resembles the tetracoordinate square-planar cation of $[Cu(tim)](BPh_4)_2$ in which the macrocycle is nearly planar, excepting the C(4) atoms (Elia, 1982). The conformation assumed is by symmetry a boat, with the C(4) carbon atoms and the axial ligand on opposite sides of the coordination plane as shown in Fig. 1.

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Structure of Tetraphenylarsonium Bis(μ_6-carbido-2,3;4,5-di-μ-carbonyl-1,1,1,2,2,3,3,4,4,5,5,6,6,6-tetradecacarbonyl-*octahedro*-hexaruthenio-*Ru*^{3},*Ru*^{4})thallate(1−)(4*Tl–Ru*), $[As(C_6H_5)_4][\{Ru_6C(CO)_{16}\}_2Tl]$

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Abstract. M_r = 2720·9, triclinic, $P1$, a = 15·325 (5), b = 17·301 (3), c = 17·356 (3) Å, α = 115·25 (1), β = 106·01 (2), γ = 94·77 (2)°, Z = 1, D_x = 2·32 g cm^{-3}, D_m not measured, graphite-monochromatized Mo $K\alpha$ radiation, λ = 0·71073 Å, μ = 48·1 cm^{-1}, T = 293 (2) K, $F(000)$ = 2532, 3634 independent reflections, for which R = 0·078. The $[\{Ru_6C(CO)_{16}\}_2Tl]^-$ anion consists of a bimetallic carbonyl cluster containing two distorted Ru_6 octahedra, each linked by two edge-related Ru atoms to the central Tl atom. Each Ru_6 octahedron encapsulates a central C atom and bears 16 carbonyl ligands (14 linear, two semi-bridged). The bimetallic anion has pseudo 222 symmetry. Within the Ru_6 octahedra Ru—Ru distances range from 2·813 (4) to 2·938 (4) Å with the exception of the edges bridged by Tl, which average 3·10 Å. Average Ru—Tl distances are 2·780 (3) and 2·864 (2) Å. The four Ru Tl bonds deviate from coplanarity (torsional angle 35·9°) because of non-bonded interactions between the O atoms of the two sets of six carbonyls associated with the Ru_2TlRu_2 region of the cluster.

Introduction. The title material was synthesized as part of an investigation of oxidative activation of transition-metal carbide clusters (Bradley, Ansell & Hill, 1980; Bradley, Pruett, Hill, Ansell, Leonowicz & Modrick, 1982).

Experimental. Title compound was crystallized from toluene. Block-shaped crystal approximately 0·1 × 0·12 × 0·1 mm. Cell dimensions from the setting angles of 25 centered reflections of various intensities. Enraf–Nonius CAD-4 diffractometer. ω—2θ scan-mode. Intensities of 7172 reflections measured, 0·0° < 2θ < 40·0°. Scan begun 0·75° below the calculated 2θ position for $K\alpha_1$ and terminated 0·75° above the calculated $K\alpha_2$ angle. Total background counting time half the scan time and evenly divided on either side of the peak. 3634

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0108-2701/84/081315-04$01.50

Table 1. *Final fractional positional coordinates and thermal parameters*

	x	y	z	B_{eq} or B_{iso}(Å^2)
Tl(1)	0·3287 (1)	0·2118 (1)	−0·0696 (1)	2·53 (4)*
Ru(1)	0·5416 (2)	0·2798 (2)	−0·1512 (2)	3·2 (1)*
Ru(2)	0·6344 (2)	0·1390 (2)	−0·1556 (2)	3·1 (1)*
Ru(3)	0·5130 (2)	0·1866 (2)	−0·0554 (2)	2·6 (1)*
Ru(4)	0·3622 (2)	0·1601 (2)	−0·2316 (2)	2·8 (1)*
Ru(5)	0·5008 (2)	0·1137 (2)	−0·3179 (2)	3·4 (1)*
Ru(6)	0·4488 (2)	0·0233 (2)	−0·2268 (2)	2·9 (1)*
Ru(1′)	0·1919 (2)	0·1838 (2)	0·1012 (2)	2·8 (1)*
Ru(2′)	0·0228 (2)	0·2351 (2)	0·0286 (3)	3·7 (1)*
Ru(3′)	0·1390 (2)	0·1815 (2)	−0·0758 (2)	3·0 (1)*
Ru(4′)	0·3044 (2)	0·3165 (2)	0·0936 (2)	3·0 (1)*
Ru(5′)	0·1697 (2)	0·3619 (2)	0·1835 (3)	3·9 (1)*
Ru(6′)	0·1442 (2)	0·3652 (2)	0·0141 (3)	3·6 (1)*
As(1)	−0·0139 (3)	0·2602 (3)	0·5023 (3)	4·2 (1)
O(1*A*)	0·435 (2)	0·411 (2)	−0·079 (2)	6·5 (9)
O(1*B*)	0·713 (2)	0·407 (2)	0·000 (2)	5·2 (8)
O(1*C*)	0·578 (3)	0·348 (3)	−0·272 (3)	10·7 (14)
O(2*A*)	0·714 (2)	0·207 (2)	0·039 (2)	5·0 (8)
O(2*B*)	0·753 (2)	0·001 (2)	−0·176 (2)	6·7 (9)
O(2*C*)	0·788 (2)	0·250 (2)	−0·164 (2)	7·1 (10)
O(3*A*)	0·505 (2)	0·096 (2)	0·057 (2)	4·1 (7)
O(3*B*)	0·580 (2)	0·365 (2)	0·109 (2)	5·2 (8)
O(4*A*)	0·185 (2)	0·026 (2)	−0·317 (2)	6·2 (9)
O(4*B*)	0·264 (2)	0·281 (2)	−0·287 (2)	7·3 (10)
O(5*A*)	0·562 (3)	−0·049 (2)	−0·413 (3)	8·8 (12)
O(5*B*)	0·592 (3)	0·192 (3)	−0·410 (3)	11·2 (15)
O(5*C*)	0·320 (2)	0·069 (2)	−0·460 (2)	6·8 (10)
O(6*A*)	0·326 (2)	−0·105 (2)	−0·412 (2)	6·3 (9)
O(6*B*)	0·560 (2)	−0·110 (2)	−0·223 (2)	7·0 (10)
O(6*C*)	0·328 (2)	−0·032 (2)	−0·142 (2)	5·7 (9)
O(1*A*′)	0·295 (2)	0·041 (2)	0·027 (2)	4·9 (8)
O(1*B*′)	0·058 (2)	0·054 (2)	0·110 (2)	5·6 (8)
O(1*C*′)	0·318 (2)	0·231 (2)	0·291 (2)	6·7 (10)
O(2*A*′)	−0·073 (2)	0·126 (2)	−0·169 (2)	5·0 (8)
O(2*B*′)	−0·106 (3)	0·356 (2)	0·059 (2)	8·0 (11)
O(2*C*′)	−0·117 (2)	0·108 (2)	0·041 (2)	7·0 (10)
O(3*A*′)	0·091 (2)	0·188 (2)	−0·250 (2)	4·9 (8)
O(3*B*′)	0·119 (2)	−0·015 (2)	−0·174 (2)	4·7 (8)
O(4*A*′)	0·423 (2)	0·475 (2)	0·110 (2)	7·0 (10)
O(4*B*′)	0·471 (2)	0·273 (2)	0·190 (2)	5·3 (8)
O(5*A*′)	0·111 (3)	0·524 (3)	0·260 (3)	11·5 (15)
O(5*B*′)	0·120 (3)	0·316 (3)	0·315 (3)	9·9 (13)
O(5*C*′)	0·363 (3)	0·458 (2)	0·305 (2)	8·0 (11)
O(6*A*′)	0·219 (2)	0·559 (2)	0·143 (2)	6·7 (10)
O(6*B*′)	−0·031 (3)	0·385 (3)	−0·098 (3)	10·0 (13)
O(6*C*′)	0·230 (2)	0·388 (2)	−0·115 (2)	6·3 (9)
C(1*A*)	0·472 (3)	0·356 (2)	−0·114 (3)	3·5 (10)
C(1*B*)	0·647 (3)	0·361 (3)	−0·056 (3)	3·7 (11)
C(1*C*)	0·547 (4)	0·313 (3)	−0·232 (3)	6·7 (15)
C(2*A*)	0·655 (3)	0·175 (2)	−0·040 (2)	2·6 (9)
C(2*B*)	0·697 (3)	0·057 (2)	−0·176 (3)	3·2 (10)
C(2*C*)	0·731 (3)	0·208 (3)	−0·155 (3)	5·8 (14)
C(3*A*)	0·504 (2)	0·131 (2)	0·011 (2)	2·2 (9)
C(3*B*)	0·548 (3)	0·296 (3)	0·042 (3)	4·0 (11)
C(4*A*)	0·258 (3)	0·079 (2)	−0·281 (2)	2·4 (9)
C(4*B*)	0·295 (4)	0·235 (4)	−0·264 (4)	8·2 (18)
C(5*A*)	0·542 (3)	0·012 (3)	−0·370 (3)	5·7 (14)
C(5*B*)	0·548 (5)	0·162 (4)	−0·383 (4)	9·8 (21)
C(5*C*)	0·372 (4)	0·091 (3)	−0·401 (4)	6·8 (15)
C(6*A*)	0·378 (3)	−0·055 (3)	−0·337 (3)	3·6 (11)
C(6*B*)	0·523 (3)	−0·055 (3)	−0·222 (3)	4·0 (11)
C(6*C*)	0·377 (3)	−0·010 (3)	−0·167 (3)	4·7 (12)
C(1*A*′)	0·250 (3)	0·095 (3)	0·052 (3)	4·7 (12)
C(1*B*′)	0·102 (3)	0·105 (2)	0·101 (3)	3·5 (11)
C(1*C*′)	0·257 (3)	0·218 (3)	0·209 (3)	4·1 (11)
C(2*A*′)	−0·013 (2)	0·168 (2)	−0·096 (2)	2·0 (9)
C(2*B*′)	−0·055 (3)	0·301 (3)	0·044 (3)	4·2 (11)
C(2*C*′)	−0·059 (3)	0·165 (3)	0·046 (3)	5·6 (13)
C(3*A*′)	0·117 (3)	0·194 (2)	−0·171 (3)	3·2 (10)
C(3*B*′)	0·132 (3)	0·057 (2)	0·136 (3)	3·4 (10)
C(4*A*′)	0·380 (3)	0·410 (3)	0·101 (3)	5·6 (13)
C(4*B*′)	0·408 (3)	0·290 (3)	0·155 (3)	4·0 (11)
C(5*A*′)	0·131 (3)	0·453 (3)	0·224 (3)	5·4 (13)
C(5*B*′)	0·140 (4)	0·333 (3)	0·262 (3)	6·3 (15)
C(5*C*′)	0·304 (5)	0·405 (4)	0·239 (5)	10·7 (22)
C(6*A*′)	0·192 (4)	0·480 (3)	0·100 (3)	6·6 (15)
C(6*B*′)	0·033 (4)	0·383 (4)	−0·038 (4)	8·9 (19)
C(6*C*′)	0·195 (3)	0·377 (3)	−0·072 (3)	4·4 (12)
CC(1)	0·503 (2)	0·153 (2)	−0·180 (2)	0·7 (7)
CC(2)	0·164 (2)	0·270 (2)	0·052 (2)	2·0 (7)
C(1)	0·076 (3)	0·210 (3)	0·462 (3)	4·6 (12)
C(2)	0·169 (3)	0·253 (3)	0·500 (3)	4·9 (12)
C(3)	0·232 (4)	0·215 (3)	0·461 (3)	6·1 (14)
C(4)	0·215 (4)	0·145 (4)	0·397 (4)	7·5 (17)
C(5)	0·117 (4)	0·091 (4)	0·345 (4)	8·5 (18)
C(6)	0·053 (3)	0·130 (3)	0·383 (3)	4·8 (12)
C(7)	0·045 (3)	0·376 (3)	0·594 (3)	4·1 (11)
C(8)	0·096 (3)	0·387 (3)	0·673 (3)	4·5 (12)
C(9)	0·142 (4)	0·474 (4)	0·744 (4)	8·2 (18)
C(10)	0·120 (4)	0·545 (4)	0·725 (4)	8·6 (18)
C(11)	0·058 (5)	0·537 (5)	0·647 (5)	11·5 (24)
C(12)	0·017 (3)	0·443 (3)	0·573 (3)	5·6 (13)
C(13)	−0·109 (3)	0·254 (3)	0·406 (3)	4·7 (12)
C(14)	−0·104 (4)	0·239 (3)	0·328 (3)	6·2 (14)
C(15)	−0·173 (4)	0·233 (3)	0·252 (3)	6·7 (15)
C(16)	−0·253 (3)	0·247 (3)	0·265 (3)	5·0 (13)
C(17)	−0·267 (4)	0·262 (4)	0·344 (4)	8·8 (19)
C(18)	−0·192 (4)	0·270 (3)	0·417 (4)	7·4 (16)
C(19)	−0·059 (3)	0·203 (3)	0·561 (3)	3·5 (11)
C(20)	−0·072 (3)	0·115 (3)	0·530 (3)	5·4 (13)
C(21)	−0·113 (3)	0·072 (3)	0·568 (3)	5·6 (13)
C(22)	−0·146 (4)	0·112 (4)	0·623 (4)	8·0 (18)
C(23)	−0·146 (4)	0·195 (4)	0·657 (4)	7·6 (17)
C(24)	−0·092 (4)	0·244 (3)	0·621 (3)	6·3 (14)

* $B_{eq} = \frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,2) + bc(\cos\alpha)B(2,3)]$.

independent reflections regarded as observed with $I > 3{\cdot}0\sigma(F)^2$ where $I = S(C-RB)$ and $\sigma(I) = [S^2(C + R^2B) + (kI)^2]^{1/2}$, where C = total counts recorded during the scan, $R = 2{\cdot}0$ = ratio of scanning time to total background B, S = scan rate (varied between 4 and 20° $\min^{-1}$) and $k = 0{\cdot}05$, a factor introduced to reflect instrumental stability. From these data structure factors and their e.s.d.'s computed using $|F_o| = (I/\mathrm{Lp})^{1/2}$ and $\sigma(F_o) = \sigma(I)/2|F_o|\mathrm{Lp}$, where Lp is the Lorentz–polarization correction. No corrections for absorption since an estimation of this factor plus ψ-scan data showed the effect to be quite small. Three check reflections, periodically monitored throughout data collection, showed a gradual decrease in intensity; data set to one scale by application of scaling factors computed from the changes in the intensities of the standard reflections. Structure solved by using a combination of Patterson syntheses, packing considerations and direct-method techniques. Isotropic refinement of the 12 Ru and one Tl atom gave a residual below 0·25. Remaining 64 carbonyl O and C atoms, the As atom and 24 phenyl C atoms then located by application of standard difference Fourier and least-squares calculations. By assigning anisotropic thermal parameters to the 13 metal atoms and isotropic ones to the 95 non-metal atoms, a residual below 0·10 was obtained. At this stage H positions were calculated for the 20 H atoms attached to the four phenyl groups. They were assigned isotropic thermal parameters of 6·5 Å^2 and their positional and thermal parameters were fixed for the remainder of the refinement. The full-matrix least-squares refinement was allowed to proceed as before with 3634 observations and finally converged when $R = 0{\cdot}078$ and $R_w = 0{\cdot}098$. In all, 483 parameters, including a scale factor and extinction coefficient, were varied, giving a data/parameter ratio of 7·52/1. During the final cycle of least squares all Δ/σ

ratios were less than 0·1. Quantity minimized $w(|F_o| - |F_c|)^2$ where $w = 1/\sigma(F_o)^2$ with $\sigma(F_o)$ defined above. The form of the extinction correction applied was $F_c \times (I + gI_c)^{-1}$ where the parameter g was refined in the least squares and converged to a value of $2·61 \times 10^{-8}$. The final difference Fourier map displayed maximum intensities of 1·5 e Å^{-3} located in positions relatively close to the metal atoms. Atomic scattering factors from Cromer & Waber (1974); anomalous-scattering corrections (Cromer, 1974) included in least-squares calculations; *SDP* (Enraf–Nonius, 1980) used for all calculations.

Discussion. The final positional and thermal parameters are listed in Table 1.*

The bimetallic cluster anion $[\{Ru_6C(CO)_{16}\}_2Tl]^-$ comprises two distorted Ru_6 octahedra, each linked by two edge-related Ru atoms to a central Tl atom (Fig. 1). Each Ru_6 octahedron encapsulates a central C atom and there are 16 carbonyl groupings (14 essentially linear, two asymmetrically bridging) (Fig. 2). Although not a crystallographic requirement, the anion has almost 222 point symmetry, with the Tl atom at the intersection of the three twofold axes. Within the directly bonded $TlRu_4$ portion of the cluster, the four Tl—Ru distances have two distinct groups of bond distances with Tl—Ru(3)(3′) [2·853 (2), 2·875 (2) Å] and Tl—Ru(4)(4′) [2·775 (3), 2·785 (3) Å]. These four Ru atoms have a distorted tetrahedral arrangement around the central Tl atom defined by a torsional angle of 35·9° and an angle of 143·9° between the planes containing TlRu(3)(4) and TlRu(3′)(4′). Displacements from the mean plane through these five atoms are Ru(3)(3′) (−0·441, −0·546 Å) and Ru(4)(4′) (0·386, 0·548 Å). This tetrahedral distortion away from a planar arrangement of the four Tl—Ru bonds appears to be the result of the close-packing arrangement of the two sets of six carbonyl groups which are bonded to this portion of the cluster (see Fig. 2). The nine unbridged Ru—Ru distances range from 2·813 (4) to 2·938 (4) Å with an average of 2·88 (1) Å. The two carbonyl-bridged values have an average value of 2·86 (1) Å. The Ru—Ru bond bridged by the Tl atom is longer [3·10 (1) Å] than any other Ru—Ru distance in the cluster and is similar to that of 3·07 (1) Å in the Cu-bridged Ru—Ru bond found in $[(CH_3CN)_2Cu_2Ru_6C(CO)_{16}]$ (Bradley, Pruett, Hill, Ansell, Leonowicz & Modrick, 1982).

The encapsulated C atoms are displaced 0·13 (3) Å from the centroids of the Ru_6 octahedra with the result that the Ru—C(carbide) values range from 1·938 (25) to 2·184 (25) Å. This displacement takes place mainly in the equatorial Tl,Ru(2),Ru(3)Ru(4),Ru(5) plane and is towards the long Tl-bridged Ru—Ru bond. The magnitude of this range in Ru—C values is much larger than that found in $Ru_6C(CO)_{14}(C_{14}H_{14})$ [2·022 (35)–2·086 (35) Å, ave. 2·06 Å] (1) (Ansell & Bradley, 1980*a*), $[Ru_6C(CO)_{16}]^{2-}$ [2·037 (50)–2·053 (50) Å, ave. 2·055 Å] (Ansell & Bradley, 1980*b*), and $Ru_6C(CO)_{17}$ (Sirigu, Bianchi & Benedetti, 1969) [2·05 (7) Å]. It is comparable with that in $Ru_6C(CO)_{14}C_6H_3Me_3$ (1·88–2·12 Å) (Mason & Robinson, 1968), however. Bond lengths and angles involving the

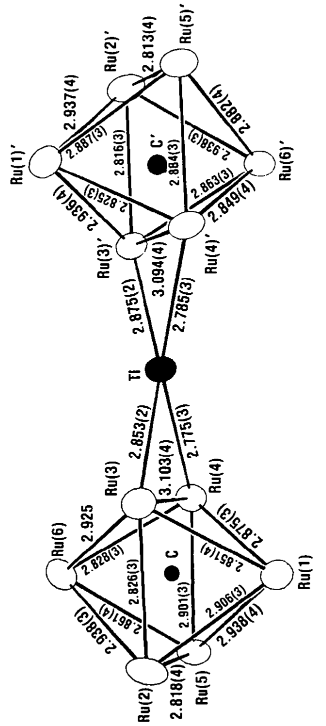

Fig. 1. The $(Ru_6)_2Tl$ skeleton. (Distances in Å.)

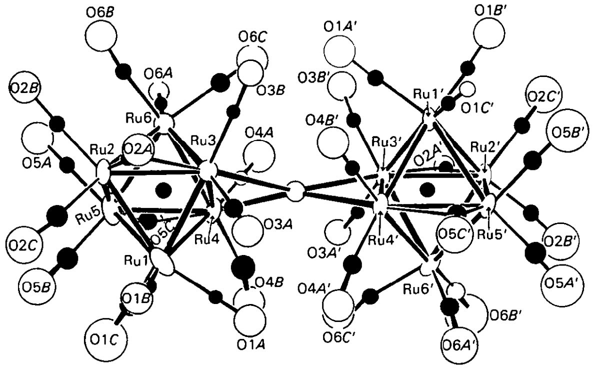

Fig. 2. The atomic arrangement within the $[\{Ru_6C(CO)_{16}\}_2Tl]^-$ anion.

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* Lists of major bond lengths and angles, hydrogen-atom coordinates, structure factors, anisotropic thermal parameters and r.m.s. radii have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39310 (41 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

almost linear Ru—carbonyl groups are similar to those found in the above-mentioned clusters. The bridged carbonyls lie within 0·08 Å of the equatorial Ru(2),-Ru(3),Ru(4),Ru(5) plane and are adjacent to the long Ru(3)—Ru(4) bond. Both are semi-bridged with a shorter Ru—C value of 1·801 (29) and 1·964 (54) Å (ave. 1·88 Å) and a longer one of 2·193 (26) and 2·519 (6) Å (ave. 2·35 Å). Bridging Ru—C—O angles range from 121·0 (2·0) to 150·5 (60)°. Bond distances and angles within the $[As(Ph)_4]^+$ counterion are normal.

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Structure of Bis[μ-(β-alanine)-*O,O′*]-disilver(I) Dinitrate, $[Ag_2(C_3H_7NO_2)_2](NO_3)_2$

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Abstract. $M_r = 517\cdot932$, monoclinic, $P2_1/n$, $a = 6\cdot656\ (5)$, $b = 8\cdot280\ (5)$, $c = 12\cdot975\ (4)$ Å, $\beta = 94\cdot90\ (3)°$, $V = 712\cdot58\ (20)$ Å^3, $Z = 2$, $D_m = 2\cdot382$, $D_x = 2\cdot414$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1\cdot54051$ Å, $\mu = 23\cdot3$ mm^{-1}, $F(000) = 504$, $T = 297$ K, $R = 0\cdot0888$ for 545 observed reflexions. The centrosymmetric dimers have an Ag–Ag separation 2·855 (4) Å. The Ag—O bond distances are 2·210 (19) and 2·198 (19) Å. The nitrate ion is bonded to the alanine moiety by two hydrogen bonds of the N—H···O type: N···O 3·09 (3) and 2·96 (3) Å. A pair of oxygen atoms from two adjacent nitrate ions are involved in weak covalent bonds with Ag, at distances of 2·58 (3) and 2·57 (3) Å.

Introduction. Alanine residues have been the subject of intensive study because of the variety of conformations in which alanine is found to be bonded in certain peptides, appearing, for instance, repetitively in the form of an Ala-Pro sequence over a segment of the light chain of rabbit skeletal muscle myosin (Kamwaya, Oster, Bradaczek, Ponnuswamy, Parthasarathy, Naraj & Balaram, 1982) and because of some interesting physical properties in complexes of metallic salts with amino acids (Tomita, 1961; Jose, Pant & Biswas, 1964; Jose & Pant, 1965; Herak, Prelesnik, Manojlović-Muir & Muir, 1974). Further, it has been observed that certain derivatives of β-alanine with $Cu(NO_3)_2.3H_2O$ form a bacteriocidal composition against *Bacillus subtilis* (Aeloney, 1982).

Experimental. Silver nitrate and β-alanine taken in stoichiometric proportion and dissolved in distilled water, filtered and then allowed to evaporate slowly; crystals slightly photosensitive; density determined by flotation in bromoform–xylene; preliminary examination by oscillation and Weissenberg photographs;

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