Laboratory, who made their automated diffractometer available for the collection of the data reported here. We are also indebted to R. A. Potter of the Metals and Ceramics Division, who participated in the preparation of the crystals.

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The Crystal Structure of Ce₅Mg₄₂

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The structure of the compound present in the Ce–Mg system at the approximate stoichiometry of CeMg₈ has been determined with the use of diffractometrically recorded single-crystal intensities. The unit cell, containing two formula units of Ce₅Mg₄₂, is body-centered tetragonal with $a = 14.78$, $c = 10.43$ Å. The calculated density is 2·51 g.cm⁻³, and the space group, as confirmed by the final structure, is $I4/m$.

Introduction

During a phase-relation study of the magnesium-rich region of the Ce–Mg system (Wood & Cramer, 1965), a new compound with a tentative composition CeMg₈.₂₅ was discovered. The composition and symmetry indicated this to be a new structure type; therefore, we have carried out a determination of this structure by conventional single-crystal X-ray diffraction techniques. Additional interest in this study resulted from the expectation that, in view of the similarity of cell constants, a simple relationship would be found to connect this structure with the other structures occurring in the magnesium-rich region (Savitskii, Terekhova, Burov, Markova & Naumkin, 1962; Evdokimenko & Kripyakevich, 1963; Johnson, Smith, Wood & Cramer, 1964; Johnson & Smith, 1966).

Experimental

The sample of Ce₅Mg₄₂ used in this investigation was kindly provided by D. Wood. Details concerning the preparation are given by Wood & Cramer (1965).

Single-crystal oscillation, Weissenberg, and precession photographs showed tetragonal symmetry. The observed extinctions ($h+k+l \neq 2n$) and $4/m$ Laue

symmetry are characteristic of space groups $I4$, $I\bar{4}$ and $I4/m$. The final structure confirms the centrosymmetric ($I4/m$) space group. Lattice constants were obtained by a least-squares fit of powder data from a Cr $K\alpha$ ($\lambda = 2\cdot 2909$ Å) powder pattern. The computer program was a modification of the Heaton, Gvildys & Mueller (1964) program. Cell constants are $a = 14\cdot 78 \pm 0\cdot 01$ and $c = 10\cdot 43 \pm 0\cdot 01$ Å.

Intensities were recorded diffractometrically with zirconium-filtered Mo $K\alpha$ radiation ($\lambda = 0\cdot 7107$ Å). 607 independent reflections up to $2\theta \le 40°$ were measured. A φ-dependent absorption correction was applied to the intensities; the maximum correction required was only 10%.

Determination of the structure

The approximate number of atoms present in the tetragonal cell could be estimated by a comparison with the corresponding data for Ce_2Mg_{17} (Johnson & Smith, 1966). Taken in conjunction with the approximate stoichiometry observed in the metallographic study (Wood & Cramer, 1965), this strongly indicated that there were ten cerium atoms in the unit cell. For the centric space group ($I4/m$), there were several combinations of special positions which would accommodate ten atoms but only the combination of $2(a)$ and $8(h)$ (*International Tables for X-ray Crystallography*, 1952) was consistent with the observed reflections and volume requirements; thus it was necessary to place five cerium atoms in the plane $z = 0$ and the other five at $z = \frac{1}{2}$. Approximate values for the two parameters of the eightfold positions ($x = \frac{2}{5}$, $y = \frac{1}{5}$) were obtained from packing considerations. A Patterson synthesis confirmed this model and yielded more accurate values for these parameters.

A 'heavy-atom' electron density synthesis calculated on the basis of a refined model sufficed to locate (after one or two false starts) all magnesium positions.

A difference map based on refined positional parameters and isotropic thermal parameters for all atoms gave evidence of anisotropic behavior for the cerium atoms. A subsequent refinement, with anisotropic thermal parameters for cerium only, resulted in a decrease in the conventional R index from 5·8% to 5·1% (all reflections). Additionally, a difference map calculated on this basis showed the electron density to be more uniform and close to zero about the cerium positions. Comparable treatment in the case of magnesium atoms resulted in no significant change; thus the parameters reported are the result of the above-mentioned refinement in which only the cerium atoms were refined anisotropically.

The final atom parameters obtained by the full-matrix least-squares program of Gantzel, Sparks & Trueblood (ACA Program No. 317, unpublished) are given in Table 1. Atomic scattering factors were those for the neutral atoms as listed in *International Tables for X-Ray Crystallography* (1962) and a weighting scheme appropriate for diffractometric data (Smith & Alexander, 1963) ($w = F_o^{1/4}$, $F_o < A$; $w = A^{5/4}F_o^{-1}$, $F_o > A$ with $A = 32$) was used. Changes in parameters for the last cycle were less than 0·01 times the estimated standard deviations. Table 2 is the list of observed and calculated structure factors.

Discussion

As stated in the introduction, a relationship was expected to be uncovered between this structure and the other magnesium-rich phases, Ce_2Mg_{17}, $CeMg_{12}(I)$, and $CeMg_{12}(II)$, which would account for the similarity in cell constants. A summary of all compounds known to date for the Ce–Mg binary system is given in Table 3. The hexagonal $TiBe_{12}$ structure reported by Miller (1960) for $CeMg_{12}$ and the cubic symmetry reported for a compound of approximate composition $CeMg_9$ by Beletskii & Galperin (1961) are not confirmed. Instead, their results are understood on the basis of the unit cells of the structures which we report.

The similarity of cell constants is noted in Table 3 by expressing these as a function of s, where s is approximately equal to 10·3 Å. The reason for this similarity in the case of the Ce_2Mg_{17} and the $CeMg_{12}$ (I and II) structures is understood following the arguments of Florio, Baenziger & Rundle (1956). These structures are merely superlattices of a hypothetical $CeMg_5$ compound with the $CaZn_5$ structure in which two magnesium atoms replace one cerium atom at certain sites to give the observed stoichiometry. No such simple scheme is appropriate for the other compounds; it is probably more instructive to consider the size of the coordination polyhedra (CP's) as essentially constant. The cell constants then mirror this fact.

There are twenty magnesium atoms in the polyhedron about Ce(1) forming a figure which is the same as that found for Th in $ThMn_{12}$ [or Ce in $CeMg_{12}(I)$]. The site symmetry is only $4/m$, as against $4/mmm$ for the 1–12 structure; nevertheless this CP departs but little from the higher site symmetry.

The CP of Ce(2) consists of eighteen magnesium atoms, two of which are Mg(5). Perpendicular to the axis formed by Mg(5)–Ce(2)–Mg(5) and passing
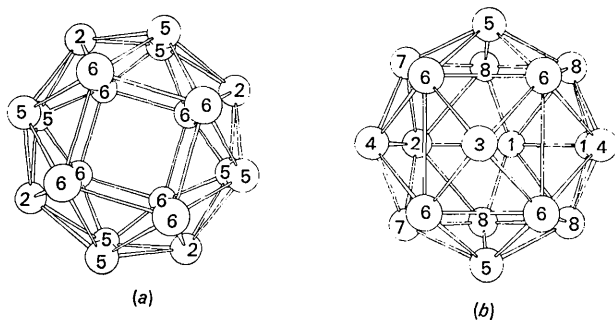

Fig. 1. (a) Ce(1) coordination polyhedron. (b) Ce(2) coordination polyhedron.

Table 1. *Final parameters*

e.s.d.'s in parentheses.

	Wyckoff notation	10^4x	10^4z	10^4z	$B(\text{Å}^2)$ or $10^4\beta_{11}$	$10^4\beta_{22}$	$10^4\beta_{33}$	$10^4\beta_{12}$
Ce(1)	(a)	0	0	0	13 (1)	13 (1)	77 (3)	0
Ce(2)	(h)	4285 (1)	2365 (1)	0	12 (1)	12 (1)	23 (1)	−2 (1)
Mg(1)	(h)	4029 (5)	−102 (5)	0	1·6 (0·2)			
Mg(2)	(h)	2217 (5)	1219 (5)	0	1·1 (0·1)			
Mg(3)	(b)	⅓	⅓	0	1·8 (0·3)			
Mg(4)	(h)	2166 (5)	3413 (4)	0	0·9 (0·1)			
Mg(5)	(i)	612 (3)	2271 (3)	1472 (4)	0·9 (0·1)			
Mg(6)	(i)	3641 (3)	4233 (3)	1901 (5)	1·1 (0·1)			
Mg(7)	(f)	¼	¼	¼	1·1 (0·1)			
Mg(8)	(i)	3674 (3)	766 (3)	2593 (5)	1·6 (0·1)			

Table 2. *Observed and calculated structure factors*

```
H,K= 0, 0      2 37 37      3 73 73      L FOB FCA    H,K= 3, 8    1 29 27     5 41 -41    0 77 77      L FOB FCA    4 21 -19     6 6 -1       L FOB FCA
L FOB FCA      4 59 55      1 9 7        L FOB FCA    L FOB FCA    3 41 42     7 39 -44    2 64 64      0 9 5        H,K=10, 1                 1 53 53
2 101 98       5 43 43      3 10 9       1 10 16      1 10 16                  H,K= 5, 7   4 56 56      H,K= 8, 9    L FCB FCA    H,K=11, 7    3 50 46
4 183 191      H,K= 0,13    5 16 -15     3 12 12      3 12 12     7 18 21      L FOB FCA   6 50 48      L FCB FCA    1 24 24      L FOB FCA    H,K=11, 7
6 131 137      L FCB FCA    7 21 21      5 1C -8      5 1C -8     H,K= 4, 8    0 62 62      H,K= 6, 7   1 22 22      3 16 -17     1 24 24      H,K=11, 8
8 123 127      1 17 14                   7 25 25      7 25 25     L FOB FCA    2 75 75      L FCB FCA   3 28 27      5 26 24      3 16 -17     1 9 -5
               3 12 10      H,K= 2,10                             0 32 -32     4 50 49      1 11 8       5 28 28      H,K=10, 2    5 26 24
H,K= 0, 1      H,K= 0,14    L FOB FCA    H,K= 3, 9    H,K= 3, 9   2 78 -80     6 49 52      3 51 -52     H,K= 8,10    L FUB FCA                 H,K=12, 0
L FOB FCA      L FCB FCA    0 10 9       L FOB FCA    L FOB FCA    4 41 -40                 5 2 -1       L FCB FCA    0 27 26      H,K=11, 8    0 62 59
1 15 -14       0 64 64      2 6 8        0 60 61      0 60 61     6 56 -55     H,K= 5, 8    7 2 -1       0 16 17      2 14 -13     1 9 -5       2 38 37
3 3 -7                     4 36 40       2 22 -20     2 22 -20                 L FOB FCA    H,K= 6, 8    2 13 10      4 12 10                   4 58 55
5 39 -39       H,K= 1, 0    6 10 -9      4 15 15      4 15 15     H,K= 4, 9    1 78 78      L FOB FCA    4 12 11                   H,K=12, 0
7 14 10        L FCB FCA                 6 20 15      6 20 15     L FOB FCA    3 57 57      0 5 -1       H,K= 9, 0    H,K=10, 6    0 62 59      H,K=12, 1
9 19 -15       1 16 -14     H,K= 1,12                             1 37 42      5 67 71      2 50 51      L FOB FCA    L FOB FCA    2 38 37      L FOB FCA
               3 7 -7       L FOB FCA    H,K= 3,1C    H,K= 3,1C    3 67 73      7 43 43      4 10 -8      1 19 -19     0 74 73      4 58 55      1 26 -23
H,K= 0, 2      5 39 -39     1 23 22      L FOB FCA    L FOB FCA    5 34 33                 6 27 28       3 25 -25     2 12 7                    3 35 -34
L FOB FCA      7 11 10      3 33 30      1 1C -14     1 1C -14     7 43 40      H,K= 5, 9    H,K= 6, 9    H,K= 9, 1    4 22 20      H,K=12, 1    5 23 -21
0 1 -4         9 18 -15     5 28 24      3 8 2        3 8 2                    L FOB FCA    L FCB FCA    L FOB FCA                 L FOB FCA
2 9 8                      H,K= 2,11     5 21 -20     5 21 -20    H,K= 4,10    0 18 -18     1 36 -36     1 91 90      H,K=10, 7    1 26 -23     H,K=12, 2
4 2 -5         H,K= 1, 1    L FCB FCA                             L FOB FCA    2 14 9       3 25 -25     3 78 79      L FOB FCA    3 35 -34     L FOB FCA
6 11 7         L FCB FCA    1 23 -24     H,K= 3,11    H,K= 3,11    0 8 8        4 15 13      5 27 -27     5 77 77      1 32 31      5 23 -21     0 14 12
8 17 -16       0 12 13      3 12 -12     L FOB FCA    L FOB FCA    2 47 50      6 -11                    7 56 58      3 34 31                   2 51 52
               2 14 12      5 16 -19     0 25 -25     0 25 -25    4 26 26                  H,K= 6,10                 H,K=10, 8    H,K=12, 2    4 19 21
H,K= 0, 3      4 17 -17                  2 16 11      2 16 11     6 33 33      H,K= 5,10    L FCB FCA    H,K= 9, 2    L FOB FCA    L FOB FCA
L FOB FCA      6 30 30      H,K= 2,12    4 24 -25                              L FOB FCA    0 73 76      L FCB FCA    0 47 46      0 14 12      H,K=12, 3
1 6 5          8 20 -21     L FCB FCA                 H,K= 4,10   H,K= 4,11    1 15 -15     2 40 40      1 7 3        2 58 59      2 51 52      1 12 -10
3 7 -9                     0 25 -25      H,K= 3,12    L FOB FCA    L FOB FCA    3 17 13      4 78 79      2 16 16      4 47 48      4 19 21      3 16 11
5 6 4          H,K= 1, 2    2 16 11      L FOB FCA    0 8 8        1 26 25      5 9 -0                   4 47 47                                H,K=12, 4
7 6 -4         L FOB FCA    4 24 -25     1 68 70      2 47 50      3 16 -14                 H,K= 6,11    7 9 -7       H,K=10, 9    H,K=12, 3    0 51 51
9 11 -10       1 24 24                   3 53 51      4 26 26                  H,K= 5,11    L FCB FCA                 L FOB FCA    1 12 -10     2 68 67
               3 25 22      H,K= 2,13                 6 33 33     H,K= 4,12    L FOB FCA    1 9 10       H,K= 9, 3    1 41 -44     3 16 11      4 72 71
H,K= 0, 4      5 22 23      L FCB FCA    H,K= 3, 0                L FOB FCA    0 33 -34     3 14 11      L FCB FCA                              H,K=12, 5
L FOB FCA      7 8 4        1 84 83      L FCB FCA    H,K= 4,11    0 15 12      2 6 -4                   1 43 -42     H,K=11, 0    H,K=12, 4    1 14 -12
0 54 52        9 20 17      3 122 125    1 2 5        L FOB FCA    2 6 -3       4 19 -18     H,K= 6,12    3 41 -42     L FCB FCA    0 51 51      3 9 4
2 80 81                    5 70 72       3 7 -9       1 26 25      4 7 -3                   L FCB FCA    5 38 -35     1 45 -42     2 68 67
4 37 36        H,K= 1, 3    7 51 53      5 6 4        3 16 -14                 H,K= 5,12    0 9 -4       6 6 5        3 21 -19     4 72 71      H,K=12, 6
6 45 44        L FOB FCA    9 56 56      7 5 -4                   H,K= 4,13    L FOB FCA    2 21 -20                 5 28 -28                  L FOB FCA
8 50 51        0 88 88                   9 9 -10      H,K= 4,12    L FOB FCA    1 79 81                  H,K= 9, 4                 H,K=12, 5     0 6 -7
               2 90 92      H,K= 2, 2                 L FOB FCA    1 2 -6       3 61 63      H,K= 7, 0    L FOB FCA    H,K=11, 1    1 14 -12     2 24 -24
H,K= 0, 5      4 61 62      L FOB FCA    H,K= 3, 1    0 15 12                  H,K= 5,13    L FCB FCA    1 27 -24     L FOB FCA    3 9 4
L FOB FCA      6 56 59      0 34 -33     L FCB FCA    2 6 -3       H,K= 5, 0    L FOB FCA    1 17 14      3 29 -28     0 31 29                  H,K=12, 7
1 102 101      8 65 67      2 27 -27     0 32 -28     4 7 -3       L FOB FCA    0 18 -18     3 46 45      5 24 -24     2 55 57      H,K=12, 6    L FOB FCA
3 61 60                    4 26 -25      2 26 -25                  1 104 101                 5 33 30                  4 35 34      0 6 -7       1 26 27
5 85 85        H,K= 1, 4    6 44 -46     4 23 23      H,K= 4,13    3 62 60      H,K= 6, 0    7 21 -7      H,K= 9, 5    6 30 31      2 24 -24
7 55 53        L FCB FCA    8 14 -13     6 43 -45     L FOB FCA    5 85 85      L FOB FCA                 L FUE FCA                              H,K=13, 0
9 44 42        1 60 -59                  8 12 -11     1 2 -6       7 55 53      0 115 -112   H,K= 7, 1    1 41 -44     H,K=11, 2    H,K=12, 7    L FOB FCA
               3 150 -151   H,K= 2, 3                              9 42 42      2 15 -12     L FCB FCA                 L FCB FCA    L FOB FCA    1 18 14
H,K= 0, 6      5 51 -49     L FCB FCA    H,K= 3, 2    H,K= 5, 0                 4 57 -55     0 7 6        H,K= 9, 6    1 36 34      1 26 27      3 13 10
L FOB FCA      7 59 -57     1 2 -1       L FCB FCA    L FOB FCA    H,K= 5, 1    6 44 -40     2 34 34      L FOB FCA    3 17 15
0 112 -112     9 63 -62     3 21 -22     1 49 49      1 104 101    L FCB FCA    8 53 -53     4 43 41      0 88 89      5 34 34      H,K=13, 0    H,K=13, 1
2 13 -12                   5 2 -3        3 82 82      3 62 60      2 59 -57                 6 11 9        2 83 84                  L FOB FCA    L FOB FCA
4 56 -55       H,K= 1, 5    7 8 -4       5 55 55      5 85 85      4 44 -44     H,K= 6, 1    8 9 7        4 86 86      H,K=11, 3    1 18 14      0 36 37
6 45 -40       L FCB FCA    9 16 -20     7 18 16      7 55 53      8 11 -7      L FOB FCA                 6 67 66      L FOB FCA    3 13 10      2 9 -2
8 51 -53       0 48 46                   9 41 41      9 42 42                   1 33 32      H,K= 7, 2                 0 56 -54
               2 66 67      H,K= 2, 4                              H,K= 5, 2    3 65 65      L FCB FCA    H,K= 9, 7    2 16 -16     H,K=13, 1    H,K=13, 2
H,K= 0, 7      4 30 29      L FCB FCA    H,K= 3, 3    H,K= 5, 1    L FOB FCA    5 34 32      1 4 -5       L FCB FCA    4 25 -22     L FOB FCA    L FOB FCA
L FOB FCA      6 35 33      0 32 36      L FCB FCA    L FCB FCA    1 21 -22     7 31 29      3 19 17      0 8 9                    0 36 37      1 53 54
1 16 14        8 52 51      2 72 72      1 49 49      2 59 -57     3 20 -20                 5 20 18       2 15 -15     H,K=11, 4    2 9 -2       3 54 53
3 46 45                    4 19 17       3 82 82      4 44 -44     5 41 -41     H,K= 6, 2    7 11 7       4 11 8       L FOB FCA
5 34 30        H,K= 1, 6    6 38 39      5 55 55      8 11 -7      7 10 -11     L FOB FCA                 H,K= 9, 8    1 15 13      H,K=13, 2    H,K=13, 3
7 21 -7        L FCB FCA    8 43 43      7 18 16                   9 20 -23     0 55 53      H,K= 7, 3    L FCB FCA    3 25 24      L FOB FCA    0 29 31
               1 30 29                   9 41 41      H,K= 5, 2                 2 29 27      L FCB FCA    1 18 -15                 1 53 54      2 11 10
H,K= 0, 8      3 17 19      H,K= 2, 5                 L FOB FCA    H,K= 5, 3    4 15 14      0 3 -6       3 12 8       H,K=11, 4    3 54 53
L FOB FCA      5 28 27      L FCB FCA    H,K= 3, 4    1 21 -22     L FOB FCA    6 23 23      2 17 -16     5 9 -4       L FOB FCA                 H,K=13, 4
0 45 42        7 15 13      1 76 77      L FOB FCA    3 20 -20     0 188 188    8 26 -27     4 20 -18                 1 15 13      H,K=13, 3    1 35 -40
2 14 16        9 10 7       3 24 27      1 86 84      5 41 -41     2 67 66                  6 6 -0        H,K= 9, 9    3 25 24      0 29 31
4 47 47                    5 43 65       3 66 64      7 10 -11     4 85 82      H,K= 6, 4    8 26 -27     L FCB FCA    5 17 18      2 11 10      H,K=13, 5
6 11 5         H,K= 1, 7    7 37 37      5 70 74      9 20 -23     6 102 104    L FOB FCA                 0 38 35                               0 35 39
8 24 22        L FCB FCA    9 26 23      7 41 44                   8 64 61      0 14 -13     H,K= 7, 4    2 6 -3       H,K=11, 7    H,K=13, 4
               0 59 58                   9 44 43      H,K= 5, 3                 2 6 -3       L FCB FCA    4 61 61      L FOB FCA    1 35 -40     H,K=14, 0
H,K= 0, 9      2 61 60      H,K= 2, 6                 L FOB FCA    H,K= 5, 4    4 49 -47     1 86 84                  1 24 24                   L FOB FCA
L FOB FCA      4 54 54      L FCB FCA    H,K= 3, 5    0 188 188    L FOB FCA    6 -3         3 122 122    H,K= 9,10    3 16 -17     H,K=13, 5    0 63 64
1 90 90        6 46 45      0 66 67      L FCB FCA    2 67 66      1 4 4        8 43 -44     5 67 68      L FOB FCA    5 26 24      0 35 39
3 77 79        8 34 31      2 15 14      0 104 -106   4 85 82      3 15 14                  7 68 69       1 29 29
5 77 77                    4 66 68       2 67 66      6 102 104    5 23 -23     H,K= 6, 5                 H,K=11, 8
7 60 58        H,K= 1, 8    6 11 -1      4 6 1        8 64 61      7 24 24      L FOB FCA    H,K= 7, 5                 1 9 -5
               L FCB FCA    8 49 48      6 34 -34                              1 28 26      L FCB FCA
H,K= 0,10      1 10 9                    8 11 -9      H,K= 5, 4    H,K= 5, 5    3 31 29      0 38 -36
L FCB FCA      3 18 16      H,K= 2, 7                 L FOB FCA    L FOB FCA    5 21 21      2 6 -3
0 35 -34       5 12 -10     L FOB FCA    H,K= 3, 6    1 4 4        0 41 38      7 12 13      4 27 25
2 25 23        7 22 21      1 53 -55     L FOB FCA    3 15 14      2 50 51                  6 12 -10
4 11 -8                    3 59 -60      1 16 16      5 23 -23     4 34 36      H,K= 6, 6
6 7 -1         H,K= 1, 9    5 56 -57     3 42 41      7 24 24      6 39 41      L FOB FCA    H,K= 7, 6
               L FCB FCA    7 38 -39     5 26 25                   8 16 13      1 53 -52     L FCB FCA
H,K= 0,11      0 19 -19                  8 9 7        H,K= 5, 5                 3 46 -46     1 76 78
L FCB FCA      2 74 -75     H,K= 2, 8                 L FOB FCA    H,K= 5, 6                 3 53 54
1 44 -42       4 39 -39     L FOB FCA    H,K= 3, 7    0 41 38      L FOB FCA                 5 71 71
3 20 -19       6 45 -43     0 87 88      L FCB FCA    2 50 51      1 53 -52
5 29 -28                    2 49 49      0 49 52      4 34 36      3 46 -46                 H,K= 7, 7
               H,K= 1,10    4 17 14      2 51 61      6 39 41                               2 8 -7
H,K= 0,12      L FCB FCA    6 81 81      4 32 33      8 16 13
L FOB FCA      1 46 46      8 18 17      6 56 57
0 60 59                                  8 18 18
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through Ce(2), there is a mirror plane containing six magnesium atoms in a girdle. Two more planes perpendicular to this same axis, containing five magnesium atoms each and related to one another by the mirror plane, complete the CP. This may be considered to be a distortion of the seventeenfold CP found about magnesium in Mg_2Zn_{11} (Samson, 1949). Here, however, the central girdle surrounding the magnesium contains only five atoms. These CP's for Ce(1) and Ce(2) are shown in Fig. 1. The central cerium atoms are omitted for the sake of perspicuity.

Since all magnesium atoms are involved in the CP's of one or the other cerium atoms, the structure is best described by a packing description of these CP's. Four of the CP's of Ce(2) form a nest which cradles the Ce(1) CP. This cluster is shown in Fig. 2(a), with the CP of Ce(1) shaded for clearness. In Fig. 2(b) four of these clusters are shown surrounding a Ce(1) polyhedron located at $(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$. The centers of these clusters are at $(0, 0, 0)$ and thus outline the unit cell (the c axis is perpendicular to the plane of the figure). The shaded area represents the region which accom-

Table 3. *Compounds of cerium and magnesium*

	a	c	M	D_x	Space group	Structure type	a/s	c/s	Reference for lattice constants
CeMg	3·912 Å		1	4·56	$Pm3m$	CsCl	$\sim\frac{1}{2}\sqrt{2}$		Iandelli (1959)
CeMg$_2$	8·733		8	3·76	$Fd3m$	MgCu$_2$	$\sim\sqrt{2/3}$		Iandelli (1959)
CeMg$_3$	7·428		4	3·45	$Fm3m$	BiF$_3$	$1/\sqrt{2}$		Iandelli (1959)
Ce$_5$Mg$_{42}$	14·78	10·43 Å	2	2·51	$I4/m$	Ce$_5$Mg$_{42}$	$\sqrt{2}$	1	This work
Ce$_2$Mg$_{17}$	10·33	10·25	2	2·42	$P6_3/mmc$	Th$_2$Ni$_{17}$	1	1	Johnson & Smith (1966)
CeMg$_{12}$(I)	10·33	5·96	2	2·25	$I4/mmm$	ThMn$_{12}$	1	$1/\sqrt{3}$	Johnson et al. (1964)
CeMg$_{12}$(II)	10·33	77·5	26	2·25	$(Immm)$	CeMg$_{12}$II	1	$13/\sqrt{3}$	Johnson et al. (1964)

(a)

(b)

(c)
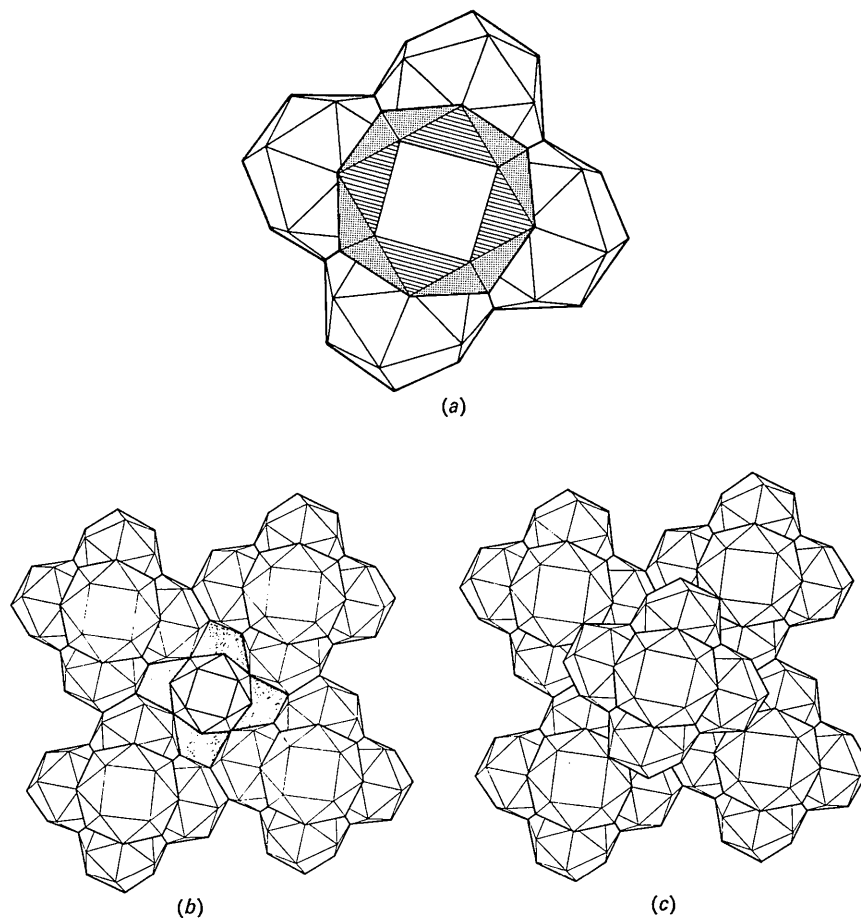
Fig. 2. (a) Cluster formed by four Ce(2) coordination polyhedra and one Ce(1) coordination polyhedron. (b) Arrangement of four clusters about a central Ce(1) coordination polyhedron. Centers of clusters outline unit cell. (c) Unit cell of Ce$_5$Mg$_{42}$ in terms of coordination polyhedra of Ce(1) and Ce(2).

modates the cluster about Ce(1) at $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$. This is shown in Fig.2(c).

The CP's for most of the magnesium atoms have been observed before. Those for Mg(4), Mg(5), and Mg(7) are icosahedra. There is one very large Mg(6)–Mg(6) distance of 3·97 Å represented in the Mg(6) CP. Including this atom, Mg(6) has thirteen neighbors in an arrangement quite similar to that found about Ni(2) in the Th₂Ni₁₇ structure (Florio et al., 1956). Mg(2) has fourteen neighbors in the same arrangement

as Ni(4) in the Th₂Ni₁₇ structure. Mg(3) has twelve neighbors in the same arrangement as Zn(3) in the Mg₂Zn₁₁ structure (Samson, 1949).

The surroundings of Mg(1) and Mg(8) appear to be novel. These CP's are best described as an envelope of atoms which surround dumbells of two Mg(1) atoms and two Mg(8) atoms. These figures are shown in Fig.3. Interatomic distances are given up to 4·5 Å in Table 4. Estimated standard deviations are 0·005 to 0·012 Å including uncertainties in lattice constants.

Table 4. *Interatomic distances in* Ce₅Mg₄₂

Kind of atom	Ligancy	Distance	Kind of atom	Ligancy	Distance	Kind of atom	Ligancy	Distance
Ce(1)	4 Mg(2)	3·739 Å	Mg(2)	2 Mg(5)	3·112 Å	Mg(6)	1 Mg(5)	2·975 Å
	8 Mg(5)	3·800		2 Mg(5)	3·225		1 Mg(5)	3·007
	8 Mg(6)	3·970		1 Mg(4)	3·243		1 Mg(3)	3·042
				2 Mg(7)	3·249		1 Mg(7)	3·130
				1 Mg(1)	3·315		1 Mg(4)	3·187
				1 Ce(2)	3·495		2 Mg(6)	3·262
Ce(2)	1 Mg(4)	3·415		2 Mg(8)	3·521		1 Mg(8)	3·462
	1 Mg(4)	3·494		2 Mg(6)	3·535		1 Ce(2)	3·505
	1 Mg(2)	3·495		1 Ce(1)	3·739		1 Ce(2)	3·530
	2 Mg(6)	3·505					1 Mg(2)	3·535
	2 Mg(6)	3·530	Mg(3)	8 Mg(6)	3·042		1 Mg(6)	3·966
	1 Mg(1)	3·666		4 Ce(2)	4·035		1 Ce(1)	3·970
	2 Mg(8)	3·667						
	2 Mg(8)	3·704	Mg(4)	2 Mg(7)	2·977	Mg(7)	2 Mg(4)	2·977
	2 Mg(7)	3·715		2 Mg(8)	3·053		2 Mg(5)	3·009
	2 Mg(5)	3·722		1 Mg(1)	3·183		2 Mg(8)	3·097
	1 Mg(3)	4·035		2 Mg(6)	3·187		2 Mg(6)	3·130
	1 Mg(1)	4·170		2 Mg(5)	3·237		2 Mg(2)	3·249
				1 Mg(2)	3·243		2 Ce(2)	3·715
				1 Ce(2)	3·415			
				1 Ce(2)	3·494	Mg(8)	1 Mg(1)	3·039
							1 Mg(4)	3·053
Mg(1)	1 Mg(1)	2·885	Mg(5)	1 Mg(6)	2·975		1 Mg(7)	3·097
	2 Mg(8)	3·039		1 Mg(6)	3·007		1 Mg(1)	3·109
	2 Mg(8)	3·109		1 Mg(7)	3·009		1 Mg(5)	3·132
	2 Mg(5)	3·111		1 Mg(5)	3·070		2 Mg(8)	3·206
	1 Mg(4)	3·183		1 Mg(1)	3·111		1 Mg(5)	3·238
	1 Mg(2)	3·315		1 Mg(2)	3·112		1 Mg(6)	3·462
	1 Ce(2)	3·666		1 Mg(8)	3·132		1 Mg(2)	3·521
	2 Mg(8)	4·165		1 Mg(2)	3·225		1 Ce(2)	3·667
	1 Ce(2)	4·170		1 Mg(4)	3·237		1 Ce(2)	3·704
	2 Mg(8)	4·449		1 Mg(8)	3·233		1 Mg(1)	4·165
				1 Ce(2)	3·722		2 Mg(1)	4·449
				1 Ce(1)	3·800			
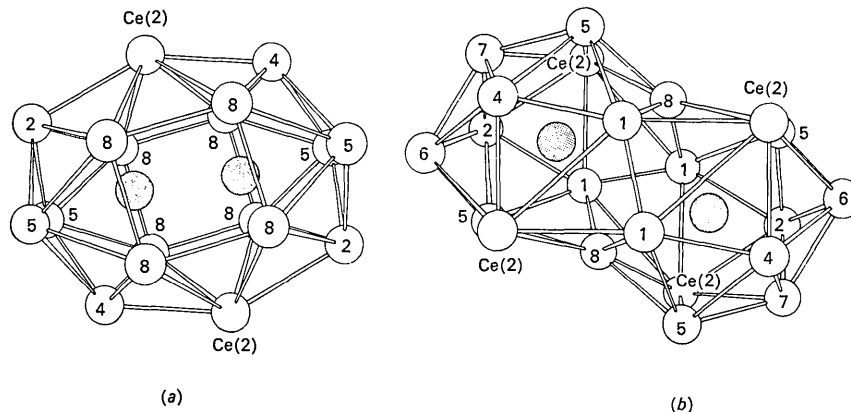
Fig.3. (a) Coordination polyhedron about two Mg(1) atoms (shaded). (b) Coordination polyhedron about two Mg(8) atoms (shaded).

The inappropriateness of the scheme of Florio *et al.* (1956) to account for this structure suggests the absence of a $CeMg_5$ compound of the $CaZn_5$-type structure. It is likely, however, that an additional compound or compounds may be discovered in this system, especially in the region $CeMg_3$–$CeMg_8$. Fig. 4 shows the densities of the observed compounds on the same plot with the end members. This plot should be useful in predicting cell volumes, and in the case of cubic compounds, cell constants. For example, if a compound Ce_5Mg_{24} with a Ti_5Re_{24}-like structure (Trzebiatowski & Niemiec, 1955) exists, its cell constant would be about 11·3 Å. Interestingly enough, there exist compounds, Er_5Mg_{24} and Dy_5Mg_{24}, with cell constants of 11·23 and 11·24 Å, respectively (Kripyakevich & Evdokimenko, 1962), so such speculation is not completely unwarranted.

Note added in proof. – The Th_2Ni_{17}-like compound referred to as Ce_2Mg_{17} in the above text has recently been shown by Johnson & Smith (1966) to have the composition $CeMg_{10.3}$.
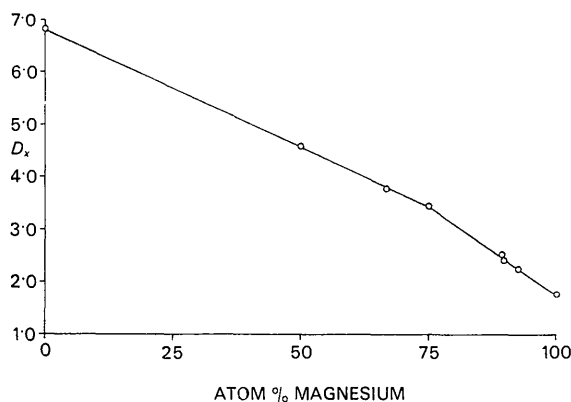
Fig. 4. Calculated densities of cerium-magnesium compounds.

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