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Two Polymorphs of 2-Bis[(2-hydroxyphenylmethylene)amino]methylphenol

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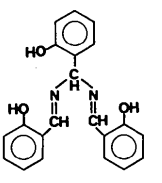
Abstract. $C_{21}H_{18}N_2O_3$, $M_r = 346{\cdot}4$, monoclinic, $C2/c$, $a = 17{\cdot}230\ (3)$, $b = 12{\cdot}322\ (2)$, $c = 19{\cdot}675\ (3)$ Å, $\beta = 121{\cdot}265\ (12)°$, $V = 3571\ (2)$ Å^3, $Z = 8$, $D_x = 1{\cdot}289$ g cm^{-3}, $\lambda(\text{Cu } K\alpha) = 1{\cdot}54184$ Å, $\mu = 6{\cdot}70$ cm^{-1}, $F(000) = 1456$, $T = 296$ K, $R = 0{\cdot}039$ for 3209 observations (of 3691 unique data); triclinic, $P\bar{1}$, $a = 7{\cdot}678\ (2)$, $b = 10{\cdot}822\ (2)$, $c = 12{\cdot}539\ (2)$ Å, $\alpha = 63{\cdot}34\ (2)$; $\beta = 74{\cdot}92\ (2)$; $\gamma = 84{\cdot}04\ (2)°$, $V = 899{\cdot}1\ (4)$ Å^3, $Z = 2$, $D_x = 1{\cdot}279$ g cm^{-3}, $\lambda(\text{Cu } K\alpha) = 1{\cdot}54184$ Å, $\mu = 6{\cdot}65$ cm^{-1}, $F(000) = 364$, $T = 299$ K, $R = 0{\cdot}036$ for 3095 observations (of 3399 unique data). Distances and angles are quite similar in the two structures. There are two strong intramolecular hydrogen bonds between a phenolic oxygen and an imino nitrogen in each structure. The intermolecular hydrogen bonds between two phenolic oxygens are closer in the monoclinic crystal than in the triclinic. This closer packing produces the higher melting point for the monoclinic polymorph.

Introduction. In an effort to synthesize a functionalized imidazole, a reaction of salicylaldehyde with ammonia and glyoxal gave the title compound (I) instead of the desired product. Formation of the title compound was not surprising because aromatic aldehydes react readily with ammonia to give diimine derivatives. (Sandler & Karo, 1971). The title compound had been prepared several times in the past (Ettling, 1840; Herzfeld, 1877; Delepine & Rivals, 1899; Hantzsch, 1906; Liggett & Diehl, 1948; Kamal, Ahmad & Ali Qureshi, 1963; Kambe, Takajo & Satto, 1975) with reported melting points ranging from 431 to 440 K, except Herzfeld's 418 K. Our melting point, 416·5–417 K, agreed with the latter. We repeated the reaction without glyoxal and obtained the higher melting material, which appeared as a different crystalline form. A brief but unsuccessful effort was made to determine the conditions required for formation of one crystalline form over the other. Infrared, ^{1}H NMR, ^{13}C NMR and elemental analyses on the two materials agreed with those reported as well as with each other. These methods did not rule out the possibility of geometric isomers, prompting us to analyze both crystals by X-ray diffraction. Single-crystal X-ray analysis revealed that both imino bonds are *anti* in both crystals; thus we had prepared two polymorphs of the title compound.



(I)

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Experimental. Both crystals isolated from their respective methanolic reaction solutions. Data collected on Enraf–Nonius CAD-4 diffractometer, Cu $K\alpha$ radiation, graphite monochromator, ω–2θ scans designed for $I = 50\sigma(I)$, subject to max. scan time = 180 s, scan rates varied 0·43–3·29° min $^{-1}$.

Triclinic. M.p. 416·5–417 K, crystal size 0·12 × 0·36 × 0·48 mm. Space group by successful refinement of centrosymmetric model; cell dimensions from setting angles of 25 reflections having $27 > \theta > 25°$. Data having $2 \le \theta \le 70°$, $0 \le h \le 9$, $-13 \le k \le 13$, $-15 \le l \le 15$ measured and corrected for background, Lorentz and polarization effects. Absorption corrections were based on ψ scans, with the minimum relative transmission coefficient 93·86%. Periodically remeasured standard reflections exhibited no decay. No redundant data were measured. Structure solved by direct methods, using *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) refined by full-matrix least squares based upon F, using data for which $I > 3\sigma(I)$, weights $w = 4F_o^2[\sigma^2(I) + (0{\cdot}02F_o^2)^2]^{-1}$ using Enraf–Nonius *SDP/VAX* (Frenz, 1978), scattering factors of Cromer & Waber (1974), anomalous coefficients of Cromer (1974), 304 unobserved data. Non-hydrogen atoms refined anisotropically; H atoms located by ΔF synthesis and refined isotropically. Final $R = 0{\cdot}036$, (0·038 for all data), $wR = 0{\cdot}059$, $S = 3{\cdot}94$ for 308 variables. Maximum shift $0{\cdot}01\sigma$ in the final cycle, max. residual density 0·18, min. −0·16 e Å^{-3}, extinction coefficient $g = 9{\cdot}9\ (5) \times 10^{-6}$ [$|F_c| = |F_o|\ (1 + gI_c)$].

Monoclinic. M.p. 436–436·5 K, crystal size 0·36 × 0·40 × 0·48 mm. Space group from systematic absences hkl with $h + k$ odd, $h0l$ with l odd and successful refinement of a centrosymmetric model; cell dimensions from setting angles of 25 reflections having $28 > \theta > 25°$. Data having $2 \le \theta \le 75°$, $0 \le h \le 21$, $0 \le k \le 15$, $-24 \le l \le 24$ measured. Data reduction, solution, and refinement as for triclinic form. Minimum relative transmission 98·04%, $R_{int} = 0{\cdot}008$ over 213 redundant data. Final $R = 0{\cdot}039$, $wR = 0{\cdot}060$, $S = 3{\cdot}53$ for 308 variables. Maximum shift $0{\cdot}01\sigma$ in the final cycle, max. residual density 0·23, min. −0·17 e Å^{-3}, extinction coefficient $g = 3{\cdot}6\ (2) \times 10^{-6}$.

Discussion. The fractional coordinates for the monoclinic crystal are given in Table 1 and those for the triclinic crystal in Table 2.* In Fig. 1, perspective drawings show the atom labels. Distances are presented in Table 3 and angles as well as selected torsion angles are given in Table 4. The only significant differences in distances (> 0·008 Å) are O2–C15, 0·018 (3) and C14–C15, 0·013 (3) Å. The largest differences in angles are N2–C8–C16, 2·7 (1) and

Table 1. *Coordinates and equivalent isotropic thermal parameters for monoclinic form*

	x	y	z	B_{eq}(Å^2)
O1	0·52841 (6)	0·2155 (1)	1·11896 (5)	4·92 (2)
O2	0·34581 (6)	0·24937 (8)	0·72020 (5)	4·46 (2)
O3	0·27476 (6)	0·08881 (8)	0·84414 (5)	4·38 (2)
N1	0·44881 (6)	0·1597 (1)	0·96925 (5)	3·63 (2)
N2	0·38124 (6)	0·11388 (9)	0·82890 (5)	3·17 (2)
C1	0·56411 (8)	0·2996 (1)	1·10005 (7)	4·11 (3)
C2	0·61855 (9)	0·3738 (2)	1·15882 (8)	5·40 (4)
C3	0·6541 (1)	0·4614 (2)	1·1409 (1)	5·99 (4)
C4	0·6379 (1)	0·4768 (2)	1·0645 (1)	5·73 (4)
C5	0·58439 (9)	0·4029 (1)	1·00594 (9)	4·83 (4)
C6	0·54617 (7)	0·3138 (1)	1·02209 (7)	3·77 (3)
C7	0·48764 (7)	0·2400 (1)	0·95822 (6)	3·65 (3)
C8	0·38838 (7)	0·0870 (1)	0·90460 (6)	3·25 (3)
C9	0·39151 (7)	0·0399 (1)	0·78831 (6)	3·17 (2)
C10	0·37894 (7)	0·0637 (1)	0·71122 (6)	3·12 (2)
C11	0·38636 (8)	−0·0197 (1)	0·66640 (7)	4·02 (3)
C12	0·37123 (9)	0·0010 (2)	0·59179 (7)	4·83 (3)
C13	0·34887 (9)	0·1054 (2)	0·56091 (7)	4·81 (4)
C14	0·34089 (9)	0·1888 (1)	0·60342 (7)	4·53 (3)
C15	0·35529 (7)	0·1689 (1)	0·67927 (6)	3·49 (3)
C16	0·29311 (7)	0·0901 (1)	0·89132 (6)	3·20 (2)
C17	0·25848 (9)	0·1817 (1)	0·90784 (7)	4·10 (3)
C18	0·17027 (9)	0·1826 (1)	0·89248 (8)	4·98 (3)
C19	0·11629 (8)	0·0919 (1)	0·86031 (8)	4·80 (3)
C20	0·14926 (8)	−0·0001 (1)	0·84362 (7)	4·24 (3)
C21	0·23791 (8)	−0·0005 (1)	0·85915 (6)	3·39 (3)

Anisotropically refined atoms are given in the form of the equivalent isotropic thermal parameter defined as:

$\frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

Table 2. *Coordinates and equivalent isotropic thermal parameters for triclinic form*

	x	y	z	B_{eq}(Å^2)
O1	−0·1408 (1)	0·18895 (9)	0·71671 (7)	5·21 (2)
O2	−0·1922 (1)	0·48793 (8)	0·13072 (7)	4·58 (2)
O3	0·4444 (1)	0·45715 (9)	0·22828 (9)	5·72 (2)
N1	−0·0464 (1)	0·34162 (8)	0·48201 (7)	3·69 (2)
N2	0·0294 (1)	0·46765 (8)	0·25983 (7)	3·50 (2)
C1	−0·3132 (2)	0·2133 (1)	0·70677 (9)	4·04 (2)
C2	−0·4516 (2)	0·1564 (1)	0·8126 (1)	5·18 (3)
C3	−0·6283 (2)	0·1789 (1)	0·8055 (1)	5·50 (3)
C4	−0·6720 (2)	0·2568 (1)	0·6936 (1)	5·39 (3)
C5	−0·5356 (2)	0·3144 (1)	0·5876 (1)	4·60 (3)
C6	−0·3545 (1)	0·2946 (1)	0·59272 (9)	3·64 (2)
C7	−0·2128 (1)	0·3559 (1)	0·48020 (9)	3·65 (2)
C8	0·0979 (1)	0·3983 (1)	0·37093 (8)	3·46 (2)
C9	0·0908 (1)	0·5882 (1)	0·18046 (9)	3·76 (2)
C10	0·0210 (1)	0·6671 (1)	0·07181 (9)	3·87 (2)
C11	0·0896 (2)	0·7996 (1)	−0·0115 (1)	5·31 (3)
C12	0·0180 (2)	0·8792 (2)	−0·1113 (1)	6·49 (4)
C13	−0·1228 (2)	0·8265 (2)	−0·1292 (1)	6·43 (4)
C14	−0·1929 (2)	0·6962 (1)	−0·0491 (1)	5·36 (3)
C15	−0·1207 (1)	0·6158 (1)	0·05142 (9)	4·03 (2)
C16	0·2263 (1)	0·2839 (1)	0·36372 (8)	3·52 (2)
C17	0·1782 (2)	0·1449 (1)	0·4292 (1)	4·43 (3)
C18	0·2984 (2)	0·0438 (1)	0·4197 (1)	5·30 (3)
C19	0·4684 (2)	0·0812 (1)	0·3434 (1)	5·41 (3)
C20	0·5201 (2)	0·2183 (1)	0·2779 (1)	4·95 (3)
C21	0·3997 (1)	0·3199 (1)	0·28895 (9)	4·04 (2)

B_{eq} is defined as in Table 1.

* Tables of H-atom coordinates, distances and angles involving H atoms, anisotropic thermal parameters and structure-factor amplitudes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44771 (58 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

C8—N2—C9, 1·7 (1)°; the other differences are 1·2° or less.

We cannot compare these structures with other diimines because a search of the Cambridge Structural Database files revealed no structures with an acyclic C=N—C—N=C fragment. The distances and angles involving this fragment are typical of monoimines. Distances C6—C7 and C9—C10 are short for sp^2—sp^2 C—C bonds, suggesting a delocalization of electron density. This delocalization is caused by the cyclic hydrogen bonding, which resembles the enol of a 1,3-dicarbonyl compound.

In both forms, each molecule has two planar six-membered cyclic intramolecular hydrogen bonds. The intramolecular interaction involving O1 and N1 has O···N distance 2·5869 (7), H···N distance 1·71 (1), O—H distance 0·95 (1) Å, and angle at H 151·5 (8)° in the triclinic form, and 2·6148 (12), 1·75 (2), 0·96 (2) Å, and 147 (2)°, respectively in the monoclinic form. The hydrogen bond involving O2 and N2 has respective values of 2·5695 (6), 1·62 (1), 1·03 (1) Å, and 152·3 (8)° in the triclinic form and 2·5255 (14), 1·49 (3), 1·10 (3) Å, and 153 (2)° in the monoclinic form. This latter intramolecular hydrogen bond has the bridging H located closer to N than does the former. This may be because O2 is part of an intermolecular hydrogen bond or because N2 is more basic than N1, which is due to the torsion angles about C16—C8 placing C8—N2 further out of the phenyl ring plane than C8—N1.

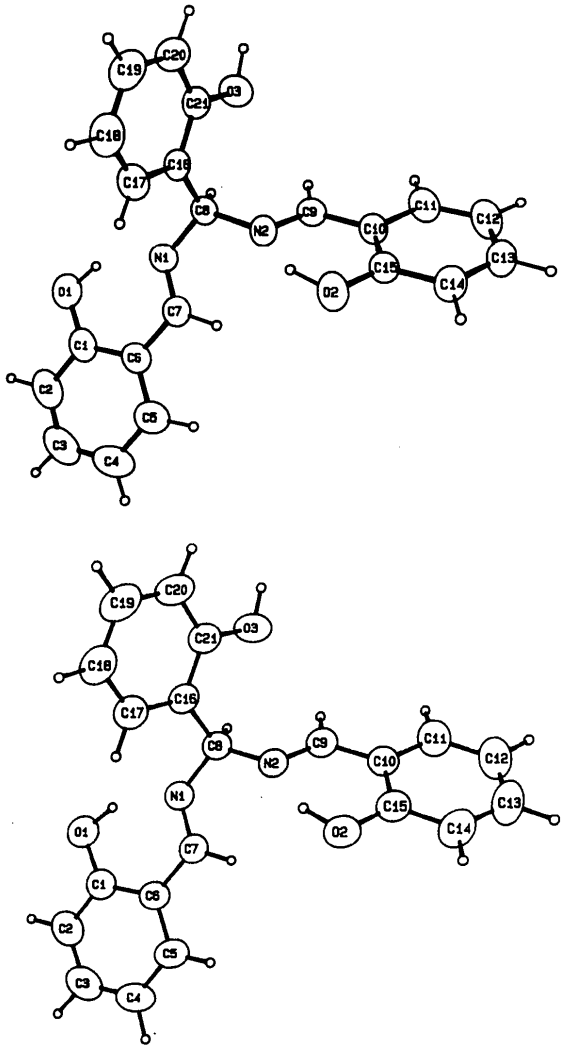

Fig. 1. *ORTEP* drawings (Johnson, 1976) of the two molecules. Monoclinic, top; triclinic, bottom.

Table 3. *Distances* (Å)

	Tri-clinic	Mono-clinic		Tri-clinic	Mono-clinic
O1—C1	1·349 (1)	1·352 (2)	C8—C16	1·521 (1)	1·523 (2)
O2—C15	1·358 (1)	1·340 (2)	C9—C10	1·454 (1)	1·447 (2)
O3—C21	1·364 (1)	1·367 (2)	C10—C11	1·397 (1)	1·402 (2)
N1—C7	1·276 (1)	1·275 (2)	C10—C15	1·398 (2)	1·405 (2)
N1—C8	1·455 (1)	1·459 (1)	C11—C12	1·379 (2)	1·375 (2)
N2—C8	1·464 (1)	1·467 (2)	C12—C13	1·382 (3)	1·389 (2)
N2—C9	1·278 (1)	1·284 (2)	C13—C14	1·376 (2)	1·376 (2)
C1—C2	1·392 (1)	1·388 (2)	C14—C15	1·389 (2)	1·402 (2)
C1—C6	1·403 (1)	1·410 (2)	C16—C17	1·387 (1)	1·392 (2)
C2—C3	1·372 (2)	1·374 (3)	C16—C21	1·391 (1)	1·387 (2)
C3—C4	1·384 (2)	1·392 (3)	C17—C18	1·383 (2)	1·387 (2)
C4—C5	1·385 (1)	1·380 (2)	C18—C19	1·377 (2)	1·379 (2)
C5—C6	1·399 (2)	1·399 (2)	C19—C20	1·376 (2)	1·382 (2)
C6—C7	1·458 (1)	1·452 (2)	C20—C21	1·393 (2)	1·394 (2)
C—H range	0·93 (1)–1·02 (1)	0·93 (2)–1·06 (2)			
O1—H10H	0·95 (1)	0·96 (2)			
O2—H20H	1·03 (1)	1·10 (3)			
O3—H30H	0·90 (1)	0·95 (2)			
N2—H20H	1·62 (1)	1·49 (3)			
N1—H10H	1·71 (1)	1·75 (2)			

Table 4. *Angles and selected torsion angles* (°)

	Tri-clinic	Mono-clinic		Tri-clinic	Mono-clinic
C7—N1—C8	122·6 (1)	121·9 (1)	C9—C10—C11	120·0 (1)	119·8 (1)
C8—N2—C9	118·7 (1)	120·4 (1)	C9—C10—C15	121·3 (1)	120·5 (1)
O1—C1—C2	118·8 (1)	118·9 (1)	C11—C10—C15	118·7 (1)	119·6 (1)
O1—C1—C6	121·3 (1)	121·4 (1)	C10—C11—C12	120·8 (1)	120·5 (1)
C2—C1—C6	119·9 (1)	119·8 (2)	C11—C12—C13	119·5 (1)	119·6 (2)
C1—C2—C3	120·2 (1)	120·2 (2)	C12—C13—C14	121·2 (1)	121·2 (1)
C2—C3—C4	120·8 (1)	121·1 (1)	C13—C14—C15	119·4 (1)	119·9 (1)
C3—C4—C5	119·6 (1)	119·0 (2)	O2—C15—C10	120·6 (1)	120·7 (1)
C4—C5—C6	120·6 (1)	121·1 (2)	O2—C15—C14	119·0 (1)	120·1 (1)
C1—C6—C5	118·8 (1)	118·8 (1)	C10—C15—C14	120·4 (1)	119·2 (1)
C1—C6—C7	121·3 (1)	121·7 (1)	C8—C16—C17	122·8 (1)	122·3 (1)
C5—C6—C7	119·9 (1)	119·5 (1)	C8—C16—C21	118·8 (1)	118·8 (1)
N1—C7—C6	121·4 (1)	121·9 (1)	C17—C16—C21	118·5 (1)	118·9 (1)
N1—C8—N2	112·3 (1)	113·1 (1)	C16—C17—C18	121·1 (1)	120·6 (1)
N1—C8—C16	109·7 (1)	110·6 (1)	C17—C18—C19	119·7 (1)	119·7 (2)
N2—C8—C16	110·5 (1)	107·8 (1)	C18—C19—C20	120·4 (1)	120·7 (1)
N2—C9—C10	121·8 (1)	120·9 (1)	C19—C20—C21	119·8 (1)	119·3 (1)
O3—C21—C16	117·0 (1)	117·0 (1)	C16—C21—C20	120·5 (1)	120·7 (1)
O3—C21—C20	122·5 (1)	122·3 (1)			

	Tri-clinic	Mono-clinic
N1—C8—C16—C17	19·7 (1)	29·1 (1)
N1—C8—C16—C21	−159·9 (1)	−153·1 (1)
N2—C8—C16—C17	−104·6 (1)	−95·0 (1)
N2—C8—C16—C21	75·8 (1)	82·7 (1)
C7—N1—C8—C16	−125·2 (1)	−118·6 (1)
C7—N1—C8—N2	−1·9 (2)	2·5 (2)
C9—N2—C8—C16	−105·5 (1)	−107·1 (1)
C9—N2—C8—N1	131·7 (1)	130·3 (1)

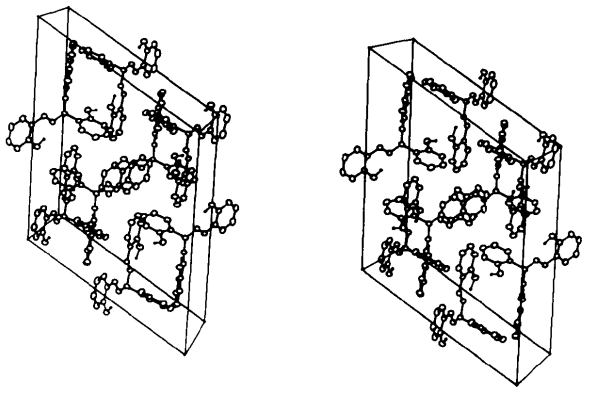

Fig. 2. Stereoview of the packing diagram for the monoclinic crystal, viewed slightly oblique to **b** with **c** vertical.

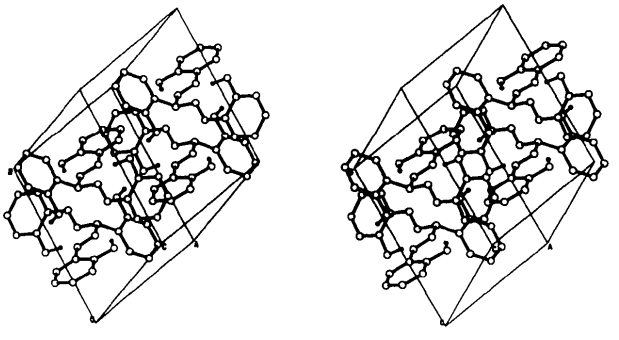

Fig. 3. Stereoview of the packing diagram for the triclinic crystal.

Both forms contain chains of intermolecular hydrogen bonds involving hydroxyl-group O3 as donor and O2 as acceptor. In the triclinic form, those chains are propagated by a simple translation along the **a** direction, with O···O distance 2·7284 (6), O···H distance 1·84 (1) Å, and angle at H 169·1 (8)°. In the monoclinic form, the chains are propagated by 2_1 axes in the **b** direction, with O···O 2·6766 (13), H···O 1·73 (2) Å, and angle 172(2)°. These interactions are illustrated in the packing diagrams, Figs. 2 and 3. The 20 K higher melting point of the monoclinic form may be partly explained by the 0·05 Å shorter O···O distance in the monoclinic polymorph.

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Structure de la Phase Triclinique (Phase II) du 4,4′ Azoxydiphénétole

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Abstract. 4,4′-Diethoxyazobenzene, $C_{16}H_{18}N_2O_3$, M_r = 286·34. Phase I: monoclinic, $C2/c$ or Cc, a = 22·78 (5), b = 5·440 (4), c = 15·95 (2) Å, β = 130·0 (1)°, V = 1514 (6) Å^3, Z = 4, D_x = 1·26 Mg m^{-3}. Phase II: triclinic, $P\bar{1}$, a = 9·014 (4), b = 9·557 (4), c = 9·861 (6) Å, α = 117·46 (8), β =

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