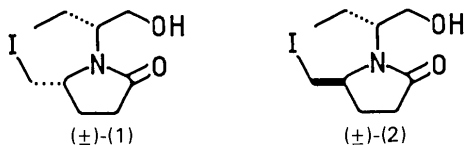


Table 2. Bond lengths (Å) and angles (°)

I—C(5)	2.147 (9)	O(1)—C(1)	1.231 (11)
O(2)—C(9)	1.407 (12)	N—C(1)	1.353 (9)
N—C(4)	1.464 (11)	N—C(6)	1.484 (9)
C(1)—C(2)	1.514 (11)	C(2)—C(3)	1.537 (11)
C(3)—C(4)	1.512 (9)	C(4)—C(5)	1.526 (14)
C(6)—C(7)	1.510 (14)	C(6)—C(9)	1.501 (12)
C(7)—C(8)	1.493 (13)		
C(1)—N—C(4)	112.3 (6)	C(1)—N—C(6)	122.2 (7)
C(4)—N—C(6)	124.9 (5)	O(1)—C(1)—N	124.3 (7)
O(1)—C(1)—C(2)	126.0 (6)	N—C(1)—C(2)	109.7 (7)
C(1)—C(2)—C(3)	101.0 (6)	C(2)—C(3)—C(4)	105.1 (6)
N—C(4)—C(3)	102.4 (6)	N—C(4)—C(5)	111.4 (6)
C(3)—C(4)—C(5)	113.5 (7)	I—C(5)—C(4)	111.9 (5)
N—C(6)—C(7)	111.5 (7)	N—C(6)—C(9)	113.9 (8)
C(7)—C(6)—C(9)	111.0 (6)	C(6)—C(7)—C(8)	115.1 (6)
O(2)—C(9)—C(6)	111.7 (6)		

$= 0.03 \text{ \AA}^2$; $R = 0.045$, $wR = 0.052$, $w = 1/[\sigma^2(F_o)]$, $S = 3.06$, $(\Delta/\sigma)_{\max} = 0.006$ for U_{33} of O(1); $(\Delta/\sigma)_{\text{av}} = 0.006$; $\Delta\rho$ excursions 1.02 and -0.98 e \AA^{-3} , ca 1.0 Å from I; atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974); computer programs from *SHELXTL* (Sheldrick, 1985). The final atomic coordinates and isotropic thermal parameters for compound (1) are given in Table 1.* Bond lengths and angles for the iodolactam (1) are given in Table 2 and a drawing with the numbering scheme is given in Fig. 1.



* Lists of structure factors, anisotropic thermal parameters and calculated H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44856 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of 2-Neopentyl-2H-isoindole

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Abstract. $C_{13}H_{17}N$, $M_r = 187.28$, monoclinic, $P2_1/c$, $a = 5.989 (5)$, $b = 16.870 (9)$, $c = 11.214 (7) \text{ \AA}$, $\beta = 97.37 (5)^\circ$, $V = 1124 (1) \text{ \AA}^3$, $Z = 4$, $D_x = 1.107 \text{ Mg m}^{-3}$, $\lambda(\text{Mo } K\alpha) = 0.71073 \text{ \AA}$, $\mu =$

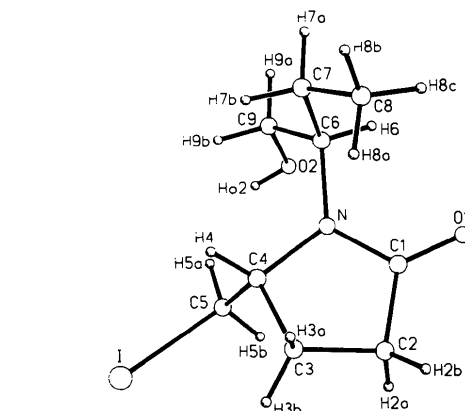


Fig. 1. A computer-generated drawing of (1) showing the relative stereochemistry and atom-numbering scheme.

Related literature. Two relevant crystal structures are those of 5-(1-methyl-2-oxacyclopropyl)pyrrolidin-2-one (Fray, Thomas & Wallis, 1983) and 2-(3-methyl-1-oxoisindolin-2-yl)butyramide (Carlström, Hacksell, Jönsson & Söderholm, 1983).

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0.06 mm^{-1} , $F(000) = 408$, $T = 291 (1) \text{ K}$, final $R = 0.044$ for 890 unique observed [$F \geq 3.0\sigma(F)$] diffractometer data. 2-Neopentyl-2H-isoindole is a typical exponent of the labile parent N heterocycle with a

conjugated cyclic 10π system. The *o*-quinonoid structure is stabilized by the alkyl group at the heteroatom and the electron density distribution is not essentially perturbed. The average bond lengths of the formal double bonds – C(4)–C(5) and C(6)–C(7) – and the formal single bonds – C(3a)–C(4) and C(7)–C(7a) – in the carbocyclic ring are 1.358 (9) and 1.412 (3) Å, respectively. The central bond C(3a)–C(7a) has a length of 1.431 (4) Å and is slightly longer than the peripheral C(5)–C(6) bond [1.406 (5) Å] due to the annelated five-membered ring. The cyclic C–N bonds [average length 1.360 (3) Å] are – as a consequence of conjugation – shorter than the exocyclic C–N bond with a distance of 1.458 (3) Å. For the angle C(1)–N(2)–C(3) a value of 110.1 (3)° is found. The distances of the C–C bonds of the *tert*-butyl group range from 1.510 (4) to 1.518 (4) Å whereas the single bond connecting the methylene group and the *tert*-butyl group has a length of 1.539 (4) Å. The general interest concerning the structure of isoindoles is documented by the independent structure investigations.

Experimental. 2-Neopentyl-2H-isoindole has been prepared *via* the *N*-oxide route through reaction of 2-neopentylisoindoline *N*-oxide with acetic anhydride in the presence of triethylamine.

Crystal size $\sim 0.61 \times 0.26 \times 0.24$ mm, $\omega/2\theta$ scan, scan speed $5.0^\circ \text{ min}^{-1}$ in θ , Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$; lattice parameters from least-squares fit with 25 reflections up to $2\theta = 27.4^\circ$; six standard reflections recorded every

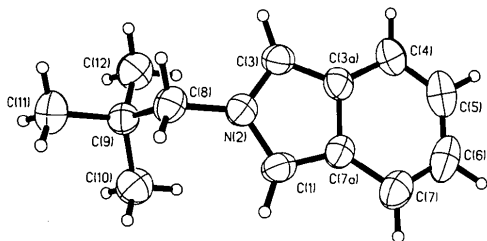


Fig. 1. General view (*SHELXTL-Plus* graphic) of the molecule, showing the atom-numbering scheme.

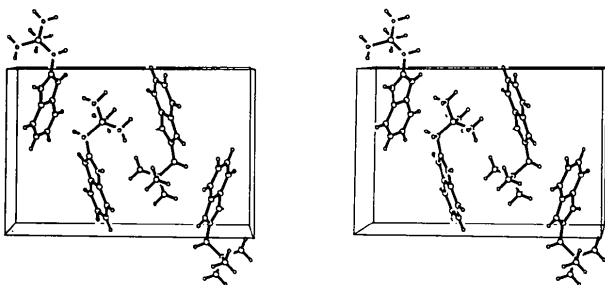


Fig. 2. Stereoscopic view (*SHELXTL-Plus* graphic) of the unit cell (**b** horizontal, **c** vertical).

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* ($\text{\AA}^2 \times 10^3$)

$$U_{\text{eq}} = \frac{1}{3}(U_{11} + U_{22} + U_{33}).$$

	x	y	z	U_{eq}
C(1)	0.7644 (5)	0.1300 (2)	0.8792 (2)	48
N(2)	0.6614 (3)	0.1684 (1)	0.9634 (2)	42
C(3)	0.4502 (4)	0.1909 (2)	0.9158 (2)	46
C(3a)	0.4136 (4)	0.1663 (2)	0.7979 (2)	44
C(4)	0.2310 (5)	0.1722 (2)	0.7066 (3)	55
C(5)	0.2490 (5)	0.1401 (2)	0.5975 (3)	64
C(6)	0.4474 (6)	0.1020 (2)	0.5735 (3)	70
C(7)	0.6298 (5)	0.0948 (2)	0.6587 (2)	59
C(7a)	0.6156 (5)	0.1272 (1)	0.7745 (2)	42
C(8)	0.7593 (4)	0.1813 (2)	1.0877 (2)	48
C(9)	0.7139 (4)	0.1156 (1)	1.1767 (2)	43
C(10)	0.8063 (5)	0.0368 (2)	1.1398 (3)	62
C(11)	0.8340 (6)	0.1400 (2)	1.2985 (3)	66
C(12)	0.4648 (5)	0.1083 (2)	1.1842 (3)	63

Table 2. *Bond distances* (Å) *and angles* ($^\circ$)

C(1)–N(2)	1.357 (4)	C(5)–C(6)	1.406 (5)
C(1)–C(7a)	1.381 (4)	C(6)–C(7)	1.362 (4)
N(2)–C(3)	1.363 (3)	C(7)–C(7a)	1.421 (4)
N(2)–C(8)	1.458 (3)	C(8)–C(9)	1.539 (4)
C(3)–C(3a)	1.376 (4)	C(9)–C(10)	1.518 (4)
C(3a)–C(4)	1.403 (4)	C(9)–C(11)	1.517 (4)
C(3a)–C(7a)	1.431 (4)	C(9)–C(12)	1.510 (4)
C(4)–C(5)	1.355 (4)		
N(2)–C(1)–C(7a)	107.8 (3)	C(6)–C(7)–C(7a)	118.0 (3)
C(1)–N(2)–C(8)	125.0 (3)	C(3a)–C(7a)–C(7)	119.7 (3)
C(1)–N(2)–C(3)	110.1 (3)	C(1)–C(7a)–C(7)	133.0 (3)
C(3)–N(2)–C(8)	124.9 (3)	C(1)–C(7a)–C(3a)	107.3 (3)
N(2)–C(3)–C(3a)	108.5 (3)	N(2)–C(8)–C(9)	115.4 (2)
C(3)–C(3a)–C(7a)	106.3 (3)	C(8)–C(9)–C(12)	110.7 (3)
C(3)–C(3a)–C(4)	133.9 (3)	C(8)–C(9)–C(11)	106.6 (3)
C(4)–C(3a)–C(7a)	119.8 (3)	C(8)–C(9)–C(10)	110.7 (3)
C(3a)–C(4)–C(5)	119.1 (3)	C(11)–C(9)–C(12)	109.3 (3)
C(4)–C(5)–C(6)	121.5 (3)	C(10)–C(9)–C(12)	109.9 (2)
C(5)–C(6)–C(7)	121.9 (3)	C(10)–C(9)–C(11)	109.6 (3)

2.5 h, only random deviations; 1541 reflections measured $1.0 \leq \theta \leq 22.0^\circ$, $-6 \leq h \leq 6$, $0 \leq k \leq 17$, $0 \leq l \leq 11$; after averaging ($R_{\text{int}} = 0.014$): 1375 unique reflections, 890 with $F \geq 3.0\sigma(F)$; Lorentz–polarization correction, no absorption correction; systematic absences ($h0l$) $l = 2n + 1$, ($0k0$) $k = 2n + 1$ conform to space group $P2_1/c$; structure solution *via* direct methods, ΔF syntheses and full-matrix least-squares refinement with anisotropic temperature factors for all non-H atoms and a common isotropic temperature factor for H atoms, which were placed in geometrically calculated positions (C–H 0.95 Å); refinement on F with 890 reflections and 128 refined parameters; $w = 4F_o^2 / [\sigma^2(F^2) + (0.085F^2)^2]$; $S = 1.03$, $R = 0.044$, $wR = 0.055$, $(\Delta/\sigma)_{\text{max}} = 0.6$, no extinction correction; largest peak in final ΔF map $\pm 0.1(1) \text{ e \AA}^{-3}$, atomic scattering factors for neutral atoms and real and imaginary dispersion terms from *International Tables for X-ray Crystallography* (1974); programs: Enraf–Nonius *SDP-Plus* (Frenz, 1985), *MULTAN80* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), *PARST* (Nardelli, 1983), *SHELXTL-Plus* (Sheldrick, 1987). The molecule and the numbering

scheme are shown in Fig. 1 and a stereoscopic view in Fig. 2. Positional parameters and the equivalent values of the anisotropic temperature factors for the non-H atoms are given in Table 1.* Bond lengths and angles are given in Table 2.

Related literature. Babichev, Kovtunenکو & Tyłtin (1981), Bonnett, Hursthouse, North & Trotter (1985), Kohl (1984), Kreher (1986), Kovtunenکو *et al.* (1984).

* Lists of H-atom coordinates, anisotropic thermal parameters and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44866 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Ethyl 3-(2-Methyl-1,3-dioxolan-2-yl)-2-(methyldiphenylsilyl)propionate

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Abstract. $C_{22}H_{28}O_4Si$, $M_r = 384.5$, triclinic, $P\bar{1}$, $a = 9.633$ (3), $b = 10.010$ (3), $c = 12.790$ (4) Å, $\alpha = 106.15$ (10), $\beta = 105.72$ (11), $\gamma = 101.16$ (15)°, $V = 1091$ (1) Å³, $Z = 2$, $D_m = 1.167$, $D_x = 1.170$ g cm⁻³, $\lambda(Cu K\alpha) = 1.5418$ Å, $\mu = 11.2$ cm⁻¹, $F(000) = 412$, $T = 297$ K, $R = 0.056$ for 3956 observed reflections (of 4478 unique data). Si–C distances are 1.876 (2) and 1.873 (2) Å (phenyl), 1.865 (2) Å (methyl) and 1.903 (2) Å (propionate). No evidence for and interaction between the Si atom and the carbonyl O atom was found.

Experimental. Colorless crystal, dimensions 0.25 × 0.32 × 0.35 mm, mounted on a glass fiber, space group from successful refinement of centrosymmetric model, cell dimensions from setting angles for 25 reflections having $36 < \theta < 45$ °. Data collection on Enraf-Nonius CAD-4 diffractometer, Cu $K\alpha$ radiation, graphite

monochromator, ω - 2θ scans at 2.1 to 16.5° min⁻¹. Data having $2\theta \leq 150$ °, $0 \leq h \leq 12$, $-12 \leq k \leq 12$, $-15 \leq l \leq 14$ measured. Three standard reflections $3\bar{2}9$, $04\bar{7}$, $3\bar{2}9$ measured every 3600s, maximum variation 3.6%. 4478 unique data, 3956 reflections with $I > 3\sigma(I)$ considered observed, corrected for background, Lorentz, polarization, no absorption correction applied. Solved by direct methods using *MULTAN11/82* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) and Fourier methods. Full-matrix least-squares methods minimized $\sum w(|F_o| - |F_c|)^2$ with $w = 4F_o^2[\sigma^2(I) + (0.05F_o^2)^2]^{-1}$. Non-H atoms refined with anisotropic thermal parameters, H atoms placed at calculated positions and not refined. Final $R = 0.056$, $wR = 0.090$, $S = 2.52$, for observed data. Max. $\Delta/\sigma = 0.01$ in final cycle, max. residual density 0.24 e Å⁻³. An empirical extinction correction was applied: $F^{corr} = F_c / (1 + 1.0 \times 10^{-6} F_c^2 Lp)$, where Lp is the Lorentz-polarization correction factor. Atomic scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystal-*

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