comparison of the dihedral angles between the Co, N(3), N(13), N(18) and Co, N(3), N(8), N(13) planes and the ring planes [176.8 (3), 92.9 (3)° and 110.1 (3), 164.6 (3)° for the N(11)-C(15) and N(1)-C(5) rings, respectively].

The structure contains a three-dimensional network of hydrogen bonds (Fig. 2) involving  $N^{\tau}$ —H, amino, water and C(12)—H groups as donors, and water O atoms, carbonate and Cl<sup>-</sup> anions as acceptors. The N(1)—H group forms a hydrogen bond, the N(1)···O(3) (-x, -y, -1-z) distance being 2.755 (4) Å. The N(8) amino group is a donor in two hydrogen bonds. With N(8)…Cl(1 + x, y, 1 + y) z) and N(8)···OW(1 + x, y, z) distances of 3.318 (4) and 2.922 (5) Å, respectively. The N(11)-H group of the second histamine ligand forms a hydrogen bond to the Cl<sup>-</sup> ion  $[N(11)\cdots Cl(1-x, 1-y, -z)] =$ 3.175 (4) Å]. The C(12)—H group acts as a donor in a bifurcated hydrogen bond, the  $C(12)\cdots O(1)$  and  $C(12)\cdots Cl(1 + x, y, z)$  distances being 2.838 (5) and 3.448 (5) Å, respectively. The N(18) amino group is a donor in two hydrogen bonds, the N(18)...Cl and  $N(18)\cdots O(3)$  (x, y, 1 + z) distances being 3.484 (5) and 2.930(5) Å, respectively. Both water O-H groups form hydrogen bonds  $[OW \cdots Cl = 3.240 (4)]$ and OW···O(2) (x, y, 1 + z) = 2.772 (4) Å]. The Cl<sup>-</sup> ion participates in five hydrogen bonds, and the carbonate ion is an acceptor in four such bonds, whereas the water O atom is a single-hydrogen-bond acceptor.

This research was partly supported by project RP.II.10.

### References

- BONNET, J. J. & IBERS, J. A. (1973). J. Am. Chem. Soc. 95, 4829-4833.
- BONNET, J. J. & JEANNIN, Y. (1970). Acta Cryst. B26, 318-326.
- DAHAN, F. (1976). Acta Cryst. B32, 2472-2475.
- DANILCZUK, E. & SURDYKOWSKI, A. (1986). Pol. J. Chem. 60, 379-387.
- International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- IUPAC-IUB COMMISSION ON BIOCHEMICAL NOMENCLATURE (1970). J. Mol. Biol. 52, 1-17.
- JASKÓLSKI, M. (1982). In Collected Abstracts of the Fourth Symposium on Organic Crystal Chemistry, Poznań, September 1982, edited by Z. KAŁUSKI, pp. 70–71. A. Mickiewicz Univ., Poznań, Poland.
- JOHNSON, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO78*. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.
- NIEDERHOFFER, E. C., MARTELL, A. E., RUDOLF, P. & CLEARFIELD, A. (1982). *Inorg. Chem.* 21, 3734–3741.
- SHELDRICK, G. M. (1976). SHELX76. Program for crystal structure determination. Univ. of Cambridge, England.
- THROUP, N. (1977). Acta Chem. Scand. Ser. A, 31, 203-207.
- WOJTCZAK, A., JASKÓLSKI, M. & KOSTURKIEWICZ, Z. (1983). Acta Cryst. C39, 545–547.
- WOJTCZAK, A., JASKÓLSKI, M. & KOSTURKIEWICZ, Z. (1985). Acta Cryst. C41, 1752–1755.
- WOJTCZAK, A., JASKÓLSKI, M. & KOSTURKIEWICZ, Z. (1987). Acta Cryst. C43, 645–648.

Acta Cryst. (1990). C46, 581-584

# Structure of *trans*-Bromodicarbonyl[*o*-phenylenebis(diphenylphosphine)]-(*p*-tolylmethylidyne)tungsten(0)

BY G. A. CARRIEDO, V. RIERA, J. M. RUBIO GONZALEZ AND M. G. SANCHEZ

Departamento de Química Organometálica, Universidad de Oviedo, 33071 Oviedo, Spain

(Received 23 January 1989; accepted 6 July 1989)

Abstract. [WBr(CO)<sub>2</sub>(C<sub>8</sub>H<sub>7</sub>)(C<sub>30</sub>H<sub>24</sub>P<sub>2</sub>)],  $M_r = 869\cdot39$ , monoclinic,  $P2_1/n$ ,  $a = 9\cdot505$  (5),  $b = 18\cdot333$  (4),  $c = 20\cdot775$  (8) Å,  $\beta = 96\cdot68$  (4)°, V = 3595 (3) Å<sup>3</sup>, Z = 4,  $D_x = 1\cdot606$  Mg m<sup>-3</sup>, Mo K $\alpha$  radiation (graphite monochromator,  $\lambda = 0.71073$  Å),  $\mu = 4\cdot50$  mm<sup>-1</sup>, F(000) = 1704, T = 291 K, final R = 0.025 for 4337 observed reflections and 509 variables. The W atom is in a distorted octahedral environment formed by the two P atoms of the chelating diphosphine, two mutually *cis* carbonyl groups and a bromide ligand *trans* to a methylidyne group. The W=C-R  $(R = C_6H_4CH_3-4)$  group deviates slightly from linearity and the short W—C distance suggests a formal metal—carbon triple bond.

**Introduction.** Very few X-ray structure determinations have been carried out on neutral sixcoordinated methylidyne complexes of tungsten(0), and the majority of them are *trans*-tetracarbonyls, having also halogens (Huttner, Lorenz & Gartzke, 1974; Neugebauer, Fischer, Dao & Schubert, 1978; Fischer, Gammel & Neugebauer, 1980) or the

0108-2701/90/040581-04\$03.00

© 1990 International Union of Crystallography

Co(CO)₄ group (Fischer, Friedrich. Lindner. Neugebauer, Kreissl, Uedelhoven, Dao & Huttner, 1983). Here we report the first crystal structure of a stable methylidyne complex of the type trans- $X(CO)_2(L-L)W(\equiv CR),$ where X = Br. L-L =*o*-phenylenebis(diphenylphosphine) and R =C<sub>6</sub>H<sub>4</sub>Me-4, prepared by Carriedo, Riera & Sánchez (1988) following a method similar to that published recently for other dicarbonyl methylidyne complexes (McDermott, Dorries & Mayr, 1987).

**Experimental.** A crystal was selected and mounted on an Enraf–Nonius CAD-4 four-circle diffractometer. The unit-cell parameters were determined from 23 reflections ( $8 \le \theta \le 12^{\circ}$ ) and refined by least-squares method. Intensities were collected, using the  $\omega$ -2 $\theta$ scan technique, up to  $\theta = 30^{\circ}$  in the *hkl* range from -13,0,0 to 13,25,19. Three reflections were measured each hour as orientation and intensity control; no significant intensity decay was observed. 9194 reflections were measured, corresponding to 8631 unique reflections ( $R_{int} = 0.024$ ), 4337 of which were assumed as observed applying the condition  $I \ge$  $3\sigma(I)$ . Lorentz and polarization corrections were applied.

The structure was solved by locating the W and Br atoms with MULTAN80 (Main et al., 1980); the other atoms were found by Fourier synthesis with SHELX76 (Sheldrick, 1976). The structure was refined by block-matrix least squares, using SHELX76 (Sheldrick, 1976). The function minimized  $\sum [w(|F_{o}| - |F_{c}|)^{2}],$ was where  $w = [\sigma^2(F_o) +$  $0.0002|F_o|^2]^{-1}$ . After the isotropic refinement, an empirical absorption correction was applied (Walker & Stuart, 1983), correction factors were in the range 0.905 to 1.090. Anisotropic thermal parameters were comparable after refinement with and without absorption correction. Except for those of the methyl group [C(10)], which were located by difference Fourier synthesis, the H atoms were inserted geometrically. All the H atoms were refined freely with an overall isotropic temperature factor (final U = $0.107 \text{ Å}^2$ ). The remaining atoms were refined with individual anisotropic temperature factors. The final R was 0.025 and wR was 0.024. Max. shift/e.s.d. was 2.43 for the overall temperature factor of H atoms. For non-H atoms the max. shift/e.s.d. was 1.47 for  $U_{11}$  of C(33). Owing to restrictions in calculation time, in each run of the SHELX program each block was refined only once. The truncation of the results in each run of the program resulted in numerical noise. Finally, successive executions of the program led to no further progress in the refinement. The final difference Fourier map showed a residual electron density between -0.42 and 0.45 e Å<sup>-3</sup>. The values of f, f' and f'' were taken from International Tables for X-ray Crystallography (1974). The geometry calculations were performed with *PARST* (Nardelli, 1983), and Fig. 1 was drawn with *PLUTO* (Motherwell, 1976).

**Discussion.** Final atomic parameters are listed in Table 1 and selected bond lengths and angles in Table 2.\* The structure consists of discrete molecules (Fig. 1) linked by van der Waals forces. The shortest intermolecular separation is 2.480 (0) Å  $[H(24)\cdots H(34^{i}); (i) = x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}]$ . The W atom is in a slightly distorted octahedral environment, with two P atoms of the chelating ligand and two carbonyl ligands in the equatorial positions. The Br atom and the methylidyne group are in the apical positions.

The Br(1)—W(1) bond distance [2.675(1) Å] is very similar to that observed in  $[Br(CO)_4W(\equiv CMe)]$ [2.648 (6) Å] (Neugebauer, Fischer, Dao & Schubert, 1978). The W(1)—C(3) distance [1.798(5) Å)] may be compared with those found in the related complexes  $[(\eta - C_5H_5)(CO)_2W \equiv C(C_6H_4Me-4)]$ [1.82 (2) Å] (Fischer, Lindner, Huttner, Friedrich, Kreissl & Besenhard, 1977) and [I(CO)<sub>4</sub>W=CPh)] [1.90 (5) Å] (Huttner, Lorenz & Gartzke, 1974). In all of these complexes the W-C separation is considerably shorter than that observed in  $[W(=CPh_2)(CO)_5]$  [2.14 (2) Å] (Casey, Burkhardt, Bunnell & Calabrese, 1977) and this has been taken to imply a W=C bond because it is significantly less than the corresponding distance [2.34(1) Å] in the  ${W[CH(OMe)Ph](CO)_5}^-$  (Casey, Polichanion nowski, Tuinstra, Albin & Calabrese, 1978). The angles Br(1)—W(1)—C(3)  $[173.4 (2)^{\circ}]$  and W(1)—  $C(3) - C(4) [171.5 (4)^{\circ}]$  deviate slightly from linearity.

The W(1)—CO bond lengths [2.012(5) Å] are shorter than those observed in  $[Br(CO)_4W(\equiv CMe)]$ [average value 2.12 (5) Å] (Neugebauer, Fischer, Dao & Schubert, 1978). This may be attributed to the presence of a P atom in a trans position to each CO group. The W(1)—C—O groups are almost linear [average value  $176.8(5)^{\circ}$ ]. Both W(1)—P distances [average value 2.513 (1) Å] are close to those found in the related complex [W(CO)<sub>3</sub>(dppe)(C=CHCO<sub>2</sub>-Me)] [average value 2.550 (3) Å] (Birdwhistell, Nieter Burgmayer & Templeton, 1983). The Br(1)-W(1)—P angles are smaller than the Br(1)— W(1)-CO angles, but all of them are about 90°. Similarly, the C(3)—W(1)—CO angles [average value]  $87.0(2)^{\circ}$  are smaller than those corresponding to the C(3)—W(1)—P angles [average value  $98.4(1)^{\circ}$ ]. The angle between the two carbonyl groups is near 90°

<sup>\*</sup> Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52399 (31 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional positional and thermal parameters Table 2. Selected bond lengths (Å) and angles (°) with  $(Å^2 \times 10^2)$  with e.s.d.'s in parentheses

## $U_{\rm eq} = (1/3) \sum_i \sum_j U_{ij} a_i^* a_i^* \mathbf{a}_j \cdot \mathbf{a}_j.$

$ \begin{array}{c} W(1) & 0.49916 (2) & 0.22404 (1) & 0.08264 (1) & 4.26 (1) \\ Br(1) & 0.49150 (6) & 0.30205 (3) & -0.02654 (3) & 6.15 (2) \\ P(1) & 0.3103 (1) & 0.30583 (7) & 0.11781 (6) & 4.40 (4) \\ P(2) & 0.2757 (1) & 0.16591 (7) & 0.02763 (6) & 4.68 (4) \\ C(1) & 0.6574 (5) & 0.2873 (3) & 0.1241 (3) & 5.8 (2) \\ O(1) & 0.7441 (4) & 0.3217 (3) & 0.1506 (2) & 9.4 (2) \\ C(2) & 0.6319 (5) & 0.1159 (3) & 0.0436 (3) & 6.4 (2) \\ O(2) & 0.7050 (5) & 0.1163 (2) & 0.0236 (3) & 9.8 (2) \\ C(3) & 0.5256 (4) & 0.1702 (3) & 0.1554 (2) & 500 (2) \\ C(4) & 0.5675 (5) & 0.1317 (3) & 0.2155 (3) & 5.7 (2) \\ C(5) & 0.7055 (6) & 0.1340 (4) & 0.2437 (3) & 9.2 (3) \\ C(6) & 0.7422 (8) & 0.0985 (5) & 0.3024 (4) & 1.3-5 (4) \\ C(7) & 0.6501 (9) & 0.0614 (4) & 0.3381 (3) & 9.9 (3) \\ C(8) & 0.5181 (8) & 0.0576 (4) & 0.3051 (4) & 11.9 (4) \\ C(9) & 0.4739 (7) & 0.0925 (4) & 0.2467 (3) & 10.5 (3) \\ C(10) & 0.698 (1) & 0.0242 (5) & 0.3978 (4) & 18.8 (6) \\ C(21) & 0.1026 (5) & 0.2200 (3) & -0.0139 (3) & 6.4 (2) \\ C(22) & 0.1306 (4) & 0.2323 (3) & 0.0249 (2) & 4.8 (2) \\ C(23) & 0.0026 (5) & 0.2200 (3) & -0.0139 (3) & 6.4 (2) \\ C(24) & -0.1046 (5) & 0.2715 (4) & -0.0157 (3) & 7.5 (3) \\ C(33) & 0.0777 (6) & 0.2623 (4) & 0.2670 (3) & 0.00 (3) \\ C(34) & 0.1746 (8) & 0.2540 (4) & 0.3176 (3) & 8.6 (3) \\ C(35) & 0.3335 (6) & 0.2738 (3) & 0.2481 (3) & 7.0 (2) \\ C(41) & 0.3364 (5) & 0.4040 (3) & 0.1245 (3) & 5.1 (2) \\ C(42) & 0.3535 (6) & 0.2738 (3) & 0.2481 (3) & 7.0 (2) \\ C(43) & 0.3740 (7) & 0.5180 (3) & 0.0720 (3) & 8.2 (3) \\ C(44) & 0.3765 (7) & 0.5546 (3) & 0.1812 (4) & 8.8 (3) \\ C(55) & 0.3181 (7) & 0.473 (4) & -0.1349 (4) & 9.6 (3) \\ C(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ C(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ C(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ C(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ C(54) & 0.2777 (7) & 0.0939 (5) & 0.1312 (4) & 1.1 (4) \\ C(46) & 0.3181 (7) & 0.0330 (3) & 0.0693 (3) & 8.2 (3) \\ C(55) & 0.3183 (7) & 0.0473 (4) & -0.7175 (3) & 6.4 (2) \\ C(54) & 0.3131 (7) & 0.0330 $		x	v	z	U.
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	W(1)	0.49916 (2)	0.22404 (1)	0.08264(1)	4.26 (1)
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Br(1)	0.49150 (6)	0.30205(3)	-0.02654(3)	6.15 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	P(1)	0.3103 (1)	0.30583(7)	0.11781(6)	4.40 (4)
C(1) $0-5574$ (5) $0-2873$ (3) $0-1241$ (3) $58$ (2)O(1) $0-7441$ (4) $0-3217$ (3) $0-1506$ (2) $9-4$ (2)C(2) $0-6319$ (5) $0-1559$ (3) $0-0436$ (3) $644$ (2)O(2) $0-7050$ (5) $0-1163$ (2) $0-0236$ (3) $9-8$ (2)C(3) $0-5256$ (4) $0-1702$ (3) $0-1554$ (2) $500$ (2)C(4) $0-5675$ (5) $0-1317$ (3) $0-2155$ (3) $5-77$ (2)C(5) $0-7055$ (6) $0-1340$ (4) $0-2437$ (3) $9-2$ (3)C(6) $0-7422$ (8) $0-0985$ (5) $0-3024$ (4) $13-5$ (4)C(7) $0-6501$ (9) $0-0614$ (4) $0-3338$ (3) $9-9$ (3)C(8) $0-5181$ (8) $0-0576$ (4) $0-3051$ (4) $11-9$ (4)C(9) $0-4739$ (7) $0-0925$ (4) $0-2467$ (3) $10-5$ (3)C(10) $0-698$ (1) $0-0242$ (5) $0-3978$ (4) $18.8$ (6)C(21) $0-1306$ (4) $0-22323$ (3) $0-0249$ (2) $4.8$ (2)C(22) $0-1306$ (4) $0-22323$ (3) $0-0249$ (2) $4.8$ (2)C(23) $0-00226$ (5) $0-2200$ (3) $-0-0139$ (3) $6-4$ (2)C(24) $-0-1046$ (5) $0-2715$ (4) $-00157$ (3) $7-6$ (2)C(23) $0-10226$ (5) $0-3881$ (3) $0-0703$ (3) $8-6$ (3)C(24) $-0-1046$ (5) $0-2715$ (4) $0-2056$ (3) $8-3$ (3)C(33) $0-0777$ (6) $0-2253$ (4) $0-2670$ (3) $10-0$ (3)C(34) $0-1746$ (8) $0-2540$ (4)<	P(2)	0.2757(1)	0.16591(7)	0.02763(6)	4.68 (4)
C(1) $0.7441$ $0.3217$ $0.7506$ $0.7506$ $0.7506$ $0.9462$ C(2) $0.6319$ $(5)$ $0.1559$ $0.04366$ $(3)$ $6.422$ O(2) $0.7050$ $(5)$ $0.1163$ $(2)$ $0.0236$ $(3)$ $9.822$ C(3) $0.5256$ $(4)$ $0.1702$ $(3)$ $0.1554$ $(2)$ $50$ $(2)$ C(4) $0.5675$ $(5)$ $0.11317$ $(3)$ $0.2155$ $(3)$ $5.772$ C(5) $0.7055$ $(6)$ $0.13404$ $0.24377$ $(3)$ $9.23$ C(6) $0.7422$ $(8)$ $0.0985$ $(5)$ $0.3024$ $(4)$ $1.544$ C(7) $0.6501$ $(9)$ $0.0614$ $(4)$ $0.3338$ $(3)$ $9.99$ $(3)$ C(8) $0.5181$ $(8)$ $0.0576$ $(4)$ $0.3051$ $(4)$ $1.944$ C(9) $0.47397$ $(7)$ $0.0925$ $(4)$ $0.2467$ $(3)$ $1.0533$ C(10) $0.69841$ $0.024242$ $(5)$ $0.397844$ $1.8.866$ C(21) $0.149044$ $0.22573$ $0.0608622$ $4.7722$ C(23) $0.002665$ $0.22003$ $-0.013933$ $6.4422$ C(23) $0.002665$ $0.22003$ $-0.0139433$ $6.4222$ C(24) $-0.104653$ $0.275344$ $0.075533$ $6.3333363$ C(24) $-0.104653$ $0.2753444$ $0.0556333$ $6.4223$ C(24) $-0.1046453$ $0.2259444$ $0.3075333$ $0.2256333$ $8-633333333337633$ </td <td>cú</td> <td>0.6574 (5)</td> <td>0.2873(3)</td> <td>0.1241(3)</td> <td>5.8 (2)</td>	cú	0.6574 (5)	0.2873(3)	0.1241(3)	5.8 (2)
$\begin{array}{cccccc} (2) & 0.431 (5) & 0.1559 (3) & 0.0436 (3) & 6.4 (2) \\ (2) & 0.7050 (5) & 0.1163 (2) & 0.0236 (3) & 9.8 (2) \\ (3) & 0.5256 (4) & 0.1702 (3) & 0.1554 (2) & 5.0 (2) \\ (4) & 0.5675 (5) & 0.1317 (3) & 0.2155 (3) & 5.7 (2) \\ (5) & 0.7055 (6) & 0.1340 (4) & 0.2437 (3) & 9.2 (3) \\ (6) & 0.7422 (8) & 0.0985 (5) & 0.3024 (4) & 1.35 (4) \\ (7) & 0.6501 (9) & 0.0614 (4) & 0.3338 (3) & 9.9 (3) \\ (7) & 0.6501 (9) & 0.0614 (4) & 0.3338 (3) & 9.9 (3) \\ (8) & 0.5181 (8) & 0.0576 (4) & 0.3051 (4) & 11.9 (4) \\ (9) & 0.4739 (7) & 0.0925 (4) & 0.2467 (3) & 10.5 (3) \\ (10) & 0.698 (1) & 0.0242 (5) & 0.3978 (4) & 18.8 (6) \\ (21) & 0.1490 (4) & 0.2257 (3) & 0.0608 (2) & 4.7 (2) \\ (22) & 0.1306 (4) & 0.2253 (3) & 0.0249 (2) & 4.8 (2) \\ (23) & 0.0026 (5) & 0.2200 (3) & -0.0139 (3) & 6.4 (2) \\ (24) & -0.1046 (5) & 0.2715 (4) & -0.0157 (3) & 7.5 (3) \\ (26) & 0.0428 (5) & 0.3353 (4) & 0.0175 (3) & 7.6 (3) \\ (23) & 0.0026 (5) & 0.2820 (3) & 0.1959 (2) & 4.9 (2) \\ (33) & 0.0777 (6) & 0.2623 (4) & 0.2670 (3) & 10.0 (3) \\ (23) & 0.0177 (6) & 0.2623 (4) & 0.23176 (3) & 8-6 (3) \\ (23) & 0.0177 (6) & 0.2623 (4) & 0.2470 (3) & 10.0 (3) \\ (24) & 0.1746 (8) & 0.2540 (4) & 0.3176 (3) & 8-6 (3) \\ (24) & 0.3535 (6) & 0.2738 (3) & 0.2481 (3) & 7.0 (2) \\ (24) & 0.3535 (6) & 0.2738 (3) & 0.2481 (3) & 7.0 (2) \\ (24) & 0.354 (5) & 0.4040 (3) & 0.1245 (3) & 5.1 (2) \\ (24) & 0.354 (5) & 0.4040 (3) & 0.1245 (3) & 5.1 (2) \\ (24) & 0.354 (5) & 0.4040 (3) & 0.1245 (3) & 5.1 (2) \\ (24) & 0.354 (5) & 0.4040 (3) & 0.1285 (4) & 8.8 (3) \\ (24) & 0.3765 (7) & 0.5546 (3) & 0.1812 (3) & 9.1 (3) \\ (55) & 0.3181 (7) & 0.473 (4) & -0.1349 (4) & 9.0 (3) \\ (54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ (55) & 0.3183 (7) & 0.0473 (4) & -0.1349 (4) & 9.0 (3) \\ (56) & 0.3134 (6) & 0.0677 (3) & -0.0717 (3) & 8.2 (3) \\ (56) & 0.3131 (7) & 0.0330 (3) & 0.0693 (3) & 8.2 (3) \\ (56) & 0.3131 (7) & 0.0330 (3) & 0.0693 (3) & 8.2 (3) \\ (56) & 0.4333 (9) & 0.0133 (6) & 0.1312 (4) & 1.2 (4) \\ (264) & 0.138 (1) & -0.0395 (5) & 0.1312 (4) & 1.1 (4) \\ (664) & 0.138 (1) & $	on	0.7441(4)	0.3217(3)	0.1506(2)	9.4 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(2)	0.6319 (5)	0.1559 (3)	0.0436(3)	6.4 (2)
C(3) $0.5256$ (4) $0.1702$ (3) $0.1554$ (2) $50$ (2)C(4) $0.5675$ (5) $0.1317$ (3) $0.2155$ (3) $5.7$ (2)C(5) $0.7055$ (6) $0.1340$ (4) $0.2437$ (3) $9.2$ (3)C(6) $0.7422$ (8) $0.0985$ (5) $0.3024$ (4) $1.35$ (4)C(7) $0.6501$ (9) $0.0614$ (4) $0.3338$ (3) $9.9$ (3)C(8) $0.5181$ (8) $0.0576$ (4) $0.3024$ (4) $1.56$ (4)C(9) $0.4739$ (7) $0.0925$ (4) $0.2467$ (3) $10.5$ (3)C(10) $0.698$ (1) $0.0242$ (5) $0.3978$ (4) $1.88$ (6)C(21) $0.1490$ (4) $0.2957$ (3) $0.0608$ (2) $4.7$ (2)C(23) $0.0026$ (5) $0.2200$ (3) $-0.0139$ (3) $6.4$ (2)C(24) $-0.1046$ (5) $0.2715$ (4) $-0.0157$ (3) $7.5$ (2)C(25) $-0.0834$ (5) $0.3353$ (4) $0.0563$ (3) $6.4$ (2)C(24) $-0.1046$ (5) $0.2715$ (4) $-0.0157$ (3) $7.8$ (3)C(26) $0.0428$ (5) $0.3481$ (3) $0.0563$ (3) $6.4$ (2)C(31) $0.2524$ (5) $0.2820$ (3) $0.1959$ (2) $4.9$ (2)C(33) $0.0777$ (6) $0.2529$ (4) $0.2056$ (3) $8.3$ (3)C(33) $0.0777$ (6) $0.2592$ (4) $0.3095$ (3) $9.2$ (3)C(34) $0.1746$ (8) $0.2594$ (4) $0.3176$ (3) $8.6$ (3)C(35) $0.3132$ (7) $0.2594$ (4) $0.3176$ (3) $8.6$ (3)C(34) $0.774$ (8) $0.2594$ (4)<	O(2)	0.7050 (5)	0.1163(2)	0.0236(3)	9.8 (2)
C(4) $0-5675$ $0-1317$ $(3)$ $0-2155$ $(3)$ $57$ $(2)$ C(5) $0-7055$ $(6)$ $0-1340$ $(4)$ $0-2437$ $(3)$ $9-2$ $(3)$ C(6) $0-7422$ $(8)$ $00985$ $(5)$ $0-3024$ $(4)$ $13-5$ $(4)$ C(7) $0-6501$ $(9)$ $0-0614$ $(4)$ $0-3338$ $(3)$ $9-9$ $(3)$ C(8) $0-5181$ $(8)$ $0-0576$ $(4)$ $0-3051$ $(4)$ $11-9$ $(4)$ C(9) $0-4739$ $(7)$ $00925$ $(4)$ $0-2467$ $(3)$ $10-5$ $(3)$ C(10) $0-698$ $(1)$ $0-0242$ $(5)$ $0-3978$ $(4)$ $18-8$ $(6)$ C(21) $0-1490$ $(4)$ $0-22577$ $(3)$ $0-0608$ $(2)$ $4.7$ $(2)$ C(22) $0-1306$ $(4)$ $0-2220$ $(3)$ $-0-0139$ $(3)$ $644$ $(2)$ C(23) $0-0026$ $(5)$ $0-2200$ $(3)$ $-0-0139$ $(3)$ $644$ $(2)$ C(24) $-0-1046$ $(5)$ $0-2715$ $(4)$ $-0.0157$ $(3)$ $7-8$ $(3)$ C(25) $-0-0834$ $(5)$ $0-3353$ $(4)$ $0-0175$ $(3)$ $7-8$ $(3)$ C(25) $-0-0834$ $(5)$ $0-3353$ $(4)$ $0-0175$ $(3)$ $7-8$ $(3)$ C(26) $0-0428$ $(5)$ $0-3353$ $(4)$ $0-0175$ $(3)$ $8-6$ $(3)$ C(31) $0-2254$ <td>C(3)</td> <td>0.5256 (4)</td> <td>0.1702(3)</td> <td>0.1554(2)</td> <td>5.0 (2)</td>	C(3)	0.5256 (4)	0.1702(3)	0.1554(2)	5.0 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(4)	0.5675 (5)	0.1317(3)	0.2155(3)	5.7 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(S)	0.7055 (6)	0.1340 (4)	0.2437(3)	9.2 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(6)	0.7422(8)	0.0985(5)	0.3024(4)	13.5 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(7)	0.6501 (9)	0.0614(4)	0.3338 (3)	0.0 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(8)	0.5181(8)	0.0576 (4)	0.3051(4)	11.9 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(9)	0.4739 (7)	0.0925 (4)	0.2467(3)	10.5 (3)
$\begin{array}{cccccc} (21) & 0.1490 (4) & 0.2957 (3) & 0.0608 (2) & 4.7 (2) \\ (22) & 0.1306 (4) & 0.2323 (3) & 0.0249 (2) & 4.8 (2) \\ (23) & 0.0026 (5) & 0.2200 (3) & -0.0139 (3) & 6.4 (2) \\ (24) & -0.1046 (5) & 0.2715 (4) & -0.0157 (3) & 7.5 (2) \\ (25) & -0.0834 (5) & 0.3353 (4) & 0.0175 (3) & 7.8 (3) \\ (26) & 0.0428 (5) & 0.3353 (4) & 0.0175 (3) & 7.8 (3) \\ (23) & 0.0777 (6) & 0.2820 (3) & 0.1959 (2) & 4.9 (2) \\ (23) & 0.1122 (6) & 0.2753 (4) & 0.2056 (3) & 8.3 (3) \\ (23) & 0.0777 (6) & 0.2623 (4) & 0.2056 (3) & 8.6 (3) \\ (23) & 0.0777 (6) & 0.2623 (4) & 0.2056 (3) & 8.6 (3) \\ (23) & 0.0777 (6) & 0.2629 (4) & 0.3176 (3) & 8.6 (3) \\ (23) & 0.1746 (8) & 0.2540 (4) & 0.3176 (3) & 8.6 (3) \\ (24) & 0.1746 (8) & 0.2540 (4) & 0.3176 (3) & 8.6 (3) \\ (24) & 0.3535 (6) & 0.2738 (3) & 0.2481 (3) & 7.0 (2) \\ (241) & 0.3364 (5) & 0.4040 (3) & 0.1245 (3) & 5.1 (2) \\ (242) & 0.3554 (6) & 0.4433 (3) & 0.0700 (3) & 7.3 (2) \\ (243) & 0.3740 (7) & 0.5180 (3) & 0.0720 (3) & 8.2 (3) \\ (244) & 0.3765 (7) & 0.5546 (3) & 0.1812 (3) & 9.1 (3) \\ (244) & 0.3765 (7) & 0.5546 (3) & 0.1812 (3) & 9.1 (3) \\ (251) & 0.2712 (5) & 0.1377 (3) & -0.0569 (3) & 5.1 (2) \\ (252) & 0.2356 (5) & 0.1862 (3) & -0.1705 (3) & 8.2 (3) \\ (253) & 0.2382 (6) & 0.1649 (4) & -0.1705 (3) & 8.2 (3) \\ (254) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ (255) & 0.3183 (7) & 0.0473 (4) & -0.1349 (4) & 9.0 (3) \\ (256) & 0.3134 (6) & 0.0677 (3) & -0.0717 (3) & 7.0 (2) \\ (261) & 0.2156 (6) & 0.0858 (3) & 0.0694 (3) & 6.0 (2) \\ (262) & 0.3131 (7) & 0.0330 (3) & 0.0893 (3) & 8.2 (3) \\ (563) & 0.2717 (10) & -0.0296 (4) & 0.1199 (4) & 11.1 (4) \\ (40) (64) & 0.138 (1) & -0.0395 (5) & 0.1312 (4) & 12.9 (5) \\ (565) & 0.0433 (9) & 0.0133 (6) & 0.0591 (3) & 5.2 (3) \\ (266) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ (566) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ (566) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ (566) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ (566) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ (566) & 0.0433 (9) & 0.0133 (6) & 0$	CUM	0.698(1)	0.0242(5)	0.3978 (4)	18-8 (6)
$\begin{array}{cccc} (22) & 0 & 1306 (4) & 0 & 2232 (3) & 0 & 0249 (2) & 48 (2) \\ (23) & 0 & 0026 (5) & 0 & 2200 (3) & - & 00139 (3) & 64 (2) \\ (24) & - & 0 & 1046 (5) & 0 & 2715 (4) & - & 0 & 0157 (3) & 7.5 (2) \\ (25) & - & 0 & 0834 (5) & 0 & 3353 (4) & 0 & 0175 (3) & 7.8 (3) \\ (26) & 0 & 0428 (5) & 0 & 3481 (3) & 0 & 0563 (3) & 64 (2) \\ (23) & 0 & 2524 (5) & 0 & 2820 (3) & 0 & 1059 (2) & 49 (2) \\ (23) & 0 & 0777 (6) & 0 & 2623 (4) & 0 & 2056 (3) & 8.3 (3) \\ (23) & 0 & 0777 (6) & 0 & 2623 (4) & 0 & 2056 (3) & 8.6 (3) \\ (23) & 0 & 0777 (6) & 0 & 2623 (4) & 0 & 2056 (3) & 8.6 (3) \\ (23) & 0 & 0777 (6) & 0 & 2599 (4) & 0 & 3095 (3) & 92 (3) \\ (23) & 0 & 0777 (6) & 0 & 2599 (4) & 0 & 3095 (3) & 92 (3) \\ (24) & 0 & 1746 (8) & 0 & 2549 (4) & 0 & 3076 (3) & 8.6 (3) \\ (24) & 0 & 3535 (6) & 0 & 2738 (3) & 0 & 2481 (3) & 7.0 (2) \\ (241) & 0 & 3364 (5) & 0 & 4040 (3) & 0 & 1245 (3) & 5.1 (2) \\ (242) & 0 & 3554 (6) & 0 & 4433 (3) & 0 & 0700 (3) & 7.3 (2) \\ (243) & 0 & 3740 (7) & 0 & 5180 (3) & 0 & 0720 (3) & 8.2 (3) \\ (244) & 0 & 3765 (7) & 0 & 5546 (3) & 0 & 1812 (4) & 11.1 (4) \\ (246) & 0 & 3381 (8) & 0 & 4410 (3) & 0 & 1812 (3) & 9.1 (3) \\ (251) & 0 & 2712 (5) & 0 & 1377 (3) & - 0 & 0569 (3) & 5.1 (2) \\ (252) & 0 & 2356 (5) & 0 & 1862 (3) & - 0 & 1705 (3) & 8.2 (3) \\ (254) & 0 & 2777 (7) & 0 & 0949 (5) & - 0 & 1843 (4) & 9.5 (3) \\ (255) & 0 & 3183 (7) & 0 & 0473 (4) & - 0 & 1349 (4) & 90 (3) \\ (256) & 0 & 3131 (7) & 0 & 0330 (3) & 0 & 0693 (3) & 8.2 (3) \\ (56) & 0 & -1313 (7) & 0 & 0330 (3) & 0 & 0693 (3) & 8.2 (3) \\ (56) & 0 & -1313 (1) & - & 0 & 0395 (5) & 0 & 1312 (4) & 12.9 (5) \\ (264) & 0 & -138 (1) & - & 0 & -0 & 0395 (5) & 0 & 1312 (4) & 12.9 (5) \\ (265) & 0 & -0 & 133 (1) & - & 0 & 0395 (5) & 0 & 1312 (4) & 12.9 (5) \\ (266) & 0 & -0 & 038 (17) & 0 & 0 & 033 (6) & 0 & 033 (3) & 8.2 (3) \\ (566) & 0 & -0 & 0381 (7) & 0 & 0 & 033 (6) & 0 & 0312 (4) & 12.9 (5) \\ (266) & 0 & -0 & 0381 (7) & 0 & 0 & 033 (6) & 0 & 0313 (6) & 0 & 021 (64) & 0 & 133 (6) & 0 & 0133 (6) & 0 & 1312 (4) & 12.9 (5) \\ (266) & 0 & -0 & 0381 (7) & 0 & 0 & $	C(21)	0.1490 (4)	0.2957(3)	0.0608(2)	4.7 (2)
$\begin{array}{cccccc} C(22) & 0 & 1300 & (7) & 0 & 2220 & (3) & -0 & 0139 & (3) & (64 & (2)) \\ C(23) & -0 & 0045 & (5) & 0 & 2200 & (3) & -0 & 0157 & (3) & 7.5 & (2) \\ C(25) & -0 & 0834 & (5) & 0 & 3353 & (4) & 0 & 0175 & (3) & 7.8 & (3) \\ C(26) & 0 & 0428 & (5) & 0 & 3481 & (3) & 0 & 0563 & (3) & 64 & (2) \\ C(31) & 0 & 2524 & (5) & 0 & 2820 & (3) & 0 & 1959 & (2) & 4.9 & (2) \\ C(32) & 0 & 1122 & (6) & 0 & 2753 & (4) & 0 & 2056 & (3) & 8.3 & (3) \\ C(34) & 0 & 0777 & (6) & 0 & 2623 & (4) & 0 & 2056 & (3) & 8.8 & (3) \\ C(34) & 0 & 0777 & (6) & 0 & 2540 & (4) & 0 & 3176 & (3) & 8.6 & (3) \\ C(35) & 0 & 3132 & (7) & 0 & 2599 & (4) & 0 & 3095 & (3) & 9.2 & (3) \\ C(41) & 0 & 3364 & (5) & 0 & 4040 & (3) & 0 & 1245 & (3) & 5.1 & (2) \\ C(42) & 0 & 3554 & (6) & 0 & 4433 & (3) & 0 & 0700 & (3) & 7.3 & (2) \\ C(43) & 0 & 7740 & (7) & 0 & 5180 & (3) & 0 & 0720 & (3) & 8.2 & (3) \\ C(44) & 0 & 3765 & (7) & 0 & 5546 & (3) & 0 & 1832 & (4) & 11.1 & (4) \\ C(46) & 0 & 3381 & (8) & 0 & 4410 & (3) & 0 & 1812 & (3) & 9.1 & (3) \\ C(51) & 0 & 2712 & (5) & 0 & 1377 & (3) & -0 & 0569 & (3) & 5.1 & (2) \\ C(53) & 0 & 2382 & (6) & 0 & 1862 & (3) & -0 & 1075 & (3) & 8.2 & (3) \\ C(54) & 0 & -7777 & (7) & 0 & 0949 & (5) & -0 & 1843 & (4) & 9.5 & (3) \\ C(54) & 0 & -7777 & (7) & 0 & 0949 & (5) & -0 & 1843 & (4) & 9.5 & (3) \\ C(55) & 0 & 3131 & (7) & 0 & 0330 & (3) & 0 & 0693 & (3) & 8.2 & (3) \\ C(56) & 0 & 3134 & (6) & 0 & 0677 & (3) & -0 & 0717 & (3) & 7.0 & (2) \\ C(61) & 0 & -2156 & (6) & 0 & 0858 & (3) & 0 & 0693 & (3) & 8.2 & (3) \\ C(64) & 0 & -138 & (1) & -0 & 02395 & (5) & 0 & 1312 & (4) & 12.9 & (5) \\ C(65) & 0 & 0433 & (9) & 0 & 0133 & (6) & 0 & 1139 & (4) & 12.9 & (5) \\ C(65) & 0 & 0433 & (9) & 0 & 0133 & (6) & 0 & 1139 & (4) & 12.9 & (5) \\ C(66) & 0 & 0831 & (7) & 0 & 00756 & (4) & 0 & 0132 & (4) & 12.9 & (5) \\ C(66) & 0 & 0831 & (7) & 0 & 00733 & (6) & 0 & 1139 & (5) & 15.1 & (5) \\ C(66) & 0 & 0831 & (7) & 0 & 0776 & (4) & 0 & 0731 & (4) & 12.9 & (5) \\ C(66) & 0 & 0831 & (7) & 0 & 0776 & (6) & 0 & 0831 & (7) & 0 & 0776 \\ C(66) & 0 & 0831 & (7) &$	C(22)	0.1306 (4)	0.2323(3)	0.0249 (2)	4.9 (2)
$\begin{array}{ccccc} C(24) & -0.1046 (5) & 0.215 (3) & -0.0157 (3) & 7.5 (2) \\ C(25) & -0.0834 (5) & 0.3353 (4) & -0.0157 (3) & 7.8 (3) \\ C(26) & 0.0428 (5) & 0.3381 (3) & 0.0563 (3) & 6.4 (2) \\ C(31) & 0.2524 (5) & 0.2820 (3) & 0.1959 (2) & 4.9 (2) \\ C(32) & 0.1122 (6) & 0.2753 (4) & 0.2056 (3) & 8.3 (3) \\ C(33) & 0.0777 (6) & 0.2623 (4) & 0.23176 (3) & 8.6 (3) \\ C(34) & 0.1746 (8) & 0.2540 (4) & 0.3176 (3) & 8.6 (3) \\ C(35) & 0.3132 (7) & 0.2599 (4) & 0.3095 (3) & 9.2 (3) \\ C(36) & 0.3535 (6) & 0.2738 (3) & 0.2481 (3) & 7.0 (2) \\ C(41) & 0.364 (5) & 0.4040 (3) & 0.1245 (3) & 5.1 (2) \\ C(42) & 0.3554 (6) & 0.4433 (3) & 0.0700 (3) & 7.3 (2) \\ C(43) & 0.3740 (7) & 0.5180 (3) & 0.0720 (3) & 8.2 (3) \\ C(44) & 0.3765 (7) & 0.5546 (3) & 0.1825 (4) & 8.8 (3) \\ C(45) & 0.3381 (8) & 0.4410 (3) & 0.1812 (3) & 9.1 (3) \\ C(51) & 0.2712 (5) & 0.1377 (3) & -0.0569 (3) & 5.1 (2) \\ C(52) & 0.2356 (5) & 0.1862 (3) & -0.1705 (3) & 8.2 (3) \\ C(53) & 0.2382 (6) & 0.1649 (4) & -0.1705 (3) & 8.2 (3) \\ C(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ C(55) & 0.3183 (7) & 0.0473 (4) & -0.1349 (4) & 9.0 (3) \\ C(56) & 0.3131 (7) & 0.0330 (3) & 0.0893 (3) & 8.2 (3) \\ C(56) & 0.3131 (7) & 0.0330 (3) & 0.0893 (3) & 8.2 (3) \\ C(56) & 0.4333 (9) & 0.0133 (6) & 0.1312 (4) & 1.1 (4) \\ C(64) & 0.138 (1) & -0.0395 (5) & 0.1312 (4) & 1.2 (4) \\ C(64) & 0.138 (1) & -0.0395 (5) & 0.1312 (4) & 1.2 (4) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 1.51 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6)$	C(23)	0.0026 (5)	0.2200 (3)	-0.0130(3)	6.4 (2)
$\begin{array}{cccc} (25) & -0.0834 (5) & 0.215 (4) & 0.0157 (5) & 7.8 (3) \\ (2(25) & -0.0834 (5) & 0.3353 (4) & 0.0157 (5) & 7.8 (3) \\ (2(31) & 0.2524 (5) & 0.2820 (3) & 0.1959 (2) & 4.9 (2) \\ (2(31) & 0.2524 (5) & 0.2820 (3) & 0.1959 (2) & 4.9 (2) \\ (2(32) & 0.1122 (6) & 0.2753 (4) & 0.2056 (3) & 8.3 (3) \\ (2(33) & 0.0777 (6) & 0.2623 (4) & 0.2056 (3) & 8.4 (3) \\ (2(34) & 0.1746 (8) & 0.2599 (4) & 0.3095 (3) & 9.2 (3) \\ (2(35) & 0.3132 (7) & 0.2599 (4) & 0.3095 (3) & 9.2 (3) \\ (2(36) & 0.3535 (6) & 0.2738 (3) & 0.2481 (3) & 7.0 (2) \\ (2(41) & 0.3364 (5) & 0.4040 (3) & 0.1245 (3) & 5.1 (2) \\ (2(42) & 0.3554 (6) & 0.4433 (3) & 0.0700 (3) & 7.3 (2) \\ (2(43) & 0.3740 (7) & 0.5180 (3) & 0.0720 (3) & 8.2 (3) \\ (2(44) & 0.3765 (7) & 0.5546 (3) & 0.1825 (4) & 8.8 (3) \\ (2(45) & 0.3592 (9) & 0.5166 (4) & 0.1832 (4) & 11.1 (4) \\ (2(46) & 0.3381 (8) & 0.4410 (3) & 0.1812 (3) & 9.1 (3) \\ (2(5) & 0.2356 (5) & 0.1862 (3) & -0.1075 (3) & 6.4 (2) \\ (2(53) & 0.2356 (5) & 0.1862 (3) & -0.1705 (3) & 8.2 (3) \\ (2(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ (2(54) & 0.2777 (7) & 0.0473 (4) & -0.1349 (4) & 9.0 (3) \\ (2(55) & 0.3133 (7) & 0.0473 (4) & -0.1705 (3) & 8.2 (3) \\ (2(54) & 0.2777 (7) & 0.0939 (5) & -0.1843 (4) & 9.5 (3) \\ (2(55) & 0.3133 (7) & 0.0473 (4) & -0.1705 (3) & 8.2 (3) \\ (2(56) & 0.3131 (7) & 0.0330 (3) & 0.0893 (3) & 8.2 (3) \\ (2(56) & 0.3131 (7) & 0.0330 (3) & 0.0893 (3) & 8.2 (3) \\ (2(56) & 0.4333 (9) & 0.0133 (6) & 0.1312 (4) & 12.9 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.1312 (4) & 12.9 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.1312 (4) & 12.9 (5) \\ (5(5) & 0.0433 (9) & 0.0133 (6) & 0.1312 (4) & 12.9 (5) \\ (5(5) & 0.0433 (9) & 0.0133 (6) & 0.132 (5) & 1.51 (5) \\ (5(5) & 0.0433 (9) & 0.0133 (6) & 0.132 (5) & 1.51 (5) \\ (5(5) & 0.0433 (9) & 0.0133 (6) & 0.132 (5) & 1.51 (5) \\ (5(6) & 0.0433 (9) & 0.0133 (6) & 0.132 (5) & 1.51 (5) \\ (5(6) & 0.0433 (9) & 0.0133 (6) & 0.132 (6) & 0.139 (5) & 1.51 (5) \\ (5(6) & 0.0433 (9) & 0.0133 (6) & 0.132 (6) & 0.139 (5) & 1.51 (5) \\ (5(6) & 0.0433 (9) & 0.0133 (6) & 0.0$	C(24)	~ 0.1046 (5)	0.2715(4)	-0.0157(3)	7.5 (2)
$\begin{array}{c} C(25) & 0.034(5) & 0.338(3) & 0.0153(3) & 0.44(2) \\ C(26) & 0.042(5) & 0.348(3) & 0.0563(3) & 6.4(2) \\ C(31) & 0.2524(5) & 0.2820(3) & 0.1959(2) & 4.9(2) \\ C(32) & 0.1122(6) & 0.2753(4) & 0.2056(3) & 8.3(3) \\ C(33) & 0.0777(6) & 0.2623(4) & 0.2670(3) & 10.0(3) \\ C(34) & 0.1746(8) & 0.2623(4) & 0.3095(3) & 9.2(3) \\ C(35) & 0.3132(7) & 0.2599(4) & 0.3095(3) & 9.2(3) \\ C(36) & 0.3535(6) & 0.2738(3) & 0.2481(3) & 7.0(2) \\ C(41) & 0.3564(5) & 0.4040(3) & 0.1245(3) & 5.1(2) \\ C(42) & 0.3554(6) & 0.4433(3) & 0.0700(3) & 7.3(2) \\ C(43) & 0.3740(7) & 0.5180(3) & 0.0720(3) & 8.2(3) \\ C(44) & 0.3765(7) & 0.5546(3) & 0.1885(4) & 8.8(3) \\ C(45) & 0.3592(9) & 0.5166(4) & 0.1832(4) & 11.1(4) \\ C(46) & 0.3381(8) & 0.4410(3) & 0.1812(3) & 9.1(3) \\ C(51) & 0.2712(5) & 0.1377(3) & -0.0569(3) & 5.1(2) \\ C(52) & 0.2356(5) & 0.1862(3) & -0.1075(3) & 8.2(3) \\ C(54) & 0.2777(7) & 0.0949(5) & -0.1843(4) & 9.6(3) \\ C(55) & 0.3183(7) & 0.0473(4) & -0.1705(3) & 8.2(3) \\ C(54) & 0.2777(7) & 0.0949(5) & -0.1843(4) & 9.6(3) \\ C(55) & 0.3183(7) & 0.0473(4) & -0.1705(3) & 8.2(3) \\ C(56) & 0.3134(6) & 0.0677(3) & -0.0717(3) & 7.0(2) \\ C(61) & 0.2156(6) & 0.0858(3) & 0.0694(3) & 6.0(2) \\ C(62) & 0.3131(7) & 0.0330(3) & 0.0893(3) & 8.2(3) \\ C(64) & 0.138(1) & -0.0296(4) & 0.119(9(4) & 11.1(4) \\ C(44) & 0.138(1) & -0.0395(5) & 0.1312(4) & 12.9(5) \\ C(55) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(56) & 0.0433(9) & 0.0133(6) & 0.1139(5) & 15.1(5) \\ C(5$	C(25)	-0.0834(5)	0.3353 (4)	0.0175(3)	7.8 (3)
$\begin{array}{ccccc} (231) & 0.123(5) & 0.2820(3) & 0.1959(2) & 4.9(2) \\ (232) & 0.1122(6) & 0.2253(4) & 0.2056(3) & 8.3(3) \\ (233) & 0.0777(6) & 0.2623(4) & 0.2670(3) & 10.0(3) \\ (234) & 0.1746(8) & 0.2540(4) & 0.3176(3) & 8.6(3) \\ (235) & 0.3132(7) & 0.2599(4) & 0.3095(3) & 9.2(3) \\ (241) & 0.3364(5) & 0.4040(3) & 0.1245(3) & 5.1(2) \\ (241) & 0.3364(5) & 0.4040(3) & 0.1245(3) & 5.1(2) \\ (242) & 0.3554(6) & 0.4433(3) & 0.0700(3) & 7.3(2) \\ (243) & 0.3740(7) & 0.5180(3) & 0.0720(3) & 8.2(3) \\ (244) & 0.3765(7) & 0.5546(3) & 0.1285(4) & 8.8(3) \\ (244) & 0.3765(7) & 0.5546(3) & 0.1285(4) & 8.8(3) \\ (245) & 0.3592(9) & 0.5166(4) & 0.1812(3) & 9.1(3) \\ (251) & 0.2712(5) & 0.1377(3) & -0.0569(3) & 5.1(2) \\ (252) & 0.2356(5) & 0.1862(3) & -0.1705(3) & 8.2(3) \\ (253) & 0.2382(6) & 0.1862(3) & -0.1705(3) & 8.2(3) \\ (254) & 0.2777(7) & 0.0949(5) & -0.1843(4) & 9.5(3) \\ (255) & 0.3183(7) & 0.0473(4) & -0.1349(4) & 9.0(3) \\ (256) & 0.3134(6) & 0.0677(3) & -0.0717(3) & 7.0(22) \\ (261) & 0.2156(6) & 0.0858(3) & 0.0694(3) & 6.0(2) \\ (262) & 0.3131(7) & 0.0330(3) & 0.0893(3) & 8.2(3) \\ (263) & 0.2717(10) & -0.0296(4) & 0.1199(4) & 1.1(4) \\ (264) & 0.138(1) & -0.0395(5) & 0.1312(4) & 1.2.9(5) \\ (265) & 0.0433(9) & 0.0133(6) & 0.139(5) & 1.51(5) \\ (566) & 0.0433(9) & 0.0133(6) & 0.139(5) & 1.51(5) \\ (566) & 0.0861(77) & 0.0766(4) & 0.0821(4) & 1.07(3) \\ (566) & 0.0433(9) & 0.0133(6) & 0.139(5) & 1.51(5) \\ (566) & 0.0861(77) & 0.0766(4) & 0.0821(4) & 10.7(3) \\ (566) & 0.0801(77) & 0.0766(4) & 0.0821(4) & 10.7(3) \\ (566) & 0.0801(77) & 0.0766(6) & 0.0821(4) & 10.7(3) \\ (566) & 0.0801(77) & 0.0766(6) & 0.0821(4) & 10.7(3) \\ (566) & 0.0801(77) & 0.0766(4) & 0.0821(4) & 10.7(3) \\ (566) & 0.0801(77) & 0.0766(4) & 0.0821(4) & 10.7(3) \\ (566) & 0.0801(77) & 0.0766(4) & 0.0821(4) & 10.7(3) \\ (566) & 0.0801(77) & 0.0766(6) & 0.0821(4) & 10.7(4) \\ (566) & 0.0801(77) & 0.0766(6) & 0.0821(4) & 10.7(4) \\ (566) & 0.0801(77) & 0.0766(7) & 0.0717(7) & 0.7(7) \\ (566) & 0.0801(77) & 0.0766(7) & 0.0821(4) & 10.7(3) \\ (566) & 0.0801(77) & 0.0766(7) & 0.0821($	C(26)	0.0428(5)	0.3481(3)	0.0563 (3)	6.4 (2)
$\begin{array}{ccccc} (232) & 0 & 1122 \ (6) & 0 & 2253 \ (4) & 0 & 2056 \ (3) & 83 \ (3) \\ (233) & 0 & 0777 \ (6) & 0 & 2623 \ (4) & 0 & -2670 \ (3) & 10 & 0 \ (3) \\ (234) & 0 & 1746 \ (8) & 0 & 2540 \ (4) & 0 & -3176 \ (3) & 86 \ (3) \\ (235) & 0 & -3132 \ (7) & 0 & 2599 \ (4) & 0 & 3095 \ (3) & 92 \ (3) \\ (236) & 0 & -3353 \ (6) & 0 & 2738 \ (3) & 0 & -2481 \ (3) & 7 & 0 \ (2) \\ (241) & 0 & -3364 \ (5) & 0 & -4040 \ (3) & 0 & -1245 \ (3) & 5 & -1 \ (2) \\ (242) & 0 & -3554 \ (6) & 0 & -4433 \ (3) & 0 & 0700 \ (3) & 7 & -3 \ (2) \\ (243) & 0 & -3740 \ (7) & 0 & 5180 \ (3) & 0 & 0720 \ (3) & 82 \ (3) \\ (243) & 0 & -3740 \ (7) & 0 & 5180 \ (3) & 0 & 0720 \ (3) & 82 \ (3) \\ (243) & 0 & -3765 \ (7) & 0 & 5546 \ (4) & 0 & -1832 \ (4) & 184 \ (3) \\ (245) & 0 & -3592 \ (9) & 0 & 5166 \ (4) & 0 & -1812 \ (3) & 9 & -1 \ (3) \\ (246) & 0 & -3381 \ (8) & 0 & 4410 \ (3) & 0 & -1812 \ (3) & 9 & -1 \ (3) \\ (251) & 0 & -2712 \ (5) & 0 & -1377 \ (3) & -0 & 0569 \ (3) & 5 & -1 \ (2) \\ (252) & 0 & -2356 \ (5) & 0 & -1862 \ (3) & -0 & -1705 \ (3) & 64 \ (2) \\ (253) & 0 & -2382 \ (6) & 0 & -0473 \ (4) & -0 & -1705 \ (3) & 82 \ (3) \\ (254) & 0 & -2777 \ (7) & 0 & 0949 \ (5) & -0 & -1843 \ (4) & 9 & -5 \ (3) \\ (255) & 0 & -3183 \ (7) & 0 & 0473 \ (4) & -0 & -0717 \ (3) & 7 & 0 \ (2) \\ (264) & 0 & -3181 \ (7) & 0 & 0330 \ (3) & 0 & 0693 \ (3) & 82 \ (3) \\ (265) & 0 & -4338 \ (1) & -0 & 0395 \ (5) & 0 & -1312 \ (4) \ 12 & 9 \ (5) \\ (265) & 0 & -4338 \ (1) & -0 & 0395 \ (5) & 0 & -1312 \ (4) \ 12 & 9 \ (5) \\ (266) & 0 & 0433 \ (9) & 0 & 0133 \ (6) & 0 & 0139 \ (5) \ 15 1 \ (5) \ (56) \ 0 & -0433 \ (9) & 0 & 0133 \ (6) \ 0 & 0.139 \ (5) \ 15 1 \ (5) \ (56) \ 0 & -0433 \ (9) \ 0 & 0.133 \ (6) \ 0 & 0.139 \ (5) \ 15 1 \ (5) \ (56) \ 0 & -0433 \ (9) \ 0 & 0.133 \ (6) \ 0 & 0.139 \ (5) \ (5) \ 0 & -1312 \ (4) \ 10 & -7 \ (3) \ 0 \ (5) \ 0 & -1139 \ (5) \ 15 1 \ (5) \ (56) \ 0 & -0433 \ (9) \ 0 & 0.133 \ (6) \ 0 & 0.139 \ (5) \ 15 1 \ (5) \ (56) \ 0 & -0833 \ (6) \ 0 & 0.139 \ (5) \ 0 & -1139 \ (5) \ 15 1 \ (5) \ (56) \ 0 & -0833 \ (6) \ 0 & -0330 \ (6) $	C(31)	0.2524 (5)	0.2820 (3)	0.1959 (2)	4.9 (2)
$\begin{array}{cccccc} (23) & 0.172 (6) & 0.253 (4) & 0.2670 (3) & 0.03 (5) \\ (2(34) & 0.1746 (8) & 0.2540 (4) & 0.3176 (3) & 8-6 (3) \\ (2(35) & 0.3132 (7) & 0.2599 (4) & 0.3095 (3) & 9-2 (3) \\ (2(36) & 0.3535 (6) & 0.2738 (3) & 0.2481 (3) & 7-0 (2) \\ (2(41) & 0.3364 (5) & 0.4040 (3) & 0.1245 (3) & 5-1 (2) \\ (2(42) & 0.3554 (6) & 0.4433 (3) & 0.0700 (3) & 7-3 (2) \\ (2(43) & 0.3765 (7) & 0.5546 (3) & 0.1285 (4) & 8-8 (3) \\ (2(44) & 0.3765 (7) & 0.5546 (3) & 0.1285 (4) & 8-8 (3) \\ (2(45) & 0.3592 (9) & 0.5166 (4) & 0.1832 (4) & 11-1 (4) \\ (2(46) & 0.3381 (8) & 0.4410 (3) & 0.1812 (3) & 9-1 (3) \\ (2(51) & 0.2712 (5) & 0.1377 (3) & -0.0569 (3) & 5-1 (2) \\ (2(52) & 0.2356 (5) & 0.1682 (3) & -0.1075 (3) & 6-4 (2) \\ (2(53) & 0.2336 (6) & 0.1649 (4) & -0.1705 (3) & 8-2 (3) \\ (2(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9-5 (3) \\ (2(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9-5 (3) \\ (2(56) & 0.3138 (7) & 0.0473 (4) & -0.1349 (4) & 90 (3) \\ (2(56) & 0.3131 (7) & 0.0330 (3) & 0.0693 (3) & 8-2 (3) \\ (2(64) & 0.138 (1) & -0.0395 (5) & 0.1312 (4) & 12.9 (5) \\ (2(65) & 0.0433 (9) & 0.0133 (6) & 0.1139 (5) & 15-1 (5) \\ (2(65) & 0.0433 (9) & 0.0133 (6) & 0.1139 (5) & 15-1 (5) \\ (2(66) & 0.0801 (7) & 0.0766 (4) & 0.0892 (4) & 0.109 (4) \\ (0,7) (3) (7) & 0.0395 (5) & 0.1312 (4) & 12.9 (5) \\ (2(65) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 15-1 (5) \\ (2(66) & 0.0801 (7) & 0.0766 (4) & 0.0892 (14) & 10.7 (3) \\ (2(66) & 0.0801 (7) & 0.0766 (4) & 0.0892 (14) & 10.7 (3) \\ (2(66) & 0.0801 (7) & 0.0766 (4) & 0.0821 (4) & 10.7 (3) \\ (2(66) & 0.0801 (7) & 0.0766 (4) & 0.0821 (4) & 10.7 (3) \\ (2(65) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 15-1 (5) \\ (2(65) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 15-1 (5) \\ (2(66) & 0.0801 (7) & 0.0766 (4) & 0.0821 (4) & 10.7 (3) \\ (2(66) & 0.0801 (7) & 0.0766 (4) & 0.0821 (4) & 10.7 (3) \\ (2(66) & 0.0801 (7) & 0.0766 (6) & 0.0821 (4) & 10.7 (3) \\ (2(66) & 0.0801 (7) & 0.0766 (6) & 0.0821 (4) & 10.7 (3) \\ (2(66) & 0.0801 (7) & 0.0766 (6) & 0.0821 (4) & 10.7 (3) \\ (2(66) & 0.0801 (7) & 0.0766 (6) & 0.0821 (4)$	C(32)	0.2324(5) 0.1122(6)	0.2753 (4)	0.2056 (3)	8.3 (3)
$\begin{array}{ccccc} C(34) & 0 & 171 (6) & 0 & 2240 (4) & 0 & 3176 (3) & 86 (3) \\ C(35) & 0 & 3132 (7) & 0 & 2599 (4) & 0 & 3095 (3) & 9 & 2 (3) \\ C(36) & 0 & 3535 (6) & 0 & 2738 (3) & 0 & 2481 (3) & 7.0 (2) \\ C(41) & 0 & 3364 (5) & 0 & 4040 (3) & 0 & 1245 (3) & 5.1 (2) \\ C(42) & 0 & 3554 (6) & 0 & 4433 (3) & 0 & 0700 (3) & 7.3 (2) \\ C(43) & 0 & 3740 (7) & 0 & 5180 (3) & 0 & 0720 (3) & 8 & 2 (3) \\ C(44) & 0 & 3765 (7) & 0 & 5546 (3) & 0 & 1832 (4) & 18.1 \\ C(45) & 0 & 3592 (9) & 0 & 5166 (4) & 0 & 1832 (4) & 11.1 (4) \\ C(46) & 0 & 3381 (8) & 0 & 4410 (3) & 0 & 1812 (3) & 9 & 1 (3) \\ C(51) & 0 & 2712 (5) & 0 & 1377 (3) & -0 & 0569 (3) & 5.1 (2) \\ C(52) & 0 & 2356 (5) & 0 & 1862 (3) & -0 & 1075 (3) & 8 & 2 (3) \\ C(53) & 0 & 2382 (6) & 0 & 1649 (4) & -0 & 1705 (3) & 8 & 2 (3) \\ C(54) & 0 & 2777 (7) & 0 & 0949 (5) & -0 & 1843 (4) & 9 & 0 (3) \\ C(56) & 0 & 3134 (6) & 0 & 0677 (3) & -0 & 0717 (3) & 7.0 (2) \\ C(61) & 0 & 2156 (6) & 0 & 0858 (3) & 0 & 0693 (3) & 8 & 2 (3) \\ C(63) & 0 & 2717 (10) & -0 & 0330 (3) & 0 & 0893 (3) & 8 & 2 (3) \\ C(64) & 0 & -138 (1) & -0 & 0395 (5) & 0 & 1312 (4) & 12.9 (4) \\ C(64) & 0 & -138 (1) & -0 & 0395 (5) & 0 & 1312 (4) & 12.9 (5) \\ C(65) & 0 & 0433 (9) & 0 & 0133 (6) & 0 & 0139 (5) & 5.1 (5) \\ C(56) & 0 & 0433 (9) & 0 & 0133 (6) & 0 & 1139 (5) & 15.1 (5) \\ C(56) & 0 & 0433 (9) & 0 & 0133 (6) & 0 & 1139 (5) & 15.1 (5) \\ C(56) & 0 & 08081 (7) & 0 & 0766 (4) & 0 & 08921 (4) & 10.7 (4) \\ C(64) & 0 & 138 (1) & -0 & 07395 (5) & 0 & 1312 (4) & 12.9 (5) \\ C(56) & 0 & 0433 (9) & 0 & 0133 (6) & 0 & 1139 (5) & 15.1 (5) \\ C(56) & 0 & 08081 (7) & 0 & 0766 (4) & 0 & 0821 (4) & 10.7 (4) \\ C(56) & 0 & 08081 (7) & 0 & 0766 (4) & 0 & 0821 (4) & 10.7 (5) \\ C(56) & 0 & 08081 (7) & 0 & 0766 (4) & 0 & 0821 (4) & 10.7 (5) \\ C(56) & 0 & 08081 (7) & 0 & 0766 (4) & 0 & 0821 (4) & 10.7 (5) \\ C(56) & 0 & 08081 (7) & 0 & 0766 (4) & 0 & 0821 (4) & 10.7 (5) \\ C(56) & 0 & 08081 (7) & 0 & 0766 (4) & 0 & 0821 (4) & 10.7 (5) \\ C(56) & 0 & 0 & 0801 (7) & 0 & 0766 (4) & 0 & 0821 (4) & 10.7 (5) \\ C(56) & 0 & 0 & 0801 (7) & 0 & 076$	C(33)	0.0777(6)	0.2623 (4)	0.2670 (3)	10.0 (3)
$\begin{array}{ccccc} (25) & 0.1132 & (7) & 0.2599 & (4) & 0.3095 & (3) & 9-2 & (3) \\ (2(36) & 0.3335 & (6) & 0.2738 & (3) & 0.2481 & (3) & 7-0 & (2) \\ (2(41) & 0.3364 & (5) & 0.4040 & (3) & 0.1245 & (3) & 5-1 & (2) \\ (2(42) & 0.3554 & (6) & 0.4433 & (3) & 0.0700 & (3) & 7-3 & (2) \\ (2(43) & 0.3740 & (7) & 0.5180 & (3) & 0.0720 & (3) & 8-2 & (3) \\ (2(44) & 0.3765 & (7) & 0.5546 & (3) & 0.1285 & (4) & 8-8 & (3) \\ (2(45) & 0.3381 & (8) & 0.5166 & (4) & 0.1832 & (4) & 11-1 & (4) \\ (2(46) & 0.3381 & (8) & 0.5166 & (4) & 0.1832 & (4) & 11-1 & (4) \\ (2(46) & 0.3381 & (8) & 0.5166 & (4) & 0.1832 & (4) & 11-1 & (4) \\ (2(46) & 0.3381 & (8) & 0.4410 & (3) & 0.1812 & (3) & 9-1 & (3) \\ (2(51) & 0.2712 & (5) & 0.1377 & (3) & -0.0569 & (3) & 5-1 & (2) \\ (2(52) & 0.2356 & (5) & 0.1862 & (3) & -0.1705 & (3) & 8-2 & (3) \\ (2(53) & 0.2382 & (6) & 0.1649 & (4) & -0.1705 & (3) & 8-2 & (3) \\ (2(54) & 0.2777 & (7) & 0.0949 & (5) & -0.1843 & (4) & 9-5 & (3) \\ (2(55) & 0.3183 & (7) & 0.0473 & (4) & -0.1349 & (4) & 9-0 & (3) \\ (2(56) & 0.3134 & (6) & 0.0677 & (3) & -0.0717 & (3) & 7-0 & (2) \\ (2(51) & 0.2156 & (6) & 0.0858 & (3) & 0.0694 & (3) & 6-0 & (2) \\ (2(52) & 0.3131 & (7) & 0.0330 & (3) & 0.0893 & (3) & 8-2 & (3) \\ (2(63) & 0.2717 & (10) & -0.0296 & (4) & 0.1199 & (4) & 11-1 & (4) \\ (2(64) & 0.138 & (1) & -0.0395 & (5) & 0.1312 & (4) & 12.9 & (5) \\ (2(55) & 0.0433 & (9) & 0.0133 & (6) & 0.139 & (5) & 15-1 & (5) \\ (5(6) & 0.0433 & (9) & 0.0133 & (6) & 0.139 & (5) & 15-1 & (5) \\ (5(6) & 0.0433 & (9) & 0.0133 & (6) & 0.139 & (5) & 15-1 & (5) \\ (5(6) & 0.0433 & (9) & 0.0133 & (6) & 0.021 & (6) & 0.021 & (6) & 0.021 & (6) & 0.021 \\ (5(6) & 0.0433 & (9) & 0.0133 & (6) & 0.021 & (4) & 10-7 & (3) \\ (5(6) & 0.0433 & (9) & 0.0133 & (6) & 0.0321 & (4) & 10-7 & (6) \\ (5(6) & 0.0801 & (7) & 0.0766 & (4) & 0.0821 & (4) & 10-7 & (6) \\ (5(6) & 0.0801 & (7) & 0.0766 & (4) & 0.0821 & (4) & 10-7 & (6) \\ (5(6) & 0.0801 & (7) & 0.0766 & (6) & 0.0821 & (4) & 10-7 & (6) \\ (5(6) & 0.0801 & (7) & 0.0766 & (4) & 0.0821 & (4) & 10-7 & (6) \\ (5(6) & 0.0801 & (7) & 0.$	C(34)	0.1746 (8)	0.2540(4)	0.3176 (3)	8.6 (3)
$\begin{array}{ccccc} (236) & 0.1325 (4) & 0.2238 (3) & 0.2481 (3) & 7.0 (2) \\ (2(41) & 0.3364 (5) & 0.4040 (3) & 0.1245 (3) & 5.1 (2) \\ (2(42) & 0.3554 (6) & 0.4433 (3) & 0.0700 (3) & 7.3 (2) \\ (2(43) & 0.3765 (7) & 0.5546 (3) & 0.1285 (4) & 8.8 (3) \\ (2(44) & 0.3765 (7) & 0.5546 (3) & 0.1285 (4) & 8.8 (3) \\ (2(45) & 0.3592 (9) & 0.5166 (4) & 0.1832 (4) & 11.1 (4) \\ (2(46) & 0.3381 (8) & 0.4410 (3) & 0.1812 (3) & 9.1 (3) \\ (2(51) & 0.2712 (5) & 0.1377 (3) & -0.0569 (3) & 5.1 (2) \\ (2(52) & 0.2356 (5) & 0.1682 (3) & -0.1075 (3) & 6.4 (2) \\ (2(53) & 0.2336 (6) & 0.1649 (4) & -0.1705 (3) & 8.2 (3) \\ (2(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ (2(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ (2(56) & 0.3138 (7) & 0.0477 (4) & -0.1349 (4) & 9.0 (3) \\ (2(56) & 0.3131 (7) & 0.0330 (3) & 0.0693 (3) & 8.2 (3) \\ (2(63) & 0.2717 (10) & -0.0296 (4) & 0.1199 (4) & 11.1 (4) \\ (2(64) & 0.138 (1) & -0.0395 (5) & 0.1312 (4) & 12.9 (5) \\ (2(55) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 15.1 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0281 (4) & 0.7 (3) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 15.1 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 15.1 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 15.1 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 15.1 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 0.1139 (5) & 15.1 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 0.1139 (5) & 15.1 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 0.1139 (5) & 15.1 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.021 (4) & 0.07 (6) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.021 (4) & 0.07 (6) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.021 (4) & 0.07 (6) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0321 (4) & 0.07 (6) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 0.511 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 0.511 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 0.511 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 0.511 (5) \\ (2(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 0.511 ($	C(35)	0.3132 (7)	0.2590 (4)	0.3095 (3)	0.2 (3)
$\begin{array}{ccccc} C(41) & 0 & 2355 (6) & 0 & 2456 (3) & 0 & 2451 (3) & 0 & 1245 (3) \\ C(42) & 0 & 3554 (6) & 0 & 4433 (3) & 0 & 0700 (3) & 7 & 3 (2) \\ C(43) & 0 & 3740 (7) & 0 & 5180 (3) & 0 & 0720 (3) & 8 & 2 & (3) \\ C(44) & 0 & 3765 (7) & 0 & 5546 (3) & 0 & 1385 (4) & 88 & (3) \\ C(45) & 0 & 3592 (9) & 0 & 5166 (4) & 0 & 1832 (4) & 11 & 1 & (4) \\ C(46) & 0 & 3381 (8) & 0 & 4410 (3) & 0 & 1812 (3) & 9 & 1 & (3) \\ C(51) & 0 & 2712 (5) & 0 & 1377 (3) & -0 & 0569 (3) & 5 & 1 & (2) \\ C(52) & 0 & 2356 (5) & 0 & 1862 (3) & -0 & 1075 (3) & 8 & 2 & (3) \\ C(53) & 0 & 2382 (6) & 0 & 1649 (4) & -0 & 1705 (3) & 8 & 2 & (3) \\ C(54) & 0 & 2777 (7) & 0 & 0949 (5) & -0 & 1843 (4) & 9 & 0 & (3) \\ C(56) & 0 & 3134 (6) & 0 & 0677 (3) & -0 & 0717 (3) & 7 & 0 & (2) \\ C(61) & 0 & 2156 (6) & 0 & 0858 (3) & 0 & 06893 (3) & 8 & 2 & (3) \\ C(63) & 0 & 2717 (10) & -0 & 02396 (4) & 0 & 119 (4) & 11 & 1 & (4) \\ C(64) & 0 & 138 (1) & -0 & 0330 (5) & 0 & 1312 (4) & 12 & 9 & (5) \\ C(65) & 0 & 0433 (9) & 0 & 0133 (6) & 0 & 1139 (5) & 15 & 1 & (5) \\ C(65) & 0 & 0433 (9) & 0 & 0133 (6) & 0 & 1139 (5) & 15 & 1 & (5) \\ \end{array}$	C(36)	0.3535 (6)	0.2738(3)	0.2481(3)	7.0 (2)
$\begin{array}{cccc} C(42) & 0.3554 (c) & 0.4433 (3) & 0.0700 (3) & 7.3 (2) \\ C(43) & 0.3740 (7) & 0.5180 (3) & 0.0720 (3) & 8.2 (3) \\ C(44) & 0.3765 (7) & 0.5546 (3) & 0.1285 (4) & 8.8 (3) \\ C(45) & 0.3592 (9) & 0.5166 (4) & 0.1832 (4) & 11.1 (4) \\ C(46) & 0.3381 (8) & 0.4410 (3) & 0.1812 (3) & 9.1 (3) \\ C(51) & 0.2712 (5) & 0.1377 (3) & -0.0569 (3) & 5.1 (2) \\ C(52) & 0.2356 (5) & 0.1862 (3) & -0.1705 (3) & 8.2 (3) \\ C(53) & 0.2382 (6) & 0.1649 (4) & -0.1705 (3) & 8.2 (3) \\ C(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9.5 (3) \\ C(55) & 0.3183 (7) & 0.0473 (4) & -0.1349 (4) & 9.0 (3) \\ C(56) & 0.3134 (6) & 0.0677 (3) & -0.0717 (3) & 7.0 (2) \\ C(61) & 0.2156 (6) & 0.0858 (3) & 0.0694 (3) & 6.0 (2) \\ C(62) & 0.3131 (7) & 0.0330 (3) & 0.0893 (3) & 8.2 (3) \\ C(64) & 0.138 (1) & -0.0395 (5) & 0.1312 (4) & 12.9 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.139 (5) & 15.1 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 15.1 (5) \\ C(56) & 0.0433 (9) & 0.0133 (6) & 0.0139 (5) & 15.1 (5) \\ \end{array}$	C(41)	0.3364(5)	0.4040 (3)	0.1245(3)	5.1 (2)
$\begin{array}{ccccc} (243) & 0.374 \ (6) & 0.413 \ (5) & 0.0720 \ (3) & 82 \ (3) \\ (243) & 0.3765 \ (7) & 0.5546 \ (3) & 0.0720 \ (3) & 82 \ (3) \\ (245) & 0.3592 \ (9) & 0.5166 \ (4) & 0.1832 \ (4) & 11.1 \ (4) \\ (246) & 0.3381 \ (8) & 0.4410 \ (3) & 0.1812 \ (3) & 9.1 \ (3) \\ (245) & 0.2356 \ (5) & 0.1377 \ (3) & -0.0569 \ (3) & 5.1 \ (2) \\ (252) & 0.2356 \ (5) & 0.1649 \ (4) & -0.1705 \ (3) & 6.4 \ (2) \\ (252) & 0.2356 \ (5) & 0.1649 \ (4) & -0.1705 \ (3) & 6.4 \ (2) \\ (253) & 0.2382 \ (6) & 0.1649 \ (4) & -0.1705 \ (3) & 8.2 \ (3) \\ (254) & 0.2777 \ (7) & 0.0949 \ (5) & -0.1843 \ (4) & 9.5 \ (3) \\ (255) & 0.3183 \ (7) & 0.0473 \ (4) & -0.1349 \ (4) & 9.0 \ (3) \\ (256) & 0.3134 \ (6) & 0.0677 \ (3) & -0.0717 \ (3) & 6.0 \ (2) \\ (261) & 0.2156 \ (6) & 0.0858 \ (3) & 0.0694 \ (3) & 6.0 \ (2) \\ (262) & 0.3131 \ (7) & 0.0330 \ (3) & 0.0893 \ (3) & 8.2 \ (3) \\ (264) & 0.138 \ (1) & -0.0395 \ (5) & 0.1312 \ (4) & 12.9 \ (5) \\ (265) & 0.0433 \ (9) & 0.0133 \ (6) & 0.0312 \ (4) & 12.9 \ (5) \\ (265) & 0.0433 \ (9) & 0.0133 \ (6) & 0.0211 \ (4) & 10.7 \ (3) \\ (56) & 0.0433 \ (9) & 0.0133 \ (6) & 0.0211 \ (4) \ (10.7) \ (5)$	C(42)	0.3554 (6)	0.4433 (3)	0.0700 (3)	7.3 (2)
$\begin{array}{cccc} C(44) & 0.7365 (7) & 0.5546 (3) & 0.128 (4) & 88 (3) \\ C(45) & 0.3592 (9) & 0.5166 (4) & 0.1832 (4) & 11\cdot1 (4) \\ C(46) & 0.3381 (8) & 0.4410 (3) & 0.1812 (3) & 9\cdot1 (3) \\ C(51) & 0.2712 (5) & 0.1377 (3) & -0.0569 (3) & 5\cdot1 (2) \\ C(52) & 0.2356 (5) & 0.1862 (3) & -0.1075 (3) & 6.4 (2) \\ C(53) & 0.2382 (6) & 0.1649 (4) & -0.1705 (3) & 8.2 (3) \\ C(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9\cdot5 (3) \\ C(55) & 0.3183 (7) & 0.0473 (4) & -0.1349 (4) & 9\cdot0 (3) \\ C(56) & 0.3134 (6) & 0.0677 (3) & -0.0717 (3) & 7\cdot0 (2) \\ C(61) & 0.2156 (6) & 0.0858 (3) & 0.0694 (3) & 6\cdot0 (2) \\ C(62) & 0.3131 (7) & 0.0330 (3) & 0.0893 (3) & 8\cdot2 (3) \\ C(64) & 0.138 (1) & -0.0395 (5) & 0.1312 (4) & 12.9 (5) \\ C(65) & 0.0433 (9) & 0.0133 (6) & 0.1139 (5) & 15\cdot1 (5) \\ C(66) & 0.0858 (17) & 0.0766 (4) & 0.0821 (4) & 10.7 (4) \\ \end{array}$	C(43)	0.3740 (7)	0.5180 (3)	0.0720 (3)	8.2 (3)
$\begin{array}{cccc} (45) & 0.1352 (4) & 0.95166 (4) & 0.1832 (4) & 11-1 (4) \\ (2(46) & 0.3381 (8) & 0.4410 (3) & 0.1812 (3) & 9-1 (3) \\ (2(51) & 0.2712 (5) & 0.1377 (3) & -0.0569 (3) & 5-1 (2) \\ (2(52) & 0.2356 (5) & 0.1862 (3) & -0.1075 (3) & 6-4 (2) \\ (2(53) & 0.2382 (6) & 0.1649 (4) & -0.1705 (3) & 8-2 (3) \\ (2(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9-5 (3) \\ (2(55) & 0.3183 (7) & 0.0473 (4) & -0.1349 (4) & 9-0 (3) \\ (2(56) & 0.3134 (6) & 0.0677 (3) & -0.0717 (3) & 7.0 (2) \\ (2(61) & 0.2156 (6) & 0.0858 (3) & 0.0694 (3) & 6-0 (2) \\ (2(62) & 0.3131 (7) & 0.0330 (3) & 0.0893 (3) & 8-2 (3) \\ (2(64) & 0.138 (1) & -0.0296 (4) & 0.1199 (4) & 11-1 (4) \\ (2(64) & 0.138 (1) & -0.0395 (5) & 0.1312 (4) & 12-9 (5) \\ (2(65) & 0.0433 (9) & 0.0133 (6) & 0.1139 (5) & 15-1 (5) \\ (2(66) & 0.0801 (7) & 0.0766 (4) & 0.0821 (4) & 10-7 (3) \\ \end{array}$	C(44)	0.3765 (7)	0.5546 (3)	0.1285 (4)	8.8 (3)
$\begin{array}{ccccc} C(46) & 0 & 3381 (8) & 0 & 4410 (3) & 0 & 1812 (3) & 9 & 1 (3) \\ C(51) & 0 & 2712 (5) & 0 & 1377 (3) & -0 & 0569 (3) & 5 & 1 (2) \\ C(52) & 0 & 2356 (5) & 0 & 1862 (3) & -0 & 1075 (3) & 64 (2) \\ C(53) & 0 & 2382 (6) & 0 & 1649 (4) & -0 & 1705 (3) & 82 (3) \\ C(54) & 0 & 2777 (7) & 0 & 0949 (5) & -0 & 1843 (4) & 9 & 5 (3) \\ C(55) & 0 & 3183 (7) & 0 & 0473 (4) & -0 & 1349 (4) & 90 (3) \\ C(56) & 0 & 3134 (6) & 0 & 0677 (3) & -0 & 0717 (3) & 70 (2) \\ C(61) & 0 & 2156 (6) & 0 & 0858 (3) & 0 & 0694 (3) & 6 & 0 (2) \\ C(62) & 0 & 3131 (7) & 0 & 0330 (3) & 0 & 0893 (3) & 82 & 2 (3) \\ C(63) & 0 & 2717 (10) & -0 & 0296 (4) & 0 & 1199 (4) & 11 & 1 (4) \\ C(64) & 0 & 138 (1) & -0 & 0395 (5) & 0 & 1312 (4) & 12 & 9 (5) \\ C(65) & 0 & 0 & 0033 (6) & 0 & 0133 (6) & 0 & 0139 (5) & 15 & 1 (5) \\ C(65) & 0 & 0 & 0031 (7) & 0 & 0766 (4) & 0 & 0821 (4) & 10 & 7 (3) \\ \end{array}$	C(45)	0.3597 (9)	0.5166 (4)	0.1832(4)	11.1 (4)
$\begin{array}{cccccc} C(51) & 0 & 2511 (5) & 0 & 4110 (5) & 0 & 1012 (5) & 0 & 11 (5) \\ C(51) & 0 & 2712 (5) & 0 & 1377 (3) & -0 & 0569 (3) & 51 (2) \\ C(52) & 0 & 2356 (5) & 0 & 1862 (3) & -0 & 1075 (3) & 8 & 2 (3) \\ C(53) & 0 & 2382 (6) & 0 & 1649 (4) & -0 & 1705 (3) & 8 & 2 (3) \\ C(54) & 0 & 2777 (7) & 0 & 0949 (5) & -0 & 1843 (4) & 9 & 5 (3) \\ C(55) & 0 & 3183 (7) & 0 & 0473 (4) & -0 & 1349 (4) & 90 & (3) \\ C(56) & 0 & 3134 (6) & 0 & 0677 (3) & -0 & 0717 (3) & 7 & 0 (2) \\ C(61) & 0 & 2156 (6) & 0 & 0858 (3) & 0 & 0694 (3) & 60 (2) \\ C(62) & 0 & 3131 (7) & -0 & 0330 (3) & 0 & 0893 (3) & 8 & 2 (3) \\ C(63) & 0 & 2717 (10) & -0 & 0296 (4) & 0 & 1199 (4) & 11 & 1 \\ C(64) & 0 & 138 (1) & -0 & 0395 (5) & 0 & 1312 (4) & 12 & 9 (5) \\ C(65) & 0 & 0433 (9) & 0 & 0133 (6) & 0 & 1139 (5) & 15 & 1 (5) \\ C(66) & 0 & 0808 (7) & 0 & 0766 (4) & 0 & 0821 (4) & 10 & 7 (3) \\ \end{array}$	C(46)	0.3381(8)	0.4410(3)	0.1812(3)	9.1 (3)
$\begin{array}{ccccc} C(52) & 0 & 2356 (5) & 0 & 1862 (3) & -0 & 1075 (3) & 64 (2) \\ C(53) & 0 & 2382 (6) & 0 & 1862 (3) & -0 & 1075 (3) & 8 & 2 (3) \\ C(54) & 0 & 2777 (7) & 0 & 0949 (5) & -0 & 1843 (4) & 9 & 5 (3) \\ C(55) & 0 & 3183 (7) & 0 & 0473 (4) & -0 & 1349 (4) & 90 (3) \\ C(56) & 0 & 3134 (6) & 0 & 0677 (3) & -0 & 0717 (3) & 7 & 0 (2) \\ C(61) & 0 & 2156 (6) & 0 & 0858 (3) & 0 & 0694 (3) & 60 (2) \\ C(62) & 0 & 3131 (7) & 0 & 0330 (3) & 0 & 0893 (3) & 8 & 2 (3) \\ C(63) & 0 & 2717 (10) & -0 & 0296 (4) & 0 & 1199 (4) & 11 & 14 \\ C(64) & 0 & 138 (1) & -0 & 0335 (5) & 0 & 1312 (4) & 12 & 9 (5) \\ C(65) & 0 & 0 & 0331 (7) & 0 & 0333 (6) & 0 & 1139 (5) & 15 & 1 (5) \\ C(65) & 0 & 0 & 0331 (7) & 0 & 0766 (4) & 0 & 0821 (4) & 10 & 7 (3) \\ \end{array}$	C(51)	0.2712(5)	0.1377(3)	-0.0569(3)	5.1 (2)
$\begin{array}{ccccc} (53) & 0-2382 \ (6) & 0-1649 \ (4) & -0-1705 \ (3) & 8-2 \ (3) \\ (54) & 0-2777 \ (7) & 0-0949 \ (5) & -0-1843 \ (4) & 9-5 \ (3) \\ (55) & 0-3183 \ (7) & 0-0473 \ (4) & -0-1349 \ (4) & 9-0 \ (3) \\ (56) & 0-3134 \ (6) & 0-0677 \ (3) & -0-0717 \ (3) & 7-0 \ (2) \\ (56) & 0-2156 \ (6) & 0-0858 \ (3) & 0-0694 \ (3) & 6-0 \ (2) \\ (62) & 0-3131 \ (7) & 0-0330 \ (3) & 0-0893 \ (3) & 8-2 \ (3) \\ (63) & 0-2717 \ (10) & -0-0296 \ (4) & 0-1199 \ (4) & 11-1 \ (4) \\ (64) & 0-138 \ (1) & -0-0395 \ (5) & 0-1312 \ (4) & 12-9 \ (5) \\ (56) & 0-0433 \ (9) & 0-0133 \ (6) & 0-0139 \ (5) & 15-1 \ (5) \\ (56) & 0-0831 \ (7) & 0-0766 \ (4) & 0.0821 \ (4) & 10-7 \ (3) \\ \end{array}$	C(52)	0.2356(5)	0.1867(3)	-0.1075(3)	6.4 (2)
$\begin{array}{ccccc} C(54) & 0.2777 (7) & 0.0949 (5) & -0.1843 (4) & 9-5 (3) \\ C(55) & 0.3183 (7) & 0.0473 (4) & -0.1349 (4) & 9-0 (3) \\ C(56) & 0.3134 (6) & 0.0677 (3) & -0.0717 (3) & 7-0 (2) \\ C(61) & 0.2156 (6) & 0.0858 (3) & 0.0694 (3) & 6-0 (2) \\ C(62) & 0.3131 (7) & 0.0330 (3) & 0.0893 (3) & 8-2 (3) \\ C(63) & 0.2717 (10) & -0.0296 (4) & 0.1199 (4) & 11\cdot1 (4) \\ C(64) & 0.138 (1) & -0.0395 (5) & 0.1312 (4) & 12.9 (5) \\ C(65) & 0.0433 (9) & 0.0133 (6) & 0.1139 (5) & 15\cdot1 (5) \\ C(66) & 0.0808 (7) & 0.0766 (4) & 0.0821 (4) & 10.7 (3) \\ \end{array}$	C(53)	0.2382 (6)	0.1649 (4)	-0.1705(3)	8.2 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(54)	0.2777(7)	0.0949 (5)	-0.1843(4)	9.5 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(55)	0.3183(7)	0.0473(4)	-0.1349(4)	9.0 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(56)	0.3134(6)	0.0677(3)	-0.0717(3)	7.0 (2)
$\begin{array}{cccc} C(62) & 0.133 & (7) & 0.0330 & (3) & 0.0893 & (3) & 8.2 & (3) \\ C(63) & 0.2717 & (10) & -0.0296 & (4) & 0.1199 & (4) & 11.1 & (4) \\ C(64) & 0.138 & (1) & -0.0395 & (5) & 0.1312 & (4) & 12.9 & (5) \\ C(65) & 0.0433 & (9) & 0.0133 & (6) & 0.1139 & (5) & 15.1 & (5) \\ C(66) & 0.0803 & (7) & 0.0766 & (4) & 0.0821 & (4) & 10.7 & (3) \\ \end{array}$	C(61)	0.2156 (6)	0.0858 (3)	0.0694 (3)	6.0 (2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(62)	0.3131(7)	0.0330 (3)	0.0893 (3)	8.2 (3)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(63)	0.2717(10)	-0.0296 (4)	0.1199 (4)	11.1 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(64)	0.138(1)	-0.0395 (5)	0.1312(4)	12.9 (5)
C(66) 0.0801 (7) 0.0766 (4) 0.0821 (4) 10.7 (3)	C(65)	0.0433 (9)	0.0133(6)	0.1139(5)	15.1 (5)
	C(66)	0.0801 (7)	0.0766 (4)	0.0821(4)	10.7 (3)



Fig. 1. Geometry and crystallographic numbering scheme for the complex  $\{trans-Br(CO)_2[o-Ph(PPh_2)_2]W(C \equiv R)\}$ . R =C<sub>6</sub>H₄Me-4.

e.s.d.'s in parentheses

	A (85 (1))		
W(I) - Br(I)	2.675(1)	W(1)—C(3)	1.798 (5)
W(1)-P(1)	2.512 (1)	C(1)—O(1)	1.128 (6)
W(1)-P(2)	2.528 (2)	C(3)—C(4)	1.449 (7)
W(1)-C(1)	2.012 (5)	P(1)-C(21)	1.834 (4)
		C(21)—C(22)	1.381 (7)
C(3)-W(1)-C(2)	88.0 (2)	P(1) - W(1) - P(2)	78.0 (1)
C(3) - W(1) - C(1)	86.1 (2)	Br(1) - W(1) - C(3)	173.4 (2)
C(1) - W(1) - C(2)	93-3 (2)	Br(1) - W(1) - C(2)	86.9 (1)
C(3)—W(1)—P(2)	100.2 (2)	Br(1) - W(1) - C(1)	89.9 (1)
C(2)-W(1)-P(2)	95·1 (2)	Br(1) - W(1) - P(2)	84.4 (1)
C(1) - W(1) - P(2)	169.6 (2)	Br(1) - W(1) - P(1)	88.7 (1)
C(3) - W(1) - P(1)	96.8 (2)	W(1) - C(1) - O(1)	176.2 (5)
P(1) - W(1) - C(2)	172-2 (2)	W(1)-C(2)-O(2)	177.5 (5)
P(1) - W(1) - C(1)	93.2 (2)	W(1)-C(3)-C(4)	171-5 (4)

 $[93\cdot3(2)^{\circ}]$ , and considerably greater than that found between the two P atoms of the chelating ligand [78·0 (1)°].

The W(1)—P(2) bond makes an angle of  $21.26(1)^{\circ}$ with the plane formed by W(1), P(1) and C(21). The plane containing the C(24), C(25) and C(26) atoms is almost perpendicular to the p-tolyl ring [dihedral angle 81.44 (1)°] and forms a dihedral angle of  $16.8 (1)^{\circ}$  with the plane formed by the W(1), P(21) and C(21) atoms.

We thank the Spanish CAICYT for financial support and the Spanish Ministerio de Educacion y Ciencia for a fellowship (to MGS).

### References

- BIRDWHISTELL, K. R., NIETER BURGMAYER, S. J. & TEMPLETON, J. L. (1983). J. Am. Chem. Soc. 105, 7789-7790.
- CARRIEDO, G. A., RIERA, J. M. & SANCHEZ, M. G. (1988). Unpublished.
- CASEY, C. P., BURKHARDT, T. J., BUNNELL, C. A. & CALABRESE, J. C. (1977). J. Am. Chem. Soc. 99, 2127-2134.
- CASEY, C. P., POLICHNOWSKI, S. W., TUINSTRA, H. E., ALBIN, L. D. & CALABRESE, J. C. (1978). Inorg. Chem. 17, 3045-3049.
- FISCHER, E. O., FRIEDRICH, P., LINDNER, T. L., NEUGEBAUER, D., KREISSL, F. R., UEDELHOVEN, W., DAO, N. Q. & HUTTNER, G. (1983). J. Organomet. Chem. 247, 239-246.
- FISCHER, E. O., GAMMEL, F. J. & NEUGEBAUER, D. (1980). Chem. Ber. 113, 1010-1019.
- FISCHER, E. O., LINDNER, T. L., HUTTNER, G., FRIEDRICH, P., KREISSL, F. R. & BESENHARD J. O. (1977). Chem. Ber. 110, 3397-3404.
- HUTTNER, G., LORENZ, H. & GARTZKE, W. (1974). Angew. Chem. 86, 667-669.
- International Tables for X-ray Crystallography (1974). Vol. IV, pp. 99-101 and 149-150. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
- MCDERMOTT, G. A., DORRIES, A. M. & MAYR, A. (1987). Organometallics, 6, 925-931.
- MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data. Univs. of York, England and Louvain, Belgium.
- MOTHERWELL, W. D. S. (1976). PLUTO. Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

Nardelli, M. (1983). Comput. Chem. 7, 95–98. NEUGEBAUER, D., FISCHER, E. O., DAO, N. Q. & SCHUBERT, U. (1978). J. Organomet. Chem. 153, C41–C44.

SHELDRICK, G. M. (1976). SHELX76. Program for crystal structure determination. Univ. of Cambridge, England.
WALKER, N. & STUART, D. (1983). Acta Cryst. A39, 158-166.

Acta Cryst. (1990). C46, 584-587

# Structure of 2-Adamantylammonium Trichloro(ethylamine)platinate(II)

BY FERNANDE D. ROCHON AND ROBERT MELANSON

Département de Chimie, Université du Québec à Montréal, CP 8888, succ.A, Montréal, Québec, Canada H3C 3P8

AND MONIQUE DOYON AND IAN S. BUTLER

Department of Chemistry, McGill University, 801 Sherbrooke Street West, Montreal, Quebec, Canada H3A 2K6

(Received 26 April 1989; accepted 19 July 1989)

Abstract. 2-Adamantylammonium trichloro(ethylamine)platinate(II),  $[C_{10}H_{18}N]$ [PtCl<sub>3</sub>(C<sub>2</sub>H<sub>7</sub>N)],  $M_r =$ 498·79, monoclinic,  $P2_1/n$ , with a = 12.401 (10), b =6·859 (15), c = 20.199 (15) Å,  $\beta = 100.72$  (6)°, V =1688 (2) Å<sup>3</sup>, Z = 4,  $D_x = 1.962$  Mg m<sup>-3</sup>,  $\lambda$ (Mo K $\alpha$ ) = 0.71069 Å,  $\mu = 8.86$  mm<sup>-1</sup>, F(000) = 960, T =

Example 1 and 200 a

**Introduction.** The cage molecule 1-adamantanamine  $(C_{10}H_{15}NH_2)$  has been the subject of some attention lately, chiefly because of its antiviral (Hay, Wolstenholme, Shehel & Smith, 1985; Widell, Hansson, Oeberg & Nordenfelt, 1986; Fletcher, Hirschfield & Forbes, 1965) and antitumor activity (Ho, Hakala & Zakrsewski, 1972). Moreover, platinum(II) complexes containing the related 1,2-adamantanediamine ligand (Shionogi & Co. Ltd, 1983) apparently possess antitumor activity comparable to that of the commercially licensed drug cisplatin, cis-Pt(NH<sub>3</sub>)<sub>2</sub>Cl<sub>2</sub> (Rosenberg, van Camp, Trosko & Mansour, 1969). A convenient synthetic route to mixed-amine platinum(II) complexes of the type  $cis-Pt(L)(L')Cl_2$  (L,L' = methylamine, ethylamine, cyclobutylamine, cyclopentylamine etc.) has been developed recently and we felt that it would be worthwhile attempting to synthesize similar complexes containing various adamantanamine ligands. It is our ultimate hope that such synthetic combina-

0108-2701/90/040584-04\$03.00

tions might result in compounds with enhanced antitumor activity and reduced toxicity.

Reaction of  $K[Pt(EtNH_2)Cl_3]$  with 2-adamantanamine (2-adam) does apparently yield the mixedamine complex  $[Pt(EtNH_2)(2-adam)Cl_2]$  but, upon treatment with dilute HCl during the work-up of the product, yellow crystals of the  $[2-adamH]^+$ .- $[Pt(EtNH_2)Cl_3]^-$  salt are also produced. This complex is probably the result of displacement of the coordinated adamantanamine ligand by Cl<sup>-</sup> and subsequent quarternization of the amine group. We have now characterized the ionic compound by X-ray diffraction and report the results here.

The crystal structure was also of interest to us in view of our ongoing work on order-disorder phase transitions in organic molecular crystals, including substituted adamantane derivatives (Bélanger-Gariépy, Brisse, Harvey, Butler & Gilson, 1987, 1990; Harvey, Gilson & Butler, 1987). The roomtemperature phases in such 'plastic crystalline' materials are usually disordered and the phase transitions take place at low temperatures or under high external pressures. The transitions are exothermic and consequently the materials are beginning to be exploited in various passive heat-storage systems. In the case of our complex, we anticipated that the adamantylammonium ion might be disordered at room temperature.

**Experimental.** 1 mmol of K[Pt(EtNH<sub>2</sub>)Cl<sub>3</sub>], synthesized by the method already reported (Rochon, Melanson & Doyon, 1987) and 1·1 mmol of 2adamantanamine were stirred together in a minimum quantity of water for 90 min. Then 0.1M HCl (10 ml) was added to the solution and the mixture was stirred for a further 10 min. The resulting yellow

© 1990 International Union of Crystallography