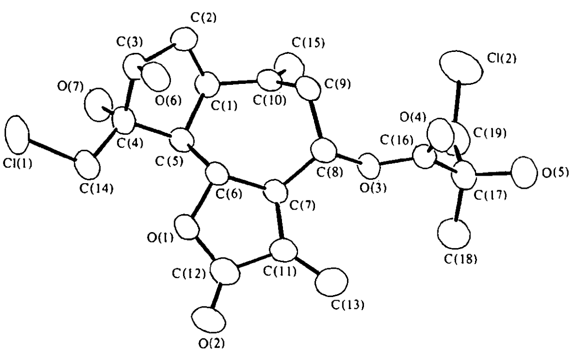

Fig. 1. The absolute configuration of centaurepensin.

with a slope of 1·01 passing through the origin. The correlation coefficient and χ^2 of the fit are 0·99 and 0·01, respectively, indicating effectively identical results.*

The present absolute configuration, shown in Fig. 1, corresponds to the enantiomorph of the one previously reported (Mason, Hewson, Kennard & Pettersen, 1972; Hewson, Pettersen & Kennard, 1972). This was confirmed after refinement of both enantiomers to give $R = 0{\cdot}044$ and 0·054 (R_w being 0·057 and 0·076, respectively). Finally a comparison of the 30 most relevant Bijvoet pairs gave the following discrepancy indices: averaged Bijvoet difference of 0·72 (3·11 for the enantiomorph) and averaged Bijvoet ratio of 0·05 (0·49).

We thank the staff of the Centro de Proceso de Datos del MEC of Spain for facilities on the Univac 1108 computer.

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* Positional and anisotropic thermal parameters for non-hydrogen atoms, bond distances, bond angles, torsion angles and lists of structure factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33565 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Acta Cryst. (1978). B**34**, 2670

4,5-Dichloro-1,3,6,8-tetrafluoro-2,7-naphthyridine: erratum.

By D. M. W. van den Ham and G. J. van Hummel, *Twente University of Technology, Chemical Physics Laboratory, PO Box* 217, *Enschede, The Netherlands*

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In the discussion of the experimental results the Cl–Cl distance of the title compound was erroneously given as 2·307 Å in the paper by van den Ham & van Hummel [*Acta Cryst.* (1977), B**33**, 3866–3868]. This value should be 3·109 Å. As this value is still smaller than twice the van der Waals radius, this error does not affect the conclusion.

All the relevant information is given in the Abstract.

Acta Cryst. (1978). B**34**, 2670–2671

Experimental and theoretical difference densities for cyanuric acid. A simple refinement of density distributions of bonding electrons VI. Erratum.

By C. Scheringer, A. Kutoglu and E. Hellner, *Institut für Mineralogie der Universität Marburg, D*-3550 *Marburg/Lahn, Federal Republic of Germany*

(*Received* 27 *June* 1978)

Owing to an error in the data transmission with respect to the form factor curve of oxygen, Fig. 1(*a*,*b*) of the paper by Scheringer, Kutoglu, Hellner, Hase, Schulte & Schweig [*Acta Cryst.* (1978). B**34**, 2162–2165] – hereafter referred to as SKHHSS – was incorrectly drawn. Similarly, the peak heights of the experimental investigation in Table 1 of SKHHSS are not correct. The corrected Fig. 1(*a*,*b*) and the full Table 1 are given. The good agreement between the experimental and theoretical peak heights mentioned in SKHHSS no longer holds for the lone-pair peaks of the oxygen atoms. The experimental peaks are considerably lower and in better agreement with the $X - N$ map of Coppens & Vos [*Acta Cryst.* (1971), B**27**, 146–158].

Table 1. *Peak heights in difference densities of cyanuric acid*

Experimental cut-off at $(\sin\theta)/\lambda = 0{\cdot}8$ Å^{-1}. ∞ means extrapolation to infinite resolution. LP stands for lone pair. AM = asphericity map of Jones, Pautler & Coppens (1972, Fig. 2*b*). $X-N = X-N$ map of Coppens & Vos (1971, Fig. 4).

	Peak heights in the difference densities (e Å^{-3})							
	Dynamic				Static			
Method	C=O	C–N	N–H	LP	C=O	C–N	N–H	LP
exp (0·8)	0·3, 0·3	0·3, 0·3, 0·3	0·4, 0·4	0·2, 0·2	0·3, 0·3	0·4, 0·3, 0·4	0·5, 0·5	0·3, 0·3
exp (∞)					0·4, 0·4	0·5, 0·4, 0·5	0·7, 0·7	0·4, 0·4
Theoretical	0·4	0·2	0·3	0·5	0·6	0·4	0·5	1·4
AM	0·4, 0·2	0·5, 0·5, 0·4	0·5, 0·5	0·3, 0·2				
$X-N$	0·5, 0·3	0·5, 0·4, 0·5	0·5, 0·4	0·5, 0·3				

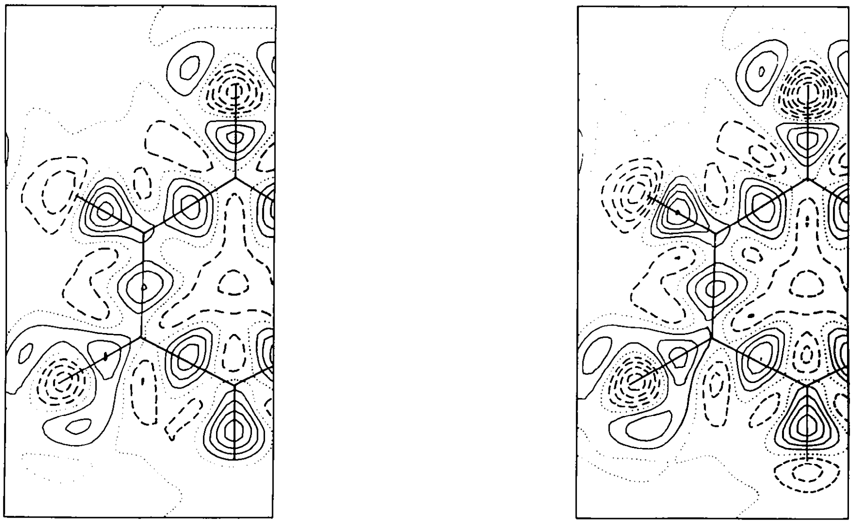
(*a*) (*b*)

Fig. 1. Observed (*a*) dynamic and (*b*) static difference density in the plane of the molecule. Contour interval 0·1 e Å^{-3}. Positive contours: full; zero: dotted; negative: dashed.

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Acta Cryst. (1978). B**34**, 2671–2672

Structure of glycylglycine hydrochloride: errata. By Y. Aka, N. Armağan and A. Aydin Uraz, *Department of Physics, Faculty of Science, University of Ankara, Ankara, Turkey*

(*Received* 20 *April* 1978; *accepted* 15 *May* 1978)

Errors in the paper of Parthasarathy [*Acta Cryst.* (1969), B**25**, 509–518] are corrected.

In the course of a survey of thermal analysis, our calculations revealed the following errors in the work of Parthasarathy (1969).

The signs of direction cosines $C3a$ of atoms Cl and O(2) should be changed to obtain three mutually orthogonal principal axes.