Table 2. *Bond distances (Å) and angles (°) with e.s.d.'s in parentheses*

| | | | | |
|---|---|---|---|---|
| O(1)—C(2) | 1·336 (3) | C(8)—C(9) | 1·546 (6) |
| O(1)—C(15) | 1·473 (5) | C(9)—C(91) | 1·534 (6) |
| C(2)—O(21) | 1·209 (4) | C(9)—C(10) | 1·526 (6) |
| C(2)—C(3) | 1·510 (6) | C(10)—N(11) | 1·483 (5) |
| C(3)—C(31) | 1·523 (6) | N(11)—C(111) | 1·477 (6) |
| C(3)—C(4) | 1·549 (6) | N(11)—C(12) | 1·495 (5) |
| C(4)—O(41) | 1·422 (5) | C(12)—C(121) | 1·547 (7) |
| C(4)—C(5) | 1·526 (5) | C(12)—C(13) | 1·537 (5) |
| C(5)—C(51) | 1·537 (6) | C(13)—O(131) | 1·438 (5) |
| C(5)—C(6) | 1·552 (6) | C(13)—C(14) | 1·562 (5) |
| C(6)—O(61) | 1·449 (5) | C(14)—O(141) | 1·455 (5) |
| C(6)—C(7) | 1·555 (6) | C(14)—C(142) | 1·513 (6) |
| C(7)—O(71) | 1·443 (5) | C(14)—C(15) | 1·544 (6) |
| C(7)—C(72) | 1·522 (7) | C(15)—C(151) | 1·529 (6) |
| C(7)—C(8) | 1·539 (6) | C(151)—C(152) | 1·518 (6) |

| | | | | |
|---|---|---|---|---|
| C(2)—O(1)—C(15) | 118·6 (3) | C(8)—C(9)—C(91) | 111·1 (3) |
| O(1)—C(2)—O(21) | 123·6 (4) | C(8)—C(9)—C(10) | 110·4 (3) |
| O(1)—C(2)—C(3) | 112·1 (3) | C(91)—C(9)—C(10) | 107·7 (4) |
| O(21)—C(2)—C(3) | 124·3 (3) | C(9)—C(10)—N(11) | 113·0 (3) |
| C(2)—C(3)—C(31) | 109·3 (3) | C(10)—N(11)—C(111) | 109·2 (3) |
| C(2)—C(3)—C(4) | 110·6 (3) | C(10)—N(11)—C(12) | 111·1 (3) |
| C(31)—C(3)—C(4) | 111·5 (4) | C(111)—N(11)—C(12) | 114·8 (3) |
| C(3)—C(4)—O(41) | 107·7 (3) | N(11)—C(12)—C(121) | 113·5 (3) |
| C(3)—C(4)—C(5) | 114·2 (3) | N(11)—C(12)—C(13) | 110·7 (3) |
| O(41)—C(4)—C(5) | 111·0 (3) | C(121)—C(12)—C(13) | 113·9 (3) |
| C(4)—C(5)—C(51) | 111·0 (3) | C(12)—C(13)—O(131) | 108·3 (3) |
| C(4)—C(5)—C(6) | 109·9 (3) | C(12)—C(13)—C(14) | 115·6 (3) |
| C(51)—C(5)—C(6) | 114·8 (3) | O(131)—C(13)—C(14) | 108·0 (3) |
| C(5)—C(6)—O(61) | 108·1 (3) | C(13)—C(14)—O(141) | 107·9 (3) |
| C(5)—C(6)—C(7) | 115·8 (3) | C(13)—C(14)—C(142) | 114·2 (3) |
| O(61)—C(6)—C(7) | 112·4 (3) | C(13)—C(14)—C(15) | 108·7 (3) |
| C(6)—C(7)—O(71) | 105·6 (3) | C(142)—C(14)—O(141) | 106·9 (3) |
| C(6)—C(7)—C(72) | 109·2 (4) | C(142)—C(14)—C(15) | 111·9 (3) |
| C(6)—C(7)—C(8) | 114·2 (4) | O(141)—C(14)—C(15) | 106·8 (3) |
| O(71)—C(7)—C(72) | 107·3 (4) | O(1)—C(15)—C(14) | 105·8 (3) |
| O(71)—C(7)—C(8) | 108·8 (3) | O(1)—C(15)—C(151) | 107·0 (3) |
| C(72)—C(7)—C(8) | 111·4 (3) | C(14)—C(15)—C(151) | 115·6 (4) |
| C(7)—C(8)—C(9) | 115·4 (4) | C(15)—C(151)—C(152) | 111·9 (4) |

mycin A and its analogous compounds such as 10,10-dihydro-10-deoxo-11-azaerythronolide A hydroiodide (Djokić, Kobrehel, Lazarevski, Lopotar, Tamburašev, Kamenar, Nagl & Vicković, 1986) and 10,10-dihydro-10-deoxo-11-methyl-11-azaerythromycin A (Djokić, Kobrehel, Lopotar, Kamenar, Nagl & Mrvoš, 1988) have been reported.

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# Structure of Ratibinolide, a Sesquiterpene Lactone*

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**Abstract.** 5a,7a-Dimethyl-3-methyleneperhydrocyclopropa[2,3]indeno[4,5-*b*]furan-2,6-dione, $C_{15}H_{18}O_3$, $M_r = 246\cdot3$, orthorhombic, $P2_12_12_1$, $a = 6\cdot779$ (4), $b = 11\cdot052$ (6), $c = 17\cdot760$ (9) Å, $V = 1331$ (2) Å$^3$, $Z = 4$, $D_x = 1\cdot23$ Mg m$^{-3}$, $\lambda$(Mo $K\alpha$) = 0·7107 Å, $\mu = 0\cdot079$ mm$^{-1}$, $F(000) = 528$, $T = 293$ K, $R = 0\cdot038$ for 1073 observed reflections. The six-membered ring adopts a chair conformation with the methyl group at C(10) in the axial position. The five-membered rings [C(1)—C(2)—C(4)—C(5)—C(10) and O(2)—C(6)—C(7)—C(11)—C(12)] are in a conformation intermediate between half-chair and $\alpha$-envelope, and in a half-chair conformation, respectively. The $\Delta$ and $\varphi$ values [Altona, Geise & Romers (1968). *Tetrahedron*, 24, 13–32] are −15·7 (3), −39·7 (3)° and −4·1 (3), −37·8 (3)°, respectively. A C—H···O intermolecular contact is present, C(6)···O(1)(1 + x, y, z) 3·412 (4) Å. The packing in the crystal is entirely due to van der Waals forces.

Table 1. *Positional and equivalent isotropic thermal parameters and their e.s.d.'s*

$$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij}a_i{}^*a_j{}^*\mathbf{a}_i.\mathbf{a}_j.$$

| | x | y | z | $B_{eq}$ (Å²) |
|---|---|---|---|---|
| O(1) | −0·1245 (3) | 0·8259 (2) | 0·8700 (1) | 6·5 (1) |
| O(2) | 0·5989 (3) | 1·1372 (2) | 0·8559 (1) | 4·7 (1) |
| O(3) | 0·8490 (4) | 1·2469 (2) | 0·9010 (1) | 7·4 (1) |
| C(1) | 0·0235 (4) | 0·8715 (3) | 0·8457 (2) | 4·7 (1) |
| C(2) | 0·0613 (5) | 0·9144 (3) | 0·7666 (2) | 5·1 (1) |
| C(3) | 0·0490 (5) | 1·0465 (3) | 0·7478 (2) | 5·7 (1) |
| C(4) | 0·2442 (5) | 0·9935 (3) | 0·7673 (2) | 4·4 (1) |
| C(5) | 0·2928 (4) | 1·0072 (2) | 0·8515 (2) | 3·5 (1) |
| C(6) | 0·4960 (4) | 1·0279 (2) | 0·8816 (1) | 3·5 (1) |
| C(7) | 0·4814 (4) | 1·0483 (2) | 0·9669 (1) | 3·8 (1) |
| C(8) | 0·4050 (5) | 0·9371 (3) | 1·0079 (2) | 5·2 (1) |
| C(9) | 0·2058 (5) | 0·9004 (3) | 0·9750 (2) | 5·2 (1) |
| C(10) | 0·2152 (4) | 0·8890 (2) | 0·8894 (1) | 3·9 (1) |
| C(11) | 0·6748 (4) | 1·1059 (3) | 0·9821 (2) | 4·6 (1) |
| C(12) | 0·7238 (5) | 1·1718 (3) | 0·9113 (2) | 4·9 (1) |
| C(13) | 0·7872 (6) | 1·1085 (3) | 1·0427 (2) | 6·3 (2) |
| C(14) | 0·3383 (5) | 0·7764 (3) | 0·8665 (2) | 4·9 (1) |
| C(15) | 0·4057 (6) | 0·9820 (3) | 0·7102 (2) | 6·3 (2) |

Table 2. *Bond lengths (Å) and angles (°) with e.s.d.'s in parentheses*

| | | | | |
|---|---|---|---|---|
| O(1)—C(1) | 1·202 (4) | | C(5)—C(6) | 1·495 (4) |
| O(2)—C(12) | 1·353 (4) | | C(5)—C(10) | 1·561 (4) |
| O(2)—C(6) | 1·468 (3) | | C(6)—C(7) | 1·535 (4) |
| O(3)  C(12) | 1·201 (4) | | C(7)—C(11) | 1·482 (4) |
| C(1)—C(2) | 1·506 (4) | | C(7)—C(8) | 1·519 (4) |
| C(1)—C(10) | 1·526 (4) | | C(8)—C(9) | 1·526 (5) |
| C(2)—C(3) | 1·500 (6) | | C(9)—C(10) | 1·527 (4) |
| C(2)—C(4) | 1·518 (5) | | C(10)—C(14) | 1·553 (4) |
| C(3)—C(4) | 1·488 (5) | | C(11)—C(13) | 1·320 (4) |
| C(4)—C(15) | 1·497 (5) | | C(11)—C(12) | 1·490 (4) |
| C(4)—C(5) | 1·539 (4) | | | |

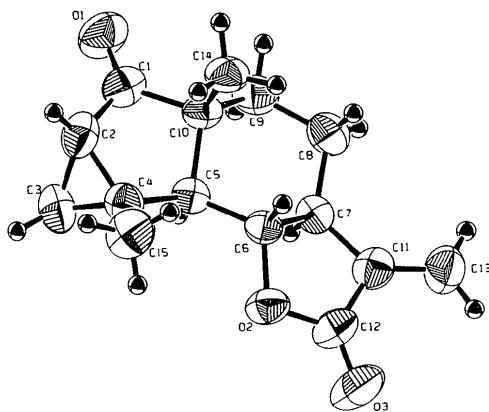| | | | | |
|---|---|---|---|---|
| C(12)—O(2)—C(6) | 107·7 (2) | | C(5)—C(6)—C(7) | 108·4 (2) |
| O(1)—C(1)—C(2) | 127·5 (3) | | C(11)—C(7)—C(8) | 124·2 (3) |
| O(1)—C(1)—C(10) | 125·6 (3) | | C(11)—C(7)—C(6) | 100·7 (2) |
| C(2)—C(1)—C(10) | 106·8 (2) | | C(8)—C(7)—C(6) | 112·0 (2) |
| C(3)—C(2)—C(1) | 120·3 (3) | | C(7)—C(8)—C(9) | 109·4 (3) |
| C(3)—C(2)—C(4) | 59·1 (2) | | C(8)—C(9)—C(10) | 111·5 (2) |
| C(1)—C(2)—C(4) | 108·3 (2) | | C(1)—C(10)—C(9) | 118·7 (2) |
| C(4)—C(3)—C(2) | 61·1 (2) | | C(1)—C(10)—C(14) | 102·9 (2) |
| C(3)—C(4)—C(15) | 121·8 (3) | | C(1)—C(10)—C(5) | 100·1 (2) |
| C(3)—C(4)—C(2) | 59·9 (2) | | C(9)—C(10)—C(14) | 110·5 (3) |
| C(3)—C(4)—C(5) | 112·2 (3) | | C(9)—C(10)—C(5) | 111·9 (2) |
| C(15)—C(4)—C(2) | 122·9 (3) | | C(14)—C(10)—C(5) | 112·2 (2) |
| C(15)—C(4)—C(5) | 120·6 (3) | | C(13)—C(11)—C(7) | 132·0 (3) |
| C(2)—C(4)—C(5) | 103·8 (2) | | C(13)—C(11)—C(12) | 123·3 (3) |
| C(6)—C(5)—C(4) | 124·1 (2) | | C(7)—C(11)—C(12) | 104·7 (2) |
| C(6)—C(5)—C(10) | 106·5 (2) | | O(3)—C(12)—O(2) | 121·8 (3) |
| C(4)—C(5)—C(10) | 105·3 (2) | | O(3)—C(12)—C(11) | 128·6 (3) |
| O(2)—C(6)—C(5) | 116·9 (2) | | O(2)—C(12)—C(11) | 109·6 (2) |
| O(2)—C(6)—C(7) | 102·5 (2) | | | |



Fig. 1. The molecular structure of the title compound showing atom numbering. The thermal ellipsoids are drawn at 50% probability level.

**Experimental.** A colourless crystal, 0·40 × 0·50 × 0·50 mm, was used for data collection. Nicolet *R*3 four-circle diffractometer, graphite-monochromated Mo *K*α radiation. Lattice parameters from 25 machine-centred reflections with $5·8 < 2\theta < 18·8°$. 1405 reflections with $3 < 2\theta < 50°$ for one octant, 1073 independent reflections with $I > 3·0\sigma(I)$, index range *h* 0–7, *k* 0–12, *l* 0–18, ω-scan mode, variable scan speed. Two standard reflections (132 and 111) monitored every 50 measurements showed no significant variation. Lp correction. Data adjusted to an approximately absolute scale and an overall *U* value of 0·046 Å², absorption ignored, $R_{int} = 0·032$. Structure solved by direct methods using the *TEXSAN* (Molecular Structure Corporation, 1988) structure-analysis package. Full-matrix least-squares refinement to minimize the function $\Sigma\sigma_f^2(|F_o| -$

$|F_c|)^2$, in which $\sigma_f = \sigma_I/2F\text{Lp}$, for the unique reflections. Anisotropic temperature factors for C and O atoms; H-atom positions calculated from the geometry of the C-atom skeleton and refined with isotropic terms. The results for the final refinement cycle were: 1073 independent observations; 163 variables; $R = 0·038$, $wR = 0·054$, $S = 1·24$, $(\Delta/\sigma)_{max} = 0·20$, $w = [\sigma^2(F_o) + 0·001(F_o)^2]^{-1}$. Maximum and minimum peaks on the final electron density difference map were $-0·19$ to $+0·18$ e Å$^{-3}$, respectively. Atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). Atomic coordinates are given in Table 1*. Fig. 1 shows the molecular conformation of the title compound. Bond distances and angles are listed in Table 2.

**Related literature.** Ratibinolide is a sesquiterpene lactone which was isolated from the whole plant, *Ratibida latipalearis* Richards (Asteraceae) (Tarahumara name: Chi'punuwa). Details of the source and chemical background of ratibinolide are given by Mata, Rojas, Soriano, Villena, Bye & Linares (1990).

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# Chloracetimin–Tetraphenylphosphoniumchlorid (1/1)

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**Abstract.** 1-Chloroacetimine–tetraphenylphosphonium chloride (1/1), $C_2H_4ClN.C_{24}H_{20}P^+.Cl^-$, $M_r = 452\cdot4$, triclinic, $P\bar{1}$, $a = 10\cdot439$ (2), $b = 10\cdot574$ (2), $c = 11\cdot583$ (2) Å, $\alpha = 74\cdot81$ (2), $\beta = 82\cdot38$ (1), $\gamma = 70\cdot72$ (2)°, $V = 1163\cdot3$ (3) Å³, $Z = 2$, $D_x = 1\cdot29$ g cm⁻³, $\lambda$(Mo $K\alpha$) = 0·7107 Å, $\mu = 3\cdot16$ cm⁻¹, $F(000) = 472$, $T = 292$ K, $R = 0\cdot051$ for 3578 unique observed reflexions. $P(C_6H_5)_4^+$ ions are arranged in zigzag chains along [001] and form layers parallel to (100). Cl⁻ ions and chloroacetimine molecules are situated between the layers, Cl⁻···H—N bridges being only weak.

**Experimentelles.** Die Verbindung entstand unbeabsichtigt in geringer Menge beim (vergeblichen) Versuch, IrCl₃ mit S(SiMe₃)₂ in einem Gemisch aus CH₂Cl₂ und CH₃CN zur Reaktion zu bringen. Einer Suspension von 0,67 g IrCl₃ in CH₂Cl₂/CH₃CN (1/1) wurden zuerst 22,52 g PPh₄Cl, dann 0,47 ml S(SiMe₃)₂ zugegeben. Das Gemisch wurde eine Woche lang mit Ultraschall behandelt. Nach Abfiltrieren des unverändert erscheinenden IrCl₃ und Einengen der Lösung wurden bei 278 K Kristalle der Titelverbindung erhalten. Elementaranalyse: Cl 69,42 (berechnet 69,10), H 5,90 (5,35), N 2,89% (3,10%). Im IR-Spektrum findet sich $\nu$NH bei 3236 cm⁻¹ und $\nu$C=N bei 1651 cm⁻¹; nach diesem Wert ist die NH-Gruppe allenfalls an schwachen Wasserstoffbrücken beteiligt.

Kristallgröße 0,19 × 0,31 × 0,38 mm; Vierkreisdiffraktometer Enraf–Nonius CAD-4, $\omega$-scan, $\Delta\omega = 1,2° + 0,35°\tan\theta$. Gitterparameter aus 23 Reflexen, $11 < \theta < 23°$. $\sin\theta_{max}/\lambda = 0,595$ Å⁻¹, $-11 \le h \le 11$, $-11 \le k \le 11$, $0 \le l \le 13$. Kontrollreflexe 302 und 442 zeigten Intensitätsschwankungen < 2%. 4239

**Tabelle 1.** *Atomkoordinaten und Parameter für den äquivalenten isotropen Temperaturfaktor* (Å²) (*Hamilton*, 1959)

|        | $x$         | $y$          | $z$          | $U_{äq}$   |
|--------|-------------|--------------|--------------|------------|
| Cl(1)  | 0,6425 (1)  | 0,6461 (1)   | 0,06337 (8)  | 0,0557 (4) |
| Cl(2)  | 0,4585 (1)  | 0,3917 (1)   | 0,3877 (1)   | 0,0747 (4) |
| N      | 0,4884 (3)  | 0,3997 (3)   | 0,1544 (3)   | 0,057 (1)  |
| C(1)   | 0,4438 (3)  | 0,3483 (4)   | 0,2617 (3)   | 0,049 (1)  |
| C(2)   | 0,3728 (4)  | 0,2440 (4)   | 0,2642 (4)   | 0,074 (2)  |
| P(1)   | 0,96836 (8) | 0,13730 (8)  | 0,20960 (7)  | 0,0302 (3) |
| C(11)  | 0,8260 (3)  | 0,3697 (3)   | 0,2893 (3)   | 0,039 (1)  |
| C(12)  | 0,7943 (3)  | 0,4550 (3)   | 0,3680 (3)   | 0,045 (1)  |
| C(13)  | 0,8787 (4)  | 0,4283 (4)   | 0,4584 (3)   | 0,051 (1)  |
| C(14)  | 0,9968 (4)  | 0,3183 (4)   | 0,4710 (3)   | 0,052 (1)  |
| C(15)  | 1,0289 (3)  | 0,2304 (3)   | 0,3937 (3)   | 0,040 (1)  |
| C(16)  | 0,9431 (3)  | 0,2555 (3)   | 0,3031 (3)   | 0,030 (1)  |
| C(21)  | 1,0126 (3)  | 0,3189 (3)   | 0,0006 (3)   | 0,044 (1)  |
| C(22)  | 0,9832 (4)  | 0,3974 (3)   | −0,1132 (3)  | 0,055 (1)  |
| C(23)  | 0,8739 (5)  | 0,3966 (4)   | −0,1688 (3)  | 0,064 (2)  |
| C(24)  | 0,7917 (4)  | 0,3182 (4)   | −0,1099 (3)  | 0,057 (2)  |
| C(25)  | 0,8208 (3)  | 0,2372 (3)   | 0,0034 (3)   | 0,043 (1)  |
| C(26)  | 0,9325 (3)  | 0,2346 (3)   | 0,0598 (3)   | 0,033 (1)  |
| C(31)  | 0,7625 (3)  | 0,0644 (3)   | 0,3609 (3)   | 0,040 (1)  |
| C(32)  | 0,6773 (3)  | −0,0171 (4)  | 0,4058 (3)   | 0,050 (1)  |
| C(33)  | 0,6816 (3)  | −0,1211 (4)  | 0,3532 (3)   | 0,052 (1)  |
| C(34)  | 0,7686 (4)  | −0,1462 (3)  | 0,2555 (3)   | 0,052 (1)  |
| C(35)  | 0,8566 (3)  | −0,0681 (3)  | 0,2119 (3)   | 0,044 (1)  |
| C(36)  | 0,8525 (3)  | 0,0385 (3)   | 0,2649 (3)   | 0,031 (1)  |
| C(41)  | 1,1656 (3)  | −0,0869 (3)  | 0,3246 (3)   | 0,043 (1)  |
| C(42)  | 1,2934 (4)  | −0,1812 (3)  | 0,3394 (3)   | 0,051 (1)  |
| C(43)  | 1,3932 (3)  | −0,1745 (4)  | 0,2515 (4)   | 0,056 (2)  |
| C(44)  | 1,3682 (3)  | −0,0707 (4)  | 0,1477 (4)   | 0,060 (2)  |
| C(45)  | 1,2399 (3)  | 0,0267 (3)   | 0,1322 (3)   | 0,047 (1)  |
| C(46)  | 1,1378 (3)  | 0,0182 (3)   | 0,2208 (3)   | 0,032 (1)  |

**Tabelle 2.** *Interatomare Abstände* (Å) *und Winkel* (°)

| C(1)—N       | 1,309 (5)  | P—C(16)         | 1,796 (3)       |
|--------------|------------|-----------------|-----------------|
| C(1)—C(2)    | 1,511 (6)  | P—C(26)         | 1,786 (3)       |
| C(1)—Cl(2)   | 1,679 (4)  | P—C(36)         | 1,800 (3)       |
| N—H(1)       | 0,72 (3)   | P—C(46)         | 1,798 (3)       |
| N···Cl(1)    | 3,371 (4)  | C—C             | 1,373–1,405 (5) |
| Cl(1)···H(1) | 2,66 (3)   |                 |                 |
| C(2)—C(1)—N  | 113,7 (3)  | C(16)—P—C(26)   | 108,3 (2)       |
| C(2)—C(1)—Cl(2) | 121,0 (3) | C(16)—P—C(36)  | 107,8 (1)       |
| Cl(2)—C(1)—N | 125,3 (3)  | C(16)—P—C(46)   | 110,5 (2)       |
| C—C—C        | 118,7–121,5 (4) | C(26)—P—C(36) | 110,4 (2)   |
|              |            | C(26)—P—C(46)   | 112,6 (2)       |
|              |            | C(36)—P—C(46)   | 107,2 (1)       |