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Nuclear magnetic resonance in crystals. By D. W. McCall and R. W. Hamming, *Bell Telephone Laboratories, Incorporated, Murray Hill, New Jersey, U.S.A.*

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Dr. J. M. Dereppe, Dr. Pedro W. Lobo and Ing. R. Touillaux, of the Laboratoire de Chimie Physique, Louvain, Belgium, have drawn our attention to a number of errors in our paper under the above title (McCall & Hamming, 1959).

The coefficient of the term ab^3c^2d, in equation (3), should be 108.

The × on the third line of equation (5) should be +.

The expressions for $h(\theta_p, 5)$ and $h(\theta_p, 6)$ are interchanged in equations (7). These quantities should be given as:

$$h(\theta_p, 5) = a_{65} \sin 2\theta_p + a_{85} \sin 4\theta_p$$

$$h(\theta_p, 6) = a_{06}(1 - \cos 4\theta_p) + a_{26} (\cos 2\theta_p - \cos 4\theta_p)$$

The statement 'A sufficient set of measurements consists of θ-dependences at $\varphi_p = 0, \pi/4, \pi/2$ and a φ-dependence at $\theta_p = \pi/2$.' (near the bottom of the first column, page 83) is incorrect. These allow for the determination af $A, B, C, L, M, R, S, U, V$ but not D, E, F, G, N, Q.

The first sentence at the top of the second column of page 83 should read: $g(\varphi_p, n) = 0$ for $n = 1, 3, 5, 7$ for any θ-dependence at constant φ and $h\ (0, m) = 0$ for $m = 1, 3, 5, 7$.

Certain errors appear in Appendix V. The correct relations for these cases are:

$$L = 6a_{26} - 8a_{06}$$

$$S = 8a_{06} - 10a_{26} - 8a_{28}$$

$$U = 8a_{06} - 10a_{26} + 8a_{28}$$

$$M = 7a_{02} + 3a_{42} - (5/2)a_{00} + (19/6)a_{20} - (7/6)a_{40} .$$

Appendix VI is sufficiently in error that it should be disregarded entirely. A corrected table for $A, B, C, L, M, R, S, U, V$ follows.

REVISED APPENDIX VI

$$A = (15/4)g(0, 0) + (21/4)g(0, 2) + (7/4)g(0, 4) - (3/2)g(\pi/2, 0) - (7/2)g(\pi/2, 4) + 2h(\pi/2, 4)$$

$$B = -(19/6)g(0, 0) - (23/6)g(0, 2) - (1/2)g(0,4) + (2/3)g(\pi/2, 0) + (10/3)g(\pi/2,4) - (4/3)h(\pi/2, 4)$$

$$C = (5/12)g(0, 0) - (5/12)g(0, 2) - (1/4)g(0, 4) + (1/6)g(\pi/2, 4) + (5/6)g(\pi/2, 0) - (2/3)h(\pi/2, 4)$$

$$L = -8g(\pi/4, 0) + 4g(0, 0) + 4g(\pi/2, 0) - 6h(\pi/2. 4) - 3h(\pi/2, 6)$$

$$M = (5/2)g(0, 4) - (11/3)g(\pi/2, 4) + (23/6)g(0, 0) - (19/3)g(\pi/2, 0) + (19/6)g(0, 2) + (8/3)h(\pi/2, 4)$$

$$R = (17/4)g(0, 0) - (1/2)h(\pi/2, 2) - 2g(\pi/2, 0) - 2h(\pi/2, 4) + (9/4)g(0, 4) - (15/4)g(0, 2)$$

$$S = 8g(\pi/4, 0) - 4g(0, 0) - 4g(\pi/2, 0) + 6h(\pi/2, 4) + 5h(\pi/2, 6) + 4h(\pi/2, 8)$$

$$U = 8g(\pi/4, 0) - 4g(0, 0) - 4g(\pi/2, 0) + 6h(\pi/2, 4) + 5h(\pi/2, 6) - 4h(\pi/2, 8)$$

$$V = (1/4)g(0, 0) - (15/4)g(0, 2) + (9/4)g(0, 4) + 2g(\pi/2, 0) - (11/2)h(\pi/2, 2) - 2h(\pi/2, 4)$$

The quantities D, E, F, G, N, Q can be found by an additional φ-dependence at $\theta_p = \pi/4$.

We are indebted to Dr. Dereppe, Dr. Lobo and Ing. Touillaux for considerable efforts in the preparation of this communication.

Reference

McCall, D. W. & Hamming, R. W. (1959). *Acta Cryst.* **12**, 81.

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A computational technique for the coincidence method of sign determination. By R. Hine, *Viriamu Jones Laboratory, University College, Cardiff, Wales*

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Introduction

It is well known that the signs of the unitary structure factors $U(\mathbf{h})$, $U(\mathbf{h}')$, $U(\mathbf{h}+\mathbf{h}')$ are related by

$$S(\mathbf{h}) \approx S(\mathbf{h}')S(\mathbf{h}+\mathbf{h}') , \quad (1)$$

where $S(\mathbf{h})$ denotes the sign of $U(\mathbf{h})$ *etc*, with a probability increasing with increasing $|U(\mathbf{h})U(\mathbf{h}')U(\mathbf{h}+\mathbf{h}')|$. One way in which this relation has been applied to certain plane groups (Grant, Howells & Rogers, 1957) uses special relations between $S(0kl)$ and $S(0\bar{k}l)$ *etc* for these groups: *e.g.* in plane group *pgg* $S(0\bar{k}l) = S(0kl)$ for $(k+l)$ even, and $S(0\bar{k}l) = -S(0kl)$ for $(k+l)$ odd. Such terms may be said to be symmetry-related. Only reflexions of high unitary structure factor are used, and a necessary step is a procedure for finding all the relations of type (1) which exist between the reflexions considered. An important part of the method is the recognition of 'coincidences'. These are two or more terms $\mathbf{h}$ occurring with the same pair of terms $\mathbf{h}'$, $\mathbf{h}+\mathbf{h}'$, or their symmetry-related terms, in a relation of type (1): *e.g.* in plane group *pgg* the (023) and (063) terms can form a coincidence since (023) can occur with (045) and (022), and (063) with (045) and (0$\bar{2}$2). The discovery of the sign relations and coincidences is followed by an iterative process to adjust and extend a tentative initial set of signs obtained from the coincidences so as to obtain best agreement with the original data. The method described by Grant, Howells & Rogers is two-dimensional. It can, with very considerable advantage, be extended to three-dimensional data (Grant, Hine & Richards, 1960)