chromated Mo $K\alpha$; lattice parameters from least-squares fit with 25 reflections up to $2\theta = 28{\cdot}0°$ equally distributed in reciprocal space; six standard reflections recorded every 2·5 h, only random deviations; 6413 reflections measured, $1{\cdot}5 \le \theta \le 25{\cdot}0°$, $-13 \le h \le 13$, $-14 \le k \le 14$, $0 \le l \le 18$; after averaging ($R_{int} = 0{\cdot}013$): 5993 unique reflections, 3466 with $F \ge 4{\cdot}0\sigma(F)$; Lorentz–polarization correction, no absorption correction; space group $P\bar{1}$; 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 1·08 Å); refinement on F with 3466 reflections and 398 refined parameters; $w = 1{\cdot}9/[\sigma^2(F) + 0{\cdot}0005F^2]$; $S = 0{\cdot}92$, $R = 0{\cdot}062$, $wR = 0{\cdot}068$, $(\Delta/\sigma)_{max}$ 0·09; no extinction correction; largest peak in final ΔF map 0·3 (2) e Å^{-3}; complex neutral-atom scattering factors from Cromer & Mann (1968) and Cromer & Liberman (1970); programs: *SHELXS* (Sheldrick, 1986) for structure solution, *SHELX*76 (Sheldrick, 1976) for structure refinement, Enraf–Nonius *Structure Determination Package* (Frenz, 1985) for data reduction, *SHELXTL PLUS* (Sheldrick, 1987) for the plot.

The molecule and the numbering scheme are shown in Fig. 1. 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. Kreher & Hildebrand (1987).

* Lists of H-atom coordinates, anisotropic thermal parameters, structure-factor amplitudes and least-squares planes, dihedral angles and angles between a perpendicular of a plane and a direction have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44375 (24 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 *r*-1-Isopropyl-*t*-2,*t*-3-diphenylaziridine

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Abstract. $C_{17}H_{19}N$, $M_r = 239{\cdot}3$, monoclinic, $P2_1/n$, $a = 11{\cdot}331$ (2), $b = 14{\cdot}690$ (3), $c = 9{\cdot}402$ (2) Å, $\beta = 113{\cdot}49$ (2)°, $V = 1435{\cdot}2$ Å^3, $Z = 4$, $D_x = 1{\cdot}107$ Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 0{\cdot}412$ mm^{-1}, $F(000) = 512$, $T = 293$ K, $R = 0{\cdot}049$ for 1281 observed reflexions. The aziridine ring has bond lengths C–N 1·444 (4), 1·449 (3), C–C 1·499 (5) Å and bond angles 62·4 (2)° at N and 58·6 (2), 58·9 (2)° at C. The phenyl rings are in *cis* conformation with an interplanar angle of 85·1 (1)°.

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Table 1. *Atomic coordinates and equivalent isotropic thermal parameters*

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

	x	y	z	U_{eq}(Å²)
N1	0·2551 (2)	0·2628 (2)	0·1115 (2)	0·061
C11	0·2850 (3)	0·3507 (2)	0·0587 (4)	0·072
C12	0·2275 (5)	0·3518 (4)	−0·1151 (4)	0·103
C13	0·2348 (5)	0·4265 (3)	0·1268 (5)	0·099
C2	0·3402 (3)	0·2329 (2)	0·2651 (3)	0·062
C3	0·3420 (3)	0·1887 (2)	0·1223 (3)	0·068
C21	0·2858 (3)	0·1942 (2)	0·3720 (3)	0·058
C22	0·3679 (4)	0·1727 (2)	0·5232 (4)	0·071
C23	0·3189 (5)	0·1418 (3)	0·6270 (4)	0·090
C24	0·1893 (5)	0·1308 (3)	0·5840 (4)	0·098
C25	0·1085 (4)	0·1522 (3)	0·4357 (4)	0·089
C26	0·1561 (3)	0·1831 (2)	0·3309 (4)	0·069
C31	0·2904 (3)	0·0968 (2)	0·0615 (3)	0·062
C32	0·3736 (3)	0·0251 (2)	0·0797 (4)	0·081
C33	0·3274 (4)	−0·0596 (2)	0·0174 (4)	0·089
C34	0·1988 (4)	−0·0736 (3)	−0·0612 (4)	0·085
C35	0·1155 (4)	−0·0032 (2)	−0·0795 (4)	0·078
C36	0·1599 (3)	0·0813 (2)	−0·0197 (4)	0·069

Table 2. *Interatomic distances* (Å) *and angles* (°)

N1–C2	1·449 (3)	C22–C23	1·378 (7)
N1–C3	1·444 (4)	C23–C24	1·369 (8)
N1–C11	1·471 (4)	C24–C25	1·364 (5)
C11–C12	1·499 (5)	C25–C26	1·375 (6)
C11–C13	1·505 (6)	C31–C32	1·377 (5)
C2–C3	1·499 (5)	C31–C36	1·386 (4)
C2–C21	1·485 (5)	C32–C33	1·386 (5)
C3–C31	1·490 (4)	C33–C34	1·361 (6)
C21–C22	1·390 (4)	C34–C35	1·364 (6)
C21–C26	1·373 (4)	C35–C36	1·373 (5)
C2–N1–C3	62·4 (2)	C2–C21–C26	122·8 (2)
C2–N1–C11	116·8 (2)	C21–C22–C23	120·4 (4)
C3–N1–C11	116·3 (3)	C22–C23–C24	121·1 (3)
C12–C11–C13	112·5 (3)	C23–C24–C25	118·6 (5)
N1–C11–C12	108·6 (3)	C24–C25–C26	120·9 (4)
N1–C11–C13	109·2 (3)	C25–C26–C21	121·3 (3)
N1–C2–C3	58·6 (2)	C3–C31–C32	120·0 (3)
N1–C2–C21	120·0 (2)	C3–C31–C36	121·9 (3)
C3–C2–C21	126·7 (3)	C32–C31–C36	118·0 (3)
N1–C3–C2	58·9 (2)	C31–C32–C33	120·6 (3)
N1–C3–C31	120·3 (2)	C32–C33–C34	120·5 (4)
C2–C3–C31	126·3 (3)	C33–C34–C35	119·4 (3)
C2–C21–C22	119·4 (3)	C34–C35–C36	120·8 (3)
C22–C21–C26	117·7 (3)	C35–C36–C31	120·7 (3)

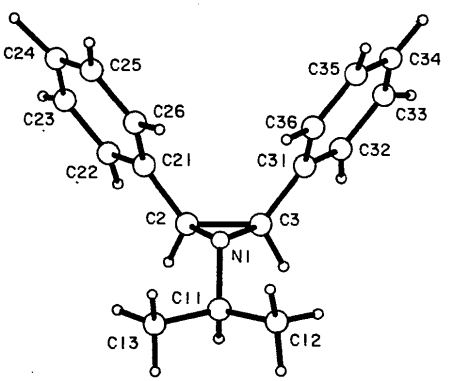

Fig. 1. View of the moelcule with the atom numbering.

Experimental. Colourless crystal, equidimensional in habit, 0·2 × 0·3 × 0·3 mm, m.p. 321–322 K, grown from ethanol, mounted in glass capillary to prevent sublimation; cell parameters and intensity data measured on Enraf–Nonius CAD-4 diffractometer with graphite monochromator; lattice parameters determined by a least-squares refinement using 25 reflexions; 3 standard reflexions, no intensity variation; 2061 independent reflexions measured to a θ limit of 75°, max. h,k,l, = 12, 14, 11; data not corrected for absorption; 1281 reflexions with $I > 3\sigma(I)$ considered observed and used in subsequent calculations; structure solved by direct methods using the *EEES* procedure of program *SHELX*76 (Sheldrick, 1976); first E map revealed positions of all non-H atoms; least-squares refinement, isotropic and then anisotropic temperature factors; H atoms located on difference Fourier maps and included in the refinement with isotropic temperature factors; weights for each reflexion in the refinement (based on F) calculated from $w = 1/[\sigma^2(F) + pF^2]$ with $p = 0{\cdot}005$, σF taken from counting statistics; refinement converged with $R = 0{\cdot}049$, $wR = 0{\cdot}056$; in the last cycle of refinement $(\Delta/\sigma)_{max}$ was 0·29 for all refined parameters; max., min. height in final difference Fourier map = 0·23, −0·21 e Å^{-3}. Scattering factors from *SHELX*76. Atomic coordinates are given in Table 1, interatomic distances and angles in Table 2. Atom numbering is shown in Fig. 1.*

Related literature. In previous studies (Bartnik & Mlostoń, 1983, 1984), we presented details of the synthesis and properties of the title compound and other related products. For structures of other aziridine derivatives see also Bruckner (1982), Quast, Jakob, Peters, Peters & von Schnering (1984), Boese, Rademacher & Treschanke (1985).

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* 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 44368 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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