

Acta Cryst. (1979). B35, 2823

Structure du carbonate d'argent: erratum. Par R. MASSE, J. C. GUITEL et A. DURIF, *Laboratoire de Cristallographie, CNRS, 166 X, 38042 Grenoble CEDEX, France*

(Reçu le 24 juillet 1979, accepté le 1 août 1979)

Abstract

A computation error has been pointed out in Tableau 2 of the paper by Masse, Guitel & Durif [*Acta Cryst.* (1979), B35, 1428–1429]. The authors apologize for this, and the revised version of Tableau 2 is given. The text and other tables require no alterations.

Référence

MASSE, R., GUITEL, J. C. & DURIF, A. (1979). *Acta Cryst.* B35, 1428–1429.

Tableau 2. Distances interatomiques (Å) et angles des liaisons (°)

Ag–O(1)	2,236 (7)	O(1)–Ag–O(2)	158,7 (2)
Ag–O(2)	2,234 (7)	O(1)–Ag–O(2)	83,8 (2)
Ag–O(2)	2,440 (7)	O(1)–Ag–O(2)	119,7 (2)
Ag–O(2)	2,741 (7)	O(2)–Ag–O(2)	90,5 (2)
Ag–Ag	2,873 (2)	O(2)–Ag–O(2)	78,7 (2)
Ag–Ag	3,165 (2)	O(2)–Ag–O(2)	77,6 (2)
Ag–Ag	3,284 (2)		

Groupement CO₃²⁻

C–O(1)	1,302 (16)	O(2)–O(1)	2,218 (11)
C–O(2)	1,268 (9)	O(2)–O(2)	2,211 (14)
O(1)–C–O(2)	119,3 (8)	O(2)–C–O(2)	121,4 (8)

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X-ray assignments of absolute configuration: recommended practice and an appeal. By D. ROGERS, *Chemical Crystallography Laboratory, Imperial College, London SW7 2AY, England* and F. H. ALLEN, *Cambridge Crystallographic Data Centre, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, England*

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Abstract

Some 900 assignments of absolute configuration have now been made by Bijvoet's X-ray anomalous-dispersion technique and a considerable number more by means of an internal reference standard. Such assignments often play a fundamental role in chemistry and biology. Application of the anomalous-dispersion technique requires some care and a few unfortunate errors or misleading presentations of results have occurred in the literature, but only two assignments have had to be reversed on re-investigation. Reports of such assignments tend increasingly to be hidden in the body of a paper, accompanied by minimal experimental details; this makes it difficult to abstract the assignment and to assess its validity should any suspicion arise.

X-ray assignments of the chirality or polarity of crystals now total *ca* 900, a figure which increases by about 100 *per annum*. The present authors began publishing bibliographic lists (Allen & Rogers, 1966; Allen, Neidle & Rogers, 1968,

1969; Neidle, Rogers & Allen, 1970), but discontinued them when the volumes of *Molecular Structures and Dimensions* began to be published by the Cambridge Crystallographic Data Centre (CCDC) (Kennard & Watson, 1970–79; Kennard, Watson, Allen, Isaacs, Motherwell, Pettersen & Town, 1973; Kennard, Allen & Watson, 1977). 'Absolute configuration' is one of the flags incorporated in the Centre's files, though the compilers regard it as somewhat less exhaustive than the rest of their flags, mainly due to problems of abstracting that are discussed below. One can now readily identify, therefore, whether an X-ray assignment has been made of the chirality of an organic compound, organometallic compound or metal complex by reference to any of the *Molecular Structures and Dimensions* volumes, especially the *Guide to the Literature*, 1935–76 (Kennard, Allen & Watson, 1977) and bibliographic volumes 9 onwards (Kennard & Watson, 1970–79) where the absolute-configuration flag is now included as an indexing term. Exhaustive current listings can be obtained by a computer search of the corresponding CCDC magnetic tape files, copies of which are held at several centres throughout the

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