

Short Communications

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Anomalous dispersion data in crystal-structure reports. By R. SRINIVASAN, *Centre of Advanced Study in Physics, University of Madras, Madras-25, India*

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Valuable information is lost when accurate measurements are so recorded that individual intensities or structure amplitudes of inverse reflexions cannot be extracted.

The anomalous-dispersion method has been used increasingly in recent years for the determination of the structure and absolute configuration of crystals. More recently it has been pointed out (Srinivasan & Chacko, 1967) that if accurate intensity measurements are available for inverse reflexions, the Fourier method could be used to study the inner electron distribution in atoms and also possibly for the determination of $\Delta f''$ values for elements. This requires particularly accurate values of the observed structure factors for the inverse reflexions. The following remarks have been prompted by our recent attempt at a literature survey to select suitable examples for which data are supplied, in order to test the above results. The survey indicates that quite often the mean intensity $[I(\mathbf{H}) + I(\bar{\mathbf{H}})]/2$ or the mean amplitude $[F(\mathbf{H}) + F(\bar{\mathbf{H}})]/2$ only are given by some authors. Quite valuable information is lost in such simplified data unless corresponding differences such as $[I(\mathbf{H}) - I(\bar{\mathbf{H}})]$ or $[F(\mathbf{H}) - F(\bar{\mathbf{H}})]$ are also given. It will be highly useful if entries are made (if possible for inverse pairs in full) in the

relevant tables, whenever the accuracy is sufficient. In certain cases the quantity $[I(\mathbf{H}) - I(\bar{\mathbf{H}})]/[I(\bar{\mathbf{H}}) + I(\mathbf{H})]$ is preferred (Zachariasen, 1965), since it is a dimensionless quantity and will be relatively free from scaling errors. In such cases more information could be added to enable one to extract $I(\mathbf{H})$ and $I(\bar{\mathbf{H}})$. The need for collecting data over the full reciprocal sphere in the presence of anomalous dispersion has recently been pointed out (Ibers, 1967). It is also necessary in this connexion to supply the data in full, without averaging.

References

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 ZACHARIASEN, W. H. (1965). *Acta Cryst.* **18**, 714.

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Stoichiometry of Ce-Mg compounds.* By QUINTIN JOHNSON and G. S. SMITH, *Lawrence Radiation Laboratory, University of California, Livermore, California 94550, U.S.A.*

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Compositions and crystal structures of compounds reported for the Ce-Mg binary system are critically reviewed.

There is a need to correct some of the compositions which have been reported for compounds in the Ce-Mg binary system.

The stoichiometry of the compound reported as $\text{Ce}_5\text{Mg}_{42}$ (Johnson & Smith, 1967*a*) is incorrect. It should be replaced by $\text{Ce}_5\text{Mg}_{41}$, a formula which can be derived from the multiplicities of the various point positions in Table 1 of that report, as given in *International Tables for X-ray Crystallography* (1952). The calculated density based on

this revised composition is 2.47 g.cm^{-3} . There is a typographical error in the title of another article dealing with a Ce-Mg compound (Johnson & Smith, 1967*b*). The stoichiometry of that compound is $\text{CeMg}_{10.3}$, not $\text{CeMg}_{1.03}$.

Three compounds are reported to occur in the Ce-Mg system up to 75 at. % Mg (see, for example, Iandelli, 1959). There is no controversy concerning these compositions or structure types which are given in Table 1.

Above 75 at. % the picture has not been so clearly presented. In order of increasing at. % Mg, the *bona fide* compounds are $\text{Ce}_5\text{Mg}_{41}$, $\text{CeMg}_{10.3}$, $\text{CeMg}_{12}(\text{I})$, and $\text{CeMg}_{12}(\text{II})$, compositions of the first two compounds hav-

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