CARLSTRÖM, D. & BERGIN, R. (1967). *Acta Cryst.* **23**, 313–319.
CAVALLERI, B. & BELLASIO, E. (1970). *Farmaco Ed. Sci.* **25**, (12), 901–911.
CHION, B., LAJZÉROWICZ, J., BORDEAUX, D., COLLET, A. & JACQUES, J. (1978). *J. Phys. Chem.* **82**, 2682–2688.
CHION, B., LAJZÉROWICZ, J., COLLET, A. & JACQUES, J. (1976). *Acta Cryst.* B**32**, 339–344.
GADRET, M., LÉGER, J. M., CARPY, A. & BERTHOD, H. (1978). *Eur. J. Med. Chem. Chim. Ther.* **13**, 367–372.
GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* A**27**, 368–376.
GUEDJ, R., NABET, R. & WADE, T. N. (1972). *C. R. Acad. Sci. Sér. C*, **274**, 1317–1320.
GUEDJ, R., NABET, R. & WADE, T. N. (1973). *Tetrahedron Lett.* **12**, 907–910.
HEARN, R. A., FREEMAN, G. R. & BUGG, C. E. (1973). *J. Am. Chem. Soc.* **95**, 7150–7154.
*International Tables for X-ray Crystallography* (1974). Vol. IV. Birmingham: Kynoch Press.
JACQUES, J., COLLET, A. & WILEN, S. (1981). *Enantiomers, Racemates and Resolutions*, p. 104. New York: Wiley Interscience.
KNOX, L. H., VELARDE, E., BERGER, S., CUADRIELLO, D. & CROSS, A. D. (1964). *J. Org. Chem.* **29**, 2187–2195.
MOUSSERON-CANET, M. & BORGNA, J. L. (1969). *Bull. Soc. Chim. Fr.* **2**, 613–617.

# SHORT COMMUNICATIONS

*Contributions intended for publication under this heading should be expressly so marked; they should not exceed about* 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

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

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

By RICHARD E. MARSH, *Arthur Amos Noyes Laboratory of Chemical Physics,* California Institute of Technology, Pasadena, California* 91125, *USA*

(*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).]

* Contribution No. 6707 from the Arthur Amos Noyes Laboratory of Chemical Physics. This work was supported by National Institutes of Health Research Grant No. GM 16966.

0108-2701/84/040712-01$01.50

**References**

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