



Crystal structure of *fac*-tricarbonyl(quinoline-2-carboxylato- κ^2N,O)(triphenylarsane- κAs)-rhenium(I)

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Received 25 November 2015

Accepted 22 December 2015

Edited by M. Weil, Vienna University of Technology, Austria

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Keywords: crystal structure; rhenium(I) tricarbonyl complex; rhenium(I) triphenylarsane and quinaldic acid complex; *trans* influence

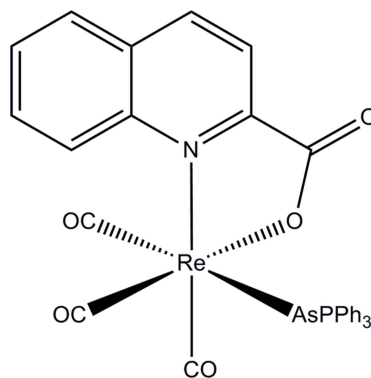
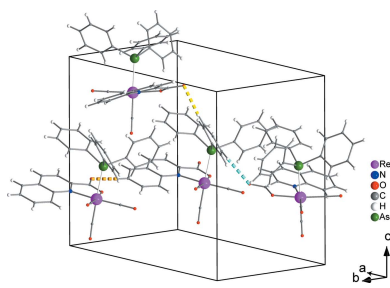
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In the title compound, $[\text{Re}(\text{C}_{10}\text{H}_6\text{NO}_2)(\text{CO})_3\{\text{As}(\text{C}_6\text{H}_5)_3\}]$, the coordination environment of Re^{I} is that of a distorted octahedron. Three coordination sites are occupied by three carbonyl groups in a facial arrangement and the remaining three sites by triphenylarsane and deprotonated quinaldic acid in *As*-mono- and *N,O*-bidentate fashions, respectively. In the crystal, the complexes are linked through weak $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a three-dimensional network. It worth noting that, as far as we know, this complex is the first Re^{I} triphenylarsane tricarbonyl compound to be reported.

1. Chemical context

In recent years, Re and Tc radiopharmaceutical chemistry with the tricarbonyl precursor *fac*- $[M(\text{CO})_3(\text{H}_2\text{O})_3]^+$ ($M = {}^{99\text{m}}\text{Tc}$, Re) has expanded continuously with the development of suitably derivatized novel ligand systems which efficiently displace the coordinating water molecules to produce complexes with high *in vivo* stability, favorable pharmacokinetic properties, and target tissue specificity (Mundwiler *et al.*, 2004; Triantis *et al.*, 2013; Jürgens *et al.*, 2014; Alberto, 2012). In this article, we describe the crystal structure of a '2 + 1' tricarbonyl rhenium(I) complex, *fac*- $[M(\text{CO})_3(L)(\text{NO-QA})]$, where *L* is triphenylarsane and NO-QA deprotonated quinaldic acid. This study is part of our ongoing research in the field of rhenium coordination compounds, particularly complexes bearing the *fac*- $[\text{Re}(\text{CO})_3]^+$ synthon, to develop new molecular radiopharmaceuticals. Related rhenium(I) tricarbonyl complexes have been reported by Schutte *et al.* (2011) and Manicum *et al.* (2015).



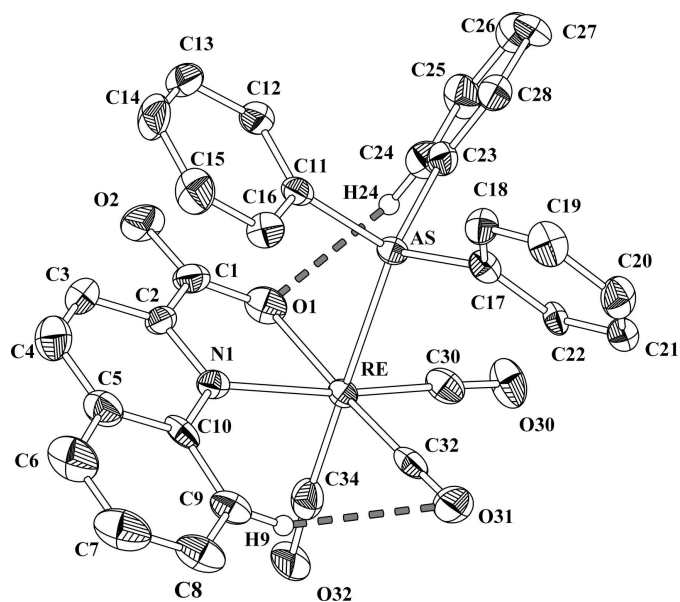


Figure 1
The molecular structure and atom-labelling scheme of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity, except for those involved in intramolecular hydrogen bonding (dashed grey lines).

2. Structural commentary

In the title compound, the Re^{I} cation is in a distorted octahedral environment (Fig. 1). The apical positions of the octahedron are occupied by the monodentate arsane ligand and one of the carbonyl groups ($\text{C}34\equiv\text{O}32$). The rhenium atom lies almost on the equatorial plane [displacement = $0.0459(6)$ Å]. The five-membered ring defined by the metal ion and the chelating bidentate NO-QA anion is almost planar [maximum deviation of $0.078(6)$ Å for atom N1]. One phenyl

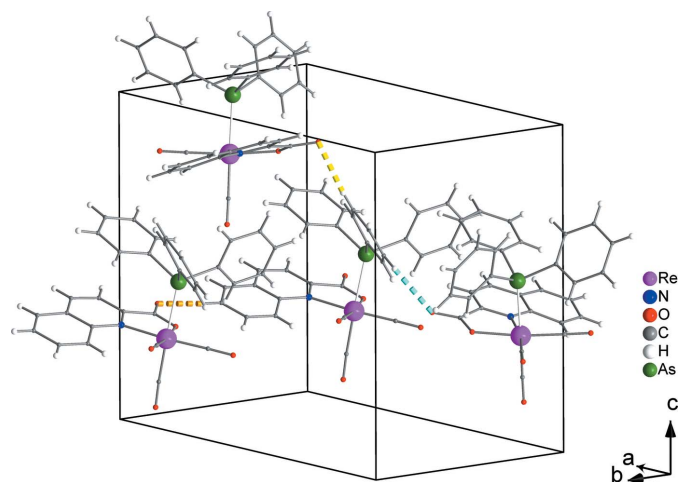


Figure 2
Weak intermolecular hydrogen bonds ($\text{C}7\text{--H}7\cdots\text{O}2$, $\text{C}19\text{--H}19\cdots\text{O}2$ and $\text{C}21\text{--H}21\cdots\text{O}2$) between neighbouring complexes indicated by dashed orange, yellow and turquoise lines, respectively. Intramolecular hydrogen bonds are not shown for clarity.

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

$D\text{--H}\cdots A$	$D\text{--H}$	$\text{H}\cdots A$	$D\cdots A$	$D\text{--H}\cdots A$
$\text{C}9\text{--H}9\cdots\text{O}31$	0.95	2.60	3.431 (11)	146
$\text{C}24\text{--H}24\cdots\text{O}1$	0.95	2.47	3.276 (12)	143
$\text{C}7\text{--H}7\cdots\text{O}2^{\text{i}}$	0.95	2.20	3.151 (11)	176
$\text{C}21\text{--H}21\cdots\text{O}2^{\text{ii}}$	0.95	2.57	3.251 (11)	128
$\text{C}19\text{--H}19\cdots\text{O}2^{\text{iii}}$	0.95	2.46	3.337 (11)	153

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

ring (C11–C16) of the triphenylarsane ligand exhibits intramolecular $\pi\text{--}\pi$ interaction with the NO-QA ligand (Fig. 1), the distance from the centroid of the phenyl ring to the plane of the NO-QA ligand being 3.495 Å and the angle between the planes being 9.1° . In addition, intramolecular hydrogen bonds are established between the phenyl rings of the NO-QA ligand ($\text{C}9\text{--H}9\cdots\text{O}31$) and between one of the phenyl rings of the triphenylarsane ligand ($\text{C}24\text{--H}24\cdots\text{O}1$) with one carbonyl oxygen atom and one carboxylate oxygen atom respectively (Fig.1; Table 1). The $\text{Re}\text{--C}\equiv\text{O}$ bond length in the apical position [$\text{Re}\text{--C}34$: $1.937(12)$ Å] is longer than those in the equatorial plane [$\text{Re}\text{--C}32$ = $1.893(8)$ Å and $\text{Re}\text{--C}30$ = $1.904(9)$ Å] because of the *trans* influence of the triphenylarsane ligands, as expected (Coe & Glenwright, 2000; Otto & Johansson, 2002). Taking into account that this is the first structurally characterized Re^{I} triphenylarsane tricarbonyl complex, there are no other Re^{I} compound to compare with, but the measured $\text{Re}\text{--As}$ distance of $2.5855(10)$ Å is close to those given by Commons & Hoskins (1975) of $2.569\text{--}2.584$ Å where the di(diphenylarsino)methane ligand is coordinating to an Re^{I} ion.

3. Supramolecular features

Weak intermolecular hydrogen bonds ($\text{C}7\text{--H}7\cdots\text{O}2$, $\text{C}19\text{--H}19\cdots\text{O}2$ and $\text{C}21\text{--H}21\cdots\text{O}2$, Table 1 and Fig. 2) are developed among the complexes in the crystal structure. Those of the $\text{C}7\text{--H}7\cdots\text{O}2$ type result in chain formation parallel to the b axis (Fig. 3). Neighbouring chains further interact through $\text{C}19\text{--H}19\cdots\text{O}2$ and $\text{C}21\text{--H}21\cdots\text{O}2$ inter-

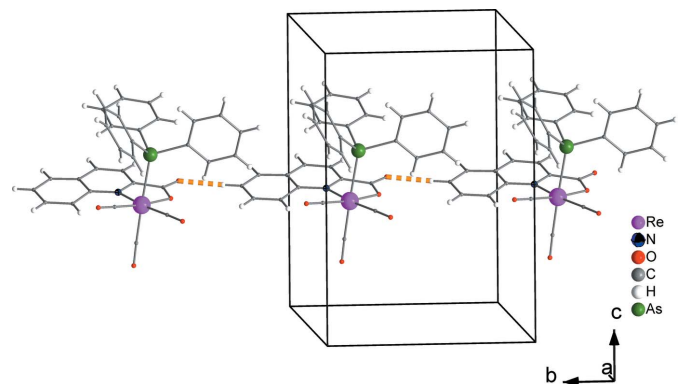


Figure 3
Chains of complexes, formed through $\text{C}7\text{--H}7\cdots\text{O}2$ hydrogen bonds (dashed orange lines), parallel to the b axis.

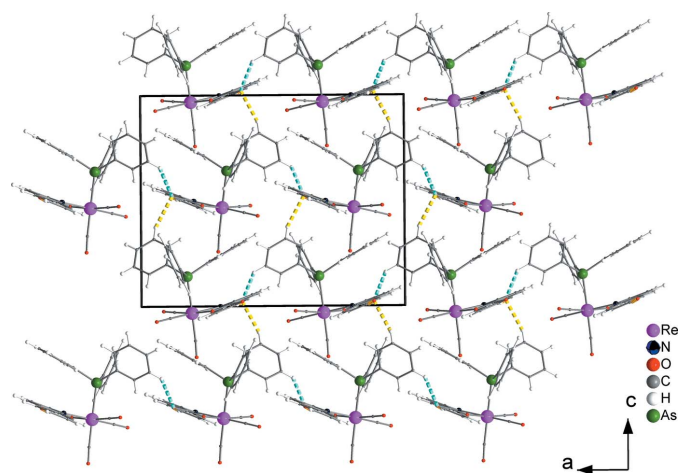


Figure 4
The three-dimensional network of neighbouring chains formed through C19–H19...O2 and C21–H21...O2 hydrogen bonds (dashed orange and dashed turquoise lines, respectively) in a view along the *b*-axis direction.

actions and build up the three-dimensional set-up of the structure (Fig. 4).

4. Synthesis and crystallization

To a stirred solution of quinaldic acid (17.3 mg, 0.1 mmol) in 5 ml methanol, a solution of $[\text{NEt}_4]_2[\text{ReBr}_3(\text{CO})_3]$ (77 mg, 0.1 mmol) in 5 ml methanol was added. The mixture was heated at 323 K and after 30 min a solution of triphenylarsane (0.1 mmol) in 3 ml methanol was added. The mixture was stirred under reflux for 2 h and the reaction progress was monitored by HPLC. The solvent was removed under reduced pressure and the solid residue was recrystallized from a dichloromethane/methanol mixture. The resulting solid was redissolved in a minimum volume of dichloromethane, layered with methanol and left to stand at room temperature. After several days crystals suitable for X-ray analysis were isolated (yield: 46.8 mg, 60%).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were placed in idealized positions and refined using a riding model with $\text{C}-\text{H} = 0.95 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Acknowledgements

CT would like to thank the State Scholarships Foundation (IKY) in Greece for financial support during his postgraduate studies in the framework of ‘IKY fellowships Excellence for postgraduate studies in Greece – Siemens program’.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[\text{Re}(\text{C}_{10}\text{H}_6\text{NO}_2)(\text{C}_{18}\text{H}_{15}\text{As})(\text{CO})_3]$
M_r	748.61
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	160
a, b, c (Å)	18.1637 (3), 10.3463 (2), 14.5322 (3)
V (Å ³)	2730.99 (9)
Z	4
Radiation type	Cu $K\alpha$
μ (mm ⁻¹)	10.40
Crystal size (mm)	0.27 × 0.27 × 0.09
Data collection	
Diffractometer	Rigaku R-AXIS SPIDER IPDS diffractometer
Absorption correction	Multi-scan (<i>CrystalClear</i> ; Rigaku, 2005)
$T_{\text{min}}, T_{\text{max}}$	0.443, 1.00
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16386, 4768, 4655
R_{int}	0.052
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.599
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.033, 0.076, 1.05
No. of reflections	4768
No. of parameters	352
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.39, -1.50
Absolute structure	Flack x determined using 2096 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.019 (7)

Computer programs: *CrystalClear* (Rigaku, 2005), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Crystal Impact, 2012) and *PLATON* (Spek, 2009).

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supporting information

Acta Cryst. (2016). E72, 114-116 [doi:10.1107/S2056989015024640]

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Computing details

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear* (Rigaku, 2005); data reduction: *CrystalClear* (Rigaku, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Crystal Impact, 2012); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

fac-Tricarbonyl(quinoline-2-carboxylato- κ^2N,O)(triphenylarsane- κAs)rhenium(I)

Crystal data

[Re(C₁₀H₆NO₂)(C₁₈H₁₅As)(CO)₃]

$M_r = 748.61$

Orthorhombic, *Pna*2₁

$a = 18.1637$ (3) Å

$b = 10.3463$ (2) Å

$c = 14.5322$ (3) Å

$V = 2730.99$ (9) Å³

$Z = 4$

$F(000) = 1448$

$D_x = 1.821$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å

Cell parameters from 17073 reflections

$\theta = 6.6$ – 71.9°

$\mu = 10.40$ mm⁻¹

$T = 160$ K

Parallelepiped, colorless

$0.27 \times 0.27 \times 0.09$ mm

Data collection

Rigaku R-AXIS SPIDER IPDS
diffractometer

Radiation source: fine-focus sealed tube

θ scans

Absorption correction: multi-scan
(*CrystalClear*; Rigaku, 2005)

$T_{\min} = 0.443$, $T_{\max} = 1.00$

16386 measured reflections

4768 independent reflections

4655 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$

$\theta_{\max} = 67.5^\circ$, $\theta_{\min} = 7.2^\circ$

$h = -20 \rightarrow 15$

$k = -12 \rightarrow 8$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.076$

$S = 1.05$

4768 reflections

352 parameters

1 restraint

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.6895P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.39$ e Å⁻³

$\Delta\rho_{\min} = -1.50$ e Å⁻³

Absolute structure: Flack x determined using
2096 quotients $[(F^+)-(F^-)]/[(F^+)+(F^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.019 (7)

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.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Re	0.19141 (2)	0.85298 (3)	0.46794 (4)	0.01930 (12)
N1	0.2993 (4)	0.9464 (7)	0.4983 (4)	0.0229 (17)
O1	0.2681 (3)	0.6990 (5)	0.4781 (5)	0.0335 (14)
O2	0.3818 (4)	0.6409 (5)	0.5218 (5)	0.0385 (18)
C1	0.3333 (5)	0.7230 (9)	0.5073 (6)	0.029 (2)
C2	0.3522 (5)	0.8626 (7)	0.5221 (6)	0.0226 (19)
C3	0.4205 (5)	0.9006 (10)	0.5543 (7)	0.038 (2)
H3	0.4555	0.8369	0.5719	0.046*
C4	0.4377 (6)	1.0254 (10)	0.5610 (7)	0.040 (2)
H4	0.4844	1.0513	0.5840	0.048*
C5	0.3859 (6)	1.1180 (9)	0.5337 (7)	0.035 (2)
C6	0.4030 (7)	1.2520 (9)	0.5344 (7)	0.049 (3)
H6	0.4499	1.2802	0.5554	0.059*
C7	0.3516 (8)	1.3419 (9)	0.5048 (8)	0.054 (3)
H7	0.3624	1.4317	0.5079	0.064*
C8	0.2841 (6)	1.2999 (7)	0.4704 (9)	0.040 (2)
H8	0.2497	1.3621	0.4489	0.048*
C9	0.2659 (5)	1.1707 (7)	0.4666 (8)	0.034 (2)
H9	0.2200	1.1438	0.4419	0.040*
C10	0.3176 (5)	1.0772 (9)	0.5008 (6)	0.027 (2)
As	0.17369 (5)	0.81237 (9)	0.64209 (6)	0.0203 (2)
C11	0.2613 (5)	0.8487 (7)	0.7149 (6)	0.024 (2)
C12	0.3060 (4)	0.7508 (10)	0.7455 (6)	0.030 (2)
H12	0.2925	0.6633	0.7349	0.037*
C13	0.3712 (5)	0.7793 (10)	0.7920 (6)	0.039 (2)
H13	0.4019	0.7115	0.8137	0.047*
C14	0.3907 (6)	0.9064 (10)	0.8063 (7)	0.042 (3)
H14	0.4353	0.9260	0.8375	0.050*
C15	0.3456 (6)	1.0064 (11)	0.7755 (7)	0.042 (3)
H15	0.3586	1.0938	0.7873	0.050*
C16	0.2817 (5)	0.9779 (9)	0.7274 (6)	0.029 (2)
H16	0.2521	1.0454	0.7031	0.035*
C17	0.0961 (5)	0.9123 (8)	0.6992 (6)	0.0245 (19)
C18	0.1054 (5)	0.9746 (8)	0.7841 (5)	0.0279 (19)
H18	0.1501	0.9653	0.8173	0.033*

C19	0.0488 (5)	1.0500 (9)	0.8192 (6)	0.036 (2)
H19	0.0552	1.0959	0.8753	0.043*
C20	-0.0172 (5)	1.0575 (9)	0.7717 (7)	0.035 (2)
H20	-0.0562	1.1083	0.7960	0.042*
C21	-0.0273 (5)	0.9923 (8)	0.6896 (6)	0.029 (2)
H21	-0.0731	0.9970	0.6581	0.035*
C22	0.0299 (4)	0.9204 (8)	0.6543 (6)	0.0208 (17)
H22	0.0233	0.8757	0.5978	0.025*
C23	0.1471 (5)	0.6365 (7)	0.6769 (6)	0.027 (2)
C24	0.1601 (5)	0.5348 (8)	0.6156 (7)	0.033 (2)
H24	0.1829	0.5514	0.5580	0.040*
C25	0.1398 (5)	0.4106 (9)	0.6385 (8)	0.038 (2)
H25	0.1484	0.3411	0.5972	0.046*
C26	0.1067 (6)	0.3891 (9)	0.7223 (8)	0.043 (3)
H26	0.0927	0.3036	0.7384	0.052*
C27	0.0935 (5)	0.4873 (9)	0.7831 (7)	0.042 (2)
H27	0.0696	0.4697	0.8399	0.050*
C28	0.1148 (5)	0.6126 (9)	0.7618 (6)	0.032 (2)
H28	0.1075	0.6808	0.8046	0.039*
C30	0.1086 (5)	0.7452 (9)	0.4440 (5)	0.031 (2)
O30	0.0571 (4)	0.6812 (7)	0.4282 (5)	0.0404 (17)
C32	0.1253 (4)	0.9943 (7)	0.4725 (7)	0.0262 (17)
O31	0.0843 (3)	1.0805 (6)	0.4766 (6)	0.0421 (16)
C34	0.2037 (5)	0.8780 (10)	0.3367 (8)	0.033 (2)
O32	0.2073 (4)	0.8903 (9)	0.2592 (5)	0.047 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Re	0.0220 (2)	0.01733 (18)	0.01854 (19)	-0.00165 (12)	0.00153 (18)	-0.00057 (19)
N1	0.026 (4)	0.022 (4)	0.020 (4)	0.003 (3)	0.002 (3)	0.001 (3)
O1	0.044 (4)	0.022 (3)	0.035 (3)	-0.004 (3)	0.000 (4)	-0.002 (3)
O2	0.044 (5)	0.026 (3)	0.046 (4)	0.018 (3)	0.004 (3)	0.004 (3)
C1	0.033 (6)	0.028 (5)	0.026 (4)	0.007 (4)	0.000 (4)	0.005 (4)
C2	0.022 (5)	0.025 (4)	0.020 (4)	0.004 (4)	-0.002 (4)	0.002 (3)
C3	0.026 (6)	0.045 (6)	0.044 (6)	0.003 (5)	-0.004 (5)	0.011 (5)
C4	0.033 (6)	0.041 (6)	0.046 (6)	-0.010 (5)	-0.005 (4)	-0.004 (5)
C5	0.040 (6)	0.030 (5)	0.035 (5)	-0.008 (5)	0.001 (4)	0.005 (4)
C6	0.066 (8)	0.033 (5)	0.050 (6)	-0.028 (6)	-0.007 (6)	-0.002 (5)
C7	0.084 (11)	0.029 (5)	0.048 (7)	-0.018 (6)	-0.004 (7)	0.003 (5)
C8	0.065 (7)	0.018 (4)	0.037 (5)	-0.001 (4)	0.011 (7)	0.001 (6)
C9	0.045 (6)	0.024 (4)	0.033 (4)	-0.005 (4)	0.005 (6)	0.006 (6)
C10	0.034 (6)	0.023 (4)	0.024 (4)	-0.013 (4)	0.007 (3)	0.003 (4)
As	0.0243 (5)	0.0170 (4)	0.0196 (4)	-0.0012 (4)	0.0007 (4)	0.0009 (4)
C11	0.027 (5)	0.024 (4)	0.021 (4)	0.001 (3)	0.004 (4)	0.004 (3)
C12	0.030 (6)	0.029 (5)	0.032 (5)	-0.003 (4)	-0.001 (4)	0.006 (4)
C13	0.032 (5)	0.054 (6)	0.032 (5)	0.007 (5)	-0.003 (4)	0.011 (5)
C14	0.024 (6)	0.056 (6)	0.045 (6)	-0.011 (5)	-0.010 (5)	-0.004 (6)

C15	0.038 (6)	0.050 (7)	0.038 (6)	-0.016 (6)	-0.008 (5)	-0.009 (5)
C16	0.033 (6)	0.026 (4)	0.028 (5)	-0.001 (4)	-0.003 (4)	-0.004 (4)
C17	0.027 (5)	0.021 (4)	0.026 (4)	-0.002 (4)	0.006 (4)	0.000 (4)
C18	0.026 (5)	0.039 (5)	0.019 (4)	-0.001 (4)	-0.002 (4)	-0.006 (4)
C19	0.041 (6)	0.036 (5)	0.030 (5)	-0.004 (4)	0.006 (4)	-0.015 (4)
C20	0.030 (6)	0.032 (5)	0.043 (6)	0.007 (5)	0.009 (4)	-0.004 (4)
C21	0.025 (5)	0.035 (5)	0.028 (5)	-0.004 (4)	0.000 (4)	0.005 (4)
C22	0.018 (4)	0.027 (4)	0.018 (4)	-0.008 (3)	0.003 (4)	-0.003 (4)
C23	0.022 (5)	0.026 (5)	0.031 (5)	-0.004 (4)	-0.002 (4)	0.002 (3)
C24	0.038 (6)	0.022 (5)	0.039 (6)	0.001 (4)	-0.002 (4)	-0.002 (4)
C25	0.035 (6)	0.023 (4)	0.057 (7)	-0.010 (4)	0.001 (6)	-0.002 (5)
C26	0.036 (6)	0.023 (4)	0.071 (8)	-0.011 (5)	-0.010 (6)	0.014 (5)
C27	0.037 (6)	0.047 (6)	0.041 (6)	-0.007 (5)	0.004 (5)	0.024 (5)
C28	0.028 (5)	0.033 (5)	0.037 (5)	0.001 (4)	-0.001 (4)	0.004 (4)
C30	0.040 (6)	0.032 (4)	0.021 (5)	-0.004 (4)	0.006 (4)	-0.002 (3)
O30	0.037 (4)	0.045 (4)	0.039 (4)	-0.022 (3)	0.003 (3)	-0.014 (3)
C32	0.032 (4)	0.027 (4)	0.019 (3)	-0.014 (4)	0.003 (4)	0.003 (5)
O31	0.039 (4)	0.038 (3)	0.049 (4)	0.017 (3)	0.009 (4)	0.012 (4)
C34	0.025 (5)	0.030 (5)	0.044 (7)	-0.005 (4)	-0.002 (5)	-0.002 (5)
O32	0.041 (4)	0.086 (6)	0.015 (4)	-0.004 (4)	0.008 (3)	0.009 (4)

Geometric parameters (Å, °)

Re—C32	1.893 (8)	C13—C14	1.378 (14)
Re—C30	1.904 (9)	C13—H13	0.9500
Re—C34	1.937 (12)	C14—C15	1.394 (14)
Re—O1	2.122 (6)	C14—H14	0.9500
Re—N1	2.229 (7)	C15—C16	1.387 (13)
Re—As	2.5855 (10)	C15—H15	0.9500
N1—C2	1.339 (10)	C16—H16	0.9500
N1—C10	1.394 (11)	C17—C22	1.371 (11)
O1—C1	1.281 (11)	C17—C18	1.403 (11)
O2—C1	1.243 (10)	C18—C19	1.388 (12)
C1—C2	1.500 (11)	C18—H18	0.9500
C2—C3	1.383 (12)	C19—C20	1.386 (13)
C3—C4	1.333 (12)	C19—H19	0.9500
C3—H3	0.9500	C20—C21	1.383 (12)
C4—C5	1.400 (13)	C20—H20	0.9500
C4—H4	0.9500	C21—C22	1.377 (11)
C5—C10	1.395 (13)	C21—H21	0.9500
C5—C6	1.422 (12)	C22—H22	0.9500
C6—C7	1.386 (17)	C23—C28	1.388 (12)
C6—H6	0.9500	C23—C24	1.399 (11)
C7—C8	1.394 (17)	C24—C25	1.377 (11)
C7—H7	0.9500	C24—H24	0.9500
C8—C9	1.378 (10)	C25—C26	1.376 (15)
C8—H8	0.9500	C25—H25	0.9500
C9—C10	1.435 (13)	C26—C27	1.367 (14)

C9—H9	0.9500	C26—H26	0.9500
As—C17	1.935 (9)	C27—C28	1.389 (12)
As—C11	1.947 (10)	C27—H27	0.9500
As—C23	1.949 (8)	C28—H28	0.9500
C11—C12	1.373 (12)	C30—O30	1.169 (10)
C11—C16	1.399 (11)	C32—O31	1.163 (9)
C12—C13	1.395 (11)	C34—O32	1.136 (12)
C12—H12	0.9500		
C32—Re—C30	87.6 (3)	C12—C11—As	121.1 (6)
C32—Re—C34	90.3 (4)	C16—C11—As	118.2 (6)
C30—Re—C34	89.4 (4)	C11—C12—C13	120.2 (9)
C32—Re—O1	173.8 (4)	C11—C12—H12	119.9
C30—Re—O1	95.2 (3)	C13—C12—H12	119.9
C34—Re—O1	95.3 (3)	C14—C13—C12	119.6 (9)
C32—Re—N1	102.5 (3)	C14—C13—H13	120.2
C30—Re—N1	169.8 (3)	C12—C13—H13	120.2
C34—Re—N1	92.0 (3)	C13—C14—C15	120.6 (9)
O1—Re—N1	74.6 (2)	C13—C14—H14	119.7
C32—Re—As	90.7 (3)	C15—C14—H14	119.7
C30—Re—As	89.1 (2)	C16—C15—C14	119.7 (9)
C34—Re—As	178.2 (3)	C16—C15—H15	120.1
O1—Re—As	83.80 (19)	C14—C15—H15	120.1
N1—Re—As	89.23 (17)	C15—C16—C11	119.4 (9)
C2—N1—C10	116.8 (7)	C15—C16—H16	120.3
C2—N1—Re	113.6 (6)	C11—C16—H16	120.3
C10—N1—Re	129.4 (6)	C22—C17—C18	119.7 (8)
C1—O1—Re	118.9 (5)	C22—C17—As	117.9 (6)
O2—C1—O1	125.4 (9)	C18—C17—As	122.4 (7)
O2—C1—C2	118.1 (9)	C19—C18—C17	119.5 (8)
O1—C1—C2	116.5 (8)	C19—C18—H18	120.2
N1—C2—C3	123.2 (8)	C17—C18—H18	120.2
N1—C2—C1	115.0 (8)	C20—C19—C18	119.3 (8)
C3—C2—C1	121.8 (8)	C20—C19—H19	120.4
C4—C3—C2	120.7 (9)	C18—C19—H19	120.4
C4—C3—H3	119.7	C21—C20—C19	121.2 (9)
C2—C3—H3	119.7	C21—C20—H20	119.4
C3—C4—C5	119.0 (9)	C19—C20—H20	119.4
C3—C4—H4	120.5	C22—C21—C20	119.0 (9)
C5—C4—H4	120.5	C22—C21—H21	120.5
C10—C5—C4	119.3 (9)	C20—C21—H21	120.5
C10—C5—C6	119.5 (10)	C17—C22—C21	121.2 (8)
C4—C5—C6	121.2 (10)	C17—C22—H22	119.4
C7—C6—C5	120.3 (11)	C21—C22—H22	119.4
C7—C6—H6	119.9	C28—C23—C24	120.2 (8)
C5—C6—H6	119.9	C28—C23—As	120.1 (6)
C6—C7—C8	119.7 (9)	C24—C23—As	119.7 (7)
C6—C7—H7	120.2	C25—C24—C23	120.2 (9)

C8—C7—H7	120.2	C25—C24—H24	119.9
C9—C8—C7	121.8 (10)	C23—C24—H24	119.9
C9—C8—H8	119.1	C26—C25—C24	118.8 (10)
C7—C8—H8	119.1	C26—C25—H25	120.6
C8—C9—C10	118.9 (9)	C24—C25—H25	120.6
C8—C9—H9	120.6	C27—C26—C25	121.9 (9)
C10—C9—H9	120.6	C27—C26—H26	119.1
N1—C10—C5	120.9 (9)	C25—C26—H26	119.1
N1—C10—C9	119.3 (8)	C26—C27—C28	120.1 (9)
C5—C10—C9	119.8 (8)	C26—C27—H27	120.0
C17—As—C11	105.0 (4)	C28—C27—H27	120.0
C17—As—C23	102.0 (4)	C23—C28—C27	118.8 (9)
C11—As—C23	104.0 (4)	C23—C28—H28	120.6
C17—As—Re	115.1 (3)	C27—C28—H28	120.6
C11—As—Re	113.5 (3)	O30—C30—Re	178.5 (8)
C23—As—Re	115.9 (3)	O31—C32—Re	179.0 (9)
C12—C11—C16	120.4 (9)	O32—C34—Re	176.5 (10)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C9—H9...O31	0.95	2.60	3.431 (11)	146
C24—H24...O1	0.95	2.47	3.276 (12)	143
C7—H7...O2 ⁱ	0.95	2.20	3.151 (11)	176
C21—H21...O2 ⁱⁱ	0.95	2.57	3.251 (11)	128
C19—H19...O2 ⁱⁱⁱ	0.95	2.46	3.337 (11)	153

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