Crystal and Molecular Structure of Hippuric Acid

By W. Harrison, S. Rettig, and J. Trotter,* Department of Chemistry, University of British Columbia, Vancouver 8, British Columbia, Canada

Hippuric acid (N-benzoylglycine) crystallizes in the orthorhombic space group $P2_12_12_1$ with $a = 10.586(1)$, $b = 9.123(5)$, $c = 8.880(2)$ Å, $Z = 4$. The structure was determined from diffractometer data by direct methods, and refined by electron-density and full-matrix least-squares techniques to R 0.034 for 750 observed reflexions. The structure consists of molecules of hippuric acid linked by a three-dimensional network of intermolecular O–H $\cdots$ O (2.68 Å) and N–H $\cdots$ O (3.02 Å) hydrogen bonds. The molecule is characterized by three planes defined by the phenyl, amide, and carboxylic acid groups, which are twisted with respect to each other.

HIPPURIC acid was one of the first natural products to be characterized. The compound was isolated from horse urine in 1829 and its composition determined in 1839 by Liebig.[1] In 1846 Dessaignes showed that it decomposed to glycine and benzoic acid when boiled with concentrated acids or bases,[2] and in 1853 he synthesized hippuric acid from benzoyl chloride and zinc glycine.[3]

The compound occurs in the urine of most mammals, including humans, large concentrations being found in that of herbivores.[1] Toluene and benzoic and cinnamic acids, when taken internally are eliminated as hippuric acid.[2]

The full three-dimensional X-ray analysis of the compound was undertaken in conjunction with an electron paramagnetic resonance study.[4]

EXPERIMENTAL

Hippuric acid (N-benzoylglycine), m.p. 187.5°,[5] crystallizes in colourless rhombic prisms. The crystal chosen for study was elongated in the b direction, dimensions $0.3 \times 0.25 \times 0.2$ mm, and was mounted with b parallel to the goniostat axis. The space group and initial unit-cell parameters were determined from precession and Weissenberg films. Accurate unit-cell parameters were later obtained by a least-squares treatment of 25 $\sin^2\theta(hkl)$ values measured on a General Electric XRD 6 diffractometer with Cu-K_α radiation.

Crystal Data.—$C_9H_9NO_3$, $M = 179.18$. Orthorhombic, $a = 10.586(1)$, $b = 9.123(5)$, $c = 8.880(2)$ Å, $U = 857.6(5)$ Å³, $D_m = 1.371$,[5] $Z = 4$, $D_c = 1.388(1)$, Space group $P2_12_12_1$ (D_2^4, No. 19) from absent spectra: $h00$ $h \neq 2n$, $0k0$ $k \neq 2n$, and $00l$, $l \neq 2n$. Cu-K_α radiation, $\lambda = 1.5418$ Å; μ(Cu-K_α) = 9 cm⁻¹.

Intensity data were collected on a Datex-automated General Electric XRD 6 diffractometer with a θ—2θ scan at 2° min⁻¹ in 2θ. All reflexions with 2θ(Cu-K_α) $\leq 146.8°$ were measured. A check reflexion was monitored every 30 reflexions throughout the data collection; the intensity of the check reflexion had fallen off by 3% of its initial

[1] V. von Richter, ' The Chemistry of the Carbon Compounds,' vol. III, Elsevier, New York, 1946, p. 301.

[2] Dessaignes, *J. prakt. Chem.* [1], 1846, **37**, 244.

[3] Dessaignes, *Annalen*, 1853, **87**, 325.

[4] C. A. McDowell and J. M. Park, unpublished work.

[5] ' Handbook of Chemistry and Physics,' 44th edn., Chemical Rubber Publishing Co., Cleveland, 1963, pp. 1038—1039.

value at the end of the data collection. Lorentz and polarization corrections were applied, and the structure amplitudes were derived; no absorption corrections were made in view of the small size of the crystal and low value of μ. Of the 1010 independent reflexions, 260 had intensities $<4\sigma(I)$ above background [$\sigma(I)$ is defined by $\sigma^2(I) = S + B + (0.05\ S)^2$ where S = scan count and B = background count] and were classified as unobserved.

Structure Analysis and Refinement.—The structure was solved by direct methods, 217 reflexions with normalized structure factor $|E| \geqslant 1.5$ being used in the symbolic addition procedure for noncentrosymmetric crystals.[6] A Σ_2 listing for the reflexions was obtained and the origin and enantiomorph were chosen by fixing the phases of the 708, 750, 021, and 830 reflexions. Using 60 reflexions with $|E| \geqslant 1.80$, the set of phases was expanded manually. The reflexions 065, 833, and 146 were assigned symbol phases to complete the basic set given in Table 1.

TABLE 1

Starting set of reflexions

	h		$|E(\mathbf{h})|$	$\phi(\mathbf{h})$
7	0	8	3·260	0
7	5	0	3·140	$\pi/2$
0	2	1	2·010	0
8	3	0	2·760	0
0	6	5	3·450	a
8	3	3	3·101	b
1	4	6	2·797	c

The manual determination gave indications for the symbol phases b and c, while the symbol a is required by space group symmetry to be 0 or π. The basic set of reflexions was split into eight starting sets by allowing the symbols to take on all combinations of their indicated values (Table 2).

TABLE 2

Results for the eight starting sets in the phase-determination procedure

Starting set	Initial a (mc)	Initial b (mc)	Initial c (mc)	t	α	Q	R
(1)	500	500	750 *	0·634	173·9	0·350	0·354
(2)	500	500	250	0·586	169·6	0·399	0·326
(3)	500	0	750 *	0·635	182·7	0·348	0·355
(4)	500	0	250	0·536	133·3	0·455	0·330
(5)	0	500	750 *	0·705	224·2	0·279	0·188
(6)	0	500	250	0·617	181·6	0·373	0·315
(7)	0	0	750 *	0·629	201·8	0·353	0·230
(8)	0	0	250	0·732	230·7	0·254	0·207

* At input stage only; the final phases are normalized to lie in the range $-\pi < \phi(\mathbf{h}) \leqslant \pi$.

The eight sets were used as input to a computer program which determines phases using the tangent formula.[7-9]

The values of overall t, overall α, Q, and R [7-9] on the final cycle for each set are given in Table 2. High values of α and t, and low values of Q and R are expected for a consistent set of phases. On this basis, E-maps were calculated using phases given by sets (5) and (8). The structure was clearly given by the thirteen highest peaks from the E-map generated by set (5). The E-map from set (8)

[6] J. Karle and I. L. Karle, *Acta Cryst.*, 1966, **21**, 849.

[7] J. Karle and H. Hauptman, *Acta Cryst.*, 1956, **9**, 635.

[8] (a) M. G. B. Drew, personal communication; see *e.g.* (b) M. G. B. Drew, D. H. Templeton, and A. Zalkin, *Acta Cryst.*, 1969, **B25**, 261.

[9] F. H. Allen and J. Trotter, *J. Chem. Soc.* (B), 1970, 166.

yielded only a partial structure as well as several intense anomalous peaks.

A structure-factor calculation based on the carbon, nitrogen, and oxygen positions obtained from the E-map from set (5), was carried out, with $B = 4.0\ \text{Å}^2$ for all atoms, and gave R 0·22. Two cycles of full-matrix least-squares refinement on the positional and isotropic thermal parameters reduced R to 0·15. A difference Fourier synthesis at this point yielded the positions of 8 of the 9 hydrogen atoms; the acidic hydrogen, H(1), was not located at this stage. The heavy atoms were all given anisotropic temperature factors and were refined for two cycles; the hydrogen atom contributions were included, but their positions and temperature factors were not refined. The anisotropic temperature factors refined were β_{ij} in the equation: $f = f^\circ \exp (\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)$ where f° is the tabulated [10] scattering factor [scattering factors for carbon, oxygen, and nitrogen were taken from ref. 10(a) and those for hydrogen from ref. 10(b)], and f is the value corrected for thermal motion. The R value was reduced to 0·088.

At this stage a weighting scheme of the form: $\sqrt{w} = 1.0$ when $|F_o| \leqslant 8.0$, $\sqrt{w} = 8.0/|F_o|$ when $|F_o| > 8.0$, and $\sqrt{w} = 0.1$ for the unobserved reflexions was found to be suitable from an analysis of $w\ (|F_o| - |F_c|)^2$ over ranges of $|F_o|$. Two cycles of anisotropic refinements, the hydrogen atoms being fixed, with this weighting scheme resulted in R 0·059. A difference Fourier synthesis gave the position of the remaining hydrogen atom. Three reflexions, 102, 021, and 022, believed to be suffering from extinction, were given zero weight in the final stages of refinement. Three cycles of isotropic refinement of the hydrogen atoms and anisotropic refinement of the other atoms concluded the

TABLE 3

Final atomic co-ordinates. Fractional co-ordinates with standard deviations in parentheses

Atom	x	y	z
O(1)	0·8526(2)	0·3715(3)	0·1276(3)
O(2)	0·6634(2)	0·4338(3)	0·0383(3)
O(3)	0·5258(2)	0·5271(2)	0·3846(2)
N	0·5453(2)	0·3010(3)	0·2871(3)
C(1)	0·7281(2)	0·3795(3)	0·1328(3)
C(2)	0·6814(3)	0·3111(4)	0·2768(4)
C(3)	0·4758(2)	0·4097(3)	0·3431(3)
C(4)	0·3360(2)	0·3898(3)	0·3545(3)
C(5)	0·2693(3)	0·4911(4)	0·4406(4)
C(6)	0·1389(3)	0·4814(4)	0·4505(4)
C(7)	0·0750(3)	0·3712(4)	0·3779(4)
C(8)	0·1400(3)	0·2700(4)	0·2927(4)
C(9)	0·2707(3)	0·2775(3)	0·2812(4)
H(1)	0·8823(40)	0·4002(49)	0·0496(61)
H(2)	0·7191(32)	0·2143(40)	0·2862(42)
H(3)	0·7141(27)	0·3672(34)	0·3643(38)
H(4)	0·5130(40)	0·2249(42)	0·2471(46)
H(5)	0·3170(29)	0·5728(36)	0·4936(41)
H(6)	0·0946(31)	0·5528(39)	0·5110(41)
H(7)	−0·0216(32)	0·3681(36)	0·3809(40)
H(8)	0·0963(29)	0·1866(41)	0·2443(38)
H(9)	0·3169(28)	0·2043(37)	0·2184(41)

refinement of the structure. Convergence was reached at R 0·034 for the 750 observed reflexions; no parameter shift was $>0.35\sigma$. The final positional and thermal parameters are given in Tables 3 and 4. A final electron-density

[10] (a) ' International Tables for X-Ray Crystallography,' vol. III, Kynoch Press, Birmingham, 1962, pp. 202—207; (b) R. F. Stewart, E. R. Davidson, and W. F. Simpson, *J. Chem. Phys.*, 1965, **42**, 3175.

TABLE 4

Final thermal parameters and estimated standard deviations

Atom	$10^5\beta_{11}$	$10^5\beta_{22}$	$10^5\beta_{33}$	$10^5\beta_{12}$	$10^5\beta_{13}$	$10^5\beta_{23}$
O(1)	616(18)	2019(38)	1355(33)	27(21)	42(21)	422(34)
O(2)	815(21)	2179(41)	1404(34)	26(23)	−125(22)	545(31)
O(3)	751(17)	1119(24)	1403(29)	−108(18)	−108(21)	−115(24)
N	591(21)	1111(31)	1271(33)	−8(20)	62(23)	−23(30)
C(1)	636(24)	1070(32)	1134(36)	−16(22)	−74(24)	−37(33)
C(2)	668(28)	1264(40)	1119(39)	92(26)	9(26)	23(36)
C(3)	647(21)	1042(33)	844(31)	−70(23)	−15(22)	131(27)
C(4)	604(21)	1025(31)	911(32)	−15(21)	7(22)	108(30)
C(5)	817(30)	1280(41)	1130(37)	4(26)	64(26)	−89(34)
C(6)	807(31)	1564(48)	1220(40)	236(31)	144(29)	−7(39)
C(7)	590(23)	1932(49)	1241(38)	53(19)	−13(27)	249(43)
C(8)	767(30)	1546(48)	1351(43)	−154(29)	−83(31)	−99(45)
C(9)	705(27)	1197(36)	1179(38)	−16(24)	47(26)	−71(38)

Atom	$B/\text{Å}^2$	Atom	$B/\text{Å}^2$
H(1)	7·17(124)	H(6)	5·03(76)
H(2)	4·33(72)	H(7)	5·08(75)
H(3)	3·81(65)	H(8)	4·36(77)
H(4)	5·30(89)	H(9)	4·02(67)
H(5)	4·99(79)		

difference map showed maximum fluctuations of $\pm 0\cdot3$ eÅ^{-3}. Measured and calculated structure factors are listed in Supplementary Publication No. SUP 20370 (4 pp., 1 microfiche).*

DISCUSSION

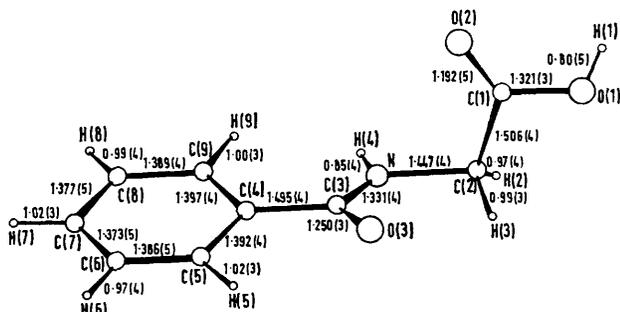Figure 1 shows the molecule of hippuric acid viewed down b. Bond lengths and angles, with their standard

FIGURE 1 The hippuric acid molecule viewed down b. Bond distances are given in Å, with standard deviations in parentheses. The bonds C(1)–O(1) and C(1)–O(2) were later corrected for thermal motion, the corrected values being 1·340(3) and 1·220(3) Å respectively
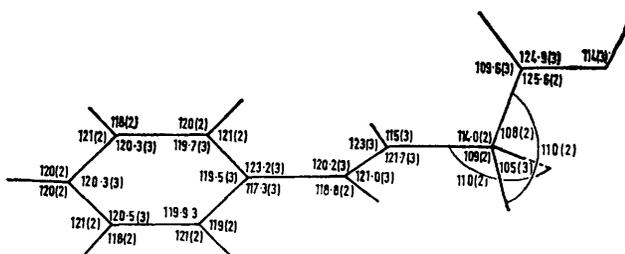

FIGURE 2 Diagram of the molecule showing bond angles, with standard deviations in parentheses

deviations, are given in Figures 1 and 2. Weighted least-squares mean planes are given in Table 5.

* For details of Supplementary Publications see Notice to Authors No. 7 in *J. Chem. Soc. (A)*, 1970, Issue No. 20 (items less than 10 pp. will be supplied as full size copies.

The molecule can be characterized by three planes defined by the phenyl, amide, and carboxylic acid groups. The phenyl and carboxylic acid groups are planar within experimental error (Table 5). The amide group is very nearly planar, the mean-deviation from the plane being 0·008 Å for the heavy atoms with individual values ranging from 0·005—0·016 Å. The deviations from the mean plane of the amide group compare well with values reported for peptide structures,[11] in which the group is planar within experimental error. In hippuric acid, owing to high accuracy, these small deviations become significant and four atoms were found to deviate significantly from the mean plane: C(3) and C(4) by 5σ, and O(3) and H(4) by 3σ.

The twist about the C(1)–C(2) bond is defined by the torsion angle O(2)[C(1)C(2)]N and is taken to be zero

TABLE 5

Equations of best least-squares planes through the molecule in the form $lX + mY + nZ = p$ where X, Y, and Z are co-ordinates in Å. Distances, d (Å), of relevant atoms from the planes are given in square brackets, together with the ratio d/σ in parentheses

	l	m	n	p

Plane (1):

O(1), O(2), C(1), C(2), H(1)   −0·0680 −0·8828 −0·4649 −4·1272

[O(1) −0·0011 (0·4), O(2) −0·0011 (0·4), C(1) 0·0035 (1·3), C(2) −0·0011 (0·3), H(1) 0·0656 (1·4), N 0·1364 (51·7)]

Plane (2):

C(2)—(4), N, O(3), H(4)   −0·1028   0·3682   −0·9240   −1·9311

[C(2) 0·0024 (1·1), C(3) 0·0145 (5·3), C(4) −0·0161 (5·1), N −0·0005 (0·2), O(3) −0·0077 (3·0), H(4) 0·1194 (3·0), C(1) 1·3334 (453·8), C(5) −0·2950 (95·0), C(9) 0·2820 (85·9)]

Plane (3):

C(4)—(9), H(5)—(9)   −0·0937   0·5811   −0·8084   −0·7930

[C(4) 0·0043 (1·7), C(5) −0·0050 (1·6), C(6) 0·0026 (0·8), C(7) −0·0017 (0·5), C(8) 0·0031 (0·9), C(9) −0·0050 (1·5), H(5) 0·0040 (0·1), H(6) −0·0054 (0·2), H(7) 0·0566 (1·6), H(8) −0·0514 (1·5), H(9) 0·0076 (0·2), C(3) 0·0520 (21·6), O(3) 0·3298 (156·7), N −0·1946 (72·2), H(4) −0·2182 (7·1)]

Angles (deg.) between planes: (1)—(2) 87·8
(2)—(3) 13·9

when the nitrogen atom is coplanar with the carboxylic acid group.[11] This angle is 6·5(3)° in hippuric acid which falls within the range of 0—27° observed in the structures of glycine derivatives and peptides in which the terminal acid group is glycine.[11]

The dihedral angles between the mean plane of the amide group and those of the phenyl and carboxylic acid groups give the rotations about the N–C(2) and C(3)–C(4) bonds as 87·8(5)° and 13·9(5)° respectively. These observations agree with values found for many dipeptide structures,[11] where the rotation about C(3)–C(4) is usually small and that about N–C(2) is often close to 90°.

[11] R. E. Marsh and J. Donohue, *Adv. Protein Chem.*, 1967, 22, 235.

The mean C–C bond length in the phenyl ring is 1·386(5) Å, with individual values ranging from 1·373(5) to 1·397(4) Å. The mean length agrees with the accepted value of 1·395(3) Å.[12]

Bond distances for the amide group are compared with corresponding values found in peptide structures,[11] benzamide,[13] and picolinamide[14] in Table 6. The

TABLE 6

Comparison of amide group bond distances (Å)

Atoms	Hippuric acid	Mean peptide[a]	Benz-amide[b]	Picolin-amide[c]
C(4)–C(3)	1·495(4)	1·51(1) *	1·48(2)	1·515(8)
C(3)–O(3)	1·250(3)	1·24(1) *	1·24(2)	1·241(7)
C(3)–N	1·331(4)	1·325(10) *	1·31(2)	1·330(7)
N–C(2)	1·447(4)	1·455(10) *		

* Approximate σ.

[a] Ref. 11.   [b] Ref. 13.   [c] Ref. 14.

N–C(3), N–C(2), and C(3)–O(3) distances agree to within experimental error. The C(3)–C(4) distance of 1·495(4) Å agrees with the 1·48(2) Å found in benzamide, and is slightly, but not significantly, shorter than the mean peptide and picolinamide distances. The value is close to the mean distance of 1·47(2) Å found for C(Ar)–CO bonds.[15]

The bond lengths O(1)–C(1) and O(2)–C(1) were corrected for thermal motion assuming the oxygen atoms ride on C(1). The corrected values are 1·220(3) Å for O(2)–C(1) and 1·340(3) Å for O(1)–C(1). The observed bond length of 1·220(3) Å for O(2)–C(1) agrees with the distance of 1·233(5) Å found for carboxy C–O double bonds.[15] The O(1)–C(1) distance is 3σ shorter than the 1·358(5) Å mean value for carboxylic acid single-bonds.[15]

The mean of the angles about all trigonally bonded carbon atoms is 120°, but there are some very significant deviations. The largest deviations are for the angles about C(1). The O(1)–C(1)–O(2) angle, 124·9(3)°, is larger than 120° by 16σ, but is normal for carboxylic acids, e.g. 125 and 124° in protonated amino-acids D-(−)-isoleucine HBr[16] and L-leucine HBr,[17] and a mean of 125·6° in amino-acid structures.[11] The two O–C–C angles in the amino-acid group tend to differ, the angle nearer the nitrogen atom usually being the larger.[11] However hippuric acid is a protonated acid, while the majority of amino-acids occur in the zwitterion form, rendering strict comparisons invalid. In hippuric acid the angle nearer the nitrogen atom, O(2)–C(1)–C(2) [109·5(3)°], is smaller than the other angle, O(1)–C(1)–C(2), 125·6(2)°, by 35σ. Figure 3 indicates that this distortion, coupled with an expansion of the C(1)–O(1)–H(1) angle, allows for a closer contact between hydrogen-bonded atoms O(1) and O(3′), while retaining the near linearity of the O(1)–H(1) · · · O(3′) hydrogen-bond (see Table 7). This distortion also allows the intramolecular

[12] Ref. 10(a), p. 276.
[13] B. R. Penfold and J. C. B. White, Acta Cryst., 1959, 12, 130.
[14] T. Takano, Y. Sasada, and M. Kakado, Acta Cryst., 1966, 21, 514.

contacts O(2) · · · C(2) (2·40 Å) and O(1) · · · C(2) (2·31 Å) to be more nearly equal. The angles about C(3) involving O(3) show small but significant deviations from
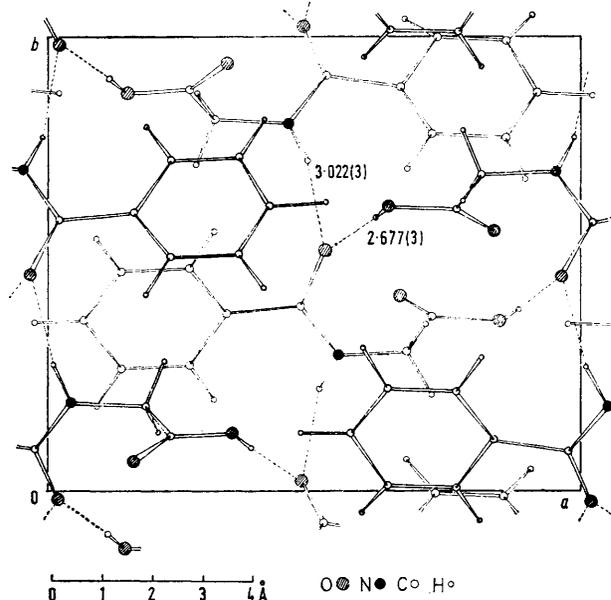

FIGURE 3 Projection of the structure along c. Hydrogen bonds are indicated by broken lines; the distances (Å) refer to O · · · O and O · · · N separations

the expected value of 120°: C(4)–C(3)–O(3) [118·8(2)°] by 6σ, and N–C(3)–O(3) [121·0(3)°] by 3σ. These deviations are in accord with the observation that in the amide group, the N–C–O angle is invariably slightly greater than the C–C–O angle.[11] The other significant

TABLE 7

Hydrogen-bond data (Å and deg.)

D–H · · · A	D · · · A	D–H	H · · · A	D–H · · · A
O(1)–H(1) · · · O(3^{I})	2·677(3)	0·80(5)	1·88(5)	171·2(46)
N–H(4) · · · O(3^{II})	3·022(3)	0·85(4)	2·19(4)	166·0(38)

O(3^{I}) · · · O(1)–H(1)	6·2(32)
O(3^{II}) · · · N–H(4)	10·1(27)
C(2)–N · · · O(3^{II})	105·6(2)
C(3)–N · · · O(3^{II})	131·8(2)
C(1)–O(1) · · · O(3^{I})	119·3(2)
C(3^{I})–O(3^{I}) · · · H(1)	138·7(14)
C(3^{II})–O(3^{II}) · · · H(4)	118·0(11)
C(3^{I})–O(3^{I}) · · · O(1)	137·5(2)
C(3^{II})–O(3^{II}) · · · N	117·0(2)
O(1^{III}) · · · O(3) · · · N^{IV}	103·9(1)
H(1^{III}) · · · O(3) · · · H(4^{IV})	102·9(18)

Roman numerals as superiors refer to the following equivalent positions relative to the reference molecule at x, y, z:

I 1½ − x, 1 − y, −½ + z   III 1½ − x, 1 − y, ½ + z
II 1 − x, −½ + y, ½ − z   IV 1 − x, ½ + y, ½ − z

deviations about trigonally bonded carbon atoms occur at C(9)–C(4)–C(3) (9σ) and C(5)–C(4)–C(3) (11σ). The angle nearer the amide oxygen C(5)–C(4)–C(3) is contracted to 117·3(3)° with a corresponding increase in

[15] Chem. Soc. Special Publ., No. 11, 1958, and No. 18, 1965.
[16] J. Trommel and J. M. Bijvoet, Acta Cryst., 1954, 7, 703.
[17] E. Subramanian, Acta Cryst., 1967, 22, 910.

C(9)–C(4)–C(3) to 123·2(3)°. This was also observed in benzamide [13] where the angles were found to be 118(1) and 121(1)°.

The geometry about the tetrahedrally bonded carbon atom, C(2), is as expected. The angle between the bulky substituents, C(1)–C(2)–N, is expanded to 114·0(2)° while the angle opposite, involving the hydrogen atoms, H(2)–C(2)–H(3), is contracted to 105(3)°. The remaining angles about C(2) are normal; the mean value of all angles at C(2) is 109(2)°. The C(2)–N–C(3) angle, 121·7(3)°, agrees with the mean value of 122° found in peptide amide groups.[11]

The molecular geometry involving the hydrogen atoms is normal except for angles at N and O(1) involving H(4) and H(1) respectively. These distortions are not significant, but they do indicate the hydrogen atoms are moved in the direction of the oxygen atom to which they are hydrogen-bonded. The angle C(1)–O(1) · · · O(3') is 119° and the C(1)–O(1)–H(1) angle is 114(3)° rather than less than the tetrahedral angle as expected. Similarly, at the nitrogen atom C(2)–N · · · O(3') is 106° while C(2)–N–H(4) is 115(3)° and C(3)–N · · · O(3') is 132° while C(3)–N–H(4) is 123(3)°. The following are as expected: mean C(Ar)–H 1·00(3), mean C(sp^3)–H 0·98(5), O–H 0·80(5), N–H 0·85(4) Å, and mean

C–C–H(Ph) 120(2)° with individual values ranging from 118—121°. The values of the bond distances are shorter than those obtained spectroscopically indicating that the hydrogen electron has been pulled toward the atom to which it is bonded.

The crystal packing arrangement, viewed down c is shown in Figure 3. The molecules are linked by a three-dimensional network of intermolecular hydrogen-bonds. Each molecule is hydrogen-bonded to four others (relevant information is given in Table 7). The O · · · O and O · · · N distances of 2·677(3) and 3·022(3) Å agree with literature values, as do the O–H · · · O and N–H · · · O angles of 171° and 166°.[18,19] The angle at O(3) between the two hydrogen bonds was found to be 103(2)° for H(1) · · · O(3) · · · H(4) and 103·9(1)° for O(1) · · · O(3) · · · N. All other intermolecular contacts correspond to van der Waals interactions, the shortest of which, not involving hydrogen atoms, are O(1) · · · C(7) 3·24 Å and N · · · C(7) 3·38 Å.

[18] J. Donohue, in 'Structural Chemistry and Molecular Biology,' eds. A. Rich and N. Davidson, Freeman, San Francisco, 1968, p. 443.

[19] W. C. Hamilton and J. A. Ibers, 'Hydrogen Bonding in Solids,' Benjamin, New York, 1968, p. 260.