minée par les méthodes directes (*MULTAN*80; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) et affinée par moindres carrés (*SHELX*76; Sheldrick, 1976); quantité minimisée $\sum(|F_o| - |F_c|)^2$ sans pondération. Hydrogènes déterminés par Fourier différence, affinement anisotrope pour les atomes lourds, pas d'affinement pour les atomes d'hydrogène. Valeur finale de $R = 0{,}043$, $wR = 0{,}043$, $w = 1$, $(\Delta/\sigma)_{max}$ du dernier cycle d'affinement $= 0{,}126$. Pour le dernier calcul de Fourier différence, $(\Delta\rho)_{max} = 0{,}15$, $(\Delta\rho)_{min} = -0{,}14$ e Å^{-3}. Facteurs de diffusion atomique issue de *SHELX*76.*

La molécule est représentée Fig. 1. Les coordonnées atomiques sont rassemblées dans le Tableau 1, les longueurs de liaison et les angles de valence dans le Tableau 2. L'examen des angles dièdres montre que cette molécule, constituée de deux cycles à six chaînons accolés par une jonction *cis*, possède une conformation chaise de la partie cyclohexanique et une conformation demi-chaise légèrement applatie pour la partie cyclohexénique (Bucourt, 1974; Viani, Lapasset, Aycard & Bodot, 1979). La valeur non nulle de l'angle autour de la double liaison [$\varphi_{89} = -1{,}1$ (4)°] est analogue à celle observée par Viani (1978) lors de l'étude du diméthyl-1,2 cyclohexènedicarbonitrile-4,5-*trans* (1,5°).

L'analyse de l'empilement montre une organisation antiparallèle des différents dipôles de la molécule susceptible de minimiser les interactions dipôle–dipôle intermoléculaire.

* Les listes des facteurs de structure, des coordonnées des atomes d'hydrogènes, des facteurs d'agitation thermique, des courtes distances interatomiques, ainsi que la figure de l'empilement moléculaire vu selon **b** mettant en évidence les interactions avec les hydrogènes ont été déposés au dépôt d'archives de la British Library Document Supply Centre (Supplementary Publication No. SUP 44197: 21 pp.). On peut en obtenir des copies en s'adressant à: The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, Angleterre.

Références

BUCOURT, R. (1974). *Top. Stereochem.* **8**, 159–224.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN*80. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. de York, Angleterre, et Louvain, Belgique.

SHELDRICK, G. M. (1976). *SHELX*76. Programme pour la détermination des structures cristallines. Univ. de Cambridge, Angleterre.

VIANI, R. (1978). Doctorat ès Sciences Physiques. Univ. de Provence (Marseille), France.

VIANI, R., LAPASSET, J., AYCARD, J. P. & BODOT, H. (1979). *J. Org. Chem.* **44**, 889–902.

Acta Cryst. (1987). C**43**, 2249–2250

Structure of 1,2-Di(nicotinoylamino)propane Monohydrate

BY YOSHIHARU NAWATA,* HITOSHI KUBONIWA, MASATOSHI HANEDA AND KIYOSHIGE OCHI

Research Laboratories, Chugai Pharmaceutical Co. Ltd, Takada, Toshima, Tokyo 171, *Japan*

(*Received* 22 *May* 1987; *accepted* 26 *June* 1987)

Abstract. *N,N'*-(Propane-1,2-diyl)dinicotinamide monohydrate, $C_{15}H_{16}N_4O_2.H_2O$, $M_r = 302{\cdot}3$, monoclinic, $P2_1/n$, $a = 16{\cdot}960$ (1), $b = 11{\cdot}311$ (1), $c = 7{\cdot}741$ (1) Å, $\beta = 100{\cdot}50$ (4)°, $V = 1460{\cdot}0$ Å^3, $Z = 4$, $D_x = 1{\cdot}375$ g cm^{-3}, λ(Cu $K\alpha$) $= 1{\cdot}5418$ Å, $\mu = 7{\cdot}7$ cm^{-1}, $F(000) = 640$, $T = 298$ K, final $R = 0{\cdot}045$ for 2498 unique reflections [$F_o^2 > 2\sigma(F_o^2)$]. The title compound adopts a *trans* (*Z*) conformation. Adjacent molecules, related by a center of symmetry, form a dimer by intermolecular hydrogen bonds through their amide groups, making a 14-membered ring, the O···N distance being 3·026 (2) Å. The H_2O molecule serves to stabilize the crystal structure by three hydrogen bonds.

Experimental. Colorless prisms of the title compound grew from an aqueous solution. Crystal size 0·50 × 0·23 × 0·08 mm, Enraf–Nonius CAD-4 κ-cradle diffractometer, Cu $K\alpha$ radiation, graphite monochromator, θ–2θ scan with scan speed 0·55–8·24° min^{-1} in θ, scan width (0·60 + 0·14tanθ)°. Range of indices, $-21 \le h \le 21$, $0 \le k \le 14$, $0 \le l \le 9$ ($2\theta < 150$°). Lattice constants determined based on 25 2θ values ($21 < 2\theta < 58$°). Variation of standard < 4·5%; 3008 reflections measured; 2546 observed reflections with $|F_o| > 2\sigma(|F_o|)$. Systematic absences *h*0*l*, *h*+*l* odd; 0*k*0, *k* odd. No corrections for absorption. Structure solved by direct methods with *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). Refined by full-matrix least squares. All H atoms found from difference synthesis. Non-H atoms refined with anisotropic thermal parameters, and H atoms with isotropic thermal parameters. $\sum w(|F_o| - |F_c|)^2$ minimized; $w = 1{\cdot}0$ for $F_o < 1341{\cdot}2$, $w = (1341{\cdot}2/F_o)^2$ for $F_o \ge 1341{\cdot}2$. Final R

* To whom all correspondence should be addressed.

0108-2701/87/112249-02$01.50

Table 1. *Final fractional coordinates and equivalent isotropic temperature factors for non-H atoms with e.s.d.'s in parentheses*

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

	x	y	z	B_{eq}(Å^2)
N(1)	0·1242 (1)	0·1971 (2)	0·9721 (3)	4·56 (5)
C(2)	0·1987 (2)	0·1844 (2)	0·9425 (4)	3·72 (5)
C(3)	0·2423 (1)	0·2739 (2)	0·8807 (3)	2·68 (4)
C(4)	0·2051 (1)	0·3826 (2)	0·8424 (3)	3·13 (5)
C(5)	0·1272 (2)	0·3970 (3)	0·8693 (4)	3·78 (6)
C(6)	0·0900 (2)	0·3038 (3)	0·9356 (4)	4·22 (6)
C(7)	0·3254 (1)	0·2452 (2)	0·8553 (3)	2·91 (5)
O(8)	0·3457 (1)	0·1410 (2)	0·8401 (3)	4·07 (4)
N(9)	0·3758 (1)	0·3362 (2)	0·8486 (3)	3·08 (4)
C(10)	0·4556 (1)	0·3178 (2)	0·8048 (3)	3·03 (5)
C(11)	0·4816 (2)	0·4275 (2)	0·7184 (4)	3·72 (5)
C(12)	0·5145 (1)	0·2815 (2)	0·9688 (3)	3·10 (5)
N(13)	0·5921 (1)	0·2478 (2)	0·9286 (3)	2·98 (4)
C(14)	0·6552 (1)	0·3207 (2)	0·9509 (3)	2·85 (5)
O(15)	0·6529 (1)	0·4230 (2)	1·0042 (3)	3·92 (4)
C(16)	0·7310 (1)	0·2722 (2)	0·9046 (3)	2·73 (4)
C(17)	0·7907 (1)	0·3520 (2)	0·8847 (4)	3·36 (5)
N(18)	0·8606 (1)	0·3216 (2)	0·8406 (3)	3·81 (5)
C(19)	0·8726 (1)	0·2057 (3)	0·8157 (4)	3·72 (6)
C(20)	0·8175 (2)	0·1198 (2)	0·8338 (4)	3·87 (6)
C(21)	0·7453 (1)	0·1527 (2)	0·8784 (4)	3·42 (5)
O(22)	0·5700 (1)	−0·0021 (2)	0·8592 (3)	5·26 (5)

Table 2. *Bond lengths* (Å) *and angles* (°) *with their e.s.d.'s in parentheses*

N(1)–C(2)	1·332 (4)	C(10)–C(12)	1·521 (3)
N(1)–C(6)	1·346 (4)	C(12)–N(13)	1·457 (3)
C(2)–C(3)	1·390 (4)	N(13)–C(14)	1·336 (3)
C(3)–C(4)	1·388 (3)	C(14)–O(15)	1·232 (3)
C(3)–C(7)	1·494 (3)	C(14)–C(16)	1·500 (3)
C(4)–C(5)	1·384 (4)	C(16)–C(17)	1·386 (3)
C(5)–C(6)	1·376 (4)	C(16)–C(21)	1·394 (4)
C(7)–O(8)	1·239 (3)	C(17)–N(18)	1·337 (3)
C(7)–N(9)	1·344 (3)	N(18)–C(19)	1·346 (4)
N(9)–C(10)	1·469 (3)	C(19)–C(20)	1·373 (4)
C(10)–C(11)	1·512 (4)	C(20)–C(21)	1·381 (4)
C(2)–N(1)–C(6)	116·5 (3)	C(11)–C(10)–C(12)	113·0 (2)
N(1)–C(2)–C(3)	124·2 (2)	C(10)–C(12)–N(13)	112·0 (2)
C(2)–C(3)–C(4)	118·0 (2)	C(12)–N(13)–C(14)	123·0 (2)
C(2)–C(3)–C(7)	117·4 (2)	N(13)–C(14)–O(15)	123·4 (2)
C(4)–C(3)–C(7)	124·5 (2)	N(13)–C(14)–C(16)	116·4 (2)
C(3)–C(4)–C(5)	118·7 (2)	O(15)–C(14)–C(16)	120·2 (2)
C(4)–C(5)–C(6)	118·8 (3)	C(14)–C(16)–C(17)	117·6 (2)
N(1)–C(6)–C(5)	123·7 (3)	C(14)–C(16)–C(21)	124·7 (2)
C(3)–C(7)–O(8)	120·3 (2)	C(17)–C(16)–C(21)	117·7 (2)
C(3)–C(7)–N(9)	117·4 (2)	C(16)–C(17)–N(18)	124·1 (2)
O(8)–C(7)–N(9)	122·3 (2)	C(17)–N(18)–C(19)	116·8 (2)
C(7)–N(9)–C(10)	121·3 (2)	N(18)–C(19)–C(20)	123·4 (3)
N(9)–C(10)–C(11)	109·9 (2)	C(19)–C(20)–C(21)	119·0 (3)
N(9)–C(10)–C(12)	109·7 (2)	C(16)–C(21)–C(20)	118·9 (2)

$= 0·045$, $wR = 0·052$, $S = 6·44$ for 272 variables; secondary-extinction factor (g) 1·48 (2) × 10^{-6} [$|F_o| = |F_c|/(1+gI_c)$]; $\Delta/\sigma < 0·1$; largest peak in final ΔF map +0·19 e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); programs: Enraf–Nonius *SDP* (Frenz, 1984), *ORTEP*II (Johnson, 1976). The structure of the title compound is shown in Fig. 1, the crystal structure in Fig. 2. Positional parameters and equivalent values of the anisotropic temperature factors are given in Table 1, bond distances and angles in Table 2.*

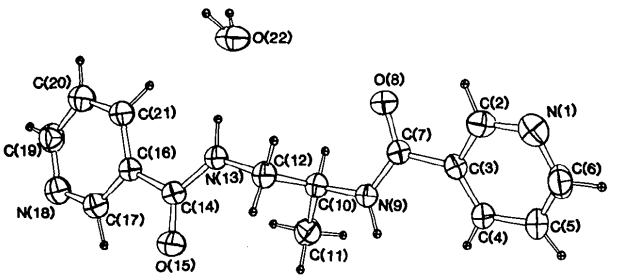

Fig. 1. A perspective view of the molecule with the numbering scheme.

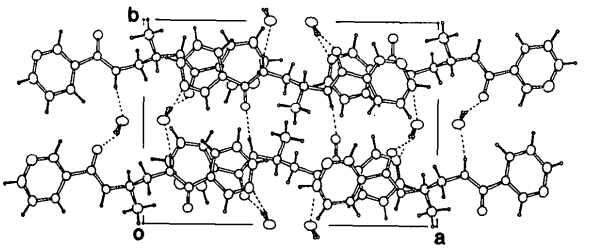

Fig. 2. Crystal structure projected along the c axis. Hydrogen bonds are indicated by dotted lines.

Related literature. Title compound has anti-thrombotic activity (Mizukami *et al.*, 1984). For the preparation see Mori *et al.* (1981).

* Lists of anisotropic thermal parameters, H-atom parameters, torsional angles and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44191 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

FRENZ, B. A. (1984). *Enraf–Nonius Structure Determination Package*. College Station, Texas, USA, and Enraf–Nonius, Delft, The Netherlands.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press. (Present distributor D. Reidel, Dordrecht.)

JOHNSON, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1982). *MULTAN*11/82. *A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.

MIZUKAMI, M., NEICHI, T., YAMAZAKI, T., KOIDE, T., NODA, Y., MATSUSHITA, H., HATA, S. & NAKANO, M. (1984). *Arzneim Forsch.* **34**(II), 764–768.

MORI, M., TAKAKU, S., MATSUURA, F., MURAKAMI, Y., NODA, Y., YAMAZAKI, T., NEICHI, T., NAKAKIMURA, H., KATAOKA, S., MATSUNO, T., HATA, S. & TAKANASHI, S. (1981). Kokai Tokkyo Koho (Japanese Patent), No. 56–75474.