angular parameters (τ,θ) or (φ,κ). But, as was pointed out by the referee, it is more significant to base the reference frame on the unit normal, N, to the aromatic moiety. It seems that the θ and φ parameters reveal changes more clearly. The four rings are then characterized by their normal N_i (Table 4) to give an idea of the overall twist (about 25° from end to end). The overall bend is described by an angle of about 5° formed between the line joining the centroids of both aromatic rings and the line joining the centroids of the other two rings.

The bonds C(1)—C(15) and C(1)—H(1) lie at 50 and 60° with respect to the plane through N(14), C(2) and C(1). However, the orientation of C(15) must be regarded as only pseudo axial since the dihedral angle between the planes [C(1),C(2),N(14)] and {N(14), C(2) and the centroid of [C(2),C(3),N(5),N(14)]} is a mere 23° instead of the ideal 54·74° (see Fig. 1).

We are grateful to Professor M. Lora-Tamayo and co-workers for suggesting the problem and supplying the material. We are also in debt to the referee for clarifying some ideas. We thank the Centro de Proceso de Datos del Ministerio de Educación y Ciencia (Madrid) for the use of the Univac 1108 computer. Most of the computations were performed with the XRAY system of crystallographic programs (Stewart, Kundell & Baldwin, 1970).

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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. (1978). B**34**, 2669–2670

Centaurepensin. A redetermination of its absolute configuration by X-ray crystallography.

By J. LÓPEZ DE LERMA, J. FAYOS, S. GARCÍA-BLANCO and M. MARTÍNEZ-RIPOLL, *Departamento de Rayos X, Instituto Rocasolano, Serrano* 119, *Madrid*-6, *Spain*

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The present study shows that the absolute configuration of centaurepensin is opposite to the one previously reported [Mason, Hewson, Kennard & Pettersen (1972). *Chem. Commun.* pp. 460–461].

The crystal structure and absolute configuration of centaurepensin (chlorohyssopifolin A) have been reported (Mason, Hewson, Kennard & Pettersen, 1972; Hewson, Pettersen & Kennard, 1972). Recently, however, chemical studies (Gonzalez, Bermejo, Bretón, Massanet, Dominguez & Amaro, 1976) indicate that the absolute configuration is the opposite of that reported. The present investigation has been undertaken in order to clarify this situation.

Crystals of $C_{19}H_{24}Cl_2O_7$ are monoclinic, space group $P2_1$, with a = 10·467 (2), b = 9·248 (1), c = 11·504 (2) Å, β = 113·12 (1)°, D_c = 1·41 g cm^{-3}, Z = 2, μ(Cu $K\alpha$) = 31·96 cm^{-1}. A spherical crystal of radius $\simeq$ 0·25 mm was used to collect the intensities of all (1812) independent Friedel pairs in the range $2 < \theta < 65°$. A four-circle automatic diffractometer and monochromated Cu $K\alpha$ radiation were used. Data were corrected for absorption effects. 1793 observed Friedel pairs were used for anisotropic full-matrix least-squares refinement (Stewart, Kundell & Baldwin, 1970) of the previously reported atomic parameters (Hewson, Pettersen & Kennard, 1972). A weighting scheme was applied to prevent bias in $w(F_o - |F_c|)^2$. The present non-hydrogen atomic coordinates have been tested against the published ones in terms of a δp half-normal probability plot (Abrahams & Keve, 1971) which shows that all the δp terms lie on a line

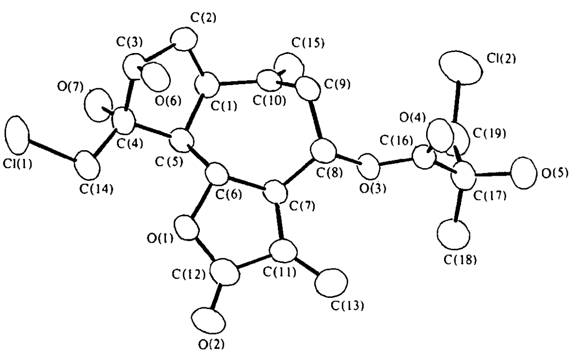

Fig. 1. The absolute configuration of centaurepensin.

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*

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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].