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The Molecular and Crystal Structure of Uric Acid

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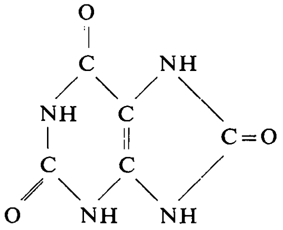
The crystals of anhydrous uric acid, 2,6,8-trioxypurine, $C_5H_4N_4O_3$, are monoclinic with four molecules in a unit cell of dimensions $a=14{\cdot}464$, $b=7{\cdot}403$, $c=6{\cdot}208$ Å, $\beta=65{\cdot}10°$, space group $P2_1/a$. The structure has been determined by trial-and-error methods and refined by three-dimensional least-squares computations. The final R value was 6·6 %. The uric acid molecule is in the triketo form. The molecules are perfectly planar and stacked nearly parallel to the (021) and (02$\bar{1}$) planes, and are kept firmly together in a close-packed system by a perfect network of hydrogen bonds.

Introduction

As part of a program of research on nitrogen-containing excretory products in biological systems, the crystal and molecular structure of uric acid, 2,6,8-trioxypurine,



has been determined.

A report on the optical and crystallographic properties of uric acid and its dihydrate has already been given (Ringertz, 1965). It should only be mentioned that the anhydrous form is biaxial positive and highly birefringent, $\gamma_D-\alpha_D=0{\cdot}31$.

Experimental

Reagent grade uric acid was recrystallized by dissolving in hot water and allowing the solution to cool and subsequently evaporate. Determination of the unit-cell dimensions was made by recording rotation photographs of a small, silicon-powder coated crystal in a 190 mm diameter precision powder camera, $a_{Si}=5{\cdot}4306$ Å. The monoclinic unit cell measured: $a=14{\cdot}464\pm0{\cdot}003$, $b=7{\cdot}403\pm0{\cdot}002$, $c=6{\cdot}208\pm0{\cdot}001$ Å, $\beta=65{\cdot}10\pm0{\cdot}05°$.

Systematic absences were $h0l$ with $h=2n+1$, $0k0$ with $k=2n+1$, space group $P2_1/a$. $D_{obs}=1{\cdot}844$ g.cm^{-3} and $D_{calc}=1{\cdot}851$ g.cm^{-3}, assuming $Z=4$.

A 0·2 mm long plate-formed crystal with a cross section of 0·16 × 0·08 mm was mounted with the rotation axis parallel to the b axis. This crystal was used in the preparation of integrated, multiple-film, equi-inclination Weissenberg photographs of layers $h0l$ through $h5l$. The same crystal was then mounted along the c axis and the $hk0$ layer was recorded. Ni-filtered Cu-radiation was used throughout. 1030 structure amplitudes were obtained of which about 110 were of zero magnitude. All intensities were recorded in a microdensitometer, the range being about 5000 to 1. Twelve of the strongest reflexions were out of the linear range and were given maximum observable intensity. The unobserved reflexions were given half the minimum observable intensity. Lorentz and polarization factor corrections were applied but the absorption in the crystal was neglected. The various k levels were placed roughly on a common scale by means of the $hk0$ data.

Determination of the structure

The high birefringence (0·31), the strength of the 021 and 02$\bar{1}$ reflexions with a d value of 3·09 Å and earlier structure determinations of related compounds indicated an essentially layered orientation of planar molecules. They also indicated that the molecules were approximately lying in the (021) and (02$\bar{1}$) planes, which assumption was supported by the size and orientation of the optical indicatrix. As uric acid has a high decomposition temperature (of about 400°C) and a comparatively high density (1·844 g.cm^{-3}) it was assumed that the molecules formed a closely packed system, probably held together by hydrogen bonding between the three oxygen and four nitrogen atoms that form the contour of the plane molecule. This was further supported by the infrared spectrum of uric acid, where there was a marked shift towards lower frequencies of the N–H band. The symmetry indicated that a hydrogen-bonding system should form alternating bonds around centres of symmetry. According to these limitations the structure factors of sixteen possible $h0l$ projections were calculated. One with $R=0{\cdot}25$ was very superior to the others with R values between 0·7 and 0·8. A two-dimensional electron density map [Fig. 1(*a*)] showed all the 12 non-hydrogen atoms of the asymmetric unit, but only four of them were well resolved in this projection.

Refinement of the structure

The y coordinates were now calculated assuming that the molecules were lying in the (021) and (02$\bar{1}$) planes, resulting in an initial three-dimensional R value of 0·44. The refinement was carried through on an IBM 7090 computer using the full-matrix least-squares program by Busing, Martin & Levy (1962) and applying the atomic scattering factors from *International Tables for X-ray Crystallography* (1962). The weighting scheme used during this part of the refinement was that of Cruickshank, Pilling, Bujosa, Lovell & Truter (1961) and seven scale factors were applied. After four cycles the R value had decreased to 0·13 with the use of individual isotropic temperature factors. All four hydrogen atoms were found from an $h0l$ difference Fourier synthesis calculated at this stage. When twelve strong reflexions given maximum observable intensity were excluded and the hydrogen atoms were introduced the R value decreased to 0·10. Using a unit weighting scheme and giving the non-hydrogen atoms anisotropic temperature factors in the form $\exp(-b_{11}h^2-b_{22}k^2-b_{33}l^2-2b_{12}hk-2b_{23}kl-2b_{13}hl)$ resulted in a final $R=\Sigma\,|F_o-F_c|/\Sigma\,|F_o|=0{\cdot}071$ and $R'=[\Sigma\,(F_o-F_c)^2/\Sigma\,F_0^2]^{0\cdot5}=0{\cdot}072$.

The hydrogen atoms were given a temperature factor equal to that of the covalently bonded nitrogen atom. Excluding the non observed reflexions and the twelve reflexions mentioned above gave $R=0{\cdot}066$ and $R'=0{\cdot}069$ for the remaining 907 structure amplitudes. The average and maximum positional shifts of the non-hydrogen atoms in the last cycle were 0·6% and 3·7% respectively of the estimated standard deviations. Observed reflexion amplitudes and fina lcalculated structure factors are given in Table 1, and a final three-dimensional electron density map projected along the b axis is seen in Fig. 1(c).

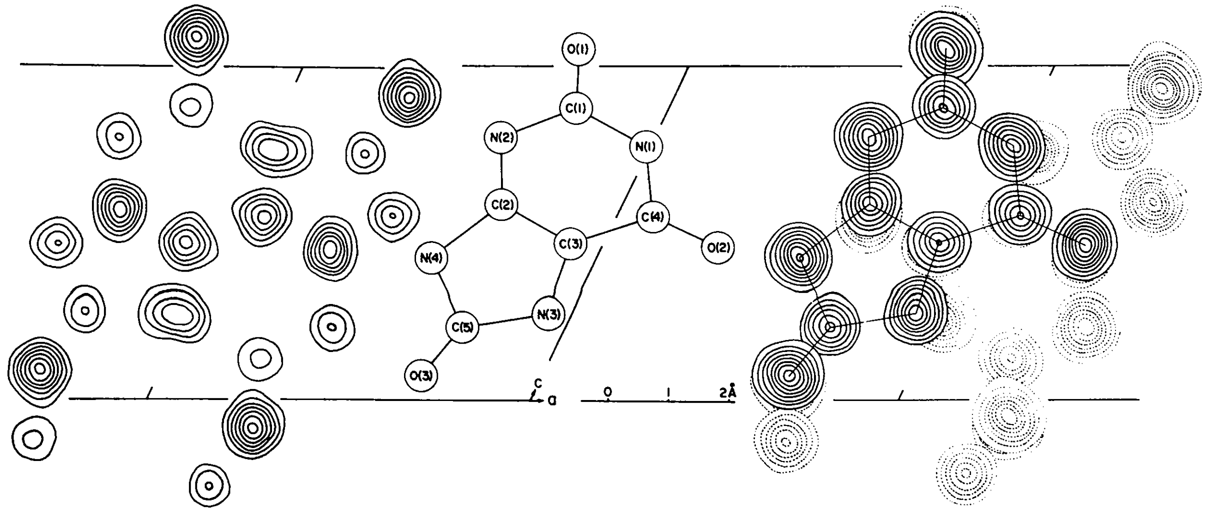
Results and discussion

Molecular arrangement

The molecules form sheets, the plane of which is normal to the molecular plane and perpendicular to the a axis. Within alternating, one-molecule-thick sheets, the molecules are oriented in the (021) and the $(02\bar{1})$ planes respectively, forming rows in which the molecules are related to each other by centres of symmetry and kept together by hydrogen bonds. Between rows within the same sheet there are no hydrogen bonds. However there is a firm hydrogen bonding system between adjacent, screw-axis related sheets (Fig. 4), which have intersecting rows of about 60°.

Molecular structure

The final fractional coordinates and anisotropic temperature factor parameters of the nonhydrogen atoms are given in Table 2. In Table 3 are tabulated the root mean square components of thermal displacement along the three principal axes of each atom and the angle between these axes and those of an orthogonal system XYZ defined by X along the a axis and Y normal to the approximate plane of the molecule $(02\bar{1})$. The calculations were performed with the 7090 Function and Error Program ORFFE (Busing, Martin & Levy, 1964). The calculated bond lengths (I) with standard deviations are given in Table 4 together with bond distances corrected for thermal motion according to Busing & Levy (1964). The values following the assumption of independent thermal motion (III) are given for comparison together with the values when one atom is assumed to 'ride' on the other (II). It is thought that the true value for intramolecular bond lengths is close to (II) especially for terminal bonds, in this case involving hydrogen (Table 7) and oxygen. Intermolecular distances and hydrogen bonds should probably be calculated according to (III) (Table 8). The bond angles are shown in Table 5 and also together with the uncorrected bond lengths in Fig. 2. It is seen that the uric acid molecule can be said to be essentially in the keto form but in resonance with a variety of mesomeric structures. Using the formula by Pauling



(a) (b) (c)

Fig. 1. (a) First electron-density projection along the b axis. Contours at equal and arbitrary intervals. (b) Same projection showing the convention adopted for the labelling of the atoms. (c) Final three-dimensional electron-density projection. Contours at equal intervals of about 1 e.Å^{-3}, zero omitted.

Table 1. *Observed and calculated structure factors*

The sign + indicates unobserved reflexions and = indicates that the photographic density of the reflexion was out of the linear range.

h00

h	Fobs	Fcal
16	8.1	7.5
14	9.9	-8.7
12	25.3	-23.7
10	14.7	-10.6
8	42.7	45.3
6	=61.5	63.7
4	=50.4	-63.8
2	=34.6	49.7

h10

h	Fobs	Fcal
15	+ 1.1	-2.0
14	5.6	5.9
13	5.6	5.4
12	15.7	16.3
11	11.9	12.0
10	4.1	-2.9
9	5.9	5.0
8	13.0	12.3
7	+ 1.0	-0.6
6	16.5	16.2
5	2.2	-1.8
4	21.3	-22.9
3	6.1	-4.9
2	=39.0	53.0
1	5.6	5.2

h20

h	Fobs	Fcal
15	+ 1.0	1.9
14	9.7	9.5
13	4.2	4.5
12	8.5	8.7
11	12.8	-12.7
10	4.1	2.4
9	14.4	-14.4
8	14.6	13.1
7	9.4	-8.2
6	14.7	-13.9
5	14.3	-13.0
4	27.5	-27.9
3	12.9	-12.9
2	15.8	-15.0
1	3.6	-4.0
0	33.9	-35.1

h30

h	Fobs	Fcal
15	+ 0.9	-0.5
14	1.8	2.3
13	15.4	-14.9
12	5.4	6.1
11	6.8	-6.3
10	14.8	15.1
9	6.4	5.9
8	4.9	5.4
7	6.6	-6.1
6	16.1	-15.1
5	11.8	-9.7
4	12.2	11.4
3	6.8	-7.1
2	33.7	-37.3
1	8.0	8.3

h40

h	Fobs	Fcal
15	3.8	-5.1
14	6.2	6.4
13	12.2	12.0
12	19.9	-19.3
11	6.1	5.2
10	20.5	-20.4
9	15.1	-14.6
8	7.5	6.9
7	13.6	12.8
6	4.3	-3.8
5	25.0	25.2
4	31.6	-31.4
3	8.4	-7.3
2	12.1	-12.7
1	4.1	-4.0
0	14.8	14.3

h50

h	Fobs	Fcal
12	6.4	-6.5
11	9.8	-10.2
10	2.3	-2.2
9	5.8	5.7
8	8.6	-8.2
7	4.4	4.2
6	10.4	-9.7
5	11.2	-10.6
4	2.4	-2.2
3	8.9	8.8
2	4.8	-4.8
1	3.3	-4.2

h60

h	Fobs	Fcal
12	8.3	9.2
11	6.1	5.5
10	2.9	1.8
9	3.9	2.6
8	5.9	-5.4
7	16.6	-16.8
6	7.5	7.6
5	+ 1.4	2.4
4	7.5	6.6
3	5.9	4.0
2	8.2	-7.3
1	11.2	-10.4
0	14.1	-12.0

h70

h	Fobs	Fcal
11	3.4	4.7
10	4.3	-4.8
9	3.7	-4.2
8	+ 1.2	0.5
7	5.0	4.2
6	5.1	4.8
5	10.8	11.0
4	6.3	-2.8
3	5.2	-4.6
2	4.9	-4.2
1	5.3	4.6

h80

h	Fobs	Fcal
8	6.6	8.0
7	10.1	11.7
6	7.4	7.9
5	10.4	11.1
4	+ 1.2	-0.6
3	3.2	-3.4
2	8.0	7.5
1	3.8	-3.1
0	14.4	14.7

h90

h	Fobs	Fcal
4	2.1	-2.6
3	+ 0.8	-1.6
2	+ 0.9	-1.0
1	3.0	-2.4

h01

h	Fobs	Fcal
16	4.2	1.0
14	8.1	5.6
12	17.5	16.0
10	25.3	26.0
8	27.9	29.1
6	10.6	-8.7
4	10.9	-9.8
2	7.9	-6.5
0	=27.3	-40.2
-2	23.3	-24.0
-4	36.2	-43.2
-6	15.5	-12.6
-8	+ 2.1	1.1
-10	15.4	-13.0
-12	12.0	10.4
-14	14.1	13.1

h11

h	Fobs	Fcal
17	3.3	2.7
16	+ 1.0	-0.7
15	2.6	-2.3
14	4.4	3.3
13	16.7	-16.7
12	7.7	7.4
11	5.5	-5.8
10	13.5	12.7
9	4.4	-4.0
8	6.2	-5.0
7	5.9	-5.5
6	11.1	-10.4
5	7.0	7.2
4	22.5	23.9
3	37.4	-40.4
2	2.2	1.3
1	18.6	-19.9
0	8.5	8.4
-1	=47.5	62.8
-2	6.6	-5.2
-3	9.6	9.0
-4	7.4	-8.1
-5	15.6	-15.7
-6	24.1	25.0
-7	5.1	5.4
-8	+ 1.2	-1.5
-9	14.9	14.9
-10	5.6	-5.1
-11	9.7	10.1
-12	15.3	15.0
-13	+ 1.2	1.2
-14	3.4	2.8

h21

h	Fobs	Fcal
16	11.5	12.3
15	8.3	-8.8
14	6.7	-6.3
13	8.3	6.6
12	34.9	-35.7
11	11.5	11.0
10	8.2	-7.5
9	+ 1.2	-0.6
8	33.5	34.0
7	41.4	42.4
6	5.3	-6.2
5	33.8	34.9
4	=55.3	-63.7
3	5.4	-4.5
2	33.1	33.9
1	=46.7	91.2
0	=49.1	125.8
-1	=55.2	66.9
-2	19.7	-18.5
-3	1.8	-1.4
-4	30.3	-29.2
-5	4.2	2.4
-6	38.5	40.1
-7	13.8	12.0
-8	12.6	10.9
-9	16.2	15.5
-10	20.3	-20.1
-11	+ 1.4	-0.0
-12	11.6	-11.0
-13	12.4	-12.2
-14	2.6	1.4

h31

h	Fobs	Fcal
16	1.9	0.9
15	+ 1.0	-1.2
14	2.4	2.4
13	12.7	12.4
12	16.4	17.0
11	+ 1.3	2.5
10	+ 1.2	1.4
9	11.0	10.7
8	9.4	-8.9
7	16.1	15.8
6	5.6	4.9
5	15.5	-15.6
4	7.4	-7.5
3	14.6	15.2
2	3.1	3.4
1	6.0	6.7
0	1.5	0.9
-1	23.2	-23.7
-2	16.9	-16.8
-3	2.2	1.7
-4	13.6	13.7
-5	12.9	-12.5
-6	1.5	0.5
-7	10.4	-10.3
-8	5.2	-5.1
-9	2.9	2.3
-10	11.6	11.3
-11	8.9	-8.8
-12	6.4	6.3
-13	4.7	-5.1
-14	2.8	-3.3

h41

h	Fobs	Fcal
15	1.6	-1.5
14	12.2	-13.1
13	2.9	-2.4
12	4.9	4.9
11	3.6	-3.6
10	10.8	-11.1
9	3.4	2.4
8	8.0	7.7
7	18.8	-18.5
6	+ 1.0	0.5
5	14.8	-14.9
4	20.0	-18.9
3	4.2	-4.3
2	4.2	-4.1
1	7.8	-8.4
0	23.2	-23.0
-1	14.1	14.6
-2	13.1	-12.9
-3	9.2	-8.4
-4	8.5	8.2
-5	11.1	-10.6
-6	5.9	-5.6
-7	17.3	16.5
-8	+ 1.3	-1.3
-9	6.7	6.3
-10	13.4	13.5
-11	+ 1.2	-1.8
-12	7.8	7.7
-13	1.6	0.8

h51

h	Fobs	Fcal
15	+ 0.6	1.4
14	6.2	-6.1
13	+ 1.0	0.9
12	10.1	9.3
11	8.6	-8.5
10	4.6	-4.1
9	3.0	-3.0
8	+ 1.1	1.1
7	+ 1.0	-0.9
6	16.4	-16.0
5	6.4	6.3
4	2.6	2.1
3	3.9	3.2
2	8.8	9.2
1	11.9	13.7
0	5.3	-6.1
-1	4.2	-3.6
-2	2.7	-2.7
-3	17.0	-16.9
-4	5.2	-4.8
-5	6.9	6.4
-6	8.8	-8.5
-7	3.2	2.4
-8	+ 1.1	1.6
-9	6.7	-6.8
-10	3.6	-3.1
-11	10.0	-6.9
-12	6.6	-7.4
-13	6.2	-8.6

h02

h	Fobs	Fcal
18	9.5	-9.5
16	22.8	22.0
14	14.5	-10.6
12	49.5	-57.4
10	+ 2.1	-0.9
8	14.3	12.0
6	=47.0	-71.4
4	=42.0	-63.5
2	2.8	-0.8
0	20.2	19.2
-2	36.3	-39.1
-4	17.8	-14.6
-6	28.1	27.7
-8	12.4	-8.9
-10	24.2	-22.8
-12	3.6	1.8
-14	6.4	6.0

h12

h	Fobs	Fcal
18	1.6	-2.5
17	+ 0.9	-0.4
16	4.3	3.2
15	+ 1.2	-2.1
14	10.8	-10.1
13	11.7	-12.2
12	+ 1.3	0.5
11	14.2	-13.4
10	8.8	-8.5
9	11.2	9.9
8	16.9	-16.6
7	13.5	13.0
6	19.4	19.0
5	15.6	-14.7
4	16.4	-16.4
3	10.8	-10.1
2	28.5	-29.2
1	8.3	-7.4
0	21.4	20.7
-1	20.4	20.8
-2	15.6	15.7
-3	5.9	5.1
-4	7.4	6.4
-5	25.4	-25.5
-6	5.9	-5.7
-7	+ 1.2	-0.5
-8	5.5	5.4
-9	8.2	7.9
-10	15.5	16.5
-11	10.9	-10.4
-12	2.7	3.2
-13	4.9	-4.6
-14	2.6	-3.2

h22

h	Fobs	Fcal
17	3.8	3.5
16	+ 1.1	-0.6
15	2.1	-1.5
14	11.3	10.9
13	3.1	-2.5
12	12.0	11.7
11	16.3	16.3
10	5.4	5.1
9	15.1	14.8
8	23.6	24.3
7	16.8	-16.6
6	6.3	6.1
5	3.5	-0.0
4	13.9	-12.2
3	5.9	5.4
2	4.0	3.3
1	4.0	-3.0
0	34.8	-35.7
-1	19.9	19.2
-2	16.5	-15.8
-3	21.4	-21.4
-4	1.5	1.4
-5	12.6	-11.4
-6	12.3	-11.7
-7	15.2	14.8
-8	7.3	-7.4
-9	6.4	-6.5
-10	3.5	3.9
-11	6.0	-5.7
-12	8.9	8.8
-13	5.5	6.2

h32

h	Fobs	Fcal
17	4.0	4.7
16	2.3	-2.1
15	3.3	3.3
14	9.8	-10.0
13	3.4	3.7
12	12.1	-12.4
11	8.5	7.9
10	3.5	3.0
9	4.3	-4.3
8	6.6	-5.8
7	9.8	8.8
6	17.1	-16.7
5	17.3	17.2
4	4.9	5.1
3	19.0	-18.7
2	10.8	-9.8
1	13.6	12.8
0	8.5	8.7
-1	19.2	19.9
-2	20.7	20.2
-3	13.9	-13.8
-4	6.3	-5.8
-5	9.0	8.7
-6	2.1	0.2
-7	8.2	6.9
-8	7.6	7.6
-9	+ 1.3	-1.4
-10	4.9	4.8
-11	6.2	6.2
-12	7.1	7.9

h42

h	Fobs	Fcal
16	9.2	10.4
15	4.2	-4.3
14	10.0	-10.5
13	3.0	3.8
12	18.5	-17.7
11	3.8	-2.6
10	7.9	7.0
9	3.2	-3.3
8	25.5	24.5
7	26.2	25.0
6	2.2	-2.0
5	3.5	2.7
4	16.4	-16.8
3	19.2	-19.5
2	49.0	49.5
1	25.9	26.2
0	64.9	66.5
-1	16.3	16.2
-2	8.2	-8.1
-3	10.6	-10.8
-4	4.4	3.3
-5	12.7	-13.0
-6	36.8	37.3
-7	4.4	-4.7
-8	9.5	9.1
-9	6.2	5.5
-10	8.9	-8.5
-11	7.6	-7.3
-12	2.3	3.0

h52

h	Fobs	Fcal
15	+ 0.7	-1.1
14	3.8	3.1
13	14.3	14.9
12	7.3	6.8
11	3.6	3.4
10	7.7	6.8
9	7.3	-6.7
8	7.2	7.2
7	2.1	1.2
6	4.5	-3.6
5	5.7	-5.3
4	+ 0.9	-0.9
3	3.2	3.0
2	4.9	4.6
1	+ 0.8	0.1
0	8.9	-8.0
-1	13.9	-13.8
-2	3.5	-3.1
-3	+ 1.0	-1.1
-4	4.2	4.0
-5	+ 1.1	1.3
-6	11.2	-11.0
-7	2.3	2.2
-8	5.7	-5.5
-9	+ 1.0	1.2
-10	5.9	6.0

h03

h	Fobs	Fcal
18	+ 1.4	-1.9
16	+ 2.1	-2.2
14	17.7	15.6
12	+ 2.4	-0.7
10	18.3	-14.9
8	30.0	30.5
6	8.9	9.4
4	22.6	-19.2
2	8.5	5.9
0	42.1	-47.7
-2	5.8	-4.9
-4	20.2	17.9
-6	23.9	-22.4
-8	10.2	-7.7
-10	13.8	12.7
-12	4.5	3.5

h13

h	Fobs	Fcal
18	2.9	-3.3
17	+ 1.0	0.6
16	4.7	-4.2
15	7.9	7.5
14	8.0	-8.2
13	5.9	5.5
12	21.8	-21.9
11	3.3	-2.7
10	8.1	7.7
9	10.9	10.1
8	7.8	7.3
7	19.4	18.1
6	33.8	-34.0
5	3.0	-2.6
4	10.2	10.0
3	3.0	-3.2
2	5.2	5.9
1	7.8	7.5
0	8.7	-8.7
-1	5.0	-4.0
-2	14.4	13.6
-3	12.9	-12.5
-4	12.1	-11.1
-5	2.2	-2.6
-6	5.2	-4.0
-7	+ 1.3	0.3
-8	5.6	5.5
-9	6.9	-6.8
-10	8.7	-8.9
-11	8.8	-9.4
-12	2.3	-2.5

h23

h	Fobs	Fcal
18	2.2	2.4
17	5.3	-4.8
16	19.3	19.6
15	3.3	3.4
14	16.6	-16.8
13	9.5	-7.8
12	32.5	-34.2
11	14.4	-12.9
10	15.6	14.7
9	8.6	-8.1
8	8.0	6.4
7	6.6	-6.3
6	38.3	-38.9
5	15.7	-14.9
4	12.7	-13.2
3	28.5	-28.5
2	30.8	29.9
1	23.2	-22.0
0	23.2	22.4
-1	8.7	-7.3
-2	16.7	-15.7
-3	8.8	-8.5
-4	11.0	10.7
-5	15.4	-15.7
-6	29.5	30.9
-7	10.8	-10.4
-8	5.5	-4.2
-9	2.8	-2.6
-10	9.8	-9.6
-11	4.0	-3.7
-12	4.9	5.4

h33

h	Fobs	Fcal
17	1.9	1.3
16	2.8	1.7
15	3.5	-3.7
14	10.2	-10.5
13	+ 1.3	-1.3
12	5.4	-5.4
11	7.0	-6.5
10	5.7	5.2
9	9.4	-9.7
8	6.2	5.7
7	6.6	5.9
6	6.0	5.9
5	5.5	-4.5
4	6.6	-6.6
3	13.5	-12.3
2	12.7	-11.5
1	3.0	2.5
0	7.7	7.5
-1	9.3	9.0
-2	13.0	12.9
-3	2.4	1.4
-4	5.3	-5.0
-5	3.4	-2.6
-6	15.5	-15.3
-7	8.9	8.5
-8	2.1	2.3
-9	5.5	5.8
-10	8.4	8.3

h43

h	Fobs	Fcal
16	+ 0.8	-1.4
15	5.5	5.1
14	+ 1.1	0.2
13	4.4	3.1
12	18.0	17.9
11	4.1	-4.2
10	20.2	19.8
9	8.4	7.7
8	2.4	2.3
7	+ 1.2	0.6
6	5.7	4.8
5	13.9	-13.6
4	13.6	11.9
3	6.1	-4.9
2	3.0	3.0
1	8.3	-7.1
0	9.3	-8.6
-1	4.5	5.1
-2	13.4	-13.1
-3	1.7	1.5
-4	11.4	-11.1
-5	+ 1.3	-0.2
-6	5.1	-4.7
-7	5.8	5.2
-8	4.6	-4.9
-9	1.4	1.1
-10	4.4	-4.2

h53

h	Fobs	Fcal
15	+ 0.7	0.7
14	+ 0.9	-0.4
13	11.2	-11.5
12	7.3	7.0
11	5.4	-5.1
10	+ 1.1	1.1
9	2.0	-1.8
8	2.2	2.4
7	7.1	-6.2
6	9.5	8.7
5	+ 1.0	1.0
4	+ 1.0	0.9
3	10.7	-10.2
2	+ 1.0	0.4
1	8.0	7.0
0	4.7	4.9
-1	18.5	19.0
-2	3.0	2.7
-3	7.7	-7.7
-4	3.8	3.3
-5	+ 1.1	-0.3
-6	+ 1.1	-0.7
-7	10.0	10.4
-8	2.7	-2.4
-9	2.5	2.7

h04

h	Fobs	Fcal
18.	13.1	14.2
16	18.0	16.2
14	19.4	-18.2
12	17.5	-15.9
10	28.2	26.3
8	7.8	6.2
6	24.2	-22.6
4	17.1	13.1
2	42.5	44.8
0	24.9	23.4
-2	10.2	-7.3
-4	24.1	22.8
-6	30.8	32.5
-8	4.6	-2.2
-10	3.1	-3.1

h14

h	Fobs	Fcal
17	2.5	2.2
16	2.4	3.3
15	7.0	7.3
14	5.0	5.0
13	14.8	15.4
12	10.3	9.7
11	4.7	-4.3
10	4.4	3.6
9	8.7	-8.4
8	8.6	8.1
7	17.2	15.7
6	18.5	17.8
5	+ 1.1	-1.3
4	5.0	-5.6
3	7.2	-7.0
2	5.5	-4.9
1	8.3	8.0
0	+ 1.2	-0.4
-1	9.7	-8.7
-2	6.5	-6.0
-3	4.3	-4.0
-4	+ 1.3	-1.1
-5	10.2	9.7
-6	10.8	-10.3
-7	4.2	3.5
-8	5.9	-5.8
-9	3.9	-3.5
-10	2.8	3.0

h24

h	Fobs	Fcal
17	+ 0.9	-2.4
16	3.0	-3.1
15	8.8	8.3
14	3.7	4.3
13	+ 1.4	-1.9
12	10.5	10.9
11	22.8	-23.1
10	4.2	4.2
9	5.2	4.8
8	8.5	8.4
7	7.8	7.2
6	11.1	10.7
5	21.3	-20.1
4	7.5	6.6
3	7.7	-6.4
2	4.7	4.2
1	11.6	-10.5
0	19.7	-19.5
-1	+ 1.3	-0.2
-2	6.8	-7.1
-3	12.8	12.5
-4	1.9	-0.4
-5	2.3	-1.9
-6	13.4	-13.5
-7	2.7	-2.7
-8	4.5	-4.9
-9	5.7	6.3

h34

h	Fobs	Fcal
17	5.1	-5.1
16	1.6	-1.2
15	3.7	3.6
14	2.9	3.2
13	17.7	-18.2
12	+ 1.3	-0.2
11	10.4	-9.8
10	5.2	4.6
9	10.3	9.8
8	10.5	9.8
7	9.3	-8.7
6	5.7	-5.3
5	7.3	-7.3
4	4.2	4.1
3	2.9	-2.1
2	4.8	4.5
1	6.1	5.3
0	10.8	-10.3
-1	10.2	9.8
-2	+ 1.3	1.1
-3	11.6	-11.4
-4	+ 1.3	-0.1
-5	4.0	-3.7
-6	5.2	-4.9
-7	8.5	9.2
-8	3.3	-3.7
-9	3.5	-4.2

h44

h	Fobs	Fcal
16	6.1	7.1
15	3.9	4.1
14	14.3	-14.4
13	11.7	-10.6
12	16.8	-16.7
11	10.0	-9.1
10	8.1	7.8
9	2.2	2.3
8	18.2	-18.1
7	19.2	19.5
6	39.1	-40.0
5	2.1	2.3
4	3.7	-3.2
3	12.9	-13.4
2	+ 1.2	0.5
1	15.1	15.2
0	14.7	-15.4
-1	10.2	10.7
-2	8.5	-8.0
-3	3.1	-3.4
-4	4.1	3.9
-5	2.4	2.5
-6	6.2	5.6
-7	2.9	-2.2
-8	2.9	-2.9

h54

h	Fobs	Fcal
15	4.2	-5.1
14	2.6	-3.1
13	4.2	-4.3
12	+ 1.0	0.6
11	1.9	1.2
10	6.6	-6.4
9	9.9	10.1
8	6.3	-6.5
7	3.8	4.0
6	11.9	11.5
5	13.4	-13.7
4	+ 1.1	-1.1
3	2.8	2.3
2	16.9	-17.1
1	9.1	9.7
0	4.9	4.3
-1	2.5	-2.4
-2	11.8	12.5
-3	2.4	-2.8
-4	+ 1.0	-1.5
-5	5.6	-5.4
-6	1.7	-1.9

h05

h	Fobs	Fcal
16	7.5	-5.9
14	+ 2.2	0.3
12	27.8	28.5
10	13.9	10.5
8	4.1	-2.7
6	23.3	20.3
4	21.1	16.7
2	10.8	7.2
0	12.3	-8.9
-2	14.6	-12.2
-4	5.5	-4.4
-6	7.9	-6.3
-8	2.2	-5.3

h15

h	Fobs	Fcal
17	1.8	-1.0
16	+ 1.0	-1.7
15	3.5	3.4
14	9.3	9.8
13	8.7	-8.4
12	5.7	5.1
11	9.4	-9.1
10	6.6	-6.8
9	3.5	-2.6
8	3.7	2.8
7	3.9	-3.2
6	3.4	-2.8
5	3.4	-3.5
4	2.2	2.0
3	3.2	-2.8
2	4.3	4.2
1	10.2	9.7
0	10.0	-9.5
-1	5.1	4.6
-2	+ 1.3	1.6
-3	6.2	-5.8
-4	7.3	8.2
-5	7.7	7.6
-6	2.9	2.5
-7	8.7	9.9

h25

h	Fobs	Fcal
17	6.0	7.2
16	5.0	4.8
15	2.7	2.1
14	12.9	-13.6
13	3.6	-3.1
12	5.5	-5.9
11	+ 1.4	0.1
10	14.8	14.3
9	10.5	10.6
8	19.0	-19.3
7	23.6	24.3
6	30.1	-30.6
5	7.4	7.0
4	11.7	11.8
3	3.8	3.1
2	9.1	8.7
1	23.7	24.9
0	8.7	-8.8
-1	8.5	8.8
-2	4.5	-3.5
-3	2.2	1.2
-4	10.5	10.4
-5	9.6	10.1
-6	11.2	11.7

h35

h	Fobs	Fcal
16	2.8	3.0
15	2.3	2.5
14	10.3	10.4
13	7.1	6.9
12	7.7	7.3
11	3.4	2.7
10	12.2	-12.0
9	9.2	9.5
8	+ 1.3	-1.4
7	5.8	5.5
6	22.0	22.3
5	12.0	-11.9
4	4.3	-3.5
3	7.6	6.8
2	14.5	-15.0
1	5.8	6.2
0	2.2	1.1
-1	14.5	-15.1
-2	3.5	3.4
-3	3.5	-3.7
-4	2.7	2.3
-5	+ 1.0	0.0
-6	2.0	-1.9

h45

h	Fobs	Fcal
15	5.8	5.9
14	3.1	3.5
13	1.8	1.0
12	3.4	-3.8
11	5.9	-4.8
10	4.6	-4.4
9	5.3	5.3
8	9.8	9.8
7	+ 1.3	-0.4
6	5.7	5.7
5	7.6	-6.8
4	+ 1.3	-1.7
3	+ 1.3	-0.4
2	1.8	-0.9
1	10.3	-10.7
0	3.9	-3.3
-1	5.4	-5.8
-2	4.9	4.4
-3	1.5	1.8
-4	+ 1.0	-0.5
-5	2.2	-2.5

h55

h	Fobs	Fcal
14	4.1	-4.7
13	5.4	-6.1
12	8.3	-9.3
11	+ 1.0	1.6
10	4.0	-3.7
9	13.4	13.7
8	3.6	-2.9
7	3.8	-3.9
6	1.1	-0.6
5	7.0	-7.1
4	+ 1.1	0.9
3	4.5	4.3
2	3.3	-3.6
1	4.1	4.4
0	+ 1.0	0.5
-1	+ 1.0	-0.8
-2	4.1	4.0
-3	5.7	-6.5
-4	2.4	-2.8

h06

h	Fobs	Fcal
16	2.9	-1.8
14	11.7	-10.1
12	+ 2.2	-1.7
10	8.1	4.8
8	36.1	-36.4
6	32.1	-31.7
4	13.1	11.1
2	15.1	-11.8
0	20.1	-19.0
-2	+ 2.0	-0.5
-4	3.4	2.3

h16

h	Fobs	Fcal
16	2.8	3.5
15	3.3	-3.1
14	2.1	-2.5
13	9.7	-9.6
12	3.4	-3.4
11	3.5	3.3
10	7.8	-7.6
9	7.9	8.5
8	3.5	-3.7
7	8.4	-7.9
6	16.9	16.6
5	8.9	-8.9
4	3.7	-3.8
3	8.2	7.8
2	9.6	-9.7
1	7.9	8.3
0	12.0	12.8
-1	5.0	-5.4
-2	3.8	3.2
-3	6.1	-6.7
-4	+ 0.8	-2.3

h26

h	Fobs	Fcal
16	5.9	-6.8
15	+ 0.9	0.2
14	+ 1.0	1.2
13	8.4	8.7
12	10.8	10.5
11	9.2	9.6
10	+ 1.3	-0.5
9	+ 1.3	-0.3
8	4.4	3.4
7	+ 1.3	-0.3
6	13.0	12.3
5	5.3	5.1
4	5.6	4.7
3	4.4	3.8
2	4.5	4.5
1	3.5	-4.0
0	+ 1.2	0.1
-1	6.3	-6.8
-2	2.1	-2.3
-3	3.0	-3.1
-4	2.1	-2.1

h36

h	Fobs	Fcal
15	4.7	5.6
14	+ 0.9	1.1
13	+ 1.0	0.2
12	4.9	-5.3
11	+ 1.1	-0.5
10	11.6	-11.7
9	7.5	7.3
8	4.2	-3.4
7	1.7	-2.6
6.	3.3	2.5
5	5.1	-5.4
4	+ 1.2	-0.4
3	5.1	5.1
2	2.3	-2.2
1	4.5	4.6
0	+ 1.1	0.4
-1	3.3	-3.1
-2	4.6	4.8
-3	2.2	-1.8

h46

h	Fobs	Fcal
14	4.2	-5.6
13	7.9	-9.0
12	5.0	4.7
11	2.0	-2.0
10	8.4	8.6
9	+ 1.1	-0.6
8	+ 1.1	0.9
7	2.3	-3.1
6	5.2	-4.2
5	3.0	2.5
4	3.7	3.8
3	2.9	2.6
2	8.5	8.8
1	4.0	4.3
0	3.0	3.4
-1	1.9	-1.9
-2	2.2	2.9

h56

h	Fobs	Fcal
11	2.9	2.9
10	3.6	-3.5
9	3.1	-2.7
8	5.9	5.7
7	4.8	4.7
6	4.9	5.2
5	+ 0.9	-0.8
4	2.0	-1.5
3	+ 0.8	-1.3
2	3.5	-3.7

h07

h	Fobs	Fcal
14	2.3	-2.3
12	4.5	-2.2
10	5.4	-4.1
8	7.4	5.7
6	8.0	5.5
4	+ 1.9	-1.9
2	5.2	4.5
0	5.2	4.6

h17

h	Fobs	Fcal
14	3.6	-3.6
13	2.2	-2.1
12	1.6	-1.6
11	7.5	8.3
10	+ 1.0	-0.2
9	10.7	11.1
8	3.7	-3.0
7	10.1	-10.9
6	8.3	-7.8
5	7.1	-7.7
4	2.1	2.1
3	9.8	10.9
2	3.1	2.8
1	+ 0.9	1.7
0	3.8	-4.6

h27

h	Fobs	Fcal
13	6.2	-7.0
12	5.2	5.2
11	2.5	-2.4
10	3.5	3.5
9	9.9	-10.4
8	11.8	-11.5
7	12.1	-13.7
6	9.5	-10.1
5	2.8	2.2
4	3.2	4.0
3	3.2	-2.7
2	3.7	-3.5
1	7.0	-8.4
0	2.9	-3.9

h37

h	Fobs	Fcal
12	4.4	-5.0
11	3.8	4.2
10	+ 0.8	0.1
9	2.9	-2.7
8	2.4	2.1
7	+ 0.9	0.8
6	4.2	4.0
5	+ 0.9	-0.0
4	+ 0.9	-1.0

h47

h	Fobs	Fcal
8	2.7	2.8
7	+ 0.7	0.7
6	8.8	9.7
5	+ 0.7	0.6
4	2.4	2.6

(1948) on the bond distances (II) gives the sum of double-bond character for bonds surrounding each of the five carbon atoms as 97–109, 96–111, 92–108, 94–105 and 93–101%. The ranges include standard deviation of the bond lengths. Adding the double-bond character of the non-hydrogen bonds for the four nitrogen and the oxygen atoms in adjacent molecules connected to each of them by hydrogen bonds gives 93–105, 92–101, 90–99 and 95–105%. In the above calculations the following standard bond lengths have been used: $C{-}C = 1{\cdot}50$, $C{=}C = 1{\cdot}33$, $C{-}N = 1{\cdot}47$, $C{=}N^+ = 1{\cdot}24$, $C{-}O^- = 1{\cdot}45$, $C{=}O = 1{\cdot}20$ Å. The C–C distance is here modified according to Pauling (1960) and the $C{=}N^+$ and $C{-}O^-$ corrected in the manner suggested by Pauling (1948) to take into account the effect of the present charges in these cases. The $C{=}O$ bond length is revised according to Vaughan & Donohue (1952) and Penfold (1953).

Table 2. *Final fractional atomic positional parameters and anisotropic temperature factor parameters, all with estimated standard errors*

All values are × 10^5.

Atom	x/a	σ_x	y/b	σ_y	z/c	σ_z	β_{11}	σ	β_{22}	σ	β_{33}	σ	β_{12}	σ	β_{13}	σ	β_{23}	σ
C(1)	39588	27	42200	57	87757	64	318	21	909	135	1879	118	−39	33	−466	40	−17	79
C(2)	36545	25	26650	55	58328	63	240	19	737	127	1811	109	−26	30	−367	36	64	76
C(3)	46484	26	21754	58	46398	63	234	19	1020	133	1797	110	2	30	−339	37	−65	77
C(4)	53826	25	26650	57	54745	63	225	18	953	133	1900	113	−47	31	−318	37	213	79
C(5)	38108	25	11110	54	26193	60	183	18	1002	133	1614	105	−17	29	−266	35	53	76
N(1)	49430	24	36422	48	75924	55	297	18	1091	120	1917	97	−69	28	−461	34	−82	66
N(2)	32883	22	36683	48	78474	53	209	17	1136	119	1913	99	28	27	−359	33	−191	67
N(3)	47474	22	12343	46	26222	52	185	16	1185	120	1694	93	−2	26	−292	31	−208	64
N(4)	31415	23	20174	46	45958	52	185	16	1102	126	1649	93	65	26	−292	30	−100	63
O(1)	36783	21	51657	45	105543	51	406	18	1701	120	2253	97	29	27	−540	34	−477	67
O(2)	63000	18	23031	42	45254	48	174	14	1765	117	2532	98	−58	24	−358	29	−17	64
O(3)	35938	19	03350	41	11202	47	271	15	1474	117	1861	84	5	24	−331	28	−400	59

Table 3. *Principal axes* (i) *of anisotropic temperature factors, referred to orthogonal axes XYZ*

X is along the crystallographic a axis and Y is normal to the approximate plane of the molecule, $(02\bar{1})$. The r.m.s. displacements $\bar{\mu}_i$ are in Å and the direction angles, V, are in degrees.

Atom	i	$\bar{\mu}_i$	(σ)	V_x	(σ)	V_y	(σ)	V_z	(σ)
C(1)	1	0·140	(6)	150	(9)	93	(13)	60	(8)
	2	0·164	(11)	104	(15)	23	(16)	108	(15)
	3	0·181	(5)	116	(7)	113	(16)	144	(11)
C(2)	1	0·132	(6)	167	(22)	78	(25)	87	(11)
	2	0·144	(12)	80	(27)	23	(18)	111	(11)
	3	0·173	(5)	83	(6)	70	(10)	21	(10)
C(3)	1	0·135	(7)	177	(8)	90	(7)	87	(8)
	2	0·167	(8)	93	(8)	85	(48)	174	(43)
	3	0·175	(6)	90	(7)	175	(48)	95	(49)
C(4)	1	0·135	(6)	171	(13)	98	(14)	94	(5)
	2	0·155	(9)	98	(14)	8	(14)	88	(12)
	3	0·185	(6)	93	(5)	92	(12)	4	(7)
C(5)	1	0·122	(6)	172	(6)	96	(6)	95	(6)
	2	0·161	(5)	82	(7)	140	(30)	129	(30)
	3	0·171	(10)	91	(7)	130	(30)	40	(30)
N(1)	1	0·131	(6)	152	(5)	95	(5)	63	(5)
	2	0·180	(7)	63	(77)	116	(58)	39	(75)
	3	0·181	(5)	82	(52)	27	(44)	65	(80)
N(2)	1	0·122	(6)	175	(6)	90	(4)	85	(6)
	2	0·164	(6)	95	(6)	80	(14)	169	(13)
	3	0·187	(6)	91	(4)	170	(14)	100	(14)
N(3)	1	0·118	(6)	173	(5)	95	(3)	85	(6)
	2	0·158	(5)	94	(6)	96	(10)	173	(8)
	3	0·188	(8)	85	(3)	172	(7)	85	(10)
N(4)	1	0·121	(6)	172	(5)	84	(4)	96	(6)
	2	0·158	(5)	85	(6)	99	(15)	170	(13)
	3	0·178	(9)	97	(4)	169	(12)	81	(15)
O(1)	1	0·152	(5)	134	(5)	89	(3)	44	(5)
	2	0·192	(4)	44	(5)	86	(5)	46	(5)
	3	0·233	(6)	88	(4)	176	(5)	87	(5)
O(2)	1	0·113	(5)	171	(2)	98	(2)	95	(2)
	2	0·204	(4)	82	(2)	123	(9)	146	(9)
	3	0·224	(7)	86	(2)	146	(9)	56	(9)
O(3)	1	0·145	(4)	154	(12)	96	(3)	65	(13)
	2	0·161	(4)	66	(13)	81	(4)	26	(12)
	3	0·218	(6)	81	(3)	169	(3)	85	(4)

Table 4. *Non-hydrogen intramolecular distances* (Å)

(I) Observed, (II) corrected for thermal motion assuming one atom to 'ride' on the other and (III) assuming the atoms to move independently.

Atoms	I	(σ)	II	(σ)	III	(σ)
C(2)-C(3)	1·360	(5)	1·364	(5)	1·396	(5)
C(3)-C(4)	1·411	(5)	1·410	(5)	1·450	(5)
C(1)-N(1)	1·367	(5)	1·369	(5)	1·404	(5)
C(1)-N(2)	1·382	(4)	1·383	(4)	1·425	(5)
C(2)-N(2)	1·356	(5)	1·360	(5)	1·389	(5)
C(2)-N(4)	1·360	(4)	1·361	(5)	1·396	(5)
C(3)-N(3)	1·387	(5)	1·388	(5)	1·423	(5)
C(4)-N(1)	1·397	(5)	1·401	(5)	1·431	(5)
C(5)-N(3)	1·359	(4)	1·361	(4)	1·401	(5)
C(5)-N(4)	1·376	(5)	1·378	(5)	1·409	(5)
C(1)-O(1)	1·223	(5)	1·237	(5)	1·278	(5)
C(4)-O(2)	1·233	(4)	1·246	(4)	1·290	(5)
C(5)-O(3)	1·241	(4)	1·252	(4)	1·288	(5)

However, it must be concluded that the bond distances of the uric acid molecule cannot be explained entirely in terms of reasonable resonance contributions. Calculations including contributions from the uncharged triketo form, seven singly charged forms, three singly charged forms with a negative charge on a carbon atom, four singly charged Dewar forms and twelve doubly charged forms did not predict the bond-lengths within observed deviations when giving plausible weights to the different types of resonance structure. This has earlier been pointed out for other purine structures by Cochran (1951) and Sutor (1958*a*, *b*). However, there are no pure double or single bonds outside the purine rings as is supposed to be the case in caffeine and theophylline nor any halogen interaction to be taken into account as in adenine hydrochloride.

Comparing the bond distances and angles of uric acid with those of other purines, pyrimidines and related compounds reveals no deviation from earlier concepts of purine structure. As the internal ring dimensions are mainly dependent of the annular attachments (Pauling & Corey, 1956) the dimensions of the pyrimidine ring of uric acid should for relevance be compared with that ring of xanthazol (Nowacki & Bürki, 1955). None of the bonds differed by more than 1·6 times the standard deviation of the difference and the differences are therefore, according to the one-parameter significance test (Cruickshank & Robertson, 1953), not significant. All the angles in the two structures are in good agreement. For comparison with the imidazole ring of uric acid no exactly equivalent structure determination has been reported. A comparison

Table 5. *Intramolecular angles including non-hydrogen atoms*

Atoms	Angle	σ	Atoms	Angle	σ
N(1)-C(1)-N(2)	116·0°	0·3°	N(1)-C(4)-C(3)	111·3°	0·3°
N(1)-C(1)-O(1)	122·6	0·3	N(1)-C(4)-O(2)	122·3	0·3
N(2)-C(1)-O(1)	121·4	0·3	C(3)-C(4)-O(2)	126·4	0·4
N(2)-C(2)-N(4)	128·3	0·3	N(3)-C(5)-N(4)	107·1	0·3
N(2)-C(2)-C(3)	124·1	0·3	N(3)-C(5)-O(3)	126·8	0·3
N(4)-C(2)-C(3)	107·5	0·3	N(4)-C(5)-O(3)	126·1	0·3
N(3)-C(3)-C(2)	108·0	0·3	C(1)-N(1)-C(4)	128·8	0·3
N(3)-C(3)-C(4)	130·8	0·3	C(1)-N(2)-C(2)	118·4	0·3
C(2)-C(3)-C(4)	121·2	0·4	C(3)-N(3)-C(5)	108·1	0·3
			C(2)-N(4)-C(5)	109·2	0·3

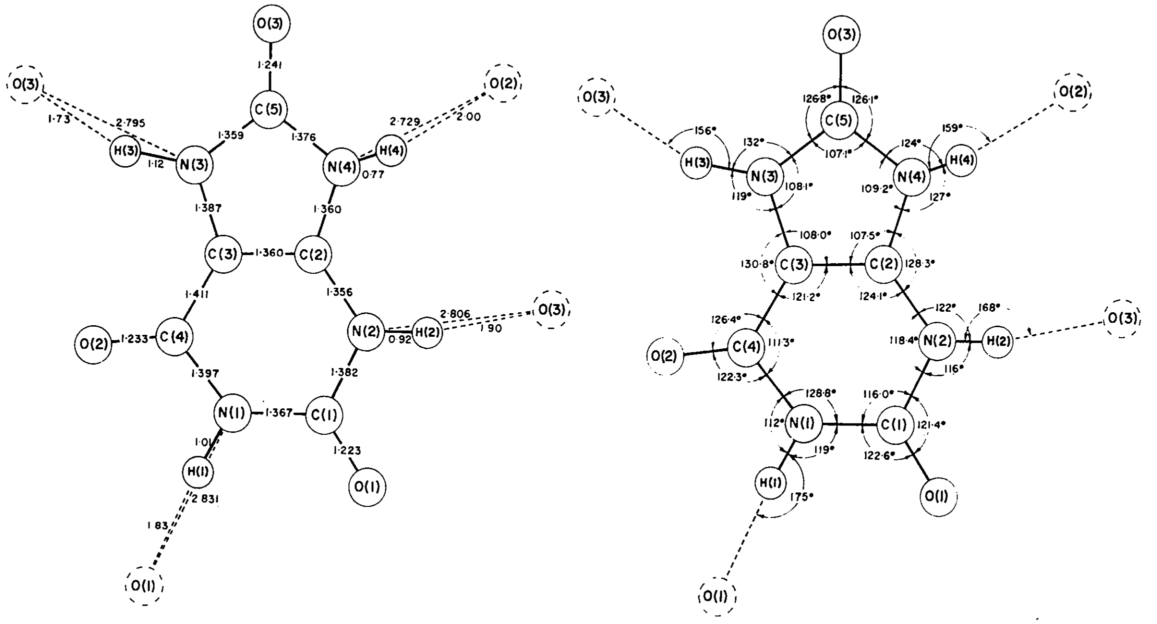


Fig. 2. Diagrams showing bond lengths and bond angles of uric acid, including the hydrogen bonds to neighbouring molecules.

with tetramethyluric acid (Sutor, 1963) shows a mean difference of comparable bond-distances and bond-angles of 0·8 and 1·1 times the standard deviation of the difference respectively. The bond-distance C(5)–N(4) and the bond-angle N(3)–C(5)–O(3) are significantly smaller and the angle C(1)–N(1)–C(4) significantly greater in uric acid.

Planarity of the molecule

The best plane through the molecule was calculated according to Blow (1960) from the orthogonal coordinates of the non-hydrogen atoms given equal weights. The deviation from that plane with equation $0{\cdot}0386X' - 0{\cdot}8410\,Y + 0{\cdot}5396\,Z' = 0{\cdot}3510$ are given in Fig. 3. It is seen that the molecule is slightly bent with the three oxygen atoms and N(3) below the plane. The significant deviation of H(2) is probably due to hydrogen bonding. The distance between the best planes of two adjacent molecules are 3·23 Å and the dihedral angle formed by such a plane and the (021) or (02$\bar{1}$) plane is 6·5°. During the study of the planarity of the five carbon atoms each with three surrounding atoms it was found that the three keto carbon groups were perfectly planar with a mean deviation of 0·0006 Å or less. The surroundings of C(2) and C(3) were less planar with a mean deviation of 0·005 and 0·004 Å respectively.

Table 6. *Fractional positional parameters for the hydrogen atoms with estimated standard deviation (both* × 10^3)

Atom	x/a	(σ)	y/b	(σ)	z/c	(σ)
H(1)	546	(4)	401	(7)	820	(9)
H(2)	268	(4)	428	(6)	837	(8)
H(3)	550	(4)	061	(6)	146	(8)
H(4)	257	(3)	213	(6)	492	(7)

Table 7. *Bond distances* (Å) *and angles including hydrogen atoms, both with estimated standard deviations*

Atoms	I	(σ)	II	(σ)
N(1)–H(1)	1·01	(5)	1·00	(5)
N(2)–H(2)	0·92	(5)	0·90	(5)
N(3)–H(3)	1·12	(5)	1·11	(5)
N(4)–H(4)	0·77	(4)	0·74	(5)

Atoms		Angle	σ
C(1)–N(1)–H(1)		119°	3°
C(4)–N(1)–H(1)		112	3
C(1)–N(2)–H(2)		116	3
C(2)–N(2)–H(2)		122	3
C(3)–N(3)–H(3)		119	2
C(5)–N(3)–H(3)		132	2
C(2)–N(4)–H(4)		127	3
C(5)–N(4)–H(4)		124	3
N(1)–H(1) - - - O(1)	$(1-x, 1-y, 2-z)$	175	4
N(2)–H(2) - - - O(3)	$(\frac{1}{2}-x, \frac{1}{2}+y, 1-z)$	168	4
N(3)–H(3) - - - O(3)	$(1-x, -y, -z)$	156	4
N(4)–H(4) - - - O(2)	$(x-\frac{1}{2}, \frac{1}{2}-y, z)$	159	4

Hydrogen bonding system

In its crystalline form uric acid has a perfect hydrogen bonding system (Fig. 4), which makes use of all the hydrogen atoms, the positional parameters of which are found in Table 6. The lengths and arrangement of these bonds can be seen in Fig. 2 and Table 8. The closest contact between atoms in two parallel molecules is between C(4) and N(3) of $(1-x, -y, 1-z)$ which is equal to 3·09 Å. All other intermolecular distances are in agreement with ordinary packing requirements. Two of the hydrogen bonds, N(1)–O(1) = 2·83 Å and N(3)–O(3) = 2·79 Å, connect the molecules in the same plane forming infinite rows in the (100) plane. N(2)–O(3) = 2·81 Å and N(4)–O(2) = 2·73 Å keep rows of adjacent sheets together.

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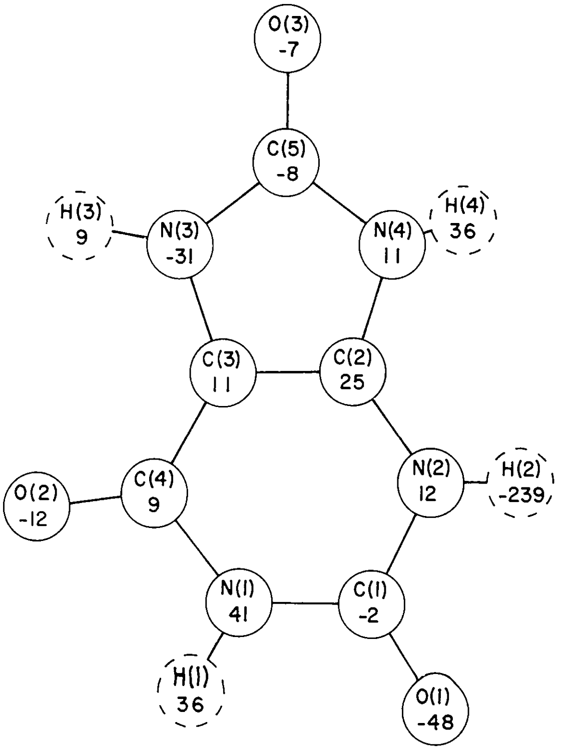

Fig. 3. The displacements in 10^{-3} Å of the atoms from the best plane through the non-hydrogen atoms.

Table 8. *Hydrogen bonds*

Atoms	I	(σ)	II	(σ)	III	(σ)
N(1)–O(1) $(1-x, 1-y, 2-z)$	2·831	(4)	2·835	(4)	2·858	(4)
N(2)–O(3) $(\frac{1}{2}-x, \frac{1}{2}+y, 1-z)$	2·806	(4)	2·808	(4)	2·829	(4)
N(3)–O(3) $(1-x, -y, -z)$	2·795	(4)	2·797	(4)	2·816	(4)
N(4)–O(2) $(x-\frac{1}{2}, \frac{1}{2}-y, z)$	2·729	(4)	2·735	(4)	2·756	(4)

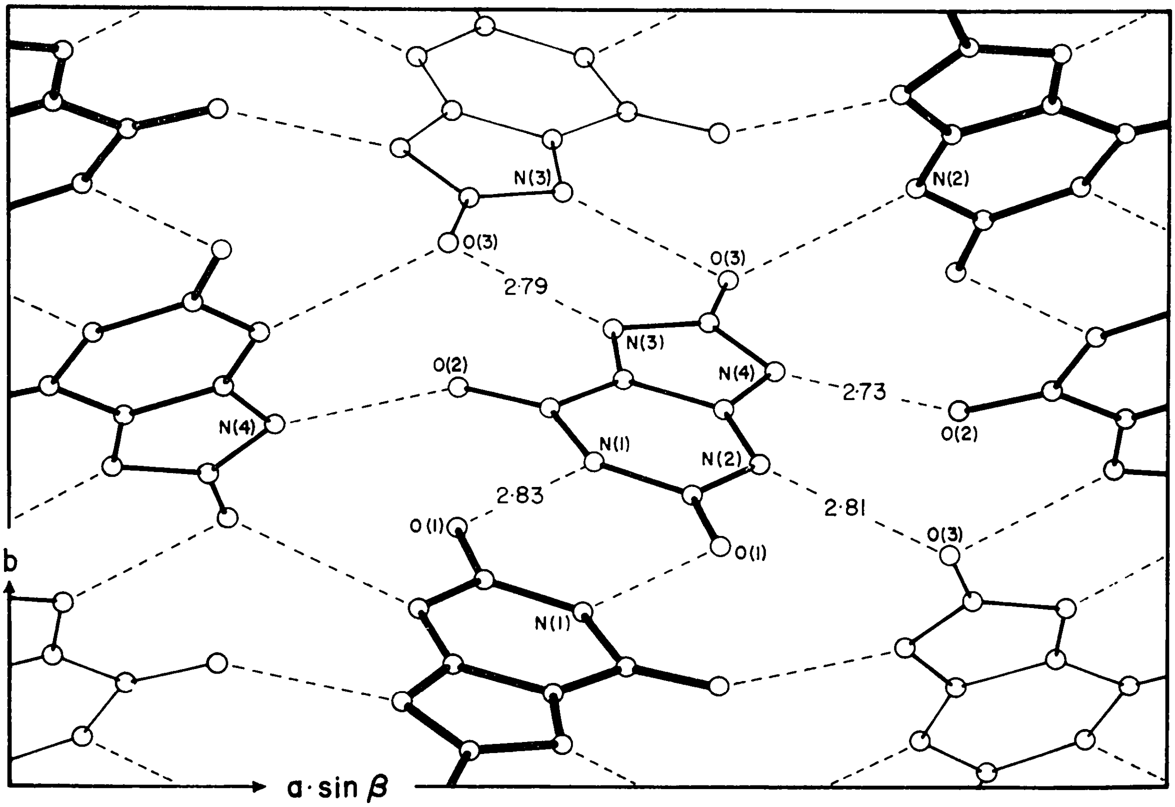

Fig. 4. A stereographic drawing of the crystal structure projected along the *c* axis showing the hydrogen bonding system.

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