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# SHORT COMMUNICATIONS

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*Acta Cryst.* (1984). C**40**, 712

## Structure of 8,5′-anhydro-8-hydroxy-9-β-D-ribofuranosyladenine (8,5′-*O*-cyclo-A) monohydrate: corrigendum.

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(*Received* 14 *September* 1983; *accepted* 21 *December* 1983)

**Abstract**

The crystal structure of $C_{10}H_{11}N_5O_4.H_2O$ should be described as orthorhombic, space group $P2_12_12_1$, with $a = 8{\cdot}485$ (1), $b = 28{\cdot}005$ (5), $c = 4{\cdot}975$ (1) Å rather than monoclinic, $P2_1$, as originally reported [Sugio, Mizuno, Kitamura, Hamada, Ikehara & Tomita (1983). *Acta Cryst.* C**39**, 745–747].

Sugio, Mizuno, Kitamura, Hamada, Ikehara & Tomita (1983) have described the structure of this compound as monoclinic, space group $P2_1$, with $a = 32{\cdot}747$ (6), $b = 4{\cdot}975$ (1), $c = 8{\cdot}485$ (1) Å, $\beta = 121{\cdot}22$ (1)°, $Z = 4$. Choosing [102] as the $a$ axis leads to an effectively orthorhombic unit cell [$\beta' = 90{\cdot}01$ (1)°] and the two independent molecules in the $P2_1$ description are related, almost within the coordinate e.s.d.'s, by the additional $2_1$ axes of space group $P2_12_12_1$. The necessary coordinate transformations are $x' = x$, $y' = y - 0{\cdot}1009$, $z' = z - 2x + 0{\cdot}25$. A permutation of axes $a'b'c' = cab$ then gives the standard setting. Successful refinement in $P2_12_12_1$ is documented in the following paper (Sugio *et al.*, 1984).

Contrary to the final sentence by Sugio *et al.* (1983), the water molecule apparently *does* participate as a hydrogen-bond donor – to N(3), at 2·923 (7) Å, and possibly to a second N(3) at $x$, $y$, $z + 1$, 3·219 (7) Å. [These numbers become 2·924 (4) and 3·215 (4) Å after the $P2_12_12_1$ refinement of Sugio *et al.* (1984).]

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0108-2701/84/040712-01$01.50

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SUGIO, S., MIZUNO, H., KITAMURA, K., HAMADA, K., IKEHARA, M. & TOMITA, K. (1984). *Acta Cryst.* C**40**, 712–713.



*Acta Cryst.* (1984). C**40**, 712–713

## Structure of 8,5′-anhydro-8-hydroxy-9-β-D-ribofuranosyladenine (8,5′-*O*-cyclo-A) monohydrate, $C_{10}H_{11}N_5O_4.H_2O$: errata.

By SHIGETOSHI SUGIO, HIROSHI MIZUNO, KUNIHIRO KITAMURA, KENSAKU HAMADA, MORIO IKEHARA and KEN-ICHI TOMITA, *Faculty of Pharmaceutical Sciences, Osaka University, Yamadaoka* 1–6, *Suita, Osaka* 565, *Japan*

(*Received* 22 *September* 1983; *accepted* 12 *December* 1983)

**Abstract**

The space group of the title compound [Sugio, Mizuno, Kitamura, Hamada, Ikehara & Tomita (1983). *Acta Cryst.* C**39**, 745–747] is not $P2_1$ but $P2_12_12_1$. The new cell parameters refined using the $2\theta$ values of 25 reflections are $a = 8{\cdot}485$ (1), $b = 28{\cdot}002$ (4), $c = 4{\cdot}975$ (4) Å, $Z = 4$. Refinement based on the correct space group gave $R = 0{\cdot}042$ for 1127 reflections.

0108-2701/84/040712-02$01.50

The final atomic coordinates with their estimated standard deviations are given in Table 1 and bond distances and angles are given in Table 2.*

The Miller indices and the fractional atomic coordinates for the $P2_12_12_1$ structure are related to those of the previous $P2_1$ structure (Sugio, Mizuno, Kitamura, Hamada, Ikehara & Tomita, 1983) by the following matrices:

(1) *Fractional atomic coordinates*

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} -2 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} + \begin{pmatrix} 0{\cdot}75 \\ 0 \\ -0{\cdot}1007 \end{pmatrix}$$

where $x$, $y$, $z$ and $x'$, $y'$, $z'$ are the $P2_12_12_1$ and $P2_1$ coordinates, respectively, and the translation (0·75, 0, −0·1007) moves the origin of coordinates of the $P2_1$ structure so that molecules $A$ and $B$ of the $P2_1$ structure can be related by the symmetry operation $(0{\cdot}5 + x, 0{\cdot}5 - y, -z)$ in the new coordinate system.

(2) *Miller indices*

$$\begin{pmatrix} h \\ k \\ l \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 2 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} h' \\ k' \\ l' \end{pmatrix}$$

where $h$, $k$, $l$ are $P2_12_12_1$ indices and $h'$, $k'$, $l'$ are $P2_1$ indices.

Observed structure-factor amplitudes of symmetry-related reflections were averaged ($R_{sym} = 0{\cdot}082$) and used for refinement. The final $R$ and $R_w$ for 1127 observed reflections [$|F_o| > 3\sigma(F_o)$] were 0·042 and 0·060, respectively, where $w = [\sigma^2(F_o) + 0{\cdot}0131|F_o| + 0{\cdot}0015|F_o|^2]^{-1}$. $S$ for 226 parameters (nine for each non-H atom, three for each H atom, an overall scale and an overall thermal parameter) was 1·116.

The results of refinement show that the present structure is consistent with the previous one within 0·020 Å in bond distances and within 1·1° in bond angles.

The authors would like to thank Dr Y. Le Page of Chemistry Division, National Research Council, Canada, for pointing out this error.

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and transformation matrices corresponding to the change in space group have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 38376 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final positional and equivalent isotropic thermal parameters for the non-*H *atoms with their estimated standard deviations in parentheses*

$B_{eq} = \frac{4}{3}\sum_i\sum_j\beta_{ij}(\mathbf{a}_i.\mathbf{a}_j)$.

| | $x$ | $y$ | $z$ | $B_{eq}$(Å$^2$) |
|---|---|---|---|---|
| N(1) | 0·5635 (3) | 0·2267 (1) | −0·2151 (7) | 4·6 (2) |
| C(2) | 0·5255 (4) | 0·1950 (1) | −0·0253 (8) | 5·2 (2) |
| N(3) | 0·6139 (3) | 0·1610 (1) | 0·0855 (6) | 5·5 (2) |
| C(4) | 0·7619 (3) | 0·1628 (1) | −0·0098 (6) | 3·1 (2) |
| C(5) | 0·8205 (3) | 0·1946 (1) | −0·1953 (7) | 2·4 (2) |
| C(6) | 0·7142 (3) | 0·2275 (1) | −0·3065 (7) | 2·6 (2) |
| N(7) | 0·9802 (3) | 0·1859 (1) | −0·2459 (6) | 2·9 (2) |
| C(8) | 1·0100 (3) | 0·1489 (1) | −0·0980 (6) | 2·7 (2) |
| N(9) | 0·8852 (3) | 0·1328 (1) | 0·0523 (6) | 3·6 (2) |
| N(6) | 0·7515 (3) | 0·2593 (1) | −0·4970 (7) | 5·3 (2) |
| O(1′) | 0·9819 (3) | 0·0861 (1) | 0·4105 (4) | 3·2 (1) |
| C(1′) | 0·8741 (3) | 0·0870 (1) | 0·1957 (6) | 3·5 (2) |
| C(2′) | 0·9177 (4) | 0·0448 (1) | 0·0107 (6) | 2·0 (2) |
| C(3′) | 1·0829 (4) | 0·0300 (1) | 0·1095 (7) | 3·0 (2) |
| C(4′) | 1·1292 (4) | 0·0704 (1) | 0·2954 (7) | 2·0 (2) |
| C(5′) | 1·2158 (4) | 0·1112 (1) | 0·1608 (8) | 2·5 (2) |
| O(2′) | 0·8079 (3) | 0·0070 (1) | 0·0453 (5) | 1·1 (1) |
| O(3′) | 1·0771 (3) | −0·0125 (1) | 0·2652 (7) | 3·4 (2) |
| O(5′) | 1·1489 (2) | 0·1261 (1) | −0·0972 (5) | 4·3 (1) |
| O(*W*) | 0·5182 (4) | 0·1038 (1) | 0·5494 (7) | 4·8 (2) |

Table 2. *Bond distances* (Å) *and angles* (°) *for the non-*H *atoms*

| | | | |
|---|---|---|---|
| N(1)–C(2) | 1·335 (5) | C(8)–O(5′) | 1·340 (4) |
| N(1)–C(6) | 1·357 (5) | N(9)–C(1′) | 1·471 (4) |
| C(2)–N(3) | 1·332 (5) | O(1′)–C(1′) | 1·407 (4) |
| N(3)–C(4) | 1·343 (4) | O(1′)–C(4′) | 1·443 (4) |
| C(4)–C(5) | 1·375 (5) | C(1′)–C(2′) | 1·543 (4) |
| C(4)–N(9) | 1·377 (4) | C(2′)–C(3′) | 1·542 (5) |
| C(5)–C(6) | 1·403 (5) | C(2′)–O(2′) | 1·421 (4) |
| C(5)–N(7) | 1·400 (4) | C(3′)–C(4′) | 1·513 (5) |
| C(6)–N(6) | 1·338 (5) | C(3′)–O(3′) | 1·421 (5) |
| N(7)–C(8) | 1·295 (4) | C(4′)–C(5′) | 1·514 (5) |
| C(8)–N(9) | 1·373 (4) | C(5′)–O(5′) | 1·464 (5) |
| | | | |
| C(2)–N(1)–C(6) | 118·4 (3) | C(4)–N(9)–C(1′) | 126·3 (3) |
| N(1)–C(2)–N(3) | 129·2 (4) | C(8)–N(9)–C(1′) | 126·9 (3) |
| C(2)–N(3)–C(4) | 110·7 (3) | C(1′)–O(1′)–C(4′) | 105·5 (2) |
| N(3)–C(4)–C(5) | 126·8 (3) | N(9)–C(1′)–O(1′) | 110·0 (2) |
| N(3)–C(4)–N(9) | 127·5 (3) | N(9)–C(1′)–C(2′) | 111·3 (3) |
| C(5)–C(4)–N(9) | 105·7 (3) | O(1′)–C(1′)–C(2′) | 106·5 (2) |
| C(4)–C(5)–C(6) | 117·2 (3) | C(1′)–C(2′)–C(3′) | 103·5 (3) |
| C(4)–C(5)–N(7) | 111·0 (3) | C(1′)–C(2′)–O(2′) | 109·9 (3) |
| C(6)–C(5)–C(7) | 131·7 (3) | C(3′)–C(2′)–O(2′) | 110·9 (3) |
| N(1)–C(6)–C(5) | 117·6 (3) | C(2′)–C(3′)–C(4′) | 103·3 (3) |
| N(1)–C(6)–N(6) | 118·1 (3) | C(2′)–C(3′)–O(3′) | 111·6 (3) |
| C(5)–C(6)–N(6) | 124·3 (3) | C(4′)–C(3′)–O(3′) | 107·6 (3) |
| C(5)–N(7)–C(8) | 103·1 (3) | O(1′)–C(4′)–C(3′) | 104·2 (3) |
| N(7)–C(8)–N(9) | 114·9 (3) | O(1′)–C(4′)–C(5′) | 111·5 (3) |
| N(7)–C(8)–O(5′) | 123·7 (3) | C(3′)–C(4′)–C(5′) | 114·8 (3) |
| N(9)–C(8)–O(5′) | 121·3 (3) | C(4′)–C(5′)–O(5′) | 114·5 (3) |
| C(4)–N(9)–C(8) | 105·3 (3) | C(8)–O(5′)–C(5′) | 118·7 (3) |

**Reference**

SUGIO, S., MIZUNO, H., KITAMURA, K., HAMADA, K., IKEHARA, M. & TOMITA, K. (1983). *Acta Cryst.* C**39**, 745–747.