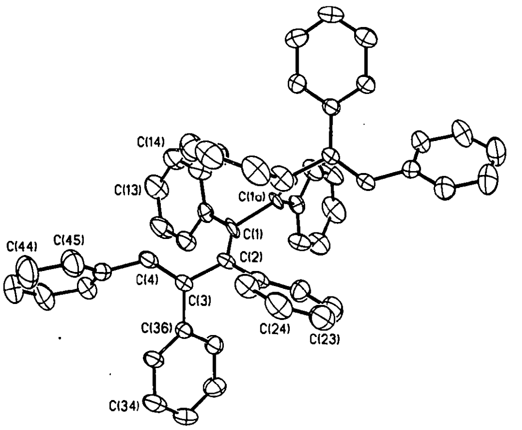

Fig. 1. Molecular structure and labeling scheme for (1) with 40% probability thermal ellipsoids. H atoms have been deleted for clarity.

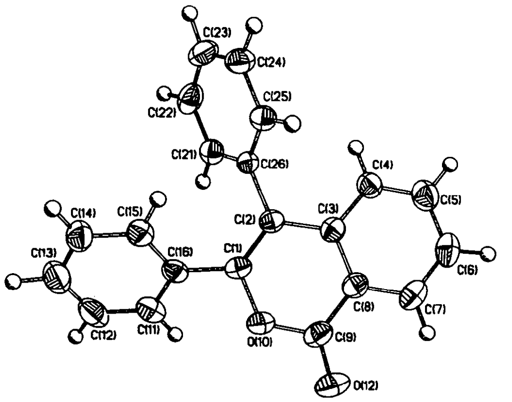

Fig. 2. Molecular structure and labeling scheme for (2) with 40% probability thermal ellipsoids. H atoms are shown with arbitrary radii.

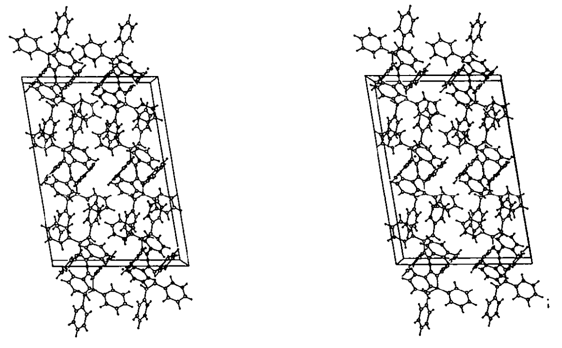

Fig. 3. Unit-cell packing diagram for (1) as viewed down the *b* axis with *a* vertical.

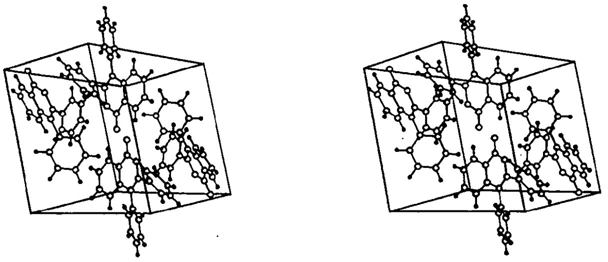

Fig. 4. Unit-cell packing diagram for (2); the *a* axis is nearly vertical and the *c* axis nearly horizontal.

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Structure of 4,5-Diphenyl-1-triphenylmethoxy-1,2,3-triazole

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Abstract. $C_{33}H_{25}N_3O$, $M_r = 479{\cdot}58$, monoclinic, $P2_1/n$, $a = 10{\cdot}599\,(5)$, $b = 14{\cdot}286\,(4)$, $c = 16{\cdot}175\,(3)$ Å, $\beta = 94{\cdot}31\,(4)°$, $V = 2442{\cdot}4\,(7)$ Å^3, $Z = 4$, $D_x = 1{\cdot}304$ g cm^{-3}, $\lambda(\text{Mo } K\overline{\alpha}) = 0{\cdot}71073$ Å, $\mu = 0{\cdot}742$ cm^{-1}, $F(000) = 1008$, $T = 105$ K, $R = 0{\cdot}034$, $wR = 0{\cdot}044$ for 3052 unique observed reflections. The triazole ring is planar. There are no unusual bond distances or angles.

Experimental. The title compound was prepared by the reaction of silver phenylcyanomethane nitronate with trityl chloride in toluene at 278 K (Boyer, Manimaran & Ramakrishnan, 1987) and recrystallized from benzene yielding colorless crystals. A tabular crystal with approximate dimensions 0·30 × 0·30 × 0·40 mm was mounted on an Enraf–Nonius CAD-4 diffractometer with graphite crystal monochromator

Table 1. *Positional parameters and equivalent isotropic thermal parameters*

	x	y	z	B(Å^2)
O1	−0·0768 (1)	0·01743 (8)	0·77895 (7)	1·55 (2)
N1	0·0222 (1)	0·0231 (1)	0·83819 (8)	1·48 (3)
N2	0·0763 (2)	0·1058 (1)	0·85709 (9)	1·77 (3)
N3	0·1607 (2)	0·0890 (1)	0·91933 (9)	1·78 (3)
C1	0·1568 (2)	−0·0043 (1)	0·9401 (1)	1·60 (3)
C2	0·0675 (2)	−0·0483 (1)	0·8872 (1)	1·52 (3)
C3	−0·0403 (2)	0·0116 (1)	0·6911 (1)	1·50 (3)
C4	0·2382 (2)	−0·0413 (1)	1·0102 (1)	1·62 (3)
C5	0·3474 (2)	0·0071 (1)	1·0384 (1)	2·10 (4)
C6	0·4256 (2)	−0·0267 (1)	1·1039 (1)	2·49 (4)
C7	0·3957 (2)	−0·1091 (1)	1·1433 (1)	2·33 (4)
C8	0·2864 (2)	−0·1567 (1)	1·1167 (1)	2·22 (4)
C9	0·2078 (2)	−0·1237 (1)	1·0511 (1)	1·89 (4)
C10	0·0273 (2)	−0·1469 (1)	0·8773 (1)	1·50 (3)
C11	0·1144 (2)	−0·2128 (1)	0·8536 (1)	1·85 (4)
C12	0·0808 (2)	−0·3064 (1)	0·8475 (1)	2·16 (4)
C13	−0·0385 (2)	−0·3351 (1)	0·8647 (1)	2·17 (4)
C14	−0·1252 (2)	−0·2702 (1)	0·8888 (1)	2·28 (4)
C15	−0·0932 (2)	−0·1758 (1)	0·8944 (1)	1·93 (4)
C16	0·0685 (2)	−0·0571 (1)	0·6832 (1)	1·54 (3)
C17	0·1916 (2)	−0·0317 (1)	0·7123 (1)	1·82 (3)
C18	0·2928 (2)	−0·0909 (1)	0·7028 (1)	2·14 (4)
C19	0·2738 (2)	−0·1767 (1)	0·6633 (1)	2·51 (4)
C20	0·1530 (2)	−0·2023 (1)	0·6342 (1)	2·41 (4)
C21	0·0513 (2)	−0·1435 (1)	0·6446 (1)	1·86 (4)
C22	−0·1661 (2)	−0·0214 (1)	0·6473 (1)	1·51 (3)
C23	−0·2442 (2)	−0·0830 (1)	0·6862 (1)	1·95 (4)
C24	−0·3547 (2)	−0·1160 (1)	0·6452 (1)	2·14 (4)
C25	−0·3894 (2)	−0·0888 (1)	0·5643 (1)	2·09 (4)
C26	−0·3131 (2)	−0·0265 (1)	0·5258 (1)	2·08 (4)
C27	−0·2032 (2)	0·0075 (1)	0·5669 (1)	1·72 (3)
C28	−0·0063 (2)	0·1095 (1)	0·6611 (1)	1·47 (3)
C29	0·0718 (2)	0·1185 (1)	0·5963 (1)	1·82 (3)
C30	0·0943 (2)	0·2056 (1)	0·5621 (1)	2·04 (4)
C31	0·0384 (2)	0·2845 (1)	0·5924 (1)	2·08 (4)
C32	−0·0402 (2)	0·2763 (1)	0·6562 (1)	2·11 (4)
C33	−0·0630 (2)	0·1891 (1)	0·6909 (1)	1·84 (4)

Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as: $(4/3)[a^2\beta(1,1) + b^2\beta(2,2) + c^2\beta(3,3) + ab(\cos\alpha)\beta(1,2) + ac(\cos\beta)\beta(1,3) + bc(\cos\alpha)\beta(2,3)]$.

and cooled to 105 (5) K with a stream of cold N_2 gas. Lattice parameters from least-squares refinement of the setting angles of 25 reflections with $30 < 2\theta < 48°$, Mo $K\alpha$ radiation. Systematic absences, $h0l$: $h + l = 2n + 1$, $0k0$: $k = 2n + 1$. Intensities measured using $\omega:2\theta$ scans within the ranges $2 < 2\theta < 50°$, $-12 \leq h \leq 0$, $0 \leq k \leq 17$, $-18 \leq l \leq 18$. The intensities of three standard reflections measured at 2 h intervals decreased by 3·2% during data collection. A linear least-squares fit to the intensities of the standards was used to correct the data. Variation in absorption as a function of ψ was observed to be minimal and no correction was applied. Lorentz and polarization corrections were applied. A total of 4370 unique reflections were measured of which 3052 were considered observed $[|F| > 3\sigma(|F|)]$.

The structure was determined by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980; modified by Frenz, 1982). Peaks corresponding to all 37 non-H atoms were located in the E map, and the positions of all 25 H atoms in a subsequent difference Fourier synthesis. Refinement was by full-matrix least-squares minimization of $\sum w(|F_o| - |F_c|)^2$, where $w = 1/\sigma^2(|F|)$ and $\sigma^2(F^2) = \sigma^2_{cs} + (0{\cdot}04F^2)^2$. Positions and anisotropic thermal parameters refined for non-H atoms, positions and isotropic thermal parameters for H atoms.

Final $R = 0{\cdot}034$, $wR = 0{\cdot}044$, $S = 1{\cdot}40$, and $(\Delta/\sigma)_{\max} = 0{\cdot}05$ for 434 variables. Maximum and

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

Numbers in parentheses are estimated standard deviations in the least significant digits.

O1—N1	1·369 (2)	C5—C6	1·382 (2)	C19—C20	1·380 (3)
O1—C3	1·503 (2)	C6—C7	1·387 (3)	C20—C21	1·387 (2)
N1—N2	1·339 (2)	C7—C8	1·384 (3)	C22—C23	1·391 (2)
N1—C2	1·357 (1)	C8—C9	1·381 (2)	C22—C27	1·393 (2)
N2—N3	1·318 (2)	C10—C11	1·392 (2)	C23—C24	1·385 (2)
N3—C1	1·376 (2)	C10—C15	1·389 (2)	C24—C25	1·388 (2)
C1—C2	1·379 (2)	C11—C12	1·386 (2)	C25—C26	1·382 (3)
C1—C4	1·471 (2)	C12—C13	1·378 (3)	C26—C27	1·385 (2)
C2—C10	1·477 (2)	C13—C14	1·382 (3)	C28—C29	1·389 (2)
C3—C16	1·527 (2)	C14—C15	1·392 (2)	C28—C33	1·389 (2)
C3—C22	1·536 (2)	C16—C17	1·402 (2)	C29—C30	1·390 (2)
C3—C28	1·532 (2)	C16—C21	1·389 (2)	C30—C31	1·380 (2)
C4—C5	1·395 (2)	C17—C18	1·382 (2)	C31—C32	1·378 (2)
C4—C9	1·399 (2)	C18—C19	1·390 (2)	C32—C33	1·396 (2)

N1—O1—C3	115·3 (1)	C10—C11—C12	120·0 (2)
O1—N1—N2	120·3 (1)	C11—C12—C13	120·5 (2)
O1—N1—C2	125·7 (1)	C12—C13—C14	119·8 (2)
N2—N1—C2	113·8 (1)	C13—C14—C15	120·3 (2)
N1—N2—N3	105·6 (1)	C10—C15—C14	119·8 (2)
N2—N3—C1	109·3 (1)	C3—C16—C17	119·7 (1)
N3—C1—C2	108·8 (1)	C3—C16—C21	122·3 (2)
N3—C1—C4	120·7 (1)	C17—C16—C21	117·9 (2)
C2—C1—C4	130·5 (1)	C16—C17—C18	121·0 (2)
N1—C2—C1	102·5 (1)	C17—C18—C19	120·2 (2)
N1—C2—C10	124·5 (1)	C18—C19—C20	119·3 (2)
C1—C2—C10	132·9 (1)	C19—C20—C21	120·4 (2)
O1—C3—C16	111·4 (1)	C16—C21—C20	121·1 (2)
O1—C3—C22	100·2 (1)	C3—C22—C23	120·7 (1)
O1—C3—C28	109·4 (1)	C3—C22—C27	120·9 (1)
C16—C3—C22	113·5 (1)	C23—C22—C27	118·3 (2)
C16—C3—C28	111·3 (1)	C22—C23—C24	120·6 (2)
C22—C3—C28	110·5 (1)	C23—C24—C25	120·8 (2)
C1—C4—C5	119·8 (2)	C24—C25—C26	118·8 (2)
C1—C4—C9	121·6 (2)	C25—C26—C27	120·6 (2)
C5—C4—C9	118·5 (2)	C22—C27—C26	120·8 (2)
C4—C5—C6	120·8 (2)	C3—C28—C29	119·4 (1)
C5—C6—C7	120·2 (2)	C3—C28—C33	121·2 (1)
C6—C7—C8	119·3 (2)	C29—C28—C33	119·0 (2)
C7—C8—C9	120·9 (2)	C28—C29—C30	120·8 (2)
C4—C9—C8	120·2 (2)	C29—C30—C31	119·9 (2)
C2—C10—C11	118·8 (1)	C30—C31—C32	119·7 (2)
C2—C10—C15	121·6 (1)	C31—C32—C33	120·7 (2)
C11—C10—C15	119·6 (2)	C28—C33—C32	119·9 (2)

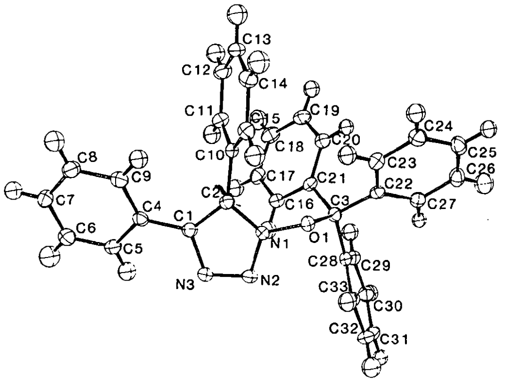

Fig. 1. *ORTEP* plot (Johnson, 1976) of the molecule showing the atomic numbering scheme.

minimum peaks in final difference Fourier synthesis, 0·18 and $-0{\cdot}22$ e Å^{-3}, respectively. Atomic scattering factors and anomalous-dispersion corrections taken from *International Tables for X-ray Crystallography* (1974), and all computer programs from the *SDP* system (Frenz, 1982).* Final atomic coordinates are listed in Table 1. Bond lengths and bond angles are given in Table 2. The molecular structure is depicted in Fig. 1 along with the atomic numbering scheme.

Related literature. The structures of several triazoles substituted with groups containing C or N atoms bonded to N(1) have been reported (Bauer, Boulton, Fedeli, Katritzky, Majid-Hamid, Mazza & Vaciago, 1972; Kokkou & Rentzeperis, 1975*a*,*b*; Murray-Rust, McManus, Lennon, Porter & Rechka, 1984; Sen & Venkatesan, 1984), as well as structures without substitution at N(1) (Kálmán, Simon, Schawartz & Horváth, 1974; Párkányi, Kálmán, Argay & Schawartz, 1977).

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* Lists of structure factors, anistropic temperature factors, H-atom positions, least-squares planes, and bond distances and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52121 (52 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 at 173 K of a Chiral, Tricyclic Aminonitrobenzene

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Abstract. R-(3aα,4aβ,7aβ,7bα)-Octahydro-4-(4-nitrophenyl)-1H,5H-dicyclopenta[b,d]pyrrole, $C_{16}H_{20}N_2O_2$, $M_r = 272{\cdot}3$, orthorhombic, $P2_12_12_1$, $a = 8{\cdot}696\ (4)$, $b = 9{\cdot}630\ (3)$, $c = 16{\cdot}428\ (5)$ Å, $V = 1375{\cdot}7\ (8)$ Å^3, $Z = 4$, $D_x = 1{\cdot}315$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 0{\cdot}82$ cm^{-1}, $F(000) = 584$, $T = 173$ K, $R = 0{\cdot}0409$ for 1220 reflections [$F_o \geq 6\sigma(F_o)$]. Crystal chirality was assigned to correspond to the known chirality of the parent amine. Pairs of neighboring molecules stack in a head-to-tail arrangement with a psuedo-inversion center.

Experimental. The title compound crystallized as yellow rods and elongated prisms by slow evaporation from ethanol. It was synthesized by aromatic substitution of the tricyclic amine (Whitesell, Minton & Chen, 1988) on p-fluoronitrobenzene. The data crystal had dimensions $0{\cdot}09 \times 0{\cdot}17 \times 0{\cdot}29$ mm. A Nicolet $R3m$/V diffractometer equipped with a graphite monochromator and a Nicolet LT-2 low-temperature delivery system (173 K) was used to collect the data. The lattice parameters were obtained from the least-squares refinement of 47 reflections with $10{\cdot}0 < 2\theta < 21{\cdot}0°$. The data were collected using the ω scan technique with a 2θ range from 3·0–55·0° and a 1·2° ω scan at 2–4° min^{-1} (three symmetry-related octants: $h = 0\rightarrow 11$, $k = 0\rightarrow 12$, $l = 0\rightarrow 21$; $h = 0\rightarrow 11$, $k = -12\rightarrow 0$, $l = -21\rightarrow 0$; $h = -11\rightarrow 0$, $k = -12\rightarrow 0$, $l = 0\rightarrow 21$). Of

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