Refinement

Refinement on F
$R = 0.0370$
$wR = 0.0424$
$S = 1.913$
1095 reflections
100 parameters
H-atom parameters not refined
$w = 4F^2/\sigma^2(F^2)$
$(\Delta/\sigma)_{\max} = 0.0072$
$\Delta\rho_{\max} = 0.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

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

	x	y	z	$U_{\rm eq}$
O(1)	0.1941 (2)	−0.1448 (2)	0.68535 (6)	0.0435 (3)
O(2)	−0.0589 (2)	0.0916 (2)	0.68345 (7)	0.0554 (4)
O(3)	−0.0157 (2)	0.0357 (2)	0.60615 (6)	0.0474 (4)
N(1)	−0.2140 (4)	−0.4225 (3)	0.5738 (1)	0.0811 (7)
C(1)	−0.0464 (4)	−0.3452 (3)	0.5674 (1)	0.0540 (6)
C(2)	0.1650 (3)	−0.2412 (3)	0.5580 (1)	0.0483 (5)
C(3)	0.1907 (3)	−0.0758 (2)	0.61182 (9)	0.0382 (4)
C(4)	0.3927 (3)	0.0512 (3)	0.6000 (1)	0.0509 (5)
C(5)	0.3898 (3)	0.2202 (3)	0.6529 (1)	0.0580 (6)
C(6)	0.3273 (3)	0.1604 (3)	0.7298 (1)	0.0537 (6)
C(7)	0.1349 (3)	0.0195 (3)	0.72563 (10)	0.0467 (5)

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

O(1)—C(3)	1.408 (2)	C(1)—C(2)	1.459 (3)
O(1)—C(7)	1.414 (2)	C(2)—C(3)	1.515 (2)
O(2)—O(3)	1.478 (2)	C(3)—C(4)	1.509 (2)
O(2)—C(7)	1.435 (2)	C(4)—C(5)	1.522 (3)
O(3)—C(3)	1.445 (2)	C(5)—C(6)	1.508 (3)
N(1)—C(1)	1.136 (2)	C(6)—C(7)	1.503 (3)
C(3)—O(1)—C(7)	102.0 (1)	O(3)—C(3)—C(4)	109.6 (1)
O(3)—O(2)—C(7)	103.8 (1)	C(2)—C(3)—C(4)	114.9 (1)
O(2)—O(3)—C(3)	104.8 (1)	C(3)—C(4)—C(5)	110.0 (1)
N(1)—C(1)—C(2)	178.3 (2)	C(4)—C(5)—C(6)	111.5 (2)
C(1)—C(2)—C(3)	111.9 (1)	C(5)—C(6)—C(7)	110.5 (2)
O(1)—C(3)—O(3)	103.3 (1)	O(1)—C(7)—O(2)	103.0 (1)
O(1)—C(3)—C(2)	109.5 (1)	O(1)—C(7)—C(6)	111.1 (1)
O(1)—C(3)—C(4)	110.9 (1)	O(2)—C(7)—C(6)	112.0 (2)
O(3)—C(3)—C(2)	108.0 (1)		

In the weighting scheme $\sigma^2(F^2) = S^2(C + R^2B) + (0.04F^2)^2/{\rm Lp}^2$, where S = scan rate, C = total integrated peak count, R = ratio of scan to background counting times, B = total background count and Lp = Lorentz–polarization factor.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992*a*). Cell refinement: *MSC/AFC Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1992*b*). Program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994). Program(s) used to refine structure: *TEXSAN*. Software used to prepare material for publication: *TEXSAN*.

Financial support from the Jacob A. and Frieda M. Hunkele Charitable Trust and the Kresge Foundation is gatefully acknowledged.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: BK1178). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1996). C**52**, 1014–1017

Two Schiff Base Ligands Derived from 1,2-Diaminocyclohexane

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(*Received 17 July 1995; accepted 10 October 1995*)

Abstract

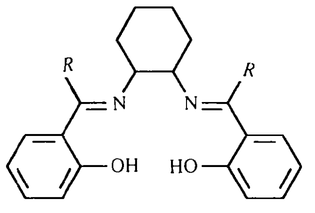
The crystal structures of the free ligands 2,2′-[(1,2-cyclohexanediyl)bis(nitrilomethylidyne)]bisphenol, $C_{20}H_{22}N_2O_2$, (I), and 2,2′-[(1,2-cyclohexanediyl)bis(nitriloethylidyne)]bisphenol, $C_{22}H_{26}N_2O_2$, (II), have been determined. In both molecules the N—O distances are indicative of intramolecular hydrogen bonding. In compound (I), the two aromatic rings are inclined at an angle of 56.5 (1)° and the O···O separation is 6.082 (3) Å; in compound (II) the corresponding values are 83.15 (8)° and 5.544 (5) Å. Thus, it is evident that the methyl groups in (II) have a very significant effect upon the overall conformation.

Comment

Relatively few crystal structures have been reported for quadridentate Schiff base ligands (Corden, Errington,

Acta Crystallographica Section C
ISSN 0108-2701 ©1996

Moore & Wallbridge, 1996). Investigations within these laboratories into the coordination chemistry of the ligands (I) and (II) have prompted us to determine the structures of these free ligands, so that subsequent changes resulting from the coordination of a metal ion may be identified.



(I) *R* = H
(II) *R* = Me

The molecular structures of these two ligands are represented in Figs. 1 and 2. The bond lengths and angles, while unexceptional, clearly indicate that the enolimine tautomer is favoured. Furthermore, the shortest N—O distances [average 2.604 (3) Å for (I); average 2.515 (3) Å for (II)] are indicative of intramolecular hydrogen bonding. Although structure (I) is non-centrosymmetric, both enantiomers are present; structure (II) is centrosymmetric.

Perhaps the most interesting comparative aspect of these two structures involves the influence of the methyl groups upon the molecular conformation. While several of the corresponding torsion angles are very similar, a large difference is noted between C7—N1—C9—C14 and C7—N1—C8—C13; the cumulative effect of the differences is that the orientation of the two aromatic rings is 56.5 (1)° in (I), but 83.15 (8)° in (II). An alternative way of expressing the significant differences between the conformations of the two molecules is to note that the O atoms are 6.082 (3) Å apart in (I), but only 5.544 (5) Å apart in (II). The overall situation is represented in Fig. 3 in which the cyclohexane rings have been superimposed for the two molecules to show the lack of coincidence in the 'wings' of the molecules.

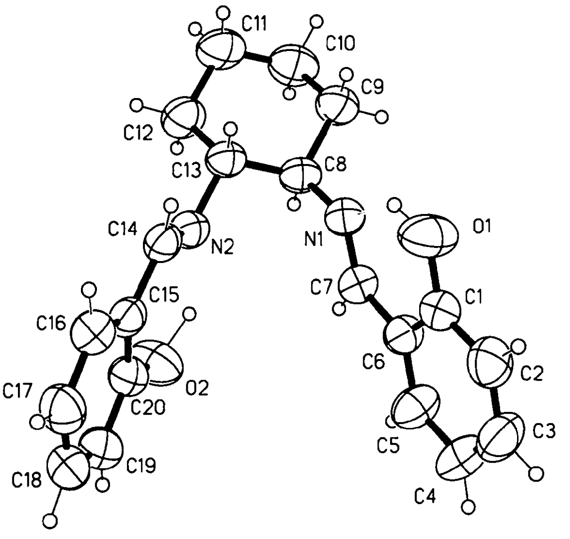


Fig. 1. View of molecule (I) showing the atomic numbering. Displacement ellipsoids are drawn at the 50% probability level.

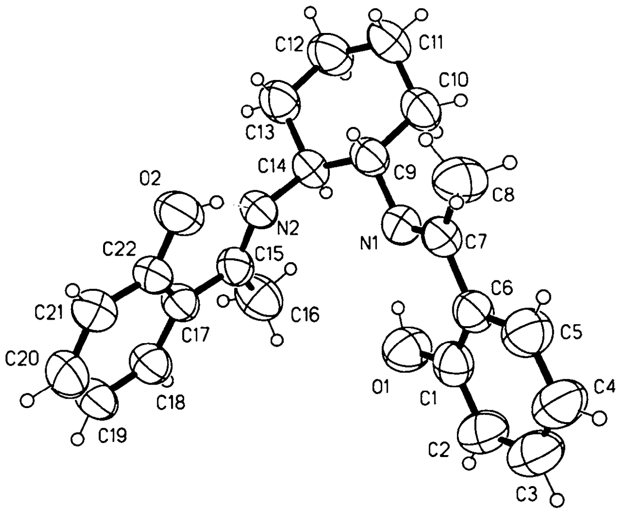


Fig. 2. View of molecule (II) showing the atomic numbering. Displacement ellipsoids are drawn at the 50% probability level.

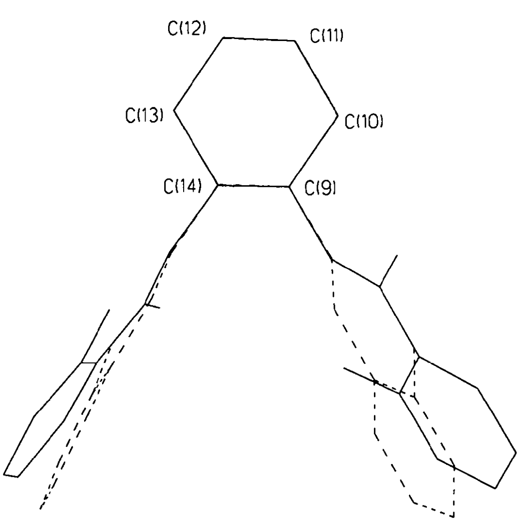


Fig. 3. Superposition of the two molecules with respect to the cyclohexane rings. The atomic numbering refers to structure (II).

Experimental

Compound (I) was prepared by the condensation of salicylaldehyde (150 mmol) with *trans*-1,2-diaminocyclohexane in 100 ml of methanol. The reaction mixture was stirred at 298 K for 20 min and then placed in a freezer for 1 h. The yellow precipitate was collected by filtration, washed with dry diethyl ether and dried *in vacuo*. Crystals of X-ray quality were obtained by the slow evaporation of a saturated methanolic solution.

Compound (II) was prepared by the condensation of 2-hydroxyacetophenone (74 mmol in 100 ml methanol) with *trans*-1,2-diaminocyclohexane (37 mmol in 40 ml methanol). The reaction mixture was stirred at 323 K for 1 h and then cooled to 253 K for 3 h. The bright yellow precipitate was washed and dried *in vacuo*. Crystals suitable for X-ray diffraction were obtained by slow evaporation from a saturated methanolic solution.

Compound (I)

Crystal data

$C_{20}H_{22}N_2O_2$
$M_r = 322.40$
Monoclinic
Cc
$a = 16.013\,(6)$ Å
$b = 11.860\,(6)$ Å
$c = 9.643\,(2)$ Å
$\beta = 98.50\,(2)°$
$V = 1811.2\,(12)$ Å^3
$Z = 4$
$D_x = 1.182$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 250 reflections
$\theta = 2.15$–$25.00°$
$\mu = 0.077$ mm^{-1}
$T = 293\,(2)$ K
Block
0.28 × 0.16 × 0.14 mm
Yellow

Data collection

Delft Instruments FAST TV area-detector diffractometer
Flat-plate detector
Absorption correction: none
3417 measured reflections
1936 independent reflections

1728 observed reflections $[I > 2\sigma(I)]$
$R_{\rm int} = 0.0461$
$\theta_{\rm max} = 25.02°$
$h = -17 \rightarrow 16$
$k = -13 \rightarrow 12$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0436$
$wR(F^2) = 0.1219$
$S = 1.022$
1932 reflections
217 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = -0.001$

$\Delta\rho_{\rm max} = 0.153$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.141$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)
Absolute configuration: Flack (1983) parameter = 1.4 (18)

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

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

	x	y	z	$U_{\rm eq}$
O1	1.0259 (2)	0.2372 (2)	−0.1151 (2)	0.0865 (7)
O2	0.8539 (2)	0.1559 (2)	0.3976 (2)	0.0845 (7)
N1	0.89210 (15)	0.1387 (2)	−0.0487 (2)	0.0556 (6)
N2	0.7976 (2)	0.2349 (2)	0.1494 (2)	0.0540 (6)
C1	1.0726 (2)	0.1683 (2)	−0.0234 (3)	0.0580 (7)
C2	1.1599 (2)	0.1739 (3)	−0.0062 (3)	0.0736 (9)
C3	1.2079 (2)	0.1053 (3)	0.0885 (4)	0.0784 (9)
C4	1.1704 (2)	0.0303 (3)	0.1688 (4)	0.0811 (10)
C5	1.0836 (2)	0.0227 (3)	0.1522 (3)	0.0709 (8)
C6	1.0326 (2)	0.0899 (2)	0.0559 (3)	0.0546 (7)
C7	0.9416 (2)	0.0787 (2)	0.0372 (3)	0.0539 (6)
C8	0.8011 (2)	0.1204 (2)	−0.0594 (3)	0.0542 (7)
C9	0.7620 (2)	0.1021 (3)	−0.2118 (3)	0.0676 (8)
C10	0.6676 (2)	0.0849 (3)	−0.2245 (4)	0.0795 (9)
C11	0.6249 (2)	0.1821 (3)	−0.1601 (3)	0.0750 (9)
C12	0.6650 (2)	0.2028 (3)	−0.0086 (3)	0.0700 (8)
C13	0.7596 (2)	0.2206 (2)	0.0021 (3)	0.0529 (7)
C14	0.8311 (2)	0.3288 (2)	0.1894 (3)	0.0498 (6)
C15	0.8746 (2)	0.3473 (2)	0.3306 (3)	0.0506 (7)
C16	0.9080 (2)	0.4527 (2)	0.3702 (3)	0.0587 (7)
C17	0.9563 (2)	0.4695 (3)	0.5003 (3)	0.0673 (8)
C18	0.9702 (2)	0.3800 (3)	0.5923 (3)	0.0685 (9)
C19	0.9359 (2)	0.2760 (3)	0.5576 (3)	0.0681 (9)
C20	0.8874 (2)	0.2588 (2)	0.4284 (3)	0.0574 (7)

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

O1—C1	1.347 (4)	N2—C13	1.470 (4)
O2—C20	1.348 (3)	C6—C7	1.447 (4)
N1—C7	1.276 (3)	C8—C13	1.524 (4)
N1—C8	1.462 (4)	C14—C15	1.452 (4)
N2—C14	1.270 (3)		
C7—N1—C8	118.7 (2)	N1—C8—C13	110.2 (2)
C14—N2—C13	119.4 (2)	N2—C13—C8	108.9 (2)
O1—C1—C6	120.1 (2)	N2—C14—C15	122.6 (2)
N1—C7—C6	123.2 (2)	O2—C20—C15	120.9 (3)
O1—C1—C6—C7	2.4 (4)	N1—C8—C13—N2	−58.6 (3)
C8—N1—C7—C6	−180.0 (2)	C13—N2—C14—C15	−175.9 (2)
C1—C6—C7—N1	−1.1 (4)	N2—C14—C15—C20	4.8 (4)
C7—N1—C8—C13	110.0 (3)	C14—C15—C20—O2	−5.2 (4)
C14—N2—C13—C8	123.4 (2)		

Compound (II)

Crystal data

$C_{22}H_{26}N_2O_2$
$M_r = 350.45$
Monoclinic
$P2_1/c$
$a = 11.832\,(9)$ Å
$b = 13.797\,(5)$ Å
$c = 12.954\,(7)$ Å
$\beta = 112.51\,(4)°$
$V = 1953.6\,(20)$ Å^3
$Z = 4$
$D_x = 1.192$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 250 reflections
$\theta = 1.86$–$24.97°$
$\mu = 0.076$ mm^{-1}
$T = 293\,(2)$ K
Block
0.30 × 0.30 × 0.15 mm
Yellow

Data collection

Delft Instruments FAST TV area-detector diffractometer
Flat-plate detector
Absorption correction: none
8708 measured reflections
2965 independent reflections

1134 observed reflections $[I > 2\sigma(I)]$
$R_{\rm int} = 0.0882$
$\theta_{\rm max} = 24.97°$
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 15$
$l = -14 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0451$
$wR(F^2) = 0.2860$
$S = 0.688$
2959 reflections
239 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\rm max} = -0.001$
$\Delta\rho_{\rm max} = 0.185$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.186$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C, Tables 4.2.6.8 and 6.1.1.4)

Table 3. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for (II)*

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

	x	y	z	U_{eq}
O1	0.0234 (2)	0.1323 (2)	0.0819 (2)	0.0892 (7)
O2	−0.4654 (2)	0.23501 (15)	−0.1220 (2)	0.0873 (7)
N1	−0.0929 (2)	0.1855 (2)	−0.1170 (2)	0.0626 (6)
N2	−0.3216 (2)	0.1064 (2)	−0.1349 (2)	0.0649 (7)
C1	0.0817 (3)	0.2181 (2)	0.0971 (3)	0.0676 (8)
C2	0.1739 (3)	0.2354 (3)	0.2011 (3)	0.0827 (10)
C3	0.2380 (3)	0.3206 (3)	0.2212 (3)	0.0954 (11)
C4	0.2107 (3)	0.3905 (3)	0.1390 (3)	0.0971 (11)
C5	0.1189 (3)	0.3736 (2)	0.0370 (3)	0.0851 (10)
C6	0.0519 (3)	0.2878 (2)	0.0115 (3)	0.0615 (7)
C7	−0.0442 (3)	0.2702 (2)	−0.0994 (2)	0.0608 (8)
C8	−0.0800 (3)	0.3517 (2)	−0.1841 (2)	0.0866 (10)
C9	−0.1871 (2)	0.1569 (2)	−0.2258 (2)	0.0615 (8)
C10	−0.1288 (3)	0.1291 (2)	−0.3080 (2)	0.0754 (9)
C11	−0.2254 (3)	0.0974 (2)	−0.4190 (2)	0.0792 (9)
C12	−0.2993 (3)	0.0135 (2)	−0.4037 (2)	0.0885 (10)
C13	−0.3548 (3)	0.0377 (2)	−0.3175 (2)	0.0782 (9)
C14	−0.2588 (2)	0.0727 (2)	−0.2072 (2)	0.0632 (8)
C15	−0.3111 (2)	0.0674 (2)	−0.0414 (3)	0.0618 (8)
C16	−0.2319 (3)	−0.0184 (2)	0.0096 (3)	0.0910 (10)
C17	−0.3833 (3)	0.1107 (2)	0.0170 (2)	0.0616 (8)
C18	−0.3814 (3)	0.0734 (2)	0.1181 (3)	0.0791 (9)
C19	−0.4496 (3)	0.1143 (3)	0.1723 (3)	0.0923 (11)
C20	−0.5215 (3)	0.1930 (3)	0.1276 (3)	0.0947 (12)
C21	−0.5278 (2)	0.2323 (2)	0.0279 (3)	0.0819 (10)
C22	−0.4578 (3)	0.1927 (3)	−0.0265 (2)	0.0683 (9)

Table 4. *Selected geometric parameters (Å, °) for (II)*

O1—C1	1.346 (3)	C6—C7	1.471 (4)
O2—C22	1.340 (3)	C7—C8	1.514 (3)
N1—C7	1.284 (3)	C9—C14	1.512 (3)
N1—C9	1.477 (3)	C15—C17	1.467 (4)
N2—C15	1.288 (3)	C15—C16	1.497 (4)
N2—C14	1.475 (3)		
C7—N1—C9	122.4 (2)	N1—C9—C14	108.5 (2)
C15—N2—C14	125.1 (2)	N2—C14—C9	108.0 (2)
O1—C1—C6	121.7 (3)	N2—C15—C17	116.7 (3)
N1—C7—C6	116.8 (3)	N2—C15—C16	124.3 (3)
N1—C7—C8	124.4 (3)	O2—C22—C17	121.9 (3)
O1—C1—C6—C7	−0.4 (4)	N1—C9—C14—N2	63.1 (3)
C9—N1—C7—C6	−177.7 (2)	C14—N2—C15—C17	−178.8 (2)
C1—C6—C7—N1	−5.3 (3)	N2—C15—C17—C22	−1.7 (4)
C7—N1—C9—C14	−157.9 (2)	C15—C17—C22—O2	−0.5 (4)
C15—N2—C14—C9	−124.0 (3)		

H atoms were added at calculated positions and refined using a riding model. Anisotropic atomic displacement parameters were used for all non-H atoms; each H atom was given an isotropic displacement parameter equal to 1.2 (or 1.5 for methyl and —OH H atoms) times the equivalent isotropic displacement parameter of the atom to which it is attached. For compound (II) the structure was solved by direct methods in *Pc* and then transformed into the space group $P2_1/c$.

For both compounds, data collection: *MADNES* (Pflugrath & Messerschmidt, 1992); cell refinement: *MADNES*; data reduction: *SHELXTL-Plus* (Sheldrick, 1990); program(s) used to solve structures: *SHELXTL-Plus*; program(s) used to refine structures: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *SHELXTL-Plus*; software used to prepare material for publication: *SHELXL*93.

We wish to thank Professor M. Hursthouse and the EPSRC X-ray Crystallographic Service (University of Wales, Cardiff) for collecting the diffraction data. We also wish to acknowledge the use of the EPSRC's Chemical Database Service (Allen *et al.*, 1991) at Daresbury. Financial assistance was provided by BP (JPC) and ICI (JCC).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KA1152). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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8-Hydroxy-7-nitroquinoline-5-sulfonic Acid Monohydrate

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(*Received 3 May 1995; accepted 23 August 1995*)

Abstract

The title compound, $C_9H_6N_2O_6S.H_2O$, is zwitterionic (*i.e.* 8-hydroxy-7-nitroquinolinium-5-sulfonate monohydrate) with a deprotonated sulfonic group and a protonated quinoline N atom which interacts with the hydroxy O atom. The H atom of the hydroxy group is distal to the N atom and is involved in an interaction with an O atom of the nitro group, which is oriented at 32.2 (1)° with respect to the quinoline ring system.

Comment

Derivatives of 8-hydroxyquinoline (oxine) are known for their anti-amoebic, antibacterial and antifungal activities, which can be correlated to their metal chelating

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