Yamasaki, Skelton & White, 1981), 6-chloro-6-cyano-1,5-dimethyl-3,8-dioxatricyclo[3.2.1.$0^{2,4}$]-octane (Cossu, Viani, Lapasset, Aycard, Marfisi & Bodot, 1982), 1-(β-D-2′,3′-anhydroribofuranosyl)-3-methyluracil and O^6,5′-anhydro-1-(β-D-2′,3′-anhydroribofuranosyl)-3,5-dimethyluracil (Marton-Merész, Kuszmann, Pelczer, Parkanyi, Koritsanszky & Kalman, 1983), and eremofortin D (Arnoux, Pascard & Moreau, 1977) have been reported. Calculation of ring conformation parameters is described by Altona & Sundaralingam (1972).

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Structure of 1*H*-Isoindole-1,3(2*H*)-dione (Phthalimide)

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Abstract. $C_8H_5NO_2$, $M_r = 147.13$, monoclinic, $P2_1/n$, $a = 3.8036$ (7), $b = 7.643$ (1), $c = 22.818$ (5) Å, $\beta = 91.36°$, $V = 663.1$ (2) Å^3, $Z = 4$, $D_x = 1.474$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 1.91$ cm^{-1}, $F(000) = 304$, $T = 298$ K, $R = 0.038$ for 770 reflections [$I \geq 3\sigma(I)$]. The flat molecule is centrosymmetrically hydrogen bonded.

Experimental. A crystal measuring approximately 0.10 × 0.20 × 0.20 mm was mounted on an Enraf–Nonius CAD-4 diffractometer. Unit-cell parameters were fixed from 25 strong reflections in the $17 \leq \theta \leq 19°$ thin shell. Intensity data were collected up to $2\theta_{max} = 50°$ (collection range: h 0–2, k 0–5, l −16–16; ω–2θ-scan mode); 1167 reflections were collected, of which 770 obeyed the $I \geq 3\sigma(I)$ criterion. Three reflections were used to monitor the intensity and showed no significant decay of the crystal. All 11 non-H atoms were located by using the *SIMPEL* (Peschar & Schenk, 1987) direct-methods program, and then refined anisotropically. A weighting scheme, $w = [\sigma(F)^2 + (0.02F)^2 + 1]^{-1}$ (Killean & Lawrence, 1969), was introduced. The H atoms were then obtained from a difference Fourier synthesis and refined isotropically. Refinement based on F converged at $R = 0.038$, $wR = 0.040$ for 120 variables refined; $\Delta/\sigma = 0.01$; $S = 0.54$; $\Delta\rho_{max} = 0.54$ (2) e Å^{-3}. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV, Tables 2.2B and 2.3.1). All computations were performed using the *MolEN* structure determination package (Fair, 1990) on a DEC MicroVAX minicomputer. The atomic coordinates are listed in Table 1* and the asymmetric unit shown in Fig. 1. Bond distances and angles are listed in Table 2.

* Lists of structure factors, anisotropic thermal parameters, H-atom positional parameters and bond distances and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55062 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS0549]

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Table 1. *Positional parameters and equivalent isotropic displacement parameters* (Å^2) *for phthalimide*

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

	x	y	z	B_{eq}
O1	0.2685 (5)	−0.0061 (3)	0.16896 (8)	4.49 (4)
O2	−0.2157 (6)	−0.2170 (3)	−0.00158 (7)	4.44 (4)
N3	0.0403 (6)	−0.0734 (3)	0.07739 (8)	3.48 (4)
C4	0.1201 (7)	−0.1060 (3)	0.1361 (1)	3.13 (5)
C5	−0.1207 (7)	−0.2130 (3)	0.0498 (1)	3.16 (5)
C6	−0.1533 (6)	−0.3506 (3)	0.0949 (1)	2.76 (5)
C7	−0.2873 (7)	−0.5174 (3)	0.0912 (1)	3.40 (5)
C8	−0.2748 (7)	−0.6176 (3)	0.1417 (1)	3.92 (6)
C9	−0.1317 (7)	−0.5534 (4)	0.1934 (1)	3.73 (6)
C10	−0.0034 (7)	−0.3858 (3)	0.1971 (1)	3.26 (5)
C11	−0.0094 (6)	−0.2860 (3)	0.1471 (1)	2.65 (4)

Table 2. *Bond distances* (Å) *and angles* (°) *for phthalimide*

O1—C4	1.202 (3)	O2—C5	1.218 (3)
N3—C4	1.388 (3)	N3—C5	1.376 (3)
C4—C11	1.485 (4)	C5—C6	1.478 (4)
C6—C7	1.374 (4)	C6—C11	1.389 (4)
C7—C8	1.385 (4)	C8—C9	1.377 (4)
C9—C10	1.382 (4)	C10—C11	1.373 (4)
C4—N3—C5	112.8 (2)	O1—C4—N3	125.2 (3)
O1—C4—C11	129.4 (3)	N3—C4—C11	105.3 (2)
O2—C5—N3	125.3 (3)	O2—C5—C6	128.6 (3)
N3—C5—C6	106.1 (2)	C5—C6—C7	130.8 (3)
C5—C6—C11	107.8 (2)	C7—C6—C11	121.3 (3)
C6—C7—C8	117.1 (3)	C7—C8—C9	121.4 (3)
C8—C9—C10	121.5 (3)	C9—C10—C11	117.2 (3)
C4—C11—C6	108.0 (2)	C4—C11—C10	130.5 (3)
C6—C11—C10	121.4 (3)		

Related literature. A search through the Cambridge Structural Database yielded the structure of phthalimide; this had been abstracted by *Chemical Abstracts* as the mineral kladnoite (Matzat, 1972*a*). The results of the present structure determination are an improvement of the published structure, which had been refined to $R = 0.072$ (Matzat, 1972*b*).

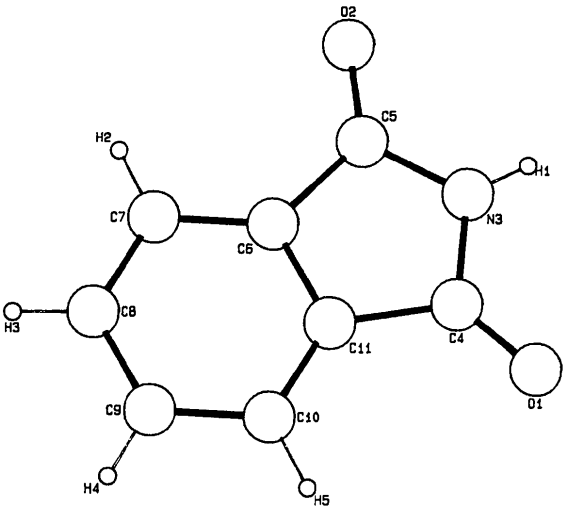

Fig. 1. Molecular structure of phthalimide.

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Structure of a Densely Oxygenated Carbocycle*

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Abstract. (3a*R*-{3aα,4α,5β[*R**(*S**)],6α,6aα})-Methyl α-(cyclohexylhydroxymethyl)-4-{[(1,1-dimethylethyl)dimethylsilyl]oxy}tetrahydro-6-hydroxy-2,2-dimethyl-4*H*-cyclopenta-1,3-dioxole-5-acetate, $C_{24}H_{44}O_7Si$, (I), $M_r = 472.69$, orthorhombic, $P2_12_12_1$, $a = 9.496$ (1), $b = 12.508$ (2), $c = 23.317$ (4) Å, $V = 2769.5$ (7) Å^3, $Z = 4$, $D_x = 1.16$ g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 1.2$ cm^{-1}, $F(000) = 1032$, $T = 298$ K, $R = 0.0475$ and $wR = 0.0579$ for 2409 reflections [$I \geq 3\sigma(I)$]. Crystal chirality was assigned on the basis of the carbohydrate D-(−)-arabinose which was used to prepare the crystals. Chiral centers C_2, C_3 and C_4 in D-(−)-arabinose are fixed in the densely oxygenated cyclopentane ring at the 1,3-dioxole ring fusion and at the C atom bearing the siloxy functionality. The

* Part 2. Part 1: Abboud, Enholm & Trivellas (1992).

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