SHORT COMMUNICATION

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. (1981). B37, 1161

X-ray structure analysis and molecular conformation of *N*-propionylproline: erratum.

By M. E. Kamwaya, O. Oster and H. Bradaczek, *Institut für Kristallographie, Freie Universität Berlin, Takustrasse* 6, *D*-1000 *Berlin* 33, *Federal Republic of Germany*

(*Received* 16 *March* 1981)

Abstract

In the paper by Kamwaya, Oster & Bradaczek [*Acta Cryst.* (1981), B37, 364–367] the first sentence on p. 367 should read: 'The N′$C_4^{\alpha}C_6^{\gamma}C_7^{\delta}$ group is fairly planar.'

All the relevant information is contained in the *Abstract*.

0567-7408/81/051161-01$01.00

International Union of Crystallography

Acta Cryst. (1981). B37, 1161

Commission on Journals

Standards for the Publication of Powder Pattern Data

Standards for the publication of powder patterns, originally compiled by a subcommittee of the American Crystallographic Association and published in *National Bureau of Standards Special Publication* 567 (1979), have been accepted by the Commission on Crystallographic Data and the Commission on Journals. Papers that present powder pattern data submitted for publication in IUCr journals are now required to follow these standards. Full details are given in *Acta Crystallographica*, Section A [*Acta Cryst.* (1981), A37, 443–444.]

Acta Cryst. (1981). B37, 1161–1162

Commission on Journals

Deposition of Macromolecular Atomic Coordinates and Structure Factors with the Protein Data Bank

The policy that all structural papers, including low-resolution protein studies, should be equally subject to the requirement of deposition of atomic coordinates and lists of structure factors was recently reaffirmed by the Commission on Journals. It was also decided that such depositions should be machine-readable, and an agreement has now been reached with the Protein Data Bank, Chemistry Department, Brookhaven National Laboratory, Upton, New York 11973, USA to incorporate these data in their system.

Authors of macromolecular structure determination manuscripts will, in future, be requested by their Co-editor to send their atomic coordinates and structure factors to the Protein Data Bank. A macromolecule is regarded as any substance containing a polypeptide, polynucleotide or polysaccharide chain longer than 25 residues. The manuscript should be accompanied by printed copies of the atomic coordinates which will be sent to the referees. The Protein Data Bank will acknowledge receipt of the machine-readable data both to the author and the Co-editor and will, at the same time, communicate to both the Reference number assigned to these data. As soon as the data have been processed into standard Data Bank format and the corresponding listings verified by the author, notification will be sent to the Co-editor. Such listings can usually be prepared in less than one month, with the cooperation of the author. Final acceptance of the manuscript requires that the atomic coordinates and structure factors have indeed been satisfactorily processed by the Data Bank. The data will also be deposited, as microfiche, with the British Library under the IUCr Supplementary Publication Scheme and may be requested from the Executive Secretary of the IUCr by quoting the Supplementary Publication Number in the usual way.

All information received by the Data Bank under this arrangement will be regarded as privileged and will not be released to others until the paper has been accepted or prior release has been authorized by the authors. Magnetic tape

with fixed line length and fixed block size in 7 track, BCD, 200, 556 or 800 CPI; or 9 track, ASCII or EBCDIC, 800 or 1600 CPI; or punched cards with IBM 026 or IBM 029 codes; or paper tape, 8-level ASCII are equally acceptable machine-readable media for deposition. Each deposition should be accompanied by sufficient information to allow ready transcription of the medium, such as a FORMAT statement and a designation of the recording equipment used.

Acta Cryst. (1981). B**37**, 1162

Commission on Journals

Submission of Manuscripts Based on Powder Diffraction Profile Fitting or Refinement (Rietveld) Methods: Deposition of Data

A steadily increasing number of manuscripts that depend on the use of either powder diffraction profile fitting or refinement (Rietveld) methods are being submitted for publication. Commission policy has recently required that figures in such manuscripts that present the experimental and calculated diffraction profiles of the material studied should also contain the difference profile (I_{obs}–I_{calc}), as an aid to the reader. It is recognized that the primary diffraction data cannot be extracted satisfactorily from such figures. The Commission has now decided that, in addition to the figure, the authors of such manuscripts should deposit the numerical intensity of each measured point on the profile, as a function of scattering angle.

The attention of authors is also drawn to notices concerning stereofigures [*Acta Cryst.* (1978). B**34**, 3846], dimensions of material for deposition [*Acta Cryst.* (1979). B**35**, 792], estimated standard deviations, SI units and anisotropic thermal parameters [*Acta Cryst.* (1979). B**35**, 1302], submission of connected computer output [*Acta Cryst.* (1979). B**35**, 2284–2285], chemical-connectivity relationships [*Acta Cryst.* (1980). B**36**, 1524], and estimated standard deviations with a zero value for varied parameters [*Acta Cryst.* (1980). B**36**, 2508], in addition to the information given in *Notes for Authors* [*Acta Cryst.* (1978). A**34**, 143–157].

Acta Cryst. (1981). B**37**, 1162

Communicated Abstracts

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