Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1068). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Dickens, J. P., Dyer, R. L., Hamil, B. J., Harrow, T. A., Bibler, R. H., Jr, Finnegan, P. M., Hendrick, K. & Owston, P. G. (1981). *J. Org. Chem.* **46**, 1781.

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

Nardelli, M. (1983). *Comput. Chem.* **7**, 95-98.

Rizzoli, C., Sangermano, V., Calestani, G. & Andreetti, G. D. (1989). *CRYSRULER*. Version 2.0. Univ. degli Studi di Parma, Italy.

Sheldrick, G. M. (1976). *SHELX*76. *Program for Crystal Structure Determination*. Univ. of Cambridge, England.

Sheldrick, G. M. (1985). *SHELXS*86. *Program for the Solution of Crystal Structures*. Univ. of Göttingen, Germany.

Stoe & Cie (1992*a*). *DIF*4. *Diffractometer Control Program*. Version 7.03. Stoe & Cie, Darmstadt, Germany.

Stoe & Cie (1992*b*). *REDU*4. *Data Reduction Program*. Version 7.03. Stoe & Cie, Darmstadt, Germany.

Acta Cryst. (1994). C**50**, 921–922

2-(5-Nitro-2-styryl-1-imidazolyl)ethanol

TOMASZ A. OLSZAK, OSWALD M. PEETERS, NORBERT M. BLATON AND CAMIEL J. DE RANTER

Laboratorium voor Analytische Chemie en Medicinale Fysicochemie, Faculteit Farmaceutische Wetenschappen, Katholieke Universiteit Leuven, Van Evenstraat 4, B-3000 Leuven, Belgium

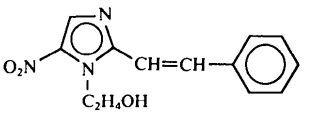
(*Received* 22 *September* 1993; *accepted* 8 *November* 1993)

Abstract

The molecules of the title compound, $C_{13}H_{13}N_3O_3$, are linked in chains through hydrogen bonds along the *a* direction.

Comment

The perspective view of the title compound (I) showing the atom-numbering scheme and hydrogen bonding is given in Fig. 1. The crystal contains well ordered molecules of 2-(5-nitro-2-styryl-1-imidazolyl)ethanol in the form previously observed in crystals of 2-(2-methyl-5-nitro-1-imidazolyl)ethanol (metronidazole) (Blaton, Peeters & De Ranter, 1979). The bond lengths and angles are in good agreement to within 0.005 Å and 1.6°, respectively, with those observed in metronidazole. More significant deviations are observed for C2—N3 (longer by 0.012 Å) and C2—C21 (shorter by 0.027 Å). These differences are undeniably a result of the conjugation effect between the C2—C21 single bond and the neighbouring C2=N3 and C21=C22 double bonds.



(I)

The five-membered ring is planar within 0.003 (2) Å. The nitro-group plane crosses the weighted least-squares imidazole plane at an angle of 4.7 (1)°. The benzene ring is planar and its weighted least-squares plane forms a dihedral angle of 5.7 (1)° with the imidazole plane. Although the molecule was expected to be planar except for the ethanol moiety, twisting is observed around the C2—C21 bond [N3—C2—C21—C22 21.9 (3)°]. This is probably caused by the molecular crowding or packing effects.

The molecules of the title compound are linked through O13—H13···N3^{i} hydrogen bonds [1.99 (3) Å, 166 (2)°; symmetry code: (i) $x-1, y, z$] forming chains along the *a* direction. Although for both the title compound and metronidazole (Blaton *et al.*, 1979) the same atoms are engaged in hydrogen bonding, the hydrogen-bonding patterns are different. This results in significant differences in the orientation of the ethanol moiety. The values of the torsion angle C5—N1—C11—C12 for the title molecule and metronidazole (Blaton *et al.*, 1979) are −106.8 (2) and 82.6 (2)°, respectively.

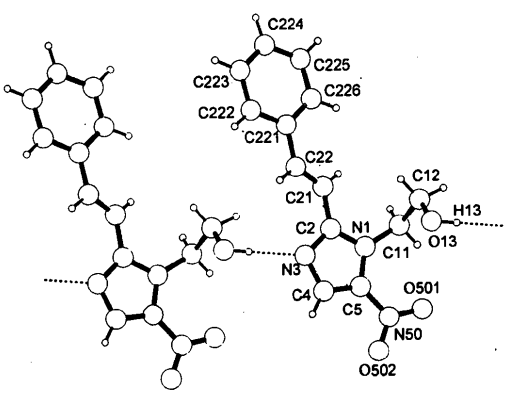


Fig. 1. The atomic numbering scheme and hydrogen bonding.

Experimental

Crystal data

$C_{13}H_{13}N_3O_3$
M_r = 259.26
Monoclinic
$P2_1/c$
a = 7.088 (1) Å
b = 7.116 (1) Å
c = 24.935 (3) Å
β = 95.03 (1)°

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 40 reflections
θ = 10.38–12.48°
μ = 0.094 mm^{-1}
T = 293 K
Prism

V = 1252.8 (3) Å^3
Z = 4
D_x = 1.375 Mg m^{-3}
0.30 × 0.30 × 0.20 mm
Light yellow

Data collection

Stoe Stadi-4 four-circle diffractometer
ω scans
Absorption correction: none
5956 measured reflections
2879 independent reflections
2014 observed reflections [$I > 2.0\sigma(I)$]
R_{int} = 0.012
θ_{max} = 27.5°
$h = -9 \rightarrow 9$
$k = -9 \rightarrow 9$
$l = 0 \rightarrow 32$
3 standard reflections
frequency: 60 min
intensity variation: 3.0%

Refinement

Refinement on F
R = 0.0361
wR = 0.0577
S = 0.970
2014 reflections
224 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F) + 0.003F^2]$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *CRYSRULER* (Rizzoli, Sangermano, Calestani & Andreetti, 1989)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
N1	0.4152 (2)	0.1911 (2)	0.0450 (1)	0.0327 (3)
C11	0.2481 (2)	0.1100 (2)	0.0676 (1)	0.0405 (5)
C12	0.1434 (2)	0.2555 (3)	0.0977 (1)	0.0473 (5)
O13	0.0892 (2)	0.4119 (2)	0.0656 (1)	0.0563 (4)
C2	0.5749 (2)	0.2478 (2)	0.0748 (1)	0.0336 (4)
C21	0.6021 (2)	0.2243 (2)	0.1328 (1)	0.0383 (4)
C22	0.7256 (2)	0.3236 (2)	0.1644 (1)	0.0391 (4)
C221	0.7616 (2)	0.3009 (2)	0.2229 (1)	0.0398 (4)
C222	0.9276 (3)	0.3713 (2)	0.2490 (1)	0.0515 (6)
C223	0.9714 (3)	0.3451 (3)	0.3036 (1)	0.0618 (7)
C224	0.8482 (3)	0.2507 (3)	0.3334 (1)	0.0602 (6)
C225	0.6807 (3)	0.1840 (3)	0.3089 (1)	0.0631 (7)
C226	0.6366 (3)	0.2078 (3)	0.2541 (1)	0.0557 (6)
N3	0.7010 (2)	0.3226 (2)	0.0438 (1)	0.0375 (3)
C4	0.6206 (2)	0.3132 (2)	−0.0072 (1)	0.0378 (4)
C5	0.4451 (2)	0.2342 (2)	−0.0075 (1)	0.0342 (4)
N50	0.3158 (2)	0.2043 (2)	−0.0534 (1)	0.0438 (4)
O501	0.1575 (2)	0.1436 (3)	−0.0486 (1)	0.0761 (6)
O502	0.3727 (2)	0.2415 (2)	−0.0972 (1)	0.0678 (5)

Table 2. *Selected geometric parameters* (Å, °)

N1—C11	1.473 (2)	C221—C226	1.396 (3)
N1—C2	1.360 (2)	C222—C223	1.382 (3)
N1—C5	1.379 (2)	C223—C224	1.371 (3)
C11—C12	1.511 (2)	C224—C225	1.371 (3)
C12—O13	1.405 (2)	C225—C226	1.385 (3)
O13—H13	0.86 (2)	N3—C4	1.349 (2)
C2—C21	1.452 (3)	C4—C5	1.365 (2)
C2—N3	1.342 (2)	C5—N50	1.418 (2)
C21—C22	1.329 (2)	N50—O501	1.218 (2)
C22—C221	1.468 (3)	N50—O502	1.226 (2)
C221—C222	1.387 (2)		
C2—N1—C5	105.2 (1)	C221—C222—C223	121.4 (2)
C11—N1—C5	130.2 (1)	C222—C223—C224	120.1 (2)
C11—N1—C2	124.5 (1)	C223—C224—C225	119.7 (2)
N1—C11—C12	111.6 (1)	C224—C225—C226	120.6 (2)
C11—C12—O13	112.4 (2)	C221—C226—C225	120.6 (2)
C12—O13—H13	107 (2)	C2—N3—C4	106.0 (1)
N1—C2—N3	111.6 (1)	N3—C4—C5	109.6 (2)
N1—C2—C21	122.8 (1)	N1—C5—C4	107.6 (2)
C21—C2—N3	125.6 (2)	C4—C5—N50	126.2 (2)
C2—C21—C22	123.5 (2)	N1—C5—N50	126.2 (1)
C21—C22—C221	125.4 (2)	C5—N50—O502	116.5 (2)
C22—C221—C226	122.8 (2)	C5—N50—O501	120.6 (2)
C22—C221—C222	119.5 (2)	O501—N50—O502	122.8 (2)
C222—C221—C226	117.6 (2)		

Data collection: *DIF*4 (Stoe & Cie, 1992*a*). Cell refinement: *DIF*4. Data reduction: *REDU*4 (Stoe & Cie, 1992*b*). Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELX*76 (Sheldrick, 1976). Molecular graphics: *PLUTON*93 (Spek, 1993). Software used to prepare material for publication: *PARST* (Nardelli, 1983).

The authors thank Eli Lilly, Benelux, Brussels, for providing the crystals. One of them (TAO) is indebted to the Research Council of the Katholieke Universiteit Leuven, Belgium, for Senior Fellowship No. F/92/32.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1069). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Blaton, N. M., Peeters, O. M. & De Ranter, C. J. (1979). *Acta Cryst.* B**35**, 2465-2467
Nardelli, M. (1983). *Comput. Chem.* **7**, 95-98.
Rizzoli, C., Sangermano, V., Calestani, G. & Andreetti, G. D. (1989). *CRYSRULER*. Version 2.0. Univ. degli Studi di Parma, Italy.
Sheldrick, G. M. (1976). *SHELX*76. *Program for Crystal Structure Determination*. Univ. of Cambridge, England.
Sheldrick, G. M. (1985). *SHELXS*86. *Program for the Solution of Crystal Structures*. Univ. of Göttingen, Germany.
Spek, A. L. (1993). *PLUTON*93. Univ. of Utrecht, The Netherlands.
Stoe & Cie (1992*a*). *DIF*4. *Diffractometer Control Program*. Version 7.03. Stoe & Cie, Darmstadt, Germany.
Stoe & Cie (1992*b*). *REDU*4. *Data Reduction Program*. Version 7.03. Stoe & Cie, Darmstadt, Germany.

Acta Cryst. (1994). C**50**, 922–924

Isopropyl Hydrogen 9,10-Dihydro-9,10-ethenoanthracene-11,12-dicarboxylate

PHANI RAJ POKKULURI, JOHN R. SCHEFFER AND JAMES TROTTER

Department of Chemistry, University of British Columbia, Vancouver, BC, Canada V6T 1Z1

(*Received* 12 *August* 1993; *accepted* 14 *December* 1993)

Abstract

The title compound, $C_{21}H_{18}O_4$, exists in the crystal as hydrogen-bonded dimers, O—H···O = 2.669 (3) Å. The molecule has normal dimensions. The C=O bond