter- and intramolecular interactions are observed (Table 1).

An interesting factor to note is the displacement of the Ag atom out of the plane defined by the three As atoms. This displacement seems to be related to the coordinating ability of the fourth/supporting (anionic) group. When describing a completely tetrhedral environment, as in $[Ag(AsPh_3)_4][PF_6]$ (Meijboom, Janse van Rensburg, Kirsten & Viljoen, 2006), this displacement is 0.8903 (3) Å. With different coordinating ligands, the distortion from tetrahedral gets larger, as expressed by this displacement. The displacement decreases from 0.7781 (3) Å for (I), 0.6438 (2) Å for $[Ag(4\text{-}MeC_6H_4SO_3)(AsPh_3)_3]$ (Meijboom, Janse van Rensburg, Senekal & Venter, 2006) unto 0.6359 (2) Å for $[Ag(NO_3)(AsPh_3)_3]$ (Nardelli *et al.*, 1985). Up to now, no trigonal planar complexes have been reported for $AsPh_3$ yet, however these are not unknown for other ligands, such as phosphines.

Experimental

A solution of triphenylarsine (57.4 mg, 0.187 mmol) in warm ethanol (3.0 ml) was added to a solution of $[Ag(CH_3CO_2)]$ (31.0 mg, 0.186 mmol) in warm ethanol (2.0 ml). Colourless crystals of the title compound were obtained in quantitative yield (based on As) on allowing the solution to cool and stand.

Refinement

H atoms were positioned geometrically and refined using a riding model, with fixed C—H distances of 0.93 Å (CH) [$U_{iso}(H) = 1.2U_{eq}$] and 0.96 Å (CH_3) [$U_{iso}(H) = 1.5U_{eq}$]. The highest residual peak is 0.73 e located 1.17 Å from atom C1 and the

deepest hole −0.70 e, 0.64 Å from Ag. A Hirschfield test failure appeared in the structure validation. Using a disordered model the U values of the As atoms were refined to an 99.2% occupancy, allowing the structure to pass the Hirschfield test. The aqua molecule was restrained to keep the refinement stable.

Figures

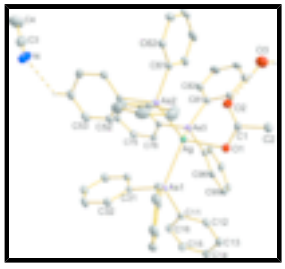


Fig. 1. The structure (I), showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity. For the C atoms, the first digit indicates ring number and the second digit indicates the position of the atom in the ring.

Acetatotris(triphenylarsine)silver(I) acetonitrile solvate monohydrate

Crystal data

$[Ag(C_2H_3O_2)(C_{18}H_{15}As)_3]\cdot C_2H_3N\cdot H_2O$	$Z = 2$
$M_r = 1144.64$	$F_{000} = 1156$
Triclinic, $P\overline{1}$	$D_x = 1.536$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 13.121$ (5) Å	Cell parameters from 7711 reflections
$b = 13.739$ (5) Å	$\theta = 2.2$–28.3°
$c = 14.051$ (5) Å	$\mu = 2.44$ mm^{-1}
$\alpha = 83.625$ (5)°	$T = 101$ (2) K
$\beta = 86.621$ (5)°	Prism, colourless
$\gamma = 79.662$ (5)°	0.39 × 0.32 × 0.29 mm
$V = 2475$ (2) Å^3	

Data collection

Bruker X8 APEXII diffractometer	11117 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.036$
$T = 101$(2) K	$\theta_{max} = 28.3^\circ$
ω and φ scans	$\theta_{min} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$h = -17\rightarrow17$
$T_{min} = 0.432$, $T_{max} = 0.495$	$k = -18\rightarrow18$
66588 measured reflections	$l = -18\rightarrow18$
12287 independent reflections	

Refinement

Refinement on F^2	3 restraints

Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.022$	$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 0.6766P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.075$	$(\Delta/\sigma)_{max} = 0.003$
$S = 1.20$	$\Delta\rho_{max} = 0.73$ e Å^{-3}
12287 reflections	$\Delta\rho_{min} = -0.70$ e Å^{-3}
603 parameters	Extinction correction: none

Special details

Experimental. The intensity data was collected on a Bruker X8 Apex II 4 K Kappa CCD diffractometer using an exposure time of 5 s/frame. A total of 2771 frames were collected with a frame width of 0.5° covering up to θ = 28.33° with 99.9% completeness accomplished.

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag	0.758824 (11)	0.195208 (10)	0.728465 (10)	0.01267 (4)
As1	0.765587 (15)	0.010529 (14)	0.806250 (14)	0.01240 (5)
As2	0.657612 (15)	0.325411 (14)	0.835151 (13)	0.01243 (5)
As3	0.684178 (15)	0.216483 (14)	0.557129 (13)	0.01226 (5)
O1	0.93657 (12)	0.19440 (12)	0.71474 (13)	0.0274 (4)
O2	0.88524 (13)	0.35687 (13)	0.69568 (16)	0.0413 (5)
C1	0.95360 (15)	0.28120 (16)	0.70034 (15)	0.0185 (4)
C2	1.06546 (18)	0.29657 (18)	0.6830 (2)	0.0306 (5)
H2A	1.0837	0.2983	0.6143	0.046*
H2B	1.1114	0.2417	0.7178	0.046*
H2C	1.0732	0.3596	0.7058	0.046*
N	0.0604 (2)	0.4127 (2)	0.9169 (2)	0.0553 (7)
C3	−0.0024 (2)	0.4715 (2)	0.8821 (2)	0.0388 (6)
C4	−0.0845 (3)	0.5446 (2)	0.8408 (3)	0.0525 (8)
H4A	−0.1235	0.5134	0.799	0.079*
H4B	−0.0549	0.598	0.8032	0.079*
H4C	−0.131	0.5722	0.892	0.079*
C11	0.84120 (15)	−0.10028 (14)	0.74123 (14)	0.0140 (4)
C12	0.94758 (15)	−0.10439 (15)	0.72360 (14)	0.0173 (4)
H12	0.9808	−0.0549	0.7442	0.021*
C13	1.00489 (16)	−0.18071 (16)	0.67599 (15)	0.0202 (4)
H13	1.0774	−0.1837	0.6646	0.024*
C14	0.95619 (17)	−0.25292 (16)	0.64493 (16)	0.0217 (4)
H14	0.9954	−0.3051	0.6123	0.026*
C15	0.85059 (17)	−0.24847 (16)	0.66174 (17)	0.0243 (5)

H15	0.8173	−0.2976	0.6404	0.029*
C16	0.79312 (16)	−0.17225 (15)	0.70979 (16)	0.0209 (4)
H16	0.7206	−0.1695	0.7211	0.025*
C21	0.82362 (15)	−0.02343 (14)	0.93176 (14)	0.0140 (4)
C22	0.85978 (16)	−0.12179 (15)	0.96811 (15)	0.0174 (4)
H22	0.8522	−0.175	0.9329	0.021*
C23	0.90675 (16)	−0.14144 (16)	1.05562 (15)	0.0192 (4)
H23	0.9313	−0.2083	1.0802	0.023*
C24	0.91812 (16)	−0.06414 (16)	1.10748 (15)	0.0199 (4)
H24	0.9512	−0.078	1.167	0.024*
C25	0.88111 (17)	0.03360 (16)	1.07243 (15)	0.0209 (4)
H25	0.888	0.0865	1.1084	0.025*
C26	0.83390 (15)	0.05398 (15)	0.98461 (15)	0.0173 (4)
H26	0.8086	0.1208	0.9607	0.021*
C31	0.62951 (15)	−0.02768 (14)	0.82364 (14)	0.0138 (4)
C32	0.59538 (16)	−0.07678 (16)	0.90805 (15)	0.0194 (4)
H32	0.6396	−0.0941	0.9607	0.023*
C33	0.49643 (17)	−0.10040 (17)	0.91527 (16)	0.0242 (5)
H33	0.4732	−0.1341	0.973	0.029*
C34	0.43107 (17)	−0.07515 (17)	0.83861 (16)	0.0233 (4)
H34	0.3636	−0.0918	0.8439	0.028*
C35	0.46450 (17)	−0.02577 (16)	0.75457 (16)	0.0207 (4)
H35	0.4201	−0.0082	0.7021	0.025*
C36	0.56342 (16)	−0.00195 (15)	0.74742 (14)	0.0170 (4)
H36	0.5862	0.0323	0.6899	0.02*
C41	0.70622 (16)	0.32578 (14)	0.96343 (14)	0.0156 (4)
C42	0.81163 (17)	0.32505 (16)	0.97131 (16)	0.0222 (4)
H42	0.8559	0.3266	0.9154	0.027*
C43	0.85215 (18)	0.32210 (18)	1.06091 (18)	0.0280 (5)
H43	0.9239	0.3224	1.0661	0.034*
C44	0.78762 (19)	0.31865 (17)	1.14311 (17)	0.0278 (5)
H44	0.8154	0.3162	1.2044	0.033*
C45	0.68339 (19)	0.31888 (17)	1.13530 (16)	0.0257 (5)
H45	0.6394	0.3167	1.1914	0.031*
C46	0.64217 (17)	0.32224 (16)	1.04540 (15)	0.0195 (4)
H46	0.5703	0.3221	1.0404	0.023*
C51	0.51136 (15)	0.31861 (14)	0.86055 (13)	0.0136 (4)
C52	0.47895 (16)	0.23102 (15)	0.84491 (15)	0.0182 (4)
H52	0.528	0.1773	0.8237	0.022*
C53	0.37538 (17)	0.22124 (17)	0.86003 (16)	0.0230 (4)
H53	0.354	0.161	0.8493	0.028*
C54	0.30339 (17)	0.29932 (17)	0.89081 (15)	0.0228 (4)
H54	0.2327	0.2926	0.9015	0.027*
C55	0.33488 (16)	0.38747 (16)	0.90598 (15)	0.0209 (4)
H55	0.2855	0.4411	0.9267	0.025*
C56	0.43817 (16)	0.39748 (15)	0.89097 (15)	0.0179 (4)
H56	0.4592	0.458	0.9013	0.021*
C61	0.64800 (14)	0.46448 (14)	0.78628 (14)	0.0147 (4)
C62	0.62752 (16)	0.54129 (15)	0.84537 (16)	0.0195 (4)

H62	0.6241	0.5265	0.913	0.023*
C63	0.61217 (17)	0.63949 (16)	0.80505 (18)	0.0251 (5)
H63	0.5973	0.692	0.8452	0.03*
C64	0.61850 (17)	0.66101 (17)	0.70649 (19)	0.0273 (5)
H64	0.606	0.7282	0.679	0.033*
C65	0.64299 (17)	0.58481 (18)	0.64777 (17)	0.0257 (5)
H65	0.6496	0.5999	0.5803	0.031*
C66	0.65778 (16)	0.48681 (16)	0.68732 (15)	0.0200 (4)
H66	0.6746	0.4346	0.647	0.024*
C71	0.53852 (15)	0.20706 (14)	0.54807 (14)	0.0142 (4)
C72	0.46556 (16)	0.27055 (16)	0.59846 (15)	0.0195 (4)
H72	0.4875	0.3185	0.6327	0.023*
C73	0.36101 (16)	0.26442 (17)	0.59916 (16)	0.0230 (4)
H73	0.3118	0.3079	0.634	0.028*
C74	0.32848 (16)	0.19511 (16)	0.54925 (16)	0.0214 (4)
H74	0.2569	0.191	0.5496	0.026*
C75	0.40016 (16)	0.13178 (16)	0.49881 (16)	0.0214 (4)
H75	0.3778	0.0843	0.4643	0.026*
C76	0.50486 (16)	0.13731 (15)	0.49845 (15)	0.0184 (4)
H76	0.5538	0.0932	0.4641	0.022*
C81	0.69607 (15)	0.33401 (14)	0.46904 (14)	0.0146 (4)
C82	0.61863 (17)	0.37928 (16)	0.40779 (15)	0.0212 (4)
H82	0.5538	0.3571	0.4119	0.025*
C83	0.63590 (19)	0.45763 (17)	0.33981 (16)	0.0259 (5)
H83	0.5826	0.489	0.2981	0.031*
C84	0.72991 (19)	0.48946 (16)	0.33319 (16)	0.0245 (5)
H84	0.7421	0.5413	0.2856	0.029*
C85	0.80700 (18)	0.44592 (17)	0.39586 (17)	0.0265 (5)
H85	0.8714	0.4688	0.3919	0.032*
C86	0.78998 (17)	0.36875 (16)	0.46441 (16)	0.0217 (4)
H86	0.8423	0.3397	0.508	0.026*
C91	0.75413 (15)	0.11608 (14)	0.47754 (14)	0.0141 (4)
C92	0.73331 (15)	0.11703 (16)	0.38087 (14)	0.0166 (4)
H92	0.6821	0.1676	0.3518	0.02*
C93	0.78775 (16)	0.04381 (16)	0.32758 (15)	0.0196 (4)
H93	0.7735	0.0443	0.262	0.024*
C94	0.86278 (16)	−0.02995 (15)	0.36955 (15)	0.0191 (4)
H94	0.8993	−0.0802	0.3329	0.023*
C95	0.88455 (16)	−0.03056 (15)	0.46499 (15)	0.0200 (4)
H95	0.9364	−0.0807	0.4937	0.024*
C96	0.83026 (16)	0.04241 (15)	0.51848 (14)	0.0176 (4)
H96	0.8453	0.042	0.5838	0.021*
O3	0.92952 (18)	0.52412 (16)	0.58411 (17)	0.0479 (5)
H3A	0.917 (3)	0.4700 (19)	0.620 (2)	0.058*
H3B	0.962 (3)	0.529 (2)	0.5288 (16)	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag	0.01282 (7)	0.01352 (7)	0.01234 (7)	−0.00327 (5)	−0.00042 (5)	−0.00269 (5)
As1	0.01405 (10)	0.01127 (9)	0.01265 (10)	−0.00450 (7)	−0.00185 (7)	−0.00013 (7)
As2	0.01327 (9)	0.01217 (9)	0.01205 (9)	−0.00211 (7)	0.00058 (7)	−0.00291 (7)
As3	0.01330 (9)	0.01365 (10)	0.01007 (9)	−0.00233 (7)	−0.00157 (7)	−0.00174 (7)
O1	0.0186 (8)	0.0202 (8)	0.0437 (10)	−0.0049 (6)	0.0023 (7)	−0.0034 (7)
O2	0.0226 (9)	0.0241 (9)	0.0746 (15)	−0.0015 (7)	0.0040 (9)	−0.0007 (9)
C1	0.0140 (9)	0.0211 (10)	0.0206 (10)	−0.0044 (8)	−0.0004 (8)	−0.0009 (8)
C2	0.0204 (11)	0.0241 (12)	0.0484 (15)	−0.0080 (9)	0.0060 (10)	−0.0056 (11)
N	0.0344 (13)	0.0447 (15)	0.086 (2)	0.0027 (12)	0.0064 (14)	−0.0222 (15)
C3	0.0342 (14)	0.0379 (15)	0.0472 (16)	−0.0100 (12)	0.0067 (12)	−0.0157 (13)
C4	0.056 (2)	0.0433 (17)	0.058 (2)	−0.0087 (15)	−0.0157 (16)	0.0038 (15)
C11	0.0164 (9)	0.0122 (9)	0.0136 (9)	−0.0043 (7)	−0.0017 (7)	0.0014 (7)
C12	0.0163 (9)	0.0205 (10)	0.0170 (9)	−0.0083 (8)	−0.0025 (8)	−0.0010 (8)
C13	0.0146 (9)	0.0237 (11)	0.0219 (10)	−0.0037 (8)	0.0003 (8)	−0.0002 (8)
C14	0.0206 (10)	0.0167 (10)	0.0268 (11)	−0.0010 (8)	0.0018 (9)	−0.0032 (8)
C15	0.0213 (11)	0.0175 (10)	0.0367 (13)	−0.0072 (8)	0.0026 (9)	−0.0097 (9)
C16	0.0155 (9)	0.0179 (10)	0.0307 (12)	−0.0048 (8)	0.0017 (8)	−0.0073 (9)
C21	0.0125 (9)	0.0163 (9)	0.0142 (9)	−0.0056 (7)	−0.0018 (7)	0.0004 (7)
C22	0.0188 (10)	0.0158 (9)	0.0187 (10)	−0.0059 (8)	−0.0023 (8)	−0.0010 (8)
C23	0.0185 (10)	0.0193 (10)	0.0187 (10)	−0.0038 (8)	−0.0014 (8)	0.0032 (8)
C24	0.0186 (10)	0.0281 (11)	0.0135 (9)	−0.0070 (8)	−0.0018 (8)	0.0006 (8)
C25	0.0240 (11)	0.0251 (11)	0.0159 (10)	−0.0079 (9)	−0.0008 (8)	−0.0063 (8)
C26	0.0171 (9)	0.0162 (9)	0.0190 (10)	−0.0038 (7)	0.0009 (8)	−0.0022 (8)
C31	0.0145 (9)	0.0125 (9)	0.0154 (9)	−0.0039 (7)	−0.0004 (7)	−0.0028 (7)
C32	0.0185 (10)	0.0222 (10)	0.0174 (10)	−0.0045 (8)	−0.0029 (8)	0.0011 (8)
C33	0.0217 (11)	0.0311 (12)	0.0205 (11)	−0.0119 (9)	0.0000 (9)	0.0057 (9)
C34	0.0168 (10)	0.0265 (11)	0.0282 (12)	−0.0092 (8)	−0.0010 (9)	−0.0010 (9)
C35	0.0195 (10)	0.0244 (11)	0.0198 (10)	−0.0064 (8)	−0.0059 (8)	−0.0018 (8)
C36	0.0201 (10)	0.0171 (10)	0.0144 (9)	−0.0047 (8)	−0.0020 (8)	−0.0010 (7)
C41	0.0187 (9)	0.0106 (9)	0.0174 (9)	−0.0008 (7)	−0.0043 (8)	−0.0027 (7)
C42	0.0198 (10)	0.0227 (11)	0.0245 (11)	−0.0023 (8)	−0.0019 (8)	−0.0066 (9)
C43	0.0224 (11)	0.0274 (12)	0.0358 (13)	−0.0022 (9)	−0.0137 (10)	−0.0074 (10)
C44	0.0370 (13)	0.0237 (11)	0.0230 (11)	0.0004 (10)	−0.0159 (10)	−0.0053 (9)
C45	0.0347 (13)	0.0263 (11)	0.0149 (10)	−0.0019 (9)	−0.0025 (9)	−0.0019 (8)
C46	0.0211 (10)	0.0206 (10)	0.0164 (10)	−0.0016 (8)	−0.0028 (8)	−0.0027 (8)
C51	0.0149 (9)	0.0159 (9)	0.0098 (8)	−0.0033 (7)	−0.0010 (7)	0.0009 (7)
C52	0.0213 (10)	0.0160 (9)	0.0174 (10)	−0.0043 (8)	−0.0015 (8)	−0.0007 (8)
C53	0.0249 (11)	0.0233 (11)	0.0228 (11)	−0.0105 (9)	−0.0039 (9)	0.0010 (9)
C54	0.0161 (10)	0.0324 (12)	0.0198 (10)	−0.0084 (9)	−0.0016 (8)	0.0042 (9)
C55	0.0157 (10)	0.0253 (11)	0.0199 (10)	−0.0009 (8)	0.0004 (8)	−0.0002 (8)
C56	0.0181 (10)	0.0176 (10)	0.0186 (10)	−0.0049 (8)	0.0006 (8)	−0.0024 (8)
C61	0.0108 (8)	0.0149 (9)	0.0183 (9)	−0.0029 (7)	0.0000 (7)	−0.0008 (7)
C62	0.0182 (10)	0.0172 (10)	0.0235 (10)	−0.0047 (8)	0.0011 (8)	−0.0028 (8)
C63	0.0205 (10)	0.0167 (10)	0.0395 (13)	−0.0058 (8)	−0.0007 (10)	−0.0048 (9)

C64	0.0179 (10)	0.0180 (10)	0.0458 (14)	−0.0093 (8)	−0.0086 (10)	0.0114 (10)
C65	0.0228 (11)	0.0304 (12)	0.0238 (11)	−0.0116 (9)	−0.0054 (9)	0.0111 (9)
C66	0.0173 (10)	0.0244 (11)	0.0193 (10)	−0.0073 (8)	−0.0005 (8)	−0.0002 (8)
C71	0.0151 (9)	0.0151 (9)	0.0120 (9)	−0.0032 (7)	−0.0009 (7)	0.0020 (7)
C72	0.0208 (10)	0.0197 (10)	0.0183 (10)	−0.0037 (8)	0.0015 (8)	−0.0042 (8)
C73	0.0174 (10)	0.0247 (11)	0.0253 (11)	−0.0005 (8)	0.0048 (8)	−0.0041 (9)
C74	0.0147 (9)	0.0243 (11)	0.0247 (11)	−0.0057 (8)	0.0012 (8)	0.0028 (9)
C75	0.0198 (10)	0.0219 (10)	0.0250 (11)	−0.0090 (8)	−0.0011 (8)	−0.0037 (9)
C76	0.0178 (10)	0.0185 (10)	0.0193 (10)	−0.0030 (8)	0.0010 (8)	−0.0055 (8)
C81	0.0176 (9)	0.0139 (9)	0.0126 (9)	−0.0029 (7)	0.0000 (7)	−0.0030 (7)
C82	0.0214 (10)	0.0216 (10)	0.0209 (10)	−0.0060 (8)	−0.0032 (8)	0.0013 (8)
C83	0.0330 (12)	0.0212 (11)	0.0212 (11)	−0.0012 (9)	−0.0067 (9)	0.0048 (9)
C84	0.0357 (13)	0.0139 (10)	0.0226 (11)	−0.0039 (9)	0.0030 (9)	0.0009 (8)
C85	0.0252 (11)	0.0223 (11)	0.0330 (13)	−0.0099 (9)	0.0043 (10)	−0.0014 (9)
C86	0.0195 (10)	0.0196 (10)	0.0261 (11)	−0.0050 (8)	−0.0031 (8)	0.0009 (8)
C91	0.0134 (9)	0.0153 (9)	0.0142 (9)	−0.0044 (7)	0.0004 (7)	−0.0015 (7)
C92	0.0134 (9)	0.0224 (10)	0.0143 (9)	−0.0029 (7)	−0.0017 (7)	−0.0031 (8)
C93	0.0175 (10)	0.0286 (11)	0.0157 (9)	−0.0085 (8)	0.0008 (8)	−0.0088 (8)
C94	0.0188 (10)	0.0165 (10)	0.0237 (10)	−0.0066 (8)	0.0059 (8)	−0.0071 (8)
C95	0.0188 (10)	0.0166 (10)	0.0228 (10)	−0.0008 (8)	0.0010 (8)	0.0018 (8)
C96	0.0194 (10)	0.0187 (10)	0.0138 (9)	−0.0036 (8)	−0.0001 (8)	0.0016 (7)
O3	0.0540 (13)	0.0364 (11)	0.0523 (14)	−0.0093 (10)	0.0106 (11)	−0.0045 (10)

Geometric parameters (Å, °)

Ag—O1	2.3269 (18)	C44—C45	1.378 (3)
Ag—As2	2.5921 (6)	C44—H44	0.95
Ag—As3	2.6190 (8)	C45—C46	1.396 (3)
Ag—As1	2.6373 (9)	C45—H45	0.95
As1—C21	1.938 (2)	C46—H46	0.95
As1—C31	1.944 (2)	C51—C52	1.390 (3)
As1—C11	1.949 (2)	C51—C56	1.400 (3)
As2—C61	1.942 (2)	C52—C53	1.391 (3)
As2—C41	1.948 (2)	C52—H52	0.95
As2—C51	1.948 (2)	C53—C54	1.386 (3)
As3—C91	1.9399 (19)	C53—H53	0.95
As3—C81	1.946 (2)	C54—C55	1.389 (3)
As3—C71	1.951 (2)	C54—H54	0.95
O1—C1	1.245 (3)	C55—C56	1.388 (3)
O2—C1	1.244 (3)	C55—H55	0.95
C1—C2	1.522 (3)	C56—H56	0.95
C2—H2A	0.98	C61—C62	1.393 (3)
C2—H2B	0.98	C61—C66	1.394 (3)
C2—H2C	0.98	C62—C63	1.388 (3)
N—C3	1.136 (4)	C62—H62	0.95
C3—C4	1.435 (4)	C63—C64	1.384 (4)
C4—H4A	0.98	C63—H63	0.95
C4—H4B	0.98	C64—C65	1.386 (4)
C4—H4C	0.98	C64—H64	0.95

C11—C16	1.387 (3)	C65—C66	1.383 (3)
C11—C12	1.395 (3)	C65—H65	0.95
C12—C13	1.388 (3)	C66—H66	0.95
C12—H12	0.95	C71—C76	1.391 (3)
C13—C14	1.393 (3)	C71—C72	1.391 (3)
C13—H13	0.95	C72—C73	1.389 (3)
C14—C15	1.383 (3)	C72—H72	0.95
C14—H14	0.95	C73—C74	1.382 (3)
C15—C16	1.391 (3)	C73—H73	0.95
C15—H15	0.95	C74—C75	1.382 (3)
C16—H16	0.95	C74—H74	0.95
C21—C26	1.393 (3)	C75—C76	1.389 (3)
C21—C22	1.399 (3)	C75—H75	0.95
C22—C23	1.386 (3)	C76—H76	0.95
C22—H22	0.95	C81—C82	1.385 (3)
C23—C24	1.387 (3)	C81—C86	1.395 (3)
C23—H23	0.95	C82—C83	1.399 (3)
C24—C25	1.389 (3)	C82—H82	0.95
C24—H24	0.95	C83—C84	1.376 (3)
C25—C26	1.391 (3)	C83—H83	0.95
C25—H25	0.95	C84—C85	1.388 (3)
C26—H26	0.95	C84—H84	0.95
C31—C32	1.389 (3)	C85—C86	1.391 (3)
C31—C36	1.393 (3)	C85—H85	0.95
C32—C33	1.389 (3)	C86—H86	0.95
C32—H32	0.95	C91—C96	1.389 (3)
C33—C34	1.391 (3)	C91—C92	1.399 (3)
C33—H33	0.95	C92—C93	1.389 (3)
C34—C35	1.384 (3)	C92—H92	0.95
C34—H34	0.95	C93—C94	1.386 (3)
C35—C36	1.390 (3)	C93—H93	0.95
C35—H35	0.95	C94—C95	1.386 (3)
C36—H36	0.95	C94—H94	0.95
C41—C46	1.387 (3)	C95—C96	1.387 (3)
C41—C42	1.392 (3)	C95—H95	0.95
C42—C43	1.389 (3)	C96—H96	0.95
C42—H42	0.95	O3—H3A	0.887 (17)
C43—C44	1.393 (4)	O3—H3B	0.865 (17)
C43—H43	0.95		
O1—Ag—As2	114.21 (4)	C42—C43—H43	120
O1—Ag—As3	109.38 (5)	C44—C43—H43	120
As2—Ag—As3	111.58 (2)	C45—C44—C43	119.9 (2)
O1—Ag—As1	97.83 (4)	C45—C44—H44	120.1
As2—Ag—As1	112.97 (2)	C43—C44—H44	120.1
As3—Ag—As1	110.077 (13)	C44—C45—C46	120.3 (2)
C21—As1—C31	103.76 (8)	C44—C45—H45	119.8
C21—As1—C11	99.53 (8)	C46—C45—H45	119.8
C31—As1—C11	100.32 (8)	C41—C46—C45	119.9 (2)
C21—As1—Ag	117.12 (6)	C41—C46—H46	120

C31—As1—Ag	112.95 (6)	C45—C46—H46	120
C11—As1—Ag	120.50 (6)	C52—C51—C56	119.12 (18)
C61—As2—C41	101.39 (8)	C52—C51—As2	117.31 (14)
C61—As2—C51	100.35 (8)	C56—C51—As2	123.55 (15)
C41—As2—C51	102.21 (8)	C51—C52—C53	120.59 (19)
C61—As2—Ag	116.99 (6)	C51—C52—H52	119.7
C41—As2—Ag	117.63 (6)	C53—C52—H52	119.7
C51—As2—Ag	115.58 (6)	C54—C53—C52	120.0 (2)
C91—As3—C81	98.54 (8)	C54—C53—H53	120
C91—As3—C71	102.62 (8)	C52—C53—H53	120
C81—As3—C71	101.76 (8)	C53—C54—C55	119.8 (2)
C91—As3—Ag	112.54 (6)	C53—C54—H54	120.1
C81—As3—Ag	120.68 (6)	C55—C54—H54	120.1
C71—As3—Ag	117.66 (6)	C56—C55—C54	120.3 (2)
C1—O1—Ag	109.98 (13)	C56—C55—H55	119.8
O2—C1—O1	124.6 (2)	C54—C55—H55	119.8
O2—C1—C2	117.15 (19)	C55—C56—C51	120.13 (19)
O1—C1—C2	118.16 (19)	C55—C56—H56	119.9
C1—C2—H2A	109.5	C51—C56—H56	119.9
C1—C2—H2B	109.5	C62—C61—C66	119.69 (19)
H2A—C2—H2B	109.5	C62—C61—As2	122.77 (15)
C1—C2—H2C	109.5	C66—C61—As2	117.48 (15)
H2A—C2—H2C	109.5	C63—C62—C61	119.8 (2)
H2B—C2—H2C	109.5	C63—C62—H62	120.1
N—C3—C4	177.9 (3)	C61—C62—H62	120.1
C3—C4—H4A	109.5	C64—C63—C62	120.1 (2)
C3—C4—H4B	109.5	C64—C63—H63	120
H4A—C4—H4B	109.5	C62—C63—H63	120
C3—C4—H4C	109.5	C63—C64—C65	120.2 (2)
H4A—C4—H4C	109.5	C63—C64—H64	119.9
H4B—C4—H4C	109.5	C65—C64—H64	119.9
C16—C11—C12	119.53 (18)	C66—C65—C64	120.0 (2)
C16—C11—As1	122.75 (15)	C66—C65—H65	120
C12—C11—As1	117.69 (14)	C64—C65—H65	120
C13—C12—C11	120.10 (19)	C65—C66—C61	120.1 (2)
C13—C12—H12	120	C65—C66—H66	120
C11—C12—H12	120	C61—C66—H66	120
C12—C13—C14	120.07 (19)	C76—C71—C72	118.81 (19)
C12—C13—H13	120	C76—C71—As3	123.57 (15)
C14—C13—H13	120	C72—C71—As3	117.53 (15)
C15—C14—C13	119.86 (19)	C73—C72—C71	120.6 (2)
C15—C14—H14	120.1	C73—C72—H72	119.7
C13—C14—H14	120.1	C71—C72—H72	119.7
C14—C15—C16	120.1 (2)	C74—C73—C72	120.07 (19)
C14—C15—H15	119.9	C74—C73—H73	120
C16—C15—H15	119.9	C72—C73—H73	120
C11—C16—C15	120.3 (2)	C75—C74—C73	119.9 (2)
C11—C16—H16	119.9	C75—C74—H74	120.1
C15—C16—H16	119.9	C73—C74—H74	120.1

C26—C21—C22	119.60 (18)	C74—C75—C76	120.2 (2)
C26—C21—As1	118.00 (15)	C74—C75—H75	119.9
C22—C21—As1	122.32 (15)	C76—C75—H75	119.9
C23—C22—C21	119.89 (19)	C75—C76—C71	120.47 (19)
C23—C22—H22	120.1	C75—C76—H76	119.8
C21—C22—H22	120.1	C71—C76—H76	119.8
C22—C23—C24	120.38 (19)	C82—C81—C86	119.72 (19)
C22—C23—H23	119.8	C82—C81—As3	122.82 (15)
C24—C23—H23	119.8	C86—C81—As3	117.33 (15)
C23—C24—C25	120.03 (19)	C81—C82—C83	120.0 (2)
C23—C24—H24	120	C81—C82—H82	120
C25—C24—H24	120	C83—C82—H82	120
C24—C25—C26	119.95 (19)	C84—C83—C82	120.2 (2)
C24—C25—H25	120	C84—C83—H83	119.9
C26—C25—H25	120	C82—C83—H83	119.9
C25—C26—C21	120.14 (19)	C83—C84—C85	120.1 (2)
C25—C26—H26	119.9	C83—C84—H84	119.9
C21—C26—H26	119.9	C85—C84—H84	119.9
C32—C31—C36	119.39 (18)	C84—C85—C86	120.0 (2)
C32—C31—As1	123.30 (15)	C84—C85—H85	120
C36—C31—As1	117.30 (15)	C86—C85—H85	120
C33—C32—C31	119.83 (19)	C85—C86—C81	119.9 (2)
C33—C32—H32	120.1	C85—C86—H86	120
C31—C32—H32	120.1	C81—C86—H86	120
C32—C33—C34	120.5 (2)	C96—C91—C92	119.31 (18)
C32—C33—H33	119.8	C96—C91—As3	117.85 (15)
C34—C33—H33	119.8	C92—C91—As3	122.81 (15)
C35—C34—C33	119.9 (2)	C93—C92—C91	119.77 (19)
C35—C34—H34	120.1	C93—C92—H92	120.1
C33—C34—H34	120.1	C91—C92—H92	120.1
C34—C35—C36	119.6 (2)	C94—C93—C92	120.37 (19)
C34—C35—H35	120.2	C94—C93—H93	119.8
C36—C35—H35	120.2	C92—C93—H93	119.8
C35—C36—C31	120.78 (19)	C93—C94—C95	120.09 (18)
C35—C36—H36	119.6	C93—C94—H94	120
C31—C36—H36	119.6	C95—C94—H94	120
C46—C41—C42	119.76 (19)	C94—C95—C96	119.7 (2)
C46—C41—As2	123.17 (16)	C94—C95—H95	120.1
C42—C41—As2	117.00 (15)	C96—C95—H95	120.1
C43—C42—C41	120.1 (2)	C95—C96—C91	120.75 (19)
C43—C42—H42	120	C95—C96—H96	119.6
C41—C42—H42	120	C91—C96—H96	119.6
C42—C43—C44	120.1 (2)	H3A—O3—H3B	130 (3)
O1—Ag—As1—C21	63.64 (8)	Ag—As2—C41—C42	49.02 (17)
As2—Ag—As1—C21	−56.89 (7)	C46—C41—C42—C43	−0.8 (3)
As3—Ag—As1—C21	177.64 (6)	As2—C41—C42—C43	−177.97 (17)
O1—Ag—As1—C31	−175.90 (7)	C41—C42—C43—C44	0.8 (3)
As2—Ag—As1—C31	63.58 (6)	C42—C43—C44—C45	−0.4 (3)
As3—Ag—As1—C31	−61.89 (6)	C43—C44—C45—C46	0.2 (3)

O1—Ag—As1—C11	−57.53 (8)	C42—C41—C46—C45	0.6 (3)
As2—Ag—As1—C11	−178.05 (7)	As2—C41—C46—C45	177.54 (16)
As3—Ag—As1—C11	56.48 (7)	C44—C45—C46—C41	−0.3 (3)
O1—Ag—As2—C61	68.85 (8)	C61—As2—C51—C52	144.80 (16)
As3—Ag—As2—C61	−55.84 (7)	C41—As2—C51—C52	−111.03 (16)
As1—Ag—As2—C61	179.51 (6)	Ag—As2—C51—C52	18.00 (17)
O1—Ag—As2—C41	−52.27 (8)	C61—As2—C51—C56	−33.53 (18)
As3—Ag—As2—C41	−176.96 (7)	C41—As2—C51—C56	70.65 (18)
As1—Ag—As2—C41	58.39 (7)	Ag—As2—C51—C56	−160.33 (15)
O1—Ag—As2—C51	−173.29 (8)	C56—C51—C52—C53	−0.6 (3)
As3—Ag—As2—C51	62.03 (6)	As2—C51—C52—C53	−178.98 (16)
As1—Ag—As2—C51	−62.63 (6)	C51—C52—C53—C54	0.1 (3)
O1—Ag—As3—C91	55.40 (8)	C52—C53—C54—C55	0.4 (3)
As2—Ag—As3—C91	−177.25 (6)	C53—C54—C55—C56	−0.4 (3)
As1—Ag—As3—C91	−50.99 (7)	C54—C55—C56—C51	−0.1 (3)
O1—Ag—As3—C81	−60.27 (8)	C52—C51—C56—C55	0.6 (3)
As2—Ag—As3—C81	67.07 (7)	As2—C51—C56—C55	178.87 (15)
As1—Ag—As3—C81	−166.67 (7)	C41—As2—C61—C62	−29.07 (18)
O1—Ag—As3—C71	174.38 (7)	C51—As2—C61—C62	75.77 (18)
As2—Ag—As3—C71	−58.27 (7)	Ag—As2—C61—C62	−158.38 (14)
As1—Ag—As3—C71	67.99 (6)	C41—As2—C61—C66	153.78 (16)
As2—Ag—O1—C1	−44.67 (16)	C51—As2—C61—C66	−101.38 (16)
As3—Ag—O1—C1	81.18 (15)	Ag—As2—C61—C66	24.47 (17)
As1—Ag—O1—C1	−164.26 (14)	C66—C61—C62—C63	3.0 (3)
Ag—O1—C1—O2	1.1 (3)	As2—C61—C62—C63	−174.05 (16)
Ag—O1—C1—C2	−176.22 (16)	C61—C62—C63—C64	−0.8 (3)
C21—As1—C11—C16	113.68 (18)	C62—C63—C64—C65	−1.8 (3)
C31—As1—C11—C16	7.68 (19)	C63—C64—C65—C66	2.2 (3)
Ag—As1—C11—C16	−116.87 (17)	C64—C65—C66—C61	0.1 (3)
C21—As1—C11—C12	−68.34 (16)	C62—C61—C66—C65	−2.7 (3)
C31—As1—C11—C12	−174.34 (15)	As2—C61—C66—C65	174.58 (16)
Ag—As1—C11—C12	61.10 (17)	C91—As3—C71—C76	3.30 (19)
C16—C11—C12—C13	−0.8 (3)	C81—As3—C71—C76	104.96 (18)
As1—C11—C12—C13	−178.84 (16)	Ag—As3—C71—C76	−120.81 (16)
C11—C12—C13—C14	0.6 (3)	C91—As3—C71—C72	179.83 (16)
C12—C13—C14—C15	−0.1 (3)	C81—As3—C71—C72	−78.51 (17)
C13—C14—C15—C16	−0.2 (4)	Ag—As3—C71—C72	55.72 (17)
C12—C11—C16—C15	0.5 (3)	C76—C71—C72—C73	0.0 (3)
As1—C11—C16—C15	178.48 (17)	As3—C71—C72—C73	−176.73 (16)
C14—C15—C16—C11	0.0 (4)	C71—C72—C73—C74	−0.2 (3)
C31—As1—C21—C26	−109.09 (16)	C72—C73—C74—C75	0.1 (3)
C11—As1—C21—C26	147.72 (15)	C73—C74—C75—C76	0.3 (3)
Ag—As1—C21—C26	16.10 (17)	C74—C75—C76—C71	−0.5 (3)
C31—As1—C21—C22	74.20 (17)	C72—C71—C76—C75	0.4 (3)
C11—As1—C21—C22	−28.98 (18)	As3—C71—C76—C75	176.91 (16)
Ag—As1—C21—C22	−160.60 (14)	C91—As3—C81—C82	94.70 (17)
C26—C21—C22—C23	−0.9 (3)	C71—As3—C81—C82	−10.19 (18)
As1—C21—C22—C23	175.77 (15)	Ag—As3—C81—C82	−142.63 (15)
C21—C22—C23—C24	0.0 (3)	C91—As3—C81—C86	−81.06 (17)

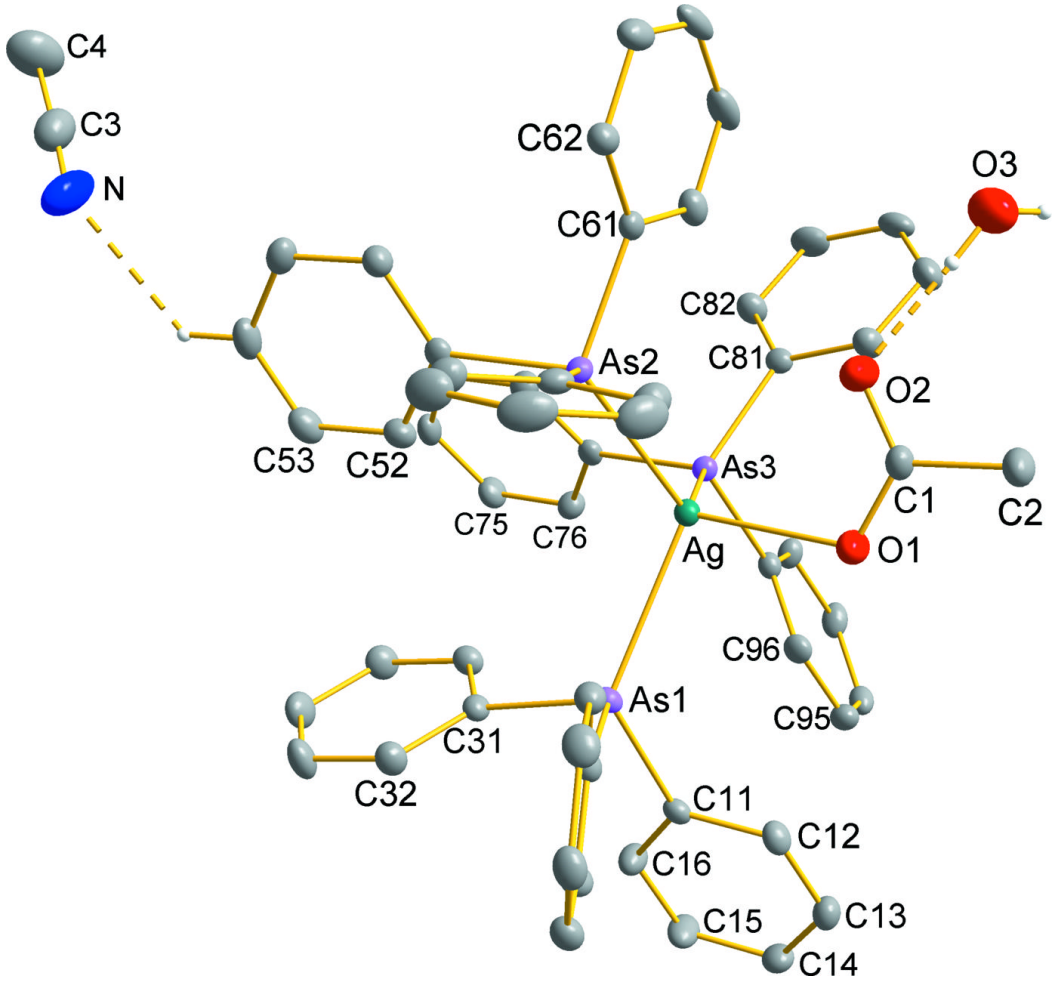
C22—C23—C24—C25	0.9 (3)	C71—As3—C81—C86	174.05 (15)
C23—C24—C25—C26	−0.9 (3)	Ag—As3—C81—C86	41.61 (17)
C24—C25—C26—C21	0.0 (3)	C86—C81—C82—C83	1.8 (3)
C22—C21—C26—C25	0.9 (3)	As3—C81—C82—C83	−173.83 (16)
As1—C21—C26—C25	−175.94 (15)	C81—C82—C83—C84	0.4 (3)
C21—As1—C31—C32	−5.59 (18)	C82—C83—C84—C85	−1.9 (3)
C11—As1—C31—C32	97.00 (17)	C83—C84—C85—C86	1.2 (3)
Ag—As1—C31—C32	−133.41 (15)	C84—C85—C86—C81	1.1 (3)
C21—As1—C31—C36	173.03 (15)	C82—C81—C86—C85	−2.6 (3)
C11—As1—C31—C36	−84.39 (16)	As3—C81—C86—C85	173.31 (16)
Ag—As1—C31—C36	45.20 (16)	C81—As3—C91—C96	131.53 (16)
C36—C31—C32—C33	0.6 (3)	C71—As3—C91—C96	−124.29 (16)
As1—C31—C32—C33	179.16 (16)	Ag—As3—C91—C96	3.15 (17)
C31—C32—C33—C34	−0.1 (3)	C81—As3—C91—C92	−46.35 (18)
C32—C33—C34—C35	−0.3 (3)	C71—As3—C91—C92	57.82 (18)
C33—C34—C35—C36	0.1 (3)	Ag—As3—C91—C92	−174.74 (15)
C34—C35—C36—C31	0.4 (3)	C96—C91—C92—C93	0.9 (3)
C32—C31—C36—C35	−0.7 (3)	As3—C91—C92—C93	178.77 (15)
As1—C31—C36—C35	−179.38 (15)	C91—C92—C93—C94	−0.2 (3)
C61—As2—C41—C46	103.09 (17)	C92—C93—C94—C95	−0.5 (3)
C51—As2—C41—C46	−0.27 (18)	C93—C94—C95—C96	0.6 (3)
Ag—As2—C41—C46	−128.00 (15)	C94—C95—C96—C91	0.1 (3)
C61—As2—C41—C42	−79.89 (17)	C92—C91—C96—C95	−0.9 (3)
C51—As2—C41—C42	176.75 (16)	As3—C91—C96—C95	−178.82 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3A···O2	0.887 (17)	1.879 (18)	2.765 (3)	177 (3)
C54—H54···N	0.95	2.56	3.307 (3)	135
O3—H3B···O3^{i}	0.865 (17)	2.17 (2)	2.973 (4)	154 (3)

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1.

Fig. 1


C4
C3
N
C62
C61
O3
C82
C81
O2
As2
C53
C52
As3
C1
C2
C75
C76
Ag
O1
C96
As1
C95
C31
C32
C11
C12
C16
C15
C13
C14