

## Short Communications

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*Acta Cryst.* (1972). B28, 2615

**Erratum: the structure of cycloalliin hydrochloride monohydrate.** By K. J. PALMER and KAY SUE LEE, *Western Regional Research Laboratory, Agricultural Research Service, U.S. Department of Agriculture, Berkeley, California 94710, U.S.A.*

(Received 27 March 1972)

A correction of the structure analysis of cycloalliin hydrochloride monohydrate is given.

The atomic parameters given in the paper with the above title (Palmer & Lee, 1965) are incorrect as they describe the stereoisomer with configuration *S*, in the notation of Cahn, Ingold & Prelog (1966), at the carbon atom bearing the carboxyl group, C(3). The configuration at C(3) should be *R* and the parameters for this stereoisomer are obtained by making negative all of the *y* parameters listed in Table 1 of the original paper. A stereographic drawing of cycloalliin with configuration *R* at C(3) made with the *ORTEP* program (Johnson, 1965) is shown in Fig. 1. Figs. 1 and 2 of

the original paper are correct as they illustrate the correct stereoisomer.

### References

- CAHN, R. S., INGOLD, C. & PRELOG, V. (1966). *Angew. Chem. Int. Ed.* **5**, 385.  
 JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794, Oak Ridge National Laboratory, Oak Ridge, Tennessee.  
 PALMER, K. J. & LEE, K. S. (1965). *Acta Cryst.* **20**, 790.

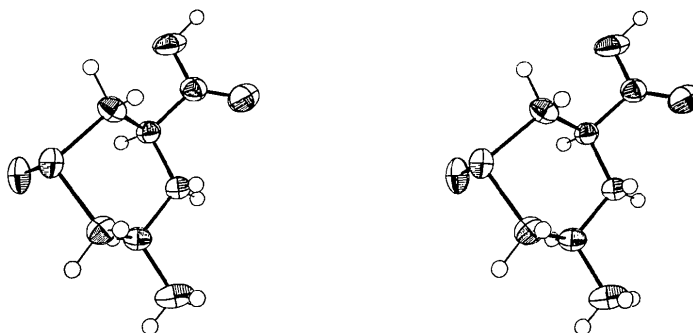


Fig. 1 A stereoscopic view of cycloalliin. The configuration at the ring carbon to which the carboxyl group is attached is *L*. The thermal ellipsoids are drawn at the 50% probability level.

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**The use of X-ray anomalous scattering to resolve the space-group ambiguity of dibenzyl disulphide.\*** By R. SRINIVASAN and B. K. VIJAYALAKSHMI, *Centre of Advanced Study in Physics, University of Madras, Guindy Campus, Madras-25, India*

(Received 14 September 1971)

The crystal structure of dibenzyl disulphide has been reinvestigated by X-ray anomalous scattering, and space group *C2/c* has been confirmed.

The crystal structure of dibenzyl disulphide which was originally reported in the space group *Cc* by Lee & Bryant (1969; hereafter LB) has been successfully refined in the centrosymmetric space group *C2/c* by two other groups of

workers (Dijk & Visser, 1971; Einspahr & Donohue, 1971; hereafter DV and ED respectively), although the original space group *Cc* is defended by Lee (1971). If the structure in the space group *Cc* were correct, it would involve an 'almost exact' twofold axis in the structure and hence the deviation from ideal centrosymmetry would be small. This may be readily estimated from the coordinates available

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