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A. Oslo University (received from Prof. O. Hassel and O. Bastiansen).
B. California Institute of Technology (received from Prof. L. Pauling and Prof. V. Schomaker).
C. Cornell University, N.Y. (received from Prof. S. H. Bauer).

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.*

Acta Cryst. (1950). **3**, 72

Corrigenda: The accuracy of electron-density maps in X-ray analysis with special reference to dibenzyl.

By D. W. J. CRUICKSHANK, *St John's College, Cambridge, England*

(*Received* 19 *July* 1949)

The estimated standard deviation of atomic co-ordinates in non-centrosymmetric structures was originally stated (Cox & Cruickshank 1948) to be $\sqrt{2}$ times the corresponding deviation in centrosymmetric structures; a revised calculation (Cruickshank, 1949*a*) gave this factor as unity; we shall revise the discussion again, now reaching by two methods a factor of 2.

The authors's papers (Cruickshank, 1949*a*, *b*, 1950) will be referred to as A, B and C; the notation of these papers will be used.

We may calculate the estimated standard deviations from the method of least squares as applied to

$$\phi = \sum_3 \frac{1}{f_r} (|F_o| - |F_c|)^2$$

in the manner of B (§3). Using C (3·7) and assuming A_{hk}, etc., small compared with A_{hh}, we have, corresponding to B (3·7) for the estimated standard deviation $\sigma(x_r)$ of the x co-ordinate of the rth atom in a non-centrosymmetric structure,

$$\sigma^2(x_r) = -2\sigma^2/(VA_{hh}), \qquad (1)$$

where σ is the estimated standard deviation of an observation of unit weight.

For a structure having only a centre of symmetry we find, corresponding to C (3·7),

$$c_{mn} = \sum_3 4\pi^2 \frac{hk}{ab} f_r \{2 \sin (\theta_r - \alpha)\}^2$$

$$= -2VA_{hk},$$

so that $$\sigma^2(x_r) = -\sigma^2/(2VA_{hh}). \qquad (2)$$

On comparing (1) and (2) we see that, for the same σ and A_{hh}, the estimated co-ordinate standard deviations of non-centrosymmetric structures are twice those of centrosymmetric structures.

This result may also be reached via the Fourier method, for by using C (§ 3·1) we see that the total error is twice that estimated by assuming errors in the $|F|$'s but none in the phase angles, which is the assumption made for centrosymmetric structures.

The mistake in the argument given previously in A occurs between equations A (11·20) and A (11·21). It was stated that the $\Delta\alpha$ occurring in the contribution of the finite-series correction error was identical with that in A (11·20). This is incorrect, the $\Delta\alpha$ of the finite-series correction error should be the difference between the phase angles of the 'calculated' structure and a 'true' structure based on the 'calculated' positions.

A mistake also occurs in equation A (11·8); the sign of $\sin(-\theta_1)$ is incorrectly given as positive.

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Increase in Q-value and reduction of aging of quartz crystal blanks.

By A. C. Prichard, M. A. A. Druesne and D. G. McCaa, *Signal Corps Engineering Laboratories, Fort Monmouth, New Jersey, U.S.A.*

(*Received* 26 *August* 1949)

The importance of quartz crystal units for frequency control derives from the very high Q (ratio of reactance to resistance) and the low frequency–temperature coefficient of quartz, and the very steep slope of the reactance curve of the crystal blank. The Q of quartz is higher than that of any other frequency-controlling device used to date.

The Q and frequency of a given quartz crystal blank change, however, with time; these changes are results of the so-called aging process. During World War II, crystal units were used in very large quantities in military communications equipment. Considerable difficulty was experienced during the first years of the war because the useful life of a crystal unit was greatly reduced by reason of its 'aging out of frequency' or 'going dead'. A usable reduction in aging was later accomplished during 1944 by etching the surfaces of the crystal blanks. This only mitigated the effect, however, and its more complete elimination was highly desirable.

A method has recently been developed at the Signal Corps Engineering Laboratories, Fort Monmouth, N.J., whereby the Q-value of the quartz blank has been materially increased, and the aging has been very greatly reduced. The method consists of annealing the quartz blank by heating it almost to the inversion temperature of quartz, or 500° C., and cooling it down extremely slowly.

This simple treatment yields values of Q which are at least double those of untreated quartz blanks, and variations in frequency and Q are minute. These improvements in Q and aging characteristics appear to be of a permanent character.

A paper describing the results in greater detail is in preparation.

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Observations on the diffuse X-ray reflexion of sodium chlorate, $NaClO_3$.

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Introduction

In the course of a systematic study of the elastic properties of cubic substances by means of diffusely reflected X-rays the authors have had occasion to study crystals of sodium chlorate. Garrido (1948) has published an account of photographic observations of X-rays diffusely reflected from this substance and we were surprised to find that our results differed considerably from his. It is, of course, possible to calculate the form of the isodiffusion surface around any reciprocal-lattice point. This only involves the elastic constants and has been worked out by Sen (1949). This calculation gives a result not in agreement with Garrido's observations. In this note we wish to put on record a direct experimental test of the variation of the intensity of diffuse reflexion round two reciprocal points, namely, 600 and 333.