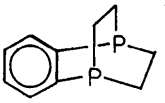
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Atomic parameters are given in Table 1, bond distances and angles in Table 2.* Fig. 1 shows a thermal-ellipsoid plot with the atom numbering.

Related literature. For the preparation and characterization of the compound see Issleib, Leissring & Schmidt (1986).



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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 51597 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

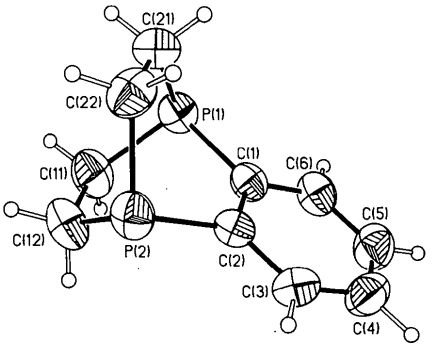

Fig. 1. A 50% thermal-ellipsoid plot with atom numbering.

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Structure of *N*-Tritylglycine Methylamide

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Abstract. $C_{22}H_{22}N_2O$, $M_r = 330{\cdot}43$, orthorhombic, $P2_12_12_1$, $a = 8{\cdot}936\ (2)$, $b = 13{\cdot}752\ (2)$, $c = 14{\cdot}611\ (2)$ Å, $V = 1795{\cdot}5\ (4)$ Å^3, $Z = 4$, $D_x = 1{\cdot}22$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}71069$ Å, $\mu = 0{\cdot}82$ cm^{-1}, $F(000) = 704$, room temperature, $R = 0{\cdot}043$ for 953 unique observed reflections. The amide bond adopts the *trans* conformation [O(23)–C(22)–N(24)–H(24) = 169·5 (8)°]. The structure is stabilized by means of intermolecular hydrogen bonding [N(24)–H(24)···O(23^i) = 1·91 (8) Å, (i) = x, y, $1+z$]. Other bond lengths and angles are normal.

Experimental. Prismatic crystal 0·26 × 0·25 × 0·22 mm. Enraf–Nonius CAD-4 diffractometer, data collection using ω–2θ scans, lattice parameters from 25 reflections in range $7 < \theta < 10°$. 5293 measured reflections in index range h 0–10, k 0–17, l ±17 up to $2\theta_{max} = 56°$, 2483 unique reflections, mean discrepancy on I 1·1% (on averaging 5105 reflections); θ scan width $(0{\cdot}7 + 0{\cdot}3\tan\theta)°$, scan rate 1·03–5·49° min^{-1}, max. scan time 60 s, aperture $(2{\cdot}4 + 0{\cdot}9\tan\theta)$ mm; reference reflections (222, 230, 006) every 2 h, intensity decrease 1·2%, orientation-control

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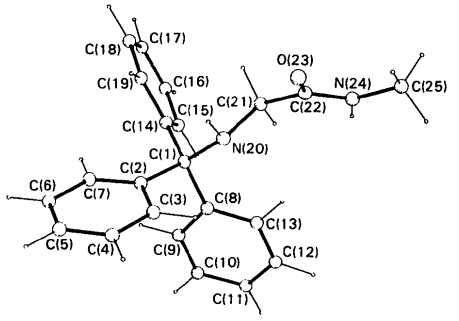

Fig. 1. Atomic numbering scheme of the molecule.

Table 1. *Final positional* ($\times 10^4$, *for* H $\times 10^3$) *and equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = \frac{4}{3}\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
C(1)	−267 (6)	958 (4)	7465 (4)	3·21
C(2)	1034 (7)	484 (4)	7984 (4)	3·48
C(3)	2238 (8)	127 (5)	7479 (5)	4·86
C(4)	3427 (8)	−331 (5)	7919 (6)	6·02
C(5)	3426 (9)	−448 (5)	8842 (6)	6·19
C(6)	2225 (10)	−134 (5)	9346 (5)	5·44
C(7)	1012 (7)	329 (5)	8918 (4)	4·16
C(8)	−1145 (6)	137 (4)	6994 (4)	3·11
C(9)	−1861 (7)	−568 (4)	7517 (4)	3·82
C(10)	−2694 (8)	−1300 (5)	7119 (5)	4·80
C(11)	−2834 (8)	−1336 (5)	6172 (6)	5·54
C(12)	−2094 (8)	−661 (5)	5648 (5)	5·56
C(13)	−1262 (7)	74 (5)	6049 (4)	4·26
C(14)	−1309 (6)	1561 (4)	8098 (3)	3·13
C(15)	−2845 (6)	1479 (5)	8084 (4)	3·54
C(16)	−3721 (7)	2110 (5)	8601 (4)	4·60
C(17)	−3106 (8)	2831 (5)	9117 (4)	5·17
C(18)	−1561 (9)	2935 (5)	9130 (4)	4·62
C(19)	−661 (7)	2315 (5)	8621 (4)	4·25
N(20)	425 (5)	1594 (4)	6766 (3)	3·51
C(21)	−547 (6)	2327 (4)	6344 (3)	3·93
C(22)	265 (6)	2732 (4)	5520 (4)	3·39
O(23)	1557 (5)	3009 (3)	5562 (3)	4·43
N(24)	−556 (6)	2787 (4)	4754 (3)	3·99
C(25)	43 (7)	3213 (5)	3920 (3)	5·70
H(20)	128 (8)	188 (5)	698 (5)	8·10
H(24)	−149 (8)	244 (5)	477 (5)	8·10

Table 2. *Selected bond lengths* (Å) *and angles* (°)

C(1)–N(20)	1·479 (7)	C(22)–N(24)	1·340 (7)
N(20)–H(20)	0·91 (7)	N(24)–H(24)	0·96 (7)
C(21)–C(22)	1·512 (7)	N(20)–C(21)	1·467 (7)
C(22)–O(23)	1·218 (6)	N(24)–C(25)	1·454 (7)

C(21)–C(22)–O(23)	122·0 (5)	O(23)–C(22)–N(24)	122·9 (5)
C(21)–C(22)–N(24)	115·1 (5)	O(23)–C(22)–N(24)–H(24)	169·5 (8)

	N–H	H···O	N···O	N–H···O
N(20)–H(20)···O(23)	0·91 (7)	2·60 (8)	2·81 (8)	86 (2)
N(24)–H(24)···O(23^i)	0·96 (7)	1·91 (8)	2·840 (8)	162 (4)

Symmetry code: (i) $x, y, 1+z$.

reflections (153, 143, 115) after 500 reflections. Refinement on F, final $R = 0{\cdot}043$ for 953 unique observed reflections with $I > 1{\cdot}5\sigma(I)$ which were used for analysis; $wR = 0{\cdot}0435$, $w = k/[\sigma^2(F) + 0{\cdot}00305F^2]$, max. Δ/σ in final cycle 0·39; residual electron density in final difference Fourier synthesis between +0·17 and −0·18 e Å^{-3}, atomic scattering factors from *SHELX*76 (Sheldrick, 1976); no absorption correction applied; heavier atoms refined with anisotropic temperature factors; H atoms positioned geometrically except for H(20) and H(24) which were located in difference Fourier syntheses and refined isotropically; computations carried out with *MULTAN*87 (Debaerdemaeker, Germain, Main, Tate & Woolfson, 1987), *SHELX*76 and *PLUTO* (Motherwell & Clegg, 1978). The molecule with the atom-numbering scheme is shown in Fig. 1. Atomic coordinates are listed in Table 1 and bond lengths and angles in Table 2.*

Related literature. *N*-Tritylglycine methylamide was prepared by the method previously described (Matsoukas, Cordopatis & Theodoropoulos, 1977). It is an intermediate in the synthesis of oxytocin analogues which differ dramatically in their biological activities (Walter, Stahl, Caplaneris, Cordopatis & Theodoropoulos, 1979; Ting, Smith, Stahl, Walter, Cordopatis & Theodoropoulos, 1980).

* Lists of structure amplitudes, anisotropic thermal parameters, H-atom coordinates, bond distances, angles and torsion angles, and equations of planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51590 (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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