Journal of
Applied
Crystallography

### letters to the editor

ISSN 0021-8898

## Comment on CRUNCH: a phase refinement program for high-resolution macromolecular structures by Langs, Blessing & Smith (2000)

#### R. A. G. de Graaff<sup>a</sup>\* and R. de Gelder<sup>b</sup>

<sup>a</sup>Gorlaeus Laboratories, Leiden Institute of Chemistry, University of Leiden, PO Box 9502, NL-2300 RA Leiden, The Netherlands, and <sup>b</sup>Crystallography Laboratory, Department of Inorganic Chemistry, Nijmegen SONphone="+31-71-527-4213" fax="+31-71-527-4537" Research Center, University of Nijmegen, Toernooiveld 1, NL-6525 ED Nijmegen, The Netherlands

Received 19 May 2000 Accepted 8 June 2000

The February issue of the *Journal of Applied Crystallography*, in the section *Computer Programs*, contains the paper entitled *CRUNCH: a phase refinement program for high-resolution macromolecular structures*, by Langs, Blessing & Smith (2000).

We would like to point out that an earlier program system *Crunch* has been available to the scientific community for a number of years now (Abrahams & de Graaff, 1998; de Graaff, 1998; Cram *et al.*, 1999; de Gelder & de Graaff, 1999). *Crunch* has been developed for the automatic solution of difficult 'small' structures.

Without discussing the various merits and demerits of the two programs, we feel that the existence of two different programs aimed at the same or a similar group of users and bearing the same name will lead to unnecessary confusion.

We hope that Dr Langs et al. will address this point as soon as possible.

#### References

Abrahams, J. P. & de Graaff, R. A. G. (1998). Curr. Op. Struct. Biol. 8, 601–605. Cram, D. J., de Graaff, R. A. G., Knobler, C. B., Lingenfelter, D. S., Maverick, E. F. & Trueblood, K. N. (1999). Acta Cryst. B55, 432–440.

Gelder, R. de & de Graaff, R. A. G. (1999). *IUCr XVIII Congress and General Assembly, Collected Abstracts*, edited by C. C. Wilson, K. Shankland & T. Csoka, p. 92.

Graaff, R. A. G. de (1998). Workshop Lecture Notes 18: Riding the Fence Between Large and Small Molecules, ACA Annual Meeting, Washington, DC, USA, pp. 1–12.

Langs, D. A., Blessing, R. H. & Smith, G. D. (2000). J. Appl. Cryst. 33, 174–175.

# Response to de Graaff & de Gelder's comment on CRUNCH: a phase refinement program for high-resolution macromolecular structures

David A. Langs, a\* Robert H. Blessing and G. David Smith A,b

<sup>a</sup>Hauptman-Woodward Medical Research Institute Inc., 73 High Street, Buffalo, New York 14203-1196, USA, and <sup>b</sup>Roswell Park Cancer Institute, Elm and Carlton Streets, Buffalo, New York 14263, USA

Received 19 May 2000 Accepted 8 June 2000

We regret that we forgot that the program name CRUNCH (Langs et al., 2000) had been associated with the direct-methods work based on Karle-Hauptman determinants as described in the above letter by de Graaff & de Gelder (2000).

We have adopted the name *CROQUE* for future reference to our program.

#### References

Graaff, R. A. G. de & de Gelder, R. (2000). J. Appl. Cryst. 33, 1194. Langs, D. A., Blessing, R. H. & Smith, G. D. (2000). J. Appl. Cryst. 33, 174–175.