C3—C4—C7	120.1 (4)	C45—C44—C47	122.6 (4)
C5—C4—C7	122.9 (3)	C44—C45—C46	122.7 (4)
C4—C5—C6	122.5 (4)	C41—C46—C45	118.3 (3)
C1—C6—C5	118.6 (4)	C41—C46—C60	122.1 (3)
C1—C6—C20	122.7 (4)	C45—C46—C60	119.4 (3)
C5—C6—C20	118.7 (3)	C44—C47—C48	110.5 (6)
C4—C7—C8	109.4 (4)	C44—C47—C49	111.2 (5)
C4—C7—C9	113.2 (4)	C44—C47—C50	113.4 (5)
C4—C7—C10	110.1 (5)	C48—C47—C49	102.3 (7)
C8—C7—C9	106.7 (4)	C48—C47—C50	107.8 (7)
C8—C7—C10	105.3 (5)	C49—C47—C50	111.1 (7)
C9—C7—C10	111.8 (5)	C46—C60—C62	118.6 (4)
C6—C20—C22	116.2 (3)	O71—C61—C62	120.3 (4)
O31—C21—C26	121.3 (4)	O71—C61—C66	118.6 (4)
O31—C21—C22	118.1 (4)	C62—C61—C66	121.1 (4)
C26—C21—C22	120.4 (4)	C60—C62—C61	122.4 (5)
C21—C26—C25	118.3 (4)	C60—C62—C63	119.4 (5)
C21—C26—C40	121.9 (4)	C61—C62—C63	118.1 (4)
C25—C26—C40	119.9 (4)	C62—C63—C64	123.4 (5)
C26—C25—C24	123.7 (4)	C63—C64—C65	115.4 (4)
C25—C24—C23	115.7 (4)	C63—C64—C67	122.9 (5)
C25—C24—C27	122.8 (4)	C65—C64—C67	121.7 (4)
C23—C24—C27	121.5 (4)	C64—C65—C66	123.8 (4)
C24—C23—C22	123.0 (4)	C61—C66—C65	118.1 (4)
C20—C22—C21	121.1 (4)	C61—C66—C80	121.4 (4)
C20—C22—C23	120.0 (4)	C65—C66—C80	120.5 (4)
C21—C22—C23	118.8 (4)	C64—C67—C68	112.2 (5)
C24—C27—C28	113.6 (4)	C64—C67—C69	111.5 (5)
C24—C27—C29	111.6 (4)	C64—C67—C70	110.5 (4)
C24—C27—C30	109.2 (4)	C68—C67—C69	104.3 (5)
C28—C27—C29	107.6 (5)	C68—C67—C70	109.6 (6)
C28—C27—C30	109.5 (5)	C69—C67—C70	108.7 (5)
C29—C27—C30	105.0 (5)	O71—C72—C73	110.0 (5)
O31—C32—C33	110.8 (6)	C2—C80—C66	117.7 (4)

Data were collected with a scan width of $(1.10 + 0.34\tan\theta)^\circ$. The intensity data were corrected for Lorentz and polarization effects, and for long-time scale variation.

The structure was solved by *MULTAN* (Germain, Main & Woolfson, 1971) and refined by full-matrix least squares. All calculations were performed with *SDP* (B. A. Frenz & Associates Inc., 1983). An *ORTEP*II (Johnson, 1976) view (Fig. 2) shows rather large thermal motion for the terminal CH_3 and CH_2 groups which may affect the *R* value.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: AB1130). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A Tautomeric Pair of 2,2-Dimethyl-6-carbamoyl-9-phenyldihydropurines

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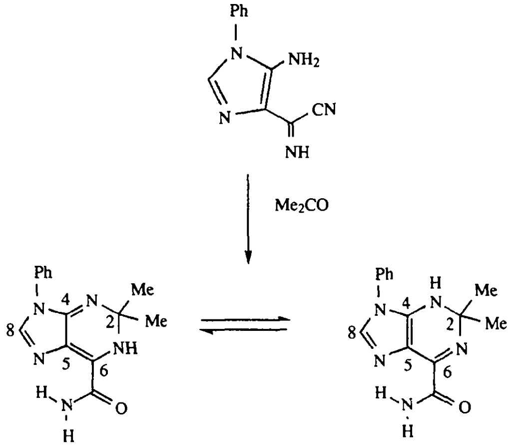
Abstract

Two tautomeric dihydropurine derivatives, $C_{14}H_{15}N_5O$, namely 2,2-dimethyl-9-phenyl-1,2-dihydropurine-6-carboxamide, (*A*) (coloured orange–red), and 2,2-dimethyl-9-phenyl-2,3-dihydropurine-6-carboxamide, (*B*) (yellow), are confirmed to have hydrogen substituents at N1 and N3, respectively. A different pattern of observed bond lengths in the purine rings of (*A*) and (*B*) illustrates differences in conjugation in accordance with the different bond alternation. The tautomerism also gives rise to differences in the hydrogen bonding, although both tautomers have an internal hydrogen bond from an amide N—H to an N atom of the five-membered ring, with N···N distances 2.84 (2) Å in (*A*) and 2.836 (6) Å in (*B*).

Comment

The two structures were determined primarily to establish the relationship between the colour and the tautomeric form, and also to establish which is the major tautomer in solution. The compounds were synthesized by the method of Alves *et al.* (1994). This method, with ethanol used in the final stage, produces a yellow solution from which the yellow form (*B*) crystallizes. For most 9-aryl derivatives, but not the 9-phenyl, the yellow form rapidly equilibrates (*e.g.* in acetone solution) with the orange form. Alves *et al.* (1994) discuss in detail the destabilization of the yellow forms. The orange form of the 9-phenyl derivative (*A*) is produced from the yellow form in acetone solution only if silica is added or if the solution is chromatographed using silica; the solution turns orange and crystals of the pure orange tautomer (*A*) can be isolated.



(*A*) (orange) (*B*) (yellow)

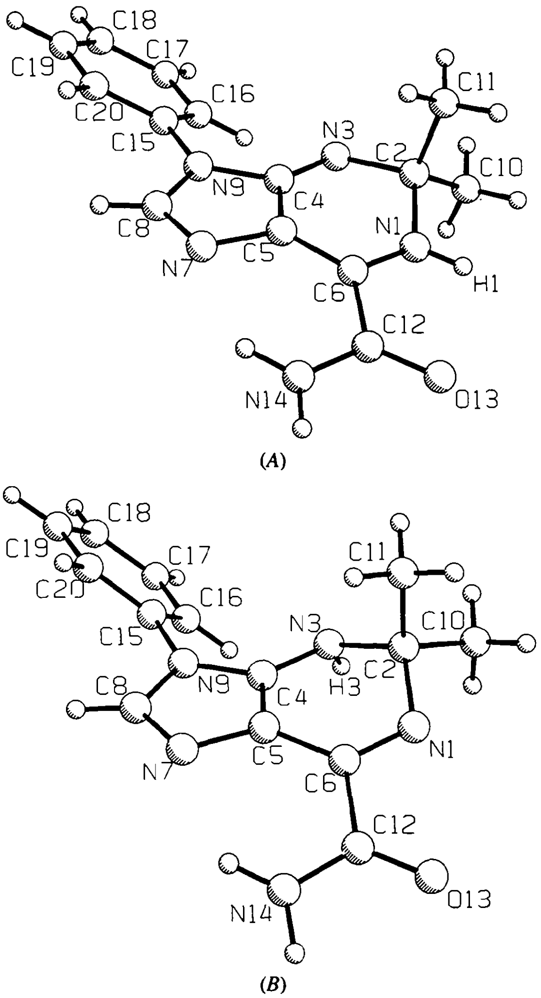


Fig. 1. The two tautomers, showing atom labelling.

The presence of an H atom on N1 in (*A*) and N3 in (*B*) was indicated by peaks in the electron-density difference maps, and was confirmed by the C—C and C—N bond lengths which are appropriate for the different patterns of conjugation in the purine rings; *e.g.* for the orange and yellow tautomers, respectively, N3—C4 = 1.291 (9), 1.376 (6) Å, C4—C5 = 1.44 (1), 1.370 (6) Å, C5—C6 = 1.352 (9), 1.420 (7) Å and C6—N1 = 1.352 (9), 1.299 (6) Å. These lengths are in keeping with the different bond alternation of the tautomers shown in the scheme. Both tautomers have an internal hydrogen bond between the amide group and N7 with N14···N7 = 2.84 (2) and 2.836 (6) Å in (*A*) and (*B*), respectively.

In the orange tautomer, the N1—H1 bond is almost coplanar with N1—C6 and N1—C2 [sum of angles at N1 = 357 (7)°], with angle C6—N1—C2 = 124.0 (7)°. This coplanarity, the molecular conjugation and the intra- and intermolecular hydrogen bonding of the orange tautomer are very similar to those found in the orange tautomer reported by Alves *et al.* (1994), in which the phenyl group is replaced by 2,4-dimethoxyphenyl, and in the orange 2,2,8,9-tetramethyldihydropurine analogue (Beagley, Booth, Pritchard & Proença, 1982). The intermolecular hydrogen bonding involves centrosymmetric dimers linked weakly through H1: N1—H1···O13 = 3.30 (2) Å (O13 of molecule at $2-x$, $1-y$, $2-z$). Stronger N···N hydrogen bonds link the dimers in strips parallel to **a**: N3···H—N14 = 3.17 (2) Å (N3 at x, $1+y$, z). Further sets of strips, not linked to the sets described, are generated by the *n*-glide operations.

The less stable yellow tautomer has a lower density implying less efficient packing. Its intermolecular hydrogen bonding involves more conventional, stronger dimerization through centrosymmetrically linked amide groups: N14—H···O13 = 2.943 (6) Å (O13 of $1-x$, $-y$, $-z$); but these dimers are weakly bound to neighbouring dimers by a bifurcated hydrogen bond, N1···H—N3 = 3.235 (6) Å and O13···H—N3 = 3.268 (6) Å, with N3 at $\frac{1}{2}-x$, $-\frac{1}{2}+y$, $\frac{1}{2}-z$. In this hydrogen-bonding network, all equivalent positions are involved, contrasting with the two unconnected networks in the orange crystals. The three bond angles at N3 sum to only 336 (6)°, with angle C2—N3—C4 = 112.0 (4)°, suggesting that the presence of H3 reduces the involvement of N3 in the ring conjugation.

Experimental

Compound (*A*) (orange)

Crystal data

$C_{14}H_{15}N_5O$
$M_r = 269.31$
Monoclinic
$P2_1/n$
$a = 12.33\ (3)$ Å
$b = 8.26\ (4)$ Å
$c = 14.25\ (3)$ Å
$\beta = 115.0\ (5)°$
$V = 1314\ (6)$ Å^3
$Z = 4$
$D_x = 1.361$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 22 reflections
$\theta = 5.79–14.64°$
$\mu = 0.086$ mm^{-1}
$T = 296$ K
Block
0.2 × 0.2 × 0.15 mm
Orange–red

Data collection

Rigaku AFC-6*S* diffractometer
ω scans
Absorption correction: none
5599 measured reflections
4972 independent reflections
738 observed reflections $[I > 2\sigma(I)]$

$R_{\rm int} = 0.086$
$\theta_{\rm max} = 25°$
$h = -6 \rightarrow 13$
$k = -5 \rightarrow 9$
$l = -14 \rightarrow 7$
3 standard reflections monitored every 150 reflections intensity decay: none

Refinement

Refinement on *F*
$R = 0.049$
$wR = 0.052$
$S = 1.49$
738 reflections
184 parameters
Weighting scheme based on measured e.s.d.'s (default scheme in *TEXSAN*)

$(\Delta/\sigma)_{\rm max} = 0.002$
$\Delta\rho_{\rm max} = 0.20$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.25$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Compound (*B*) (yellow)

Crystal data

$C_{14}H_{15}N_5O$
$M_r = 269.31$
Monoclinic
$P2_1/n$
$a = 11.130\ (8)$ Å
$b = 7.999\ (8)$ Å
$c = 15.162\ (8)$ Å
$\beta = 95.81\ (5)°$
$V = 1343\ (2)$ Å^3
$Z = 4$
$D_x = 1.332$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 13 reflections
$\theta = 7.45–11.8°$
$\mu = 0.084$ mm^{-1}
$T = 296$ K
Cube
0.3 × 0.3 × 0.3 mm
Yellow

Data collection

Rigaku AFC-6*S* diffractometer
ω scans
Absorption correction: none
2694 measured reflections
2558 independent reflections
1203 observed reflections $[I > 3\sigma(I)]$

$R_{\rm int} = 0.12$
$\theta_{\rm max} = 25°$
$h = 0 \rightarrow 13$
$k = 0 \rightarrow 9$
$l = -17 \rightarrow 17$
3 standard reflections monitored every 150 reflections intensity decay: none

Refinement

Refinement on *F*
$R = 0.066$
$wR = 0.078$
$S = 2.51$
1203 reflections
184 parameters
Weighting scheme based on measured e.s.d.'s (default scheme in *TEXSAN*)

$(\Delta/\sigma)_{\rm max} = 0.005$
$\Delta\rho_{\rm max} = 0.23$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.29$ 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)

$$B_{\rm eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	$B_{\rm eq}$
(*A*) (orange)				
O13	0.9519 (5)	0.6847 (6)	0.8994 (4)	4.8 (3)
N1	0.9371 (6)	0.3665 (8)	0.8477 (5)	3.4 (3)
N3	0.9037 (5)	0.1411 (7)	0.7272 (4)	2.5 (3)
N7	0.9303 (6)	0.5078 (8)	0.6027 (5)	3.8 (3)
N9	0.8809 (6)	0.2450 (8)	0.5605 (5)	2.9 (3)
N14	0.9376 (6)	0.7597 (8)	0.7409 (5)	3.8 (3)
C2	0.9531 (7)	0.1902 (9)	0.8374 (5)	2.8 (4)
C4	0.9090 (7)	0.2545 (10)	0.6671 (6)	2.6 (4)
C5	0.9381 (7)	0.4224 (9)	0.6907 (6)	2.8 (4)
C6	0.9439 (7)	0.4794 (9)	0.7818 (6)	2.8 (4)
C8	0.8977 (8)	0.3998 (10)	0.5308 (6)	3.7 (4)
C15	0.8490 (7)	0.1068 (10)	0.4948 (5)	2.3 (4)
C16	0.7870 (8)	−0.0192 (11)	0.5126 (5)	3.3 (4)
C17	0.7555 (8)	−0.1518 (10)	0.4473 (7)	4.4 (5)
C18	0.7856 (9)	−0.1569 (12)	0.3653 (7)	4.9 (5)
C19	0.8471 (8)	−0.0311 (12)	0.3480 (6)	4.5 (5)
C20	0.8799 (7)	0.1027 (9)	0.4126 (6)	3.5 (4)
C10	0.8840 (7)	0.1028 (9)	0.8886 (5)	3.3 (4)
C11	1.0858 (8)	0.1500 (9)	0.8884 (5)	3.7 (4)
C12	0.9446 (7)	0.6528 (10)	0.8131 (7)	3.2 (4)
H1	0.949 (6)	0.396 (8)	0.909 (5)	3.5
(*B*) (yellow)				
O13	0.4380 (4)	−0.0703 (6)	0.1021 (3)	4.9 (2)
N1	0.2559 (4)	−0.0092 (5)	0.2032 (3)	3.0 (2)
N3	0.0798 (4)	0.1710 (5)	0.2328 (3)	2.7 (2)
N7	0.0993 (4)	0.1764 (6)	−0.0004 (3)	3.4 (2)
N9	−0.0157 (4)	0.2933 (5)	0.0950 (3)	2.9 (2)
N14	0.3407 (4)	0.0711 (7)	−0.0111 (3)	4.9 (3)
C2	0.1503 (4)	0.0172 (6)	0.2562 (3)	2.7 (2)
C4	0.0653 (4)	0.1982 (6)	0.1427 (3)	2.4 (2)
C5	0.1366 (5)	0.1264 (6)	0.0846 (3)	2.7 (2)
C6	0.2405 (5)	0.0374 (6)	0.1207 (3)	2.6 (2)
C8	0.0069 (6)	0.2762 (7)	0.0060 (4)	3.7 (3)
C15	−0.1164 (5)	0.3898 (7)	0.1230 (4)	3.1 (2)
C16	−0.0922 (5)	0.4876 (7)	0.1988 (4)	3.8 (3)
C17	−0.1917 (7)	0.5840 (8)	0.2227 (5)	5.3 (4)
C18	−0.3005 (6)	0.5792 (9)	0.1744 (5)	5.4 (4)
C19	−0.3196 (5)	0.4806 (9)	0.1013 (4)	5.1 (3)
C20	−0.2243 (5)	0.3833 (8)	0.0776 (4)	4.0 (3)
C10	0.1982 (5)	0.0285 (7)	0.3522 (4)	4.0 (3)
C11	0.0661 (5)	−0.1337 (7)	0.2376 (4)	3.6 (3)
C12	0.3508 (5)	0.0062 (7)	0.0691 (3)	3.1 (2)
H3	0.115 (5)	0.265 (6)	0.267 (3)	3.5

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

(*A*)			
O13—C12	1.223 (8)	C2—C10	1.52 (1)
N1—C2	1.48 (1)	C2—C11	1.52 (1)
N1—C6	1.352 (9)	C4—C5	1.44 (1)
N1—H1	0.86 (6)	C5—C6	1.352 (9)
N3—C2	1.48 (1)	C6—C12	1.50 (1)
N3—C4	1.291 (9)	C15—C16	1.38 (1)
N7—C5	1.408 (9)	C15—C20	1.378 (9)
N7—C8	1.29 (1)	C16—C17	1.38 (1)
N9—C4	1.411 (9)	C17—C18	1.37 (1)
N9—C8	1.39 (1)	C18—C19	1.37 (1)
N9—C15	1.42 (1)	C19—C20	1.38 (1)
N14—C12	1.332 (9)		
C2—N1—C6	124.0 (7)	C4—C5—C6	117.8 (7)
C2—N3—C4	113.1 (7)	N1—C6—C5	115.7 (8)
C5—N7—C8	104.1 (8)	N1—C6—C12	116.5 (7)
C4—N9—C8	106.2 (6)	C5—C6—C12	127.4 (7)
C4—N9—C15	128.7 (6)	N7—C8—N9	115.5 (7)
C8—N9—C15	125.0 (7)	N9—C15—C16	120.5 (7)
N1—C2—N3	111.1 (6)	N9—C15—C20	118.6 (7)
N1—C2—C10	107.2 (6)	C16—C15—C20	120.9 (8)
N1—C2—C11	109.1 (6)	C15—C16—C17	119.7 (8)
N3—C2—C10	108.5 (7)	C16—C17—C18	119.9 (8)
N3—C2—C11	108.9 (8)	C17—C18—C19	120.2 (8)
C10—C2—C11	112.1 (7)	C18—C19—C20	120.9 (8)
N3—C4—N9	128.2 (7)	C15—C20—C19	118.4 (8)
N3—C4—C5	128.6 (8)	O13—C12—N14	126.0 (9)
N9—C4—C5	103.2 (6)	O13—C12—C6	119.5 (7)
N7—C5—C4	111.1 (7)	N14—C12—C6	114.5 (8)
N7—C5—C6	129.6 (8)		
(*B*)			
O13—C12	1.212 (6)	C2—C10	1.501 (7)
N1—C2	1.505 (6)	C2—C11	1.537 (7)
N1—C6	1.299 (6)	C4—C5	1.370 (6)
N3—C2	1.483 (6)	C5—C6	1.420 (7)
N3—C4	1.376 (6)	C6—C12	1.543 (6)
N3—H3	0.98 (5)	C15—C16	1.393 (7)
N7—C5	1.373 (6)	C15—C20	1.324 (8)
N7—C8	1.313 (7)	C16—C17	1.425 (8)
N9—C4	1.335 (6)	C17—C18	1.35 (1)
N9—C8	1.404 (6)	C18—C19	1.359 (9)
N9—C15	1.459 (6)	C19—C20	1.393 (8)
N14—C12	1.316 (6)		
C2—N1—C6	116.1 (4)	N7—C5—C6	131.7 (4)
C2—N3—C4	112.0 (4)	C4—C5—C6	117.6 (4)
C2—N3—H3	110 (3)	N1—C6—C5	122.6 (4)
C4—N3—H3	114 (3)	N1—C6—C12	114.0 (5)
C5—N7—C8	105.8 (4)	C5—C6—C12	123.0 (5)
C4—N9—C8	106.8 (4)	N7—C8—N9	110.3 (5)
C4—N9—C15	129.7 (4)	N9—C15—C16	116.6 (5)
C8—N9—C15	123.3 (4)	N9—C15—C20	120.7 (5)
N1—C2—N3	114.3 (4)	C16—C15—C20	122.7 (5)
N1—C2—C10	107.9 (4)	C15—C16—C17	115.0 (6)
N1—C2—C11	106.6 (4)	C16—C17—C18	121.6 (6)
N3—C2—C10	108.0 (4)	C17—C18—C19	121.1 (6)
N3—C2—C11	108.0 (4)	C18—C19—C20	118.3 (6)
C10—C2—C11	112.1 (4)	C15—C20—C19	121.2 (6)
N3—C4—N9	129.3 (4)	O13—C12—N14	124.8 (5)
N3—C4—C5	123.7 (5)	O13—C12—C6	121.1 (5)
N9—C4—C5	107.0 (4)	N14—C12—C6	114.0 (5)
N7—C5—C4	110.0 (5)		

The data for the orange tautomer were collected on the basis of a monoclinic unit cell of twice the volume of the current one and Miller indices were transformed to conform with the smaller cell during data reduction. During refinement, H atoms were fixed in calculated positions except H1, whose coordinates were refined. During refinement of the yellow tautomer, H atoms were fixed in calculated positions except H3, whose coordinates were refined. Thus, the same number of variables was refined for both tautomers.

For both compounds, data collection: *TEXSAN* (Molecular Structure Corporation, 1985); cell refinement: *TEXSAN*; data reduction: *TEXSAN*; program(s) used to solve structures: *MITHRIL* (Gilmore, 1984); program(s) used to refine structures: *TEXSAN*; molecular graphics: *PLUTO* (Motherwell & Clegg, 1978); software used to prepare material for publication: *CIF* (Hall, Allen & Brown, 1991).

The EPSRC is thanked for funding the Chemical Databank Service *CSSR* used for crystallographic literature searches.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HA1128). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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(*Z*)-*N*-4-Fluorophenyl-*C*-phenylnitrone. Confirmation that the Exclusive Product of the Reaction Between Benzaldehyde and 4-Fluorophenylhydroxylamine is the *Z* Isomer

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Abstract

The benzaldehyde nitrone moiety in the title molecule, *N*-benzylidene-4-fluoroaniline *N*-oxide, $C_{13}H_{10}FNO$, like that in *N*-(benzylidene)methylamine *N*-oxide [Bed-

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