Short Communications

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Anomalous dispersion data in crystal-structure reports.

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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

Ibers, J. A. (1967). *Acta Cryst.* **22**, 604.
Srinivasan, R. & Chacko, K. K. (1967). *Curr. Sci.* **36**, 279.
Zachariasen, W. H. (1965). *Acta Cryst.* **18**, 714.

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Stoichiometry of Ce–Mg compounds.*

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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 Ce_5Mg_{42} (Johnson & Smith, 1967*a*) is incorrect. It should be replaced by Ce_5Mg_{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 $2{\cdot}47$ 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 $CeMg_{10{\cdot}3}$, not $CeMg_{1{\cdot}03}$.

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 Ce_5Mg_{41}, $CeMg_{10{\cdot}3}$, $CeMg_{12}$(I), and $CeMg_{12}$(II), compositions of the first two compounds hav-

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Table 1. *Structure types of cerium–magnesium compounds*

	a	*c*	*M*	Space group	Structure type	Reference for lattice constants
CeMg	3·912 Å		1	*Pm*3*m*	CsCl	Iandelli (1959)
$CeMg_2$	8·733		8	*Fd*3*m*	$MgCu_2$	Iandelli (1959)
$CeMg_3$	7·428		4	*Fm*3*m*	BiF_3	Iandelli (1959)
Ce_5Mg_{41}	14·78	10·43 Å	2	*I*4/*m*	Ce_5Mg_{41}	Johnson & Smith (1967*a*)
$CeMg_{10\cdot3}$	10·33	10·25	3·42	$P6_3/mmc$	Th_2Ni_{17}*	Johnson & Smith (1967*b*)
$CeMg_{12}$(I)	10·33	5·96	2	*I*4/*mmm*	$ThMn_{12}$	Johnson *et al.* (1964)
$CeMg_{12}$(II)†	10·33	77·5	26	(*Immm*)	$CeMg_{12}$(II)	Johnson *et al.* (1964)

* The Th_2Ni_{17} structure type is probably not yet known; see Johnson & Smith (1967*b*).
† Composition of this phase has not been established with certainty.

ing been determined by single-crystal structure analysis. Three other compositions, Ce_2Mg_{17}, $CeMg_9$, and Ce_2Mg_{23}, have also been reported.

Crosby & Holman (1966) describe a powder pattern of an alloy of composition Ce_2Mg_{17} (their Table 5). We have confirmed this to be the powder pattern of Ce_5Mg_{41} and note the closeness of their metallographically determined composition $AB_{8\cdot5}$ to the composition $AB_{8\cdot2}$ which was determined by a single-crystal structure determination. Evdokimenko & Kripyakevich (1963) and Lashko & Morozova (1964) also reported a compound of composition Ce_2Mg_{17}, based on their observation that some of their powder patterns indicated a structure of the Th_2Ni_{17} type. Their structure analysis is correct but this compound is richer in magnesium than the 2–17 formulation suggests. Again using single-crystal analysis, Johnson & Smith (1967*b*) established a more accurate formula, $CeMg_{10\cdot3}$. In part, the above confusion stems from the fact that there is a compound ($CeMg_{10\cdot3}$) with an A_2B_{17} structure type but not with that composition, while a compound with nearly that composition ($CeMg_{41}$) does not have a crystal structure of the type usually referred to as A_2B_{17} (Johnson, Smith & Wood, 1969).

Beletzkii & Gal'perin (1961) reported a composition $CeMg_9$ with a cubic structure. This interpretation is incorrect; instead we note their powder pattern is in excellent agreement with that calculated for $CeMg_{12}$(I) (Johnson, Smith, Wood & Cramer, 1964). The $ThMn_{12}$ structure type for this compound has also been recognized by Lashko & Morozova (1964).

The composition Ce_2Mg_{23} was reported by Crosby & Holman (1966). The powder pattern for an alloy of this composition (their Table 3) which they incorrectly attributed to a tetragonal cell of unknown structure, can be accounted for by the hexagonal $CeMg_{10\cdot3}$ structure (Johnson & Smith, 1967*b*).

Composition ranges, if any, have not been determined for the four most Mg-rich compounds; nevertheless the formulas of Table 1, based on structure types, are considered more accurate descriptions and are more appropriate labels for these compounds than labels derived from the more approximate metallographic method or from incorrect structure type determinations. We cannot, in fact, state the precise composition of $CeMg_{12}$(II), a formula inferred from an approximate structure based on single-crystal evidence (Johnson *et al.*, 1964). Nor can we be certain that the formula $CeMg_{10\cdot3}$ is necessarily an accurate representation of the average composition of the Th_2Ni_{17}-like phase; this formula was deduced from a single-crystal structure determination which, while accurately reflecting the composition of the particular crystal used, may not necessarily reflect that of the bulk material. It is not anticipated that an appreciable difference exists, however (see Wood & Cramer, 1965).

Finally, it is not impossible that other compounds might be found in the Ce–Mg binary system. To our knowledge, however, each compound so far reported can be reconciled with one of those shown in Table 1.

We thank Dr K. Gschneidner for drawing our attention to the error in the Ce_5Mg_{42} formulation.

References

Beletskii, M. S. & Gal'perin, E. L. (1961). *Fiz. Metal. Metallov.* **11**, 698.

Crosby, R. L. & Holman, J. L. (1966). U.S. Dept. of the Interior, Bureau of Mines Report No. 6866.

Evdokimenko, V. I. & Kripyakevich, P. I. (1963). *Kristallografiya*, **8**, 186.

Iandelli, A. (1959). *The Physical Chemistry of Metallic Solutions and Intermetallic Compounds*, National Physical Laboratory, Teddington, England. Proc. Symp. 1, Paper 3F.

International Tables for X-ray Crystallography (1952). Vol. I. Birmingham: Kynoch Press.

Johnson, Q. & Smith, G. S. (1967*a*). *Acta Cryst.* **22**, 360.

Johnson, Q. & Smith, G. S. (1967*b*). *Acta Cryst.* **23**, 327.

Johnson, Q., Smith, G. S. & Wood, D. H. (1969). *Acta Cryst.* **B25**, 464.

Johnson, Q., Smith, G. S., Wood, D. H. & Cramer, E. M. (1964). *Nature, Lond.* **201**, 600.

Lashko, N. F. & Morozova, G. I. (1964). *Kristallografiya*, **9**, 269.

Wood, D. H. & Cramer, E. M. (1965). *J. Less-Common Metals*, **9**, 321.