

$\delta p_i = \frac{|p(1)_i - p(2)_i|}{[\sigma^2 p(1)_i + \sigma^2 p(2)_i]^{\frac{1}{2}}}$, where $p(1)_i$ and $p(2)_i$ are the two sets of parameters refined in the structure analysis and the σ 's are the corresponding standard deviations.

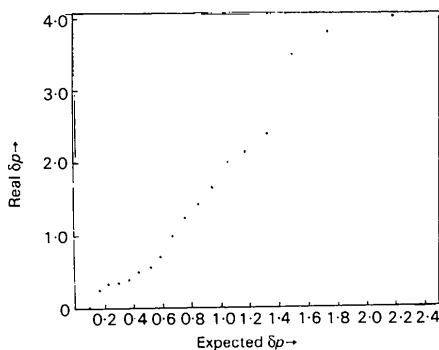


Fig. 1. Half-normal probability plot with real δp and expected δp as ordinate and abscissa.

A least-squares straight-line fit of the plot ignoring two points (16th and 17th in the figure) gave a slope of 1.83 (4) and an intercept of -0.16 (3). The non-zero intercept indicates systematic errors in the data. The slope of the straight line deviates from the ideal value of 1 by 0.85 indicating that either the $\Delta p_i = p(1)_i - p(2)_i$ are large or the corresponding standard deviations $\sigma(p_i)$ are small. The near linearity of the plot excludes the first possibility since for Δp_i to be large $p(1)_i$ and $p(2)_i$ must differ from the true value in opposite directions. The second possibility is more likely, which could arise if both sets of data are refined by least squares to a greater degree than warranted by the accuracy of the data.

References

- ABRAHAMS, S. C. & KEVE, E. T. (1971). *Acta Cryst.* **A27**, 157–165.
 APPA RAO, G. V. N., SESHASAYEE, M., ARAVAMUDAN, G., NAGESWARA RAO, T. & VENKATASUBRAMANIAN, P. N. (1982). *Acta Cryst.* **B38**, 2852–2855.
 PROUT, K. (1982). *Acta Cryst.* **B38**, 338–340.

International Union of Crystallography

Chemical nomenclature

The attention of authors is drawn to the following recommendations of the IUPAC Commission on Nomenclature of Organic Chemistry: *The Designation of Non-Standard Classical Valence Bonding in Organic Nomenclature* [*Pure Appl. Chem.* (1982), **54**, 217–227], *Revision of the Extended Hantzsch–Widman System of Nomenclature for Heteromonocycles* [*Pure Appl. Chem.* (1983), **55**, 409–416]; and to the following recent recommendations of the IUPAC–IUB Joint Commission on Biochemical Nomenclature: *Symbols for Specifying the Conformation of Polysaccharide Chains* [*Eur. J. Biochem.* (1983), **131**, 5–7], *Abbreviations and Symbols for the Description of Conformations of Polynucleotide Chains* [*Eur. J. Biochem.* (1983), **131**, 9–15].

Authors are reminded that, wherever possible, chemical nomenclature in the Union's journals should conform to IUPAC rules. Basic rules for the nomenclature of inorganic chemistry are given in *Nomenclature of Inorganic Chemistry* (1970) ('The Red Book'), London: Butterworths and, for organic chemistry, in the two volumes *Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, & H* (1979) ('The Blue Book'), Oxford: Pergamon Press and *Biochemical Nomenclature and Related Documents* (1978), London: Biochemical Society. For additional details on nomenclature requirements see p. 179 of *Notes for Authors* [*Acta Cryst.* (1983), **A39**, 174–186].

An index to all IUPAC nomenclature publications is available from the IUPAC Secretariat, Bank Court Chambers, 2–3 Pound Way, Cowley Centre, Oxford OX4 3YF.