UNCLASSIFIED

ISC-812

UNITED STATES ATOMIC ENERGY COMMISSION

# Tabulation, Bibliography, and Structure of Binary Intermetallic Compounds. II. Compounds of Beryllium, Magnesium, and Calcium

by

K. A. Gschneidner, D. J. Beerntsen, R. W. Vest,
J. A. Kingston, and J. F. Smith

December 27, 1956

Ames Laboratory
at
Iowa State College
F. H. Spedding, Director
Contract W-7405 eng-82

UNCLASSIFIED

This report is distributed according to the catagory Metallurgy and Ceramics, as listed in TID-4500, July 15, 1956.



Printed in the USA. Price 30 cents. Available from the

Office of Technical Services
U. S. Department of Commerce
Washington 25, D. C.

TABLE OF CONTENTS

This report is the second in a series. ISC-795, the first in this series, listed the compounds of lithium, sodium, potassium, and rubidium.

PART I: TABULATION OF COMPOUNDS

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS (Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $BeCu_2$ | cubic | a=2.80 (750°C) | A2 | Exists only above 575°C; disordered atomic arrangement. | 1 |
| BeCu | cubic | a=2.703 0.007 | B2 | X-ray powder data, with comparison of observed and calculated intensities; some disordering noted; after annealing at 830° for two hours completely ordered. | 2,3,11, 32 |
| BeCu | tetragonal | a=2.79 c=2.54 | | Intermediate phases during precipitation; single crystal x-ray data. | 3 |
| BeCu | monoclinic | a=2.54 b=2.54 c=3.24 $\beta$=85°25' | | " | 3 |
| $Be_3Cu$ | cubic | a=5.952 (at $CuBe_2$) to 5.899 (at $CuBe_3$) | C15 | Maximum solubility range $CuBe_2$ ⟶ $CuBe_4$ at 933°C; at room temperature ranges from $CuBe_{2.35}$ ⟶ $CuBe_4$; maximum in liquidus occurs at $CuBe_3$; structure determined at Cu:Be of 1:2.354; x-ray powder data, with comparison of observed and calculated intensities. | 2,4 |
| $Be_2Ag$ | cubic | a=6.300 | C15 | | 5,6 |
| $BeAu_3$ | | | | Determined from microscopic data and thermal analysis (6); x-ray powder data indicates these exist; no structures yet determined (7). | 6,7 |
| $BeAu_2$ | | | | " | 6,7 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Be_3Au_4$ | | | | Determined by thermal analysis and microscopic data; exists only between 550-600°C. | 6 |
| BeAu | cubic | a=4.668 ±0.001 | B20 | X-ray powder data, with comparison of calculated and observed intensities. | 8 |
| $Be_3Au$ | | | | X-ray data indicates this compound exists, but structure not yet determined. | 7 |
| $Be_5Au$ | cubic | a=6.699 ±0.007 | C15 | X-ray powder data, with comparison of calculated and observed intensities; lattice parameter also reported as 6.083 by (36). | 9,36 |
| $Be_{13}Mg$ | cubic | a=10.166 ±0.005 | $D2_3$ | X-ray powder data, with comparison of calculated and observed intensities. | 10 |
| $Be_{13}Ca$ | cubic | a=10.312 ±0.001 | $D2_3$ | " | 10,37 |
| $Be_2B$ | cubic | a=4.3 | C1 | Possibly $B_2Be_5$. | 38 |
| $Be_{13}Ce$ | cubic | a=10.375 ±0.001 | $D2_3$ | X-ray powder data, with comparison of calculated and observed intensities. | 12 |
| $Be_{13}Th$ | cubic | a=10.395 ±0.001 | $D2_3$ | " | 12 |
| $Be_{13}U$ | cubic | a=10.256 ±0.001 | $D2_3$ | X-ray powder data, with comparison of calculated and observed intensities; Be parameter verified by neutron diffraction. | 12,13 |
| $Be_{13}Pu$ | cubic | a=10.253 | $D2_3$ | | 121 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Be_{13}Np$ | cubic | a=10.266 (Be rich) a=10.256 (Np rich) | $D2_3$ | X-ray powder data with comparison of calculated and observed intensities; lattice constants accurate to ±0.001. | 14 |
| $Be_2C$ | cubic | a=4.3420 ±0.005 | C1 | X-ray powder data with comparison of calculated and observed intensities. | 15,34 |
| BeTi | | | | X-ray data indicates that the compound exists, but structure not determined. | 16 |
| $Be_2Ti$ | cubic | a=6.427 | C15 | X-ray powder data with comparison of calculated and observed intensities. | 5,16 |
| $Be_4Ti$ | | | | X-ray data indicates that the compound exists, but structure not determined. | 16 |
| $Be_{12}Ti$ | hexagonal | a=29.44 c=7.33 | $\overline{D}^1_{6h}$ -- P6/mmm | True cell dimensions; single crystal x-ray data; structure of pseudo-cell given, dimensions are a=4.23, c= 7.33; possible that actual composition is $TiBe_{13}$, but x-ray data favors $TiBe_{12}$. | 17 |
| BeZr | | | | Existence questionable. | 5,18 |
| $Be_2Zr$ | hexagonal | a=3.82 c=3.24 | C32 | X-ray powder data. | 19 |
| $Be_4Zr$ | | | | Tentative assignment from work on phase diagram; x-ray data indicates one phase at this composition. | 18 |
| $Be_7Zr$ | | | | Tentative assignment from work on phase diagram; x-ray data indicates one phase at this composition; solubility limits vary from 38-41 w/o Be. | 18 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Be_{13}Zr$ | cubic | a=10.047 ±0.001 | $D2_3$ | Single crystal x-ray data with comparison of calculated and observed intensities. | 12 |
| $Be_3N_2$ | cubic | a=8.15 ±0.01 | $D5_3$ | X-ray powder data with comparison of calculated and observed intensities. | 20 |
| $Be_3P_2$ | cubic | a=10.17 ±0.03 | $D5_3$ | " | 20 |
| $Be_2V$ | hexagonal | a=4.394 c=7.144 | C14 | " | 5 |
| $Be_{12}V$ | | a=7.251 c=4.168 | | | 33 |
| $Be_{12}Nb$ | | a=7.357 c=4.247 | | | 33 |
| ~$Be_{12}Ta$ | | | | Misch reported a high Be content compound with Ta similar to the molybdenum compound. | 5 |
| BeS | cubic | a=4.863 | B3 | X-ray powder data with comparison of calculated and observed intensities. | 21 |
| BeSe | cubic | a=5.139 ±0.004 | B3 | " | 22 |
| BeTe | cubic | a=5.626 ±0.006 | B3 | " | 23 |
| $Be_2Cr$ | hexagonal | a=4.259 ±0.001 c=6.975 ±0.001 | C14 | " | 24,35 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(A°) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Be_2Mo$ | hexagonal | a=4.433 c=7.341 | C14 | Powder and single crystal x-ray data. | 25 |
| $Be_{12}Mo$ | tetragonal | a=7.271 ±0.005 c=4.234 ±0.005 | $D_{4h}^{17}$ -- I4/mmm | Based on work of Raeuchle and Batchelder; single crystal x-ray data with comparison of calculated and observed intensities; also reported as $MoBe_{13}$ by Gordon; lattice constants of the two determinations are in agreement if unit cells are converted; chemical analysis and spatial considerations strongly support the formula $MoBe_{12}$. | 5,25,26 |
| $Be_2W$ | hexagonal | a=4.446 c=7.289 | C14 | X-ray powder data with comparison of calculated and observed intensities. | 5 |
| ~$Be_{12}W$ | | | | Misch reported a high Be content compound with W, similar to the molybdenum compound. | 5 |
| $Be_2Mn$ | hexagonal | a=4.240 c=6.923 | C14 | X-ray powder data with comparison of calculated and observed intensities. | 5 |
| $Be_{8.1}Mn$ | cubic | a=5.92 ±0.01 (89.0 a/o Be) | C15 | | 27 |
| $Be_2Re$ | hexagonal | a=4.354 c=7.101 | C14 | X-ray powder data with comparison of calculated and observed intensities. | 5 |
| $Be_2Fe$ | hexagonal | a=4.221 ±0.005 c=6.848 ±0.005 | C14 | " | 28 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Be_5Fe$ | cubic | a=5.884 | C15 | X-ray powder data with comparison of observed and calculated intensities. | 2,29 |
| $Be_{11}Fe$ | hexagonal | a=4.13 c=10.71 | | X-ray powder data. | 29 |
| BeCo | cubic | a=2.611 | B2 | X-ray powder data with comparison of calculated and observed intensities. | 5 |
| $Be_{21}Co_5$ | cubic | a=7.66 | A12 | Structure questionable since this compound has six atoms per unit cell less than required by A12 structure. | 30 |
| BeNi | cubic | a=2.621 (13.4% Be) a=2.609 (18.1% Be) | B2 | Structure worked out by (2) by x-ray powder data with calculated and observed intensities comparison; lattice for solubility limits by (31). | 2,31 |
| $Be_{21}Ni_5$ | cubic | a=7.625 | $D8_{1-3}$ | Possibly related to $\gamma$-brass structure. | 2,31 |
| $Be_2Ru$ | | | | Misch reports one phase existing at this composition, having a complex powder pattern. | 5 |
| $Be_2Rh$ | | | | " | 5 |
| $BePd_3$ | | | | Reported on basis of thermal analysis and microscopic evidence. | 6 |
| $BePd_2$ | | | | " | 6 |
| $Be_2Pd_3$ | | | | Reported on basis of thermal analysis. | 6 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Be_{10}Pd_{13}$ | | | | Reported on basis of thermal analysis. | 6 |
| $Be_{25}Pd_{27}$ | | | | " | 6 |
| BePd | cubic | a=2.819 | B2 | X-ray powder data with comparison of calculated and observed intensities. | 5 |
| $Be_5Pd$ | cubic | a=5.99 | C15 | " | 9 |
| $Be_2Os$ | | | | Shows a complex x-ray powder pattern. | 5 |
| $Be_2Ir$ | | | | " | 5 |
| $Be_{21}Pt_5$ | | | $D8_{1-3}$ | Possibly related to the $\gamma$-brass structure. | 2,5 |
| $Mg_2Li$ | | | | Only one compound in system; formula reported by different authors not in agreement ($Li_2Mg_5$, $\sim Li_{20}Mg_{80}$); evidence that structure can be derived in a continuous transition from B. C. C. with no phase transition. | 39,40,41 |
| $Mg_5Li_3$ | cubic | $\tilde{a}$=9.7 | | Structure evidently stabilized by oxide contamination, and not a binary Li-Mg compound. | 41,42,43 |
| $Mg_2Cu$ | orthorhombic | a=5.28<br>b=9.07<br>c=18.25 | $\left[D_{2h}^{24}\right.$--<br>Fddd] | Thermal analysis; x-ray powder and microscopic data. | 44 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $MgCu_2$ | cubic | a=7.04 | C15 | Rotation and Laue x-ray data. | 45 |
| $Mg_3Ag$ | | | | Previously reported as hexagonal with a=4.93 and c=7.81; complicated structure of lower symmetry. | 46,47 |
| MgAg | cubic | a=3.29 | B2 | | 46,48 |
| $MgAg_3$ | cubic | a=4.111 (disordered) a=4X4.108 (ordered) | | Powder and Weissenberg x-ray data. | 49 |
| MgAu | cubic | a=3.27 | B2 | | 50 |
| $Mg_3Au$ | hexagonal | a=4.64 c=8.46 | $DO_{18}$ | Powder and single crystal x-ray data; $Mg_2Au$ reported by (96,97) and $Mg_5Au_2$ reported by (95), both on basis of thermal analysis, are probably this compound. | 97, 51,95,96 |
| $Mg_2Ca$ | hexagonal | a=6.22 c=10.10 | C14 | Powder and single crystal x-ray data. | 53 |
| MgSr | cubic | a=3.908 | B2 | | 54 |
| $Mg_2Sr$ | hexagonal | a=6.939 c=10.494 | C14 | Debye-Scherrer x-ray powder data. | 55 |
| $Mg_9Sr$ | | | | Thermal analysis; congruently melting compound. | 57 |
| $Mg_4Sr$ | | | | Thermal analysis; incongruently melting compound. | 57 |
| $Mg_2Ba$ | hexagonal | a=6.649 c=10.676 | C14 | Debye-Scherrer x-ray powder data. | 55 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Mg_4Ba$ | | | | Thermal analysis; incongruently melting compound. | 56,57 |
| $Mg_9Ba$ | | | | Thermal analysis; congruently melting compound. | 56,57 |
| MgZn | hexagonal | a=5.33 c=8.58 | | X-ray powder data. | 58,59 |
| $MgZn_2$ | hexagonal | a=5.16 c=8.50 | C14 | Laue and rotation x-ray data. | 60 |
| $Mg_2Zn_{11}$ | cubic | a=8.552 | $\left[T_h^1\text{--}\right.$ Pm3] | Powder and Weissenberg x-ray data, Patterson and Fourier analysis. | 61 |
| $Mg_3Cd$ | hexagonal | a=6.313 c=5.074 | $DO_{19}$ | X-ray powder data. | 62 |
| MgCd | orthorhombic | a=5.0051 b=3.2217 c=5.2700 | B19 | X-ray powder data. | 63 |
| $MgCd_3$ | hexagonal | a=6.2334 c=5.0450 | $DO_{19}$ | " | 62 |
| $Mg_3Hg$ | hexagonal | a=4.87 c=8.66 | $DO_{18}$ | Powder and Weissenberg x-ray data. | 64 |
| $Mg_2Hg$ | | | | Thermal analysis, x-ray powder data. | 98 |
| $Mg_5Hg_3$ | hexagonal | a=8.26 c=5.93 | $D8_8$ | Powder and Weissenberg x-ray data. | 64 |
| MgHg | cubic | a=3.449 | B2 | | 50 |
| $MgHg_2$ | tetragonal | a=3.84 c=8.80 | $\left[D_{4h}^{17}\text{--}\right.$ I/mmm] | Powder and single crystal x-ray data. | 98 |
| $Mg_5Hg_2$ | | | | At 28 a/o Hg the phase is homogeneous; x-ray powder data, could not be indexed. | 98 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS (Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Mg_3B_2$ | | | | Questionable; article deals with the reaction of $B_2Mg_3$ with water. | 66 |
| $MgB_2$ | hexagonal | a=3.083 c=3.521 | C32 | | 67 |
| $Mg_2Al_3$ | cubic | a=28.22 | $O_h^7$ -- Fd3m | Complicated structure with 1166 atoms/cell; earlier reported as hexagonal with a=11.38 and c=17.87. | 68,70 |
| $\sim Mg_{17}Al_{12}$ | cubic | a=10.54 | A12 | | 70,71 |
| ~MgAl | | | A12 (deformed) | 45-50 a/o Mg; exists >420°C. | 69 |
| $Mg_{43-44}Al_{57-56}$ | | | | Probably peritectic; exists <410°C; phase diagram in this region somewhat uncertain. | 69 |
| $Mg_2Ga$ | hexagonal | a=7.85 c=6.94 | C22 | Incongruently melting compound. | 72,73 |
| $Mg_5Ga_2$ | orthorhombic | a=13.72 b=7.0 c=6.02 | $D_{2h}^{26}$ -- Ibam | Congruently melting compound. | 72 |
| MgGa | | | | | 72,74 |
| $MgGa_2$ | | | | | 72,74 |
| MgIn | tetragonal | a=3.24 c=4.38 | L10 | Superlattice <300°C. | 72 |
| MgIn | cubic | | A1 | Exists >300°C; evidently no phase boundary between this structure and tetragonal indium, indicating a continuous change in c/a to the limit of unity. | 80 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS (Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| ~MgIn | ortho-rhombic | | | Narrow region ~300°C between Al and L10 structures with b/a ~1. | 80 |
| ~$MgIn_2$ or 3 | cubic | a=4.60 | L12 | Superlattice. | 72 |
| ~$Mg_7In_3$ | cubic | | L12 | Superlattice <~300°C. | 80 |
| $Mg_2In$ | hexag-onal | a=8.40 c=6.96 | C22 | Structure may be more complex. | 72,80 |
| $Mg_5In_2$ | | | | Reported by (72) as isomorphous with $Mg_5Ga_2$, but possibly a more complex structure. | 72,80 |
| MgTl | cubic | a=3.628 | B2 | | 72,75 |
| $Mg_2Tl$ | hexag-onal | a=8.11 c=7.34 | C22 | | 72 |
| $Mg_5Tl_2$ | ortho-rhombic | a=15.17 b=7.30 c=6.16 | $D_{2h}^{26}$--Ibam | Isostructural with $Mg_5Ga_2$ and $Mg_5In_2$. | 72 |
| $Mg_2Th$ | cubic | a=8.570 | C15 | Weissenberg x-ray data; structure <700°C. | 76 |
| $Mg_2Th$ | hexag-onal | a=6.086 c=19.64 | C36 | Weissenberg and precession x-ray data; structure >700°C. | 76 |
| $Mg_2C_3$ | hexag-onal | a=7.43 c=10.59 | | X-ray powder data. | 52 |
| $MgC_2$ | tetrag-onal | a=5.54 c=5.02 | | X-ray powder data; possibly isomorphous with $ThC_2$ | 52 |
| $Mg_2Si$ | cubic | a=6.39 | C1 | | 99 |
| $Mg_2Ge$ | cubic | a=6.39 | C1 | X-ray powder data. | 77 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS (Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Mg_2Sn$ | cubic | a=6.76 | C1 | X-ray powder data. | 77 |
| $Mg_2Pb$ | cubic | a=6.82 | C1 | " | 77 |
| $Mg_3N_2$ | cubic | a=9.93 | $D5_3$ | " | 78 |
| $Mg_3P_2$ | cubic | a=12.01 | $D5_3$ | " | 79 |
| $Mg_3As_2$ | cubic | a=12.35 | $D5_3$ | " | 79 |
| $Mg_3Sb_2$ | hexagonal | a=4.573 c=7.229 | $D5_2$ | " | 79 |
| $Mg_3Bi_2$ | hexagonal | a=4.687 c=7.416 | $D5_2$ | " | 79 |
| MgS | cubic | a=5.1913 | B1 | | 81 |
| MgSe | cubic | a=5.45 | B1 | | 82 |
| MgTe | hexagonal | a=4.53 c=7.38 | B4 | | 83 |
| $Mg_2Co$ | | | | Thermal analysis; density, hardness, metallographic, and x-ray data. | 84 |
| $MgNi_2$ | hexagonal | a=4.81 c=7.95 | C36 | | 85 |
| $Mg_2Ni$ | hexagonal | a=5.18 c=13.19 | $[D_6^4 (D_3^5)$-- $P6_222$ $(P6_422)]$ | | 51 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Mg_2Pt$ | | | | Doubtful; crystalline product from reaction of Mg vapor in hydrogen with Pt. | 87 |
| $Mg_9La$ | | | | Thermal analysis. | 88 |
| $Mg_3La$ | cubic | a=7.49 | $DO_3$ | X-ray powder data. | 89 |
| $Mg_2La$ | cubic | a=8.79 | C15 | | 90 |
| MgLa | cubic | a=3.973 | B2 | | 54 |
| $Mg_9Ce$ | | | | Density, magnetic, and thermomagnetic data. | 88,91,92 |
| $Mg_3Ce$ | cubic | a=7.373 | $DO_3$ | X-ray powder data. | 89 |
| $Mg_2Ce$ | cubic | a=8.73 | C15 | | 90 |
| MgCe | cubic | a=3.906 | B2 | | 54 |
| $Mg_9Pr$ | | | | Thermal analysis. | 93 |
| $Mg_3Pr$ | cubic | a=7.37 | $DO_2$ | X-ray powder data. | 89 |
| MgPr | cubic | a=3.88 | B2 | | 100 |
| $MgPr_4$ | | | | (93) (1943) reported $XMg_9$, $XMg_3$, XMg, and $X_4Mg$ for La, Ce, and Pr; later work showed only $XMg_9$, $XMg_3$, $XMg_2$, XMg for La and Ce; it is possible that $PrMg_9$, $PrMg_3$, $PrMg_2$, and PrMg are also the correct compounds for Pr. | 93 |
| $Mg_9Gd$ | | | | Magnetic data; the first three compounds are probably isomorphous with the corresponding compounds of the other rare earths. | 94 |
| $Mg_3Gd$ | | | | " | 94 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| MgGd | | | | (See Remarks for $Mg_9Gd$). | 94 |
| $MgGd_9$ | | | | Magnetic data. | 94 |
| ∝Ca | cubic | a=5.57 | A1 | Stable below 460°C; x-ray powder data. | 101 |
| ⁄ßCa | cubic | a=4.48 | A2 | Stable above 460°C; x-ray powder data; a hexagonal (A3) form also reported, and is believed to stabilized by impurities. | 65,101 |
| $CaLi_2$ | hexagonal | a=6.260 ±0.008 c=10.25 ±0.02 | Cl4 | X-ray powder data. | 55 |
| $CaCu_5$ | hexagonal | a=5.092 c=4.086 | $D^1_{6h}$ -- C6/mmm | X-ray powder data; previously thought to be $CaCu_4$. | 102 |
| CaAg | cubic | a=9.07 | | X-ray powder data. | 103 |
| $CaAg_2$ | hexagonal | a=5.72 c=9.35 | Cl4 | X-ray powder data; a trace of Mg must be present. | 104 |
| $CaAg_3$ | tetragonal | a=11.3 c=9.96 | | X-ray powder data. | 103 |
| $CaAg_4$ | | | | Potential measurements. | 105 |
| $Ca_2Ag$ | | | | Thermal analysis and x-ray powder data. | 86 |
| $Ca_4Au_3$ | | | | Thermal analysis. | 106 |
| CaAu | | | | " | 106 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS (Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $CaAu_2$ | | | | Thermal analysis. | 106 |
| $CaAu_3$ | | | | " | 106 |
| $CaAu_4$ | | | | " | 106 |
| $CaZn_5$ | hexagonal | a=5.405 c=4.183 | $D_{6h}^1$ -- C6/mmm | X-ray powder data; previously thought to be $CaZn_4$. | 102 |
| $CaZn_{13}$ | cubic | a=12.13 ±0.005 | $D2_3$ | X-ray powder data; compared to $KCd_{13}$. | 107 |
| CaZn | | | | Thermal analysis. | 108 |
| $Ca_2Zn_3$ | | | | " | 108 |
| $Ca_4Zn$ | | | | " | 108 |
| CaCd | | | | " | 108 |
| $CaCd_2$ | hexagonal | a=5.99 c=9.65 | $C1_4$ | X-ray powder data. | 104 |
| $CaCd_3$ | | | | Thermal analysis. | 108 |
| $CaB_6$ | cubic | a=4.145 ±0.005 | $D2_1$ | X-ray powder data, with comparison of calculated and observed intensities. | 109 |
| $CaAl_2$ | cubic | a=8.02 | $C1_5$ | X-ray powder data. | 110 |
| $CaAl_4$ | tetragonal | a=4.35 c=11.07 | $D1_3$ | " | 111 |
| $CaGa_2$ | hexagonal | a=4.323 ±0.005 c=4.323 ±0.005 | C32 | X-ray powder data; c/a = 1.00. | 90 |
| CaTl | cubic | a=3.847 ±0.004 | B2 | X-ray powder data. | 75 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS(Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| $Ca_3Tl_4$ | | | | Thermal analysis. | 112 |
| $CaTl_3$ | cubic | a=4.794 ±0.003 | L12 | X-ray powder data. | 113 |
| $Ca_2Si$ | cubic | a=4.71 | | X-ray powder data. | 114 |
| CaSi | orthorhombic | a=3.91±0.04 b=4.59±0.05 c=10.795±0.008 | $[D_{2h}^{17}$ -- Cmmc] | Single crystal x-ray data; Laue photographs, good agreement with c alculated and observed intensities. | 115 |
| $CaSi_2$ | rhombohedral | a=10.4 $\alpha$=21°30' | C12 | Single crystal x-ray data. | 116 |
| $CaGe_2$ | rhombohedral | a=10.51 $\alpha$=21°42' | C12 | " | 117 |
| $Ca_2Sn$ | | | | Thermal analysis. | 108 |
| CaSn | | | | " | 108 |
| $CaSn_3$ | cubic | a=4.732 ±0.003 | L12 | X-ray powder data. | 113 |
| $Ca_2Pb$ | | | | Thermal analysis. | 112 |
| CaPb | | | | " | 112 |
| $CaPb_3$ | cubic | a=4.891 ±0.003 | L12 | X-ray powder data. | 113 |
| $\alpha$-$Ca_3N_2$ | cubic | a=11.40 ±0.01 | $D5_3$ | High temperature form; x-ray powder data; undergoes an irreversible transformation to $\beta$-$Ca_3N_2$ at ~700°C. | 118 |
| $\beta$-$Ca_3N_2$ | pseudohexagonal | a=3.553 c=4.11 | | Stable up to about 700°C; x-ray powder data at 300°C for lattice parameters. | 119 |

| COMPOUND | CRYSTAL CLASS | LATTICE PARAMETERS (Å) | STRUCTURE | REMARKS | REFERENCES |
|---|---|---|---|---|---|
| CaS | cubic | a=5.683 | B1 | X-ray powder data. | 120 |
| CaSe | cubic | a=5.91 | B1 | " | 120 |
| CaTe | cubic | a=6.34 | B1 | " | 120 |
| $CaNi_5$ | hexagonal | a=4.960<br>c=3.948 | $D^1_{6h}$ -- C6/mmm | " | 54 |

## PART II: REFERENCES


1. Kossolapow and Trapesnikow, Metallwirtschaft 14, 45-46 (1935).
2. Misch, L., Z. physik. Chem. B29, 42-58 (1935).
3. Geisler, Mallery, and Steigert, J. Metals 4, 307-316 (1952).
4. Losana and Venturello, Alluminio 11, 8-16 (1942).
5. Misch, L., Metallwirtschaft 15, 163-166 (1936).
6. Winkler, O., Z. Metallkunde 30, 162-173 (1938).
7. Chatterjee and Sidhu, Phys. Rev. 76, 175 (1949).
8. Cullity, B., Trans. Am. Inst. Mining Met. Engrs. 171, 396-400 (1947).
9. Misch, L., Metallwirtschaft 14, 897-899 (1935).
10. Baker and Williams, Acta Cryst. 8, 519 (1955).
11. Guinier and Jacquet, Rev. mét. 41, 1-16 (1944), and Compt. rend. 217, 22-24 (1943).
12. Baenziger and Rundle, Acta Cryst. 2, 258 (1949).
13. Koehler, Singer, and Coffinberry, Acta Cryst. 5, 394 (1952).
14. Runnalls, O., Acta Cryst. 7, 222-223 (1954).
15. Stackelberg and Quatrum, Z. physik. Chem. B27, 50-52 (1934).
16. Ehrlich, P., Z. anorg. Chem. 259, 1-41 (1949).
17. Raeuchle and Rundle, Acta Cryst. 5, 85-93 (1952) and 6, 107 (1953).
18. Hausner and Kalish, Trans. Am. Inst. Mining Met. Engrs. 188, 59 (1950).
19. Nielsen and Baenziger, Acta Cryst. 7, 132-133 (1954).
20. Stackelberg and Paulus, Z. physik. Chem. B22, 305-322 (1933).
21. Zachariasen, W., Z. physik. Chem. 119, 201-213 (1926).
22. ibid., 124, 436-448 (1926).
23. ibid., 124, 277-284 (1926).

24. Zakharova and Dalnov, Technical Physics of the USSR (Leningrad) 5, 184-188 (1938).

25. Gordon, McGurty, and Klein, J. Inst. Metals 3, 637-638 (1951) and U. S. Atomic Energy Comm. Report No. NEPA--1686 (1951).

26. Raeuchle and von Batchelder, Acta Cryst. 8, 691-694 (1955).

27. Kripyakevich and Gladyshevskii, Dopovodki Akad. Nauk Ukr. R. S. R. 1955, no. 2, 154-155 (1955), from Chem. Abstracts 50, 1561i (1956).

28. Misch, L., Naturwissenschaften 23, 287-288 (1935).

29. Teitel and Cohen, Trans. Am. Inst. Mining Met. Engrs. 185, 285-296 (1949).

30. Venturello and Burdese, Alluminio 20, 558 (1951).

31. Losana and Goria, Alluminio 11, 17-22 (1942).

32. Bowles and Tegart, Acta Met. 3, 590 (1955).

33. Kripyakevich and Gladyshevskii, Doklady Akad. Nauk. S. S. S. R. 103, 82-84 (1955), from Chem. Abstracts 50, 7538a (1956). [Note: the quoted primary reference does not correspond to the paper abstracted.]

34. Staritzky, E., Ann. Chem., Justus Liebigs 28, 915 (1956).

35. Edwards and Johnstone, J. Inst. Metals 84, 313-317 (1955-56).

36. Sidhu and Henry, J. Appl. Phys. 21, 1037 (1950).

37. Baenziger and Rundle, Acta Cryst. 2, 258 (1949).

38. Smithells, C., "Metals Reference Book" 1, 197 (1955), Interscience Publishers Inc., New York.

39. Soldau and Schamrey, Z. anorg. u. allgem. Chem. 224, 388-398 (1935).

40. Grube, von Zeppelin, and Bumm, Z. Elektrochem. 40, 160 (1934).

41. Hume-Rothery, Gaynor, and Butchers, J. Inst. Metals 71, 589-602 (1945).

42. Berry and Raynor, Nature 171, 1078-1079 (1953).

43. Herbstein and Averbach, U. S. Atomic Energy Comm. Report No. NYO--7046, 1-8 (May 31, 1954).

44. Schubert and Anderko, Z. Metallkunde 42, 321-325 (1951).

45. Friauf, J., J. Am. Chem. Soc. 49, 3107 (1927).

46. Letner and Sidhu, J. Appl. Phys. 18, 833 (1947).

47. Ageew and Kuznezow, Bull. Acad. Sci. U. S. R. R., Classe sci. math. nat., Ser.. chem., 289-309 (1937).

48. Owen and Preston, Phil. Mag. 2, 1266-1270 (1926).

49. Clarebrough and Nicholas, Australian J. Sci. Research 3A, 284-289 (1950).

50. Brauer and Haucke, Z. physik. Chem. 33, 304-310 (1936).

51. Schubert and Anderko, Z. Metallkunde 42, 321 (1951).

52. Irmann, F., Helv. Chim. Acta 31, 1584 (1948).

53. Witte, D., Naturwissenschaften 25, 795 (1937).

54. Nowotny, Hans, Z. Metallkunde 34, 247-252 (1942).

55. Hellner and Laves, Z. Krist. 105, 134-143 (1943).

56. Grube and Dietrich, Z. Elektrochem. 44, 755 (1938).

57. Klemm and Dinkelacker, Z. anorg. Chem. 255, 2 (1947).

58. Tanschisch, L., Z. Krist. 86, 423 (1933).

59. McKeehan, L., Z. Krist. 91, 501 (1935).

60. Friauf, J., Phys. Rev. 29, 34 (1937).

61. Samson, Sten, Acta Chem. Scand. 3, 835-843 (1949).

62. Edwards, Wallace, and Craig, J. Am. Chem. Soc. 74, 5256-5261 (1952).

63. Steeple, H., Acta Cryst. 5, 247-249 (1952).

64. Brauer, Nowotny, and Rudolph, Metallforschung 2, 81-84 (1947).

65. Melsert, Tiedema, Burgess, Acta Cryst. 9, 525 (1956).

66. Mikheeva and Surs, Doklady Akad. Nauk S. S. S. R. 91, 1133-1135 (1953).

67. Russell, Hirst, Kanda, and King, Acta Cryst. 6, 870 (1953).

68. Perlitz, H., Chalmers Tek. Högskol. Handl. 50, 6 (1946).

69. Eickhoff and Vosskühler, Z. Metallkunde 44, 223-231 (1953).

70. Riederer, K.,Z. Metallkunde 28, 312-317 (1936).

71. Laves, Löhberg, and Rahlfs, Nachr. Ges. Wiss. Göttingen, Math.-physik. Kl., Fachgruppen II, 1, 67-71 (1934).

72. Haucke, W., Naturwissenschaften 26, 577-578 (1938).

73. Pusin and Micic, Z. anorg. Chem. 234, 229-232 (1937).

74. Graber and Hauk, Z. Metallkunde 41, 480 (1950).

75. Zintl and Brauer, Z. physik. Chem. B20, 245-258 (1933).

76. Peterson, Diljack, and Vold, unpublished information (to be published in Acta Cryst.).

77. Brauer and Tiesler, Z. anorg. Chem. 262, 319-327 (1950).

78. Hagg, G., Z. Krist. 74, 95-99 (1930).

79. Zintl and Husemann, Z. physik. Chem. 21, 138-155 (1933).

80. Raynor, G., Trans. Faraday Soc. 44, 15 (1948).

81. Primak, Kaufman, and Ward, J. Am. Chem. Soc. 70, 2043-2046 (1948).

82. Goldschmidt, V., Geochemische Verteilungsgesetze VII, (1926).

83. Klemm and Wahl, Z. anorg. Chem. 266, 289-292 (1951).

84. Cramer, Nielsen, and Schonfield, Light Metal Age 5, 6-9 (1947).

85. Laves and Löhberg, Nachr. Ges. Wiss. Göttingen, Math.-physik Kl., KlNeue Folge 1, 59-66 (1934).

86. Hansen, M. "Aufbau der Zweistofflegierungen," p. 16 (Edwards Brothers, Inc., Ann Arbor, Michigan, 1943).

87. Hodgkinson, Waring, and Desborough, Chem. News 80, 185 (1899).

88. Vogel and Heumann, Metallforschung 2, 1-8 (1947).

89. Rossi and Iandelli, Chem. Zentr. 105, 1264-1265 (1934).

90. Laves, F., Naturwissenschaften 31, 96-145 (1943).

91. Mahn, F., Ann. phys. 3, 393- 458 (1948).

92. Mahn. F., Rev. mét. 46, 365-369 (1949).

93. Rolla, Iandelli, Canneri, and Vogel, Z. Metallkunde 35, 29 (1943).

94. Gaume-Mahn, Francoise, Compt. rend. 237, 702-704 (1953).

95. Urazov and Vogel, Z. anorg. u. allgem. Chem. 67, 442-447 (1910).

96. Vogel, R., Z. anorg. u. allgem. Chem. 63, 169-183 (1909).

97. Urazov, G., Z. anorg. u. allgem. Chem. 64, 375-396 (1909).

98. Brauer and Rudolph, Z. anorg. Chem. 248, 405-424 (1941).

99. Owen and Preston, Proc. Phys. Soc. (London) 36, 341 (1924).

100. Rossi and Iandelli, Atti R. Accad. Lincei, Roma 18, 156-161 (1933).

101. Smith, Carlson, and Vest, J. Electrochem. Soc. 103, 409 (1956).

102. Haucke, W., Z. anorg. allgem. Chem. 244, 17 (1940).

103. Degard, C., Z. Krist. 90, 399 (1935).

104. Howotny, H., Metallforschung 1, 31 (1946).

105. Kremann, Wostall, and Schopfer, Forschungsarb. Metallkunde u. Röntgenmetallog. 5, 1 (1922).

106. Weibke and Bartels, Z. anorg. u. allgem. Chem 218, 241 (1934).

107. Ketelaar, J., J. Chem. Phys. 5, 668 (1937).

108. Donski, L., Z. anorg. Chem. 57, 185 (1908).

109. Pauling and Weinbaum, Z. Krist. 87, 181 (1934).

110. Nowotny and Mohrnheim, Z. Krist. 100, 540 (1939).

111. Nowotny, Wormnes, and Mohrnheim, Z. Metallkunde 32, 39 (1940).

112. Barr, N., Z. anorg. Chem. 70, 352 (1911).

113. Zintl and Neumayr, Z. Elektrochem. 39, 86 (1933).

114. The Dow Chemical Company; X-Ray Diffraction Data Card 3-0798 (The American Society for Testing Materials, Philadelphia, 1950).

115. Hellner, E., Z. anorg. Chem. 261, 226 (1950).

116. Böhm and Hassel, Z. anorg. Chem 160, 152 (1927).

117. Wallbaum, H., Naturwissenschaften 32, 76 (1944).

118. Paulus, R., Z. physik. Chem. B22, 305 (1933).

119. Hartmann and Frohlich, Z. anorg. u. allgem. Chem. 218, 190 (1934).

120. Oftedal, I., Z. physik. Chem. 128, 154 (1927).

121. Könobeevskii, S., Conf. Acad. Sci. U. S. S. R., Div. Chem. Sci. 1955, 207-214 (1955).

## PART III: STRUCTURE DETAILS

A 1: $O_h^5$--Fm3m

A=4: Cu structure
with 4 Cu ($O_h$): $000;\frac{1}{2}0\frac{1}{2};\frac{11}{22}0;0\frac{11}{22}$

Reported compounds: MgIn, $\alpha$-Ca

Remarks: MgIn must have Mg and In atoms randomly distributed to exist in this structure.

A 2: $O_h^9$--Im3m

A=2: W structure
with 2 W ($O_h$): $000;\frac{111}{222}$

Reported compounds: $BeCu_2$, $\beta$-Ca

Remarks: $BeCu_2$ must have Be and Cu atoms randomly distributed to exist in this structure. Calcium has also been reported in the hexagonal closest packed structure. Best current evidence is that the hexagonal form is stabilized by minor impurity content.

A 12: $T_d^3$--$I\bar{4}3m$

A=58: $\alpha$-Mn structure (isomorphous with chi phase, $Fe_{36}Cr_{12}Mo_{10}$)
with 2 Mn ($T_d$): 000 + B. C.
8 Mn ($C_{3v}$): xxx;$\bar{x}\bar{x}x$; ; + B. C.: x=0.32
24 Mn ($C_s$): xxz; ↻;$\bar{x}\bar{x}z$; ↻ ;$\bar{x}xz$; ↻ ;$x\bar{x}\bar{z}$; ↻ ; + B. C.: x=0.36, z=0.04
24 Mn ($C_s$) with similar coordinates + B. C., but with x=0.09, z=0.28
[B. C. = add 000 and $\frac{111}{222}$ to all coordinates; ↻ = permutations]

Reported compounds: $Be_{21}Co_5$, ~$Mg_{17}Al_{12}$

Remarks: The structure of the compound occurring with the approximate formula ~MgAl is probably closely related to this structure.

B 1: $O_h^5$--Fm3m

A=8: NaCl structure
with 4 Na ($O_h$): 000 + F. C.
4 Cl ($O_h$): $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ + F. C.
/F. C. = add 000; $\frac{1}{2}0\frac{1}{2}$; $\frac{1}{2}\frac{1}{2}0$; and $0\frac{1}{2}\frac{1}{2}$ to all coordinates/

Reported compounds: MgS, MgSe, CaS, CaSe, CaTe.

B 2: $O_h^1$--Pm3m

A=1: ordered $\beta$-brass or CsCl structure
with Cs ($O_h$): 000
Cl ($O_h$): $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

Reported compounds: BeCu, BeCo, BeNi, BePd, MgAg, MgAu, MgSr, MgHg, MgTl, MgCe, MgPr, MgLa, CaTl.

B 3: $T_d^2$--F$\bar{4}$3m

A=8: Sphalerite structure, ZnS
with 4 Zn ($T_d$): 000 + F. C.
4 S ($T_d$): $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ + F. C.

Reported compounds: BeS, BeSe, BeTe.

B 4: $C_{6v}^4$--P6$_3$mc

A=4: Wurtzite structure, ZnS
with 2 Zn ($C_{3v}$): 1/3,2/3,0; 2/3,1/3,1/2
2 S ($C_{3v}$): 1/2,2/3,z; 2/3,1/3,($\frac{1}{2}$+z): z≈3/8

Reported compounds: MgTe.

B 19: $D_{2h}^5$--Pmcm

A=4: AuCd structure
with 2 Au ($C_{2v}$): $\pm(0y\frac{1}{4})$: y=0.805
2 Cd ($C_{2v}$): $\pm(\frac{1}{2}y\frac{1}{4})$: y=0.315

Reported compounds: MgCd with y(Mg)=0.818, y(Cd)=0.323.

B 20: $T^4$--$P2_13$

A=8: FeSi structure
with 4 Fe ($C_3$): xxx;$(\frac{1}{2}+x)(\frac{1}{2}-x)\bar{x}$; ↻ : x=0.137
4 Si ($C_3$): the same with x=0.842

Reported compounds: BeAu with x(Au)=0.150±0.005, x(Be)=0.844.

C 1: $O_h^5$--$Fm3m$

A=12: fluorite structure, $CaF_2$
with 4 Ca ($O_h$): 000 + F. C.
8 F ($T_d$): $\pm(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ + F. C.

Reported compounds: $Be_2B$, $Be_2C$, $Mg_2Si$, $Mg_2Ge$, $Mg_2Sn$, $Mg_2Pb$.

C 12: $D_{3d}^5$--$R\bar{3}m$

A=6: $CaSi_2$ structure
with 2 Ca ($C_{3v}$): ±(xxx): x=0.083
2 Si ($C_{3v}$): the same with x=0.185
2 Si ($C_{3v}$): the same with x=0.352

Reported compounds: $CaSi_2$, $CaGe_2$.

C 14: $D_{6h}^4$--$P6_3/mmc$

A=12: Laves Phase--$MgZn_2$ structure
with 4 Mg ($C_{3v}$): $\pm(1/3,2/3,z;\ 1/3,2/3,\frac{1}{2}-z)$: z≈1/16
2 Zn ($D_{3d}$): 000;$00\frac{1}{2}$
6 Zn ($C_{2v}$): $\pm(x,2x,\frac{1}{4};\ \bar{2}x,\bar{x},\frac{1}{4};\ x,\bar{x},\frac{1}{4})$: x≈5/6

Reported compounds: $FeBe_2$ with z=0.063 and x=0.833, $MnBe_2$ with z=0.053, $Be_2Mo$, $Be_2W$, $Be_2Re$, $Be_2V$, $Be_2Cr$, $Mg_2Ca$, $Mg_2Sr$, $Mg_2Ba$, $MgZn_2$, $CaLi_2$, $CaAg_2$, $CaCd_2$.

C 15: $O_h^7$--Fd3m

A=24: Laves Phase--$MgCu_2$ structure
with 8 Mg ($T_d$): $000;\frac{1}{4}\frac{1}{4}\frac{1}{4}$ + F. C.
16 Cu ($D_{3d}$): 5/8,5/8,5/8; 7/8,7/8,5/8; 7/8,5/8,7/8; 5/8,7/8,7/8 + F. C.

Reported compounds: $Be_3Cu$, $Be_2Ag$, $Be_5Au$, $Be_2Ti$, $Be_{8.1}Mn$, $Be_5Fe$, $Be_5Pd$, $MgCu_2$, $Mg_2Th$, $Mg_2La$, $Mg_2Ce$, $CaAl_2$ ($CaAl_2$ may possibly be C 14 instead).

Remarks: Those compounds which deviate from the $AB_2$ formula evidently have some atomic sites which are occupied statistically by both atomic species.

C 22: $D_3^2$--P321

A=9: $Fe_2P$ structure
with 3 Fe ($C_2$): $\bar{x}00;0\bar{x}0;xx0$: x=0.26
3 Fe ($C_2$): $x0\frac{1}{2};0x\frac{1}{2};\bar{x}x\frac{1}{2}$: x=0.40
1 P ($D_3$): $00\frac{1}{2}$
2 P ($C_3$): ±(1/3,2/3,z): z≈1/3=0.125

Reported compounds: $Mg_2Ga$, $Mg_2In$, $Mg_2Tl$.

C 32: $D_{6h}^1$--P6/mmm

A=3: $AlB_2$ structure
with 1 Al ($D_{6h}$): 000
2 B ($D_{3h}$): 1/3,2/3,1/2; 2/3,1/3,1/2

Reported compounds: $Be_2Zr$, $MgB_2$, $CaGa_2$.

C 36: $D_{6h}^4$--$P6_3/mmc$

A=Laves Phase--$MgNi_2$ structure
with 4 Mg ($C_{3v}$): ±(1/3,2/3,z); ±(2/3,1/3,½+z): z≈27/32
4 Mg ($C_{3v}$): ±(00z); ±(0,0,½+z): z≈3/32
6 Ni ($C_{2h}$): $\frac{1}{2}00;0\frac{1}{2}0;\frac{1}{2}\frac{1}{2}0;\frac{1}{2}0\frac{1}{2};0\frac{1}{2}\frac{1}{2};\frac{1}{2}\frac{1}{2}\frac{1}{2}$
6 Ni ($C_{2v}$): $\pm(x,2x,\frac{1}{4};\ 2\bar{x},\bar{x},\frac{1}{4};\ x,\bar{x},\frac{1}{4})$: x≈1/6
4 Ni ($C_{3v}$): ±(1/3,2/3,z); ±(2/3,1/3,½+z): z≈1/8

Reported compounds: $Mg_2Th$, $MgNi_2$.

D $O_2$: $T_h^5$--Im3

A=32: $CoAs_3$ structure
with 8 Co ($C_{3i}$): 1/4,1/4,1/4; 3/4,3/4,1/4; ↻ + B. C.
24 As ($C_s$): ±(xy0; ↻)±(x$\bar{y}$0; ↻) + B. C.: x=0.35, y=0.15

Reported compounds: $Mg_3Pr$.

D $O_3$: $O_h^5$--Fm3m

A=16: $BiLi_3$ structure
with 4 Bi ($O_h$): 000 + F. C.
4 Li ($O_h$): $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ + F. C.
8 Li ($T_d$): ±($\frac{1}{4}\frac{1}{4}\frac{1}{4}$) + F. C.

Reported compounds: $Mg_3La$, $Mg_3Ce$.

D $O_{18}$: $D_{6h}^4$--$P6_3/mmc$

A=8: $Na_3As$ structure
with 2 As ($D_{3h}$): ±(1/3,2/3,1/4)
2 Na ($D_{3h}$): ±(00$\frac{1}{4}$)
4 Na ($C_{3v}$): ±(1/3,2/3,z; 2/3,1/3,$\frac{1}{2}$+z): z=0.583

Reported compounds: $Mg_3Au$, $Mg_3Hg$.

D $O_{19}$: $D_{6h}^4$--$P6_3/mmc$

A=8: $Mg_3Cd$ structure
with 2 Cd ($D_{3h}$): ±(1/3,2/3,1/4)
6 Mg ($C_{2v}$): ±(2x,x,$\frac{1}{4}$; $\bar{x}$,x,$\frac{1}{4}$; $\bar{x}$,2x,$\frac{1}{4}$): x≈1/6

Reported compounds: $Mg_3Cd$, $MgCd_3$.

D $l_3$: $D_{4h}^{17}$--I4/mmm

A=10: $BaAl_4$ structure
with 2 Ba ($D_{4h}$): 000 + B. C.
4 Al ($C_{4v}$): ±(00z) + B. C.: z=0.380
4 Al ($D_{2d}$): 0$\frac{1}{2}\frac{1}{4}$;$\frac{1}{2}$0$\frac{1}{4}$ + B. C.

Reported compounds: $CaAl_4$.

D $2_1$: $O_h^1$--Pm3m

A=7: $CaB_6$ structure
with 1 Ca ($O_h$): 000
6 B ($C_{4v}$): $\pm(\frac{1}{2}\frac{1}{2}x;$ ↻ ): x=0.293±0.001

Reported compounds: $CaB_6$.

D $2_3$: $O_h^6$--Fm3c

A=112: $NaZn_{13}$ structure
with 8 Na (O): $\pm(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ + F. C.
8 Zn ($T_h$): $000;\frac{1}{2}\frac{1}{2}\frac{1}{2}$ + F. C.
96 Zn ($C_s$): $\pm(0yz;$ ↻ $;\frac{1}{2}zy;$ ↻ $;0y\bar{z};$ ↻ $;\frac{1}{2}\bar{z}y;$ ↻ ) + F. C.

Reported compounds: $CeBe_{13}$, $ThBe_{13}$, $UBe_{13}$, $ZrBe_{13}$, $Be_{13}Mg$, $Be_{13}Ca$, $Be_{13}Pu$, $Be_{13}Np$, $CaZn_{13}$

Remarks: For the first four compounds listed, y=0.178, z=0.112. For the remaining compounds the adjustable parameters are reported to be the same as those for $NaZn_{13}$.

D $5_2$: $D_{3d}^3$--P$\bar{3}$m1

A=5: $La_2O_3$ structure
with 2 La ($C_{3v}$): $1/3,2/3,z;\ 2/3,1/3,\bar{z}$: z≈0.63
1 O ($D_{3d}$): 000
2 O ($C_{3v}$): $1/3,2/3,z;\ 2/3,1/3,\bar{z}$: z≈0.63

Reported compounds: $Mg_3Bi_2$, $Mg_3Sb_2$.

D $5_3$: $T_h^7$--Ia3

A=80: $Mn_2O_3$ structure
with 8 Mn ($C_{3i}$): $1/4,1/4,1/4;\ 1/4,3/4,3/4;$ ↻ + B. C.
24 Mn ($C_2$): $\pm(x,0,1/4;$ ↻ $);\ \pm(x,1/2,3/4;$ ↻ ): x=0.970 + B. C.
48 O ($C_1$): $\pm(xyz;$ ↻ $);\ \pm(x,\bar{y},\frac{1}{2}-z;$ ↻ $);\ \pm(\frac{1}{2}+x,\bar{y},z;$ ↻ $);$ $\pm(x,\frac{1}{2}+y,\bar{z};$ ↻ ): x=0.39, y=0.15, z=0.38: + B. C.

Reported compounds: $Be_3N_2$ with $x_1$=0.985, $x_2$=0.385, y=0.145, and z=0.380; $Be_3P_2$ with $x_1$=0.997, $x_2$=0.385, y=0.145, and z=0.380; $Mg_3N_2$, $Mg_3P_2$, $Mg_3As_2$, $\alpha$-$Ca_3N_2$.

D $8_{1-3}$: $O_h^9$--Im3m; $T_d^3$--I$\bar{4}$3m; and $T_d^1$--P$\bar{4}$3m

A=52: $\gamma$-brass structures. The basic structure consists of a cubic unit cell whose edge is three times the edge of a simple body-centered cubic cell. From this large cell of 54 atomic sites is abstracted 2 atomic sites with small attendant shifts in parameters of some of the 52 occupied sites. The space group depends upon the formula of the compound and the atomic species occupying the various atomic sites.

Reported compounds: $Ni_5Be_{21}$, $Pt_5Be_{21}$

Remarks: $\gamma$-brass structures usually exhibit extensive composition variation.

D $8_8$: $D_{6h}^3$--$P6_3/mcm$

A=16: $Mn_5Si_3$ structure
with 4 Mn ($D_3$): 1/3,2/3,0; 2/3,1/3,0; 1/3,2/3,1/2; 2/3,1/3,1/2
6 Mn ($C_{2v}$): $\pm(x0\frac{1}{4};0x\frac{1}{4};\bar{x}\bar{x}\frac{1}{4})$: x=0.23
6 Si ($C_{2v}$): the same with x=0.60

Reported compounds: $Mg_5Hg_3$ with x(Mg)=0.25, x(Hg)=0.615.

L 10: $D_{4h}^1$--C4/mmm

A=4: CuAu structure
with 2 Cu ($D_{4h}$): 000 + B. C.
2 Au ($D_{4h}$): $\frac{1}{2}0\frac{1}{2}$ + B. C.

Reported compounds: MgIn

L 12: $O_h^1$--Pm3m

A=4: $Cu_3Au$ structure
with 1 Au ($O_h$): 000
3 Cu ($D_{4h}$): $\frac{1}{2}0\frac{1}{2}$; $0\frac{1}{2}\frac{1}{2}$; $\frac{1}{2}\frac{1}{2}0$

Reported compounds: $\sim MgIn_{2\text{ or }3}$, $\sim Mg_7In_3$, $CaTl_3$, $CaSn_3$, $CaPb_3$.

--- $D_{6h}^{1}$--P6/mmm

A=13: $TiBe_{12}$ structure--pseudocell
with 1 Ti ($D_{6h}$): in 000 or in $00\frac{1}{2}$
2 Be ($C_{6v}$): 00z;00z: z=0.28 when Ti is at 000, z=0.22 when Ti is at $00\frac{1}{2}$
6 Be ($C_{2v}$): $\pm(\frac{1}{2}0z)$; $\pm(0\frac{1}{2}z)$; $\pm(\frac{11}{22}z)$: z=0.25
2 Be ($D_{3d}$): 1/3,2/3,0; 2/3,1/2,0
2 Be ($D_{3d}$): 1/3,2/3,1/2; 2/3,1/3,1/2

Reported compounds: $Be_{12}Ti$.

--- $D_{4h}^{17}$--I4/mmm

A=26: $ThMn_{12}$ structure
with 2 Th ($D_{4h}$): 000 + B. C.
8 Mn ($C_{2h}$): 1/4,1/4,1/4; 3/4,3/4,1/4; $\frac{1}{2}$ + B. C.
8 Mn ($C_{2h}$): $\pm(x00)$; $\pm(0x0)$: $x_1$=0.361: + B. C.
8 Mn ($C_{2v}$): $\pm(x\frac{1}{2}0)$; $\pm(\frac{1}{2}x0)$: $x_2$=0.277: + B. C.

Reported compounds: $Be_{12}Mo$ with $x_1$=0.344 and $x_2$=0.284.

--- $D_{4h}^{17}$--I/mmm

A=6: $MgHg_2$ structure
with 2 Mg: $000;\frac{1}{2}\frac{1}{2}\frac{1}{2}$
4 Hg: 00z; $\frac{11}{22}(\frac{1}{2}+z)$; $00\bar{z}$; $\frac{11}{22}(\frac{1}{2}-z)$: $z=\frac{1}{2}$

Remarks: isomorphous with $MoSi_2$.

--- $D_6^4$ ($D_6^5$)--$P6_222$ ($P6_422$)

A=18: $Mg_2Ni$ structure
with 3 Ni ($D_2$): 0,0,1/6; 0,0,3/6; 0,0,5/6
3 Ni ($D_2$): 0,1/2,1/6; 1/2,0,3/6; 1/2,1/2,5/6
6 Mg ($C_2$): $\pm(1/2,0,z)$; 1/2,1/2,(1/3+z); 1/2,1/2,(1/3-z); $\bar{0}$,1/2,(2/3+z); 0,1/2,(2/3-z): z=1/9
6 Mg ($C_2$): $\pm(x,2x,0)$; $x,\bar{x},1/3$; $\bar{x},x,1/3$; 2x,x,2/3; 2x,x,2/3: x=1/6

Reported compounds: $Mg_2Ni$.

--- $D_{2h}^{24}$--Fddd

A=48: $Mg_2Cu$ structure
with 16 Cu ($C_2$): $+(00z); \frac{11}{44}(\frac{1}{4}+z); \frac{11}{44}(\frac{1}{4}-z)$: z=0.128: + F. C.
16 Mg ($C_2$): $\bar{+}$the same with z=0.411: + F. C.
16 Mg ($C_2$): $\pm(0y0); \frac{1}{4}(\frac{1}{4}+y)\frac{1}{4}; \frac{1}{4}(\frac{1}{4}-y)\frac{1}{4}$: y=0.161: + F. C.

Reported compounds: $Mg_2Cu$.

--- $T_h^1$--$Pm_3$

A=39: $Mg_2Zn_{11}$ structure
with 6 Mg ($C_{2v}$): $\pm(x0\frac{1}{2}; 2)$: x=0.32
6 Zn ($C_{2v}$): $\pm(x00; 2)$: x=0.235
12 Zn ($C_s^2$): $\pm(\frac{1}{2}yz; 2); \pm(\frac{1}{2}y\bar{z}; 2)$: y=0.234, z=0.343
1 Zn ($T_h$): $\frac{111}{222}$
6 Zn ($C_{2v}$): $\pm(x\frac{1}{2}0; 2)$: x=0.160
8 Zn ($C_3^2$): $\pm(xxx; x\bar{x}\bar{x}; 2)$: x=0.222

Reported compounds: $Mg_2Zn_{11}$.

--- $D_{2h}^{26}$--Ibam

A=28: $Mg_5Ga_2$ structure
with 8 Ga ($C_s$): $\pm(xy0); \pm(x\bar{y}\frac{1}{2})$: x=0.122, y=0.262: + B. C.
8 Mg ($C_s$): the same with x=0.080, y=0.660: + B. C.
8 Mg ($C_2$): $+(x0\frac{1}{4}); \pm(\bar{x}0\frac{1}{4})$: x=0.242: + B. C.
4 Mg ($D_2$): $\bar{+}(00\frac{1}{4})$ + B. C.

Reported compounds: $Mg_5Ga_2$, $Mg_5Tl_2$.

--- $D_{2h}^{17}$--Cmmc

A=8: CaSi structure
with 4 Ca ($C_{2v}$): $\pm(\frac{1}{4}0z)$: z=0.36: + B. C.
4 Si ($C_{2v}$): the same with z=0.07: + B. C.

Reported compounds: CaSi.

--- $D_{6h}^1$--C6/mmm

A=6: $CaCu_5$ structure
with 1 Ca ($D_{6h}$): 000
2 Cu ($D_{3h}$): 1/3,2/3,0; 2/3,1/3,0
3 Cu ($D_{2h}$): $\frac{1}{2}0\frac{1}{2}; 0\frac{11}{22}; \frac{111}{222}$

Reported compounds: $CaCu_5$, $CaZn_5$, $CaNi_5$.