inorganic compounds

The Heusler-type alloy MgZn$_2$Ce

Volodymyr Pavlyuk,[a,b] Pavlo Solokha,[a]* Grygorij Dmytriv,[a] Bernard Marciniak[b] and Valerie Paul-Boncour[c]

[a]Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla i Mefodiya Street 6, 79005 Lviv, Ukraine, [b]Institute of Chemistry and Environment Protection, Jan Dlugosz University, al. Armii Krajowej 13/15, 42-200 Czestochowa, Poland, and [c]Laboratoire de Chimie Métallurgique des Terres Rares, Sciences Chimiques, Centre National de la Recherche Scientifique, rue Henri Dunant 2-8, 94320 Thiais, France
Correspondence e-mail: solokha_pavlo@yahoo.com

Single crystals of the MgZn$_2$Ce alloy (magnesium dizinc cerium) were synthesized by a two-step method which couples the thermal treatment of pressed pellets of the pure elements with subsequent arc melting. The compound crystallizes in a Heusler-type (MnCu$_2$Al) structure in the space group $Fm\overline{3}m$, with one Zn site (site symmetry $\overline{4}3m$), one Ce and one Mg site (both with $m\overline{3}m$ site symmetry). All interatomic distances indicate metallic type bonding.

Related literature

Other ternary alloys in the system RE–T–Mg (RE = rare earth metal and T = transition metal) and their properties have been studied by: Kadir *et al.* (1997); Solokha *et al.* (2006, 2007); Aono *et al.* (2000); Guénée *et al.* (2003); Lukachuk & Pöttgen (2003); Renaudin *et al.* (2003); De Negri *et al.*, (2005, 2007). Tests for centrosymmetric or non-centrosymmetric space groups were performed using the *WinGX* program (Farrugia, 1999), following the advice of Marsh (1995). Atomic radii for the elements were taken from Emsley (1991) and the atomic coordinates were standardized using the *STRUCTURE-TIDY* program (Gelato & Parthé, 1987).

Experimental

Crystal data

MgZn$_2$Ce	$Z = 4$
$M_r = 295.17$	Mo $K\alpha$ radiation
Cubic, $Fm\overline{3}m$	$\mu = 26.40$ mm^{-1}
$a = 7.0358$ (4) Å	$T = 295$ (2) K
$V = 348.29$ (3) Å^3	$0.10 \times 0.08 \times 0.06$ mm

Data collection

Oxford Diffraction Xcalibur CCD diffractometer	764 measured reflections
	55 independent reflections
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2005)	55 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.053$
$T_{min} = 0.11$, $T_{max} = 0.198$	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.016$	5 parameters
$wR(F^2) = 0.045$	$\Delta\rho_{max} = 0.95$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -1.32$ e Å^{-3}
55 reflections	

Table 1
Selected bond lengths (Å).

Ce—Zn	3.04659 (17)	Zn—Mg	3.04659 (17)
Ce—Mg^i	3.5179 (2)		

Symmetry code: (i) $x - 1, y - \frac{1}{2}, z - \frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2125).

References

Aono, K., Orimo, S. & Fujii, H. (2000). *J. Alloys Compd.* **309**, L1–L4.
Brandenburg, K. (1999). *DIAMOND*. Release 2.1c. Crystal Impact GbR, Bonn, Germany.
De Negri, S., Giovannini, M. & Saccone, A. (2005). *J. Alloys Compd.* **397**, 126–134.
De Negri, S., Giovannini, M. & Saccone, A. (2007). *J. Alloys Compd.* **427**, 134–141.
Emsley, J. (1991). *The Elements*, 2nd ed. Oxford: Clarendon Press.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.
Guénée, L., Favre-Nicolin, V. & Yvon, K. (2003). *J. Alloys Compd.* **348**, 129–137.
Kadir, K., Sakai, T. & Uehara, I. (1997). *J. Alloys Compd.* **257**, 115–121.
Lukachuk, M. & Pöttgen, R. (2003). *Z. Kristallogr.* **218**, 767–787.
Marsh, R. E. (1995). *Acta Cryst.* B**51**, 897–907.
Oxford Diffraction (2004). *CrysAlis CCD*. Version 1.170. Oxford Diffraction Ltd., Abingdon, Oxfordshire, England.
Oxford Diffraction (2005). *CrysAlis RED*. Version 1.171. Oxford Diffraction Ltd., Abingdon, Oxfordshire, England.
Renaudin, G., Guénée, L. & Yvon, K. (2003). *J. Alloys Compd.* **350**, 145–150.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Solokha, P., De Negri, S., Saccone, A., Pavlyuk, V., Marciniak, B. & Tedenac, J.-C. (2007). *Acta Cryst.* C**63**, i13–i16.
Solokha, P., Pavlyuk, V., Saccone, A., De Negri, S., Prochwicz, W., Marciniak, B. & Różycka-Sokołowska, E. (2006). *J. Solid State Chem.* **179**, 3073–3081.

supplementary materials

The Heusler-type alloy MgZn$_2$Ce

V. Pavlyuk, P. Solokha, G. Dmytriv, B. Marciniak and V. Paul-Boncour

Comment

Rare-earth transition metal intermetallics are intensively studied due to their useful physical properties. Mg-containing alloys tend to be particularly effective because of their high hydrogen uptake capacity at low density and cost. Among RE–T–Mg alloys (RE = rare earth, T = 3d transition metal), the most studied are Ni-containing alloys. Ternary phases with a 1:9:2 stoichiometry were studied by Kadir *et al.* (1997) and Solokha *et al.* (2006). Hydrogen uptake capacities of RENi$_4$Mg (RE = Y, La, Nd) compounds with the MgCu$_4$Sn structure type were determined by Aono *et al.* (2000) and Guénée *et al.* (2003). The crystal structure, chemical bonding and physical properties of RE$_2${Cu,Ni,Pd}$_2$Mg ternaries with the Mo$_2$FeB$_2$ structure type were investigated by Lukachuk & Pöttgen (2003). It was shown that the Heusler-type alloy LaNi$_2$Mg adsorbs H$_2$ under formation of the quaternary metal hydride LaMg$_2$NiH$_7$ (Renaudin *et al.*, 2003). Detailed investigations of fundamental properties of La–Ni–Mg (De Negri *et al.*, 2005) and La–Cu–Mg (De Negri *et al.*, 2006) phases at 673 K have indicated a great number of novel ternary phases in these systems. Recently, Solokha *et al.* (2007) studied the crystal structure of the novel phase Tb$_2$Ni$_2$Mg$_3$ which does not form with the ligher rare earth metals.

The accurate determination of the crystal structure of new intermetallics is the basic requirement for a more detailed understanding of their properties. Here, we report the crystal structure of the ternary compound MgZn$_2$Ce (I) based on single-crystal X-ray diffraction data.

The title compound (I) belongs to the Heusler-type alloys (MnCu$_2$Al structure), with the Al site [Wyckoff position 4a] now occupied by Ce atoms, and the Mn [4b] and Cu [8c] atoms replaced by Mg and Zn atoms, respectively. The unit cell projection of (I) is shown in Fig. 1. The first coordination spheres of all atoms are the same as for the cubic close packed (c.c.p.) structures, *viz.* a rhombododecahedron with a coordination number of 14. The interatomic distances are in good correlation with the sums of the atomic radii (Emsley, 1991) and indicate a typical metallic type bonding, with the shortest Ce–Zn distance of 3.04659 (17) Å which is 96.2% of the sum of the atomic radii.

Experimental

With the purpose to avoid losses of magnesium and zinc due to their low vapour pressure at higher temperatures, the alloys were prepared in two steps. In a first step the powders of the pure elements (stoichiometry Mg:Zn:Ce = 1:2:1) were pressed into a pellet and enclosed in evacuated silica ampoules (pressure inside 10^{-5} to 10^{-6} Pa), which were then placed in a resistance furnace with a thermocouple controller. The heating process was carried out in consecutive order. Firstly, the ampoule was heated at 673 K for four d, then the temperature was increased to 873 K and held for two d. The ampoules were then heated up to 1073 K (held for four h and slowly cooled down to room temperature). In a second step, the pellets were remelted in an arc furnace. The samples were stable against air and moisture, irrespective whether they were in the form of compact pellets or as fine-grained powders. Wavelength dispersive spectrometry and electron probe microanalysis (CAMECA SX100 analyser) were used to control the number of phases and their content in the samples. An average result of the microprobe analysis for the title compound is 25.6%$_{at}$ Ce, 25.8%$_{at}$ Zn and 48.6%$_{at}$ Mg which compares well with

the composition obtained from the structure refinement. Irregularly shaped single crystals, exhibiting metallic luster, were isolated by mechanical fragmentation from the alloys.

Refinement

Systematic absences indicated possible space groups $F23$ (#196), $Fm\overline{3}$ (#202), $F432$ (#209), $F\overline{4}3m$ (#216), and centrosymmetric $Fm\overline{3}m$ (#225). The statistical test of the distribution of the E values (Farrugia, 1999) suggested that the structure is centrosymmetric with a probability of 55.1%. However, following the advice of Marsh (1995) the structure solution and refinement were also performed in non-centrosymmetric space groups. The results clearly indicated that compound (I) crystallizes in the centrosymmetric space group $Fm\overline{3}m$. The s.o.f. parameters were refined for this structure in order to check the deviations from the ideal stoichiometry, but no significant deviations were found. Therefore in the final refinement cycles the full occupancy parameters were retained and all atoms were refined with anisotropic displacement parameters. Finally, the atomic coordinates were standardized using the *STRUCTURE-TIDY* program (Gelato & Parthé, 1987). The final difference Fourier syntheses revealed no significant residual peaks - the highest maximum electron density is 0.95 Å from Ce and the deepest hole is 1.32 Å from Zn.

Figures
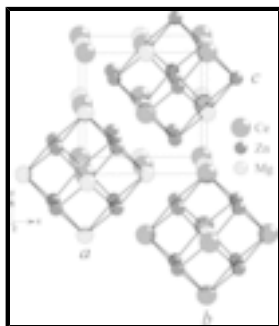
Fig. 1. Perspective view of the unit-cell projection of (I) on the (001) plane. Coordination polyhedra of Ce (*a*), Zn (*b*) and Mg (*c*) are shown.

Magnesium dizinc cerium

Crystal data

$MgZn_2Ce$	$Z = 4$
$M_r = 295.17$	$F_{000} = 520$
Cubic, $Fm\overline{3}m$	$D_x = 5.629$ Mg m^{-3}
Hall symbol: -F 4 2 3	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.0358$ (4) Å	Cell parameters from 764 reflections
$b = 7.0358$ (4) Å	$\theta = 5.0–33.0°$
$c = 7.0358$ (4) Å	$\mu = 26.40$ mm^{-1}
$\alpha = 90°$	$T = 295$ (2) K
$\beta = 90°$	Irregular, metallic dark-grey
$\gamma = 90°$	$0.10 \times 0.08 \times 0.06$ mm
$V = 348.29$ (3) Å^3	

Data collection

Oxford Diffraction Xcalibur CCD diffractometer	55 independent reflections
Radiation source: fine-focus sealed tube	55 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.053$
$T = 295(2)$ K	$\theta_{max} = 33.0º$
ω scans	$\theta_{min} = 5.0º$
Absorption correction: analytical (CrysAlis RED; Oxford Diffraction, 2005)	$h = -10 \rightarrow 7$
$T_{min} = 0.11$, $T_{max} = 0.198$	$k = -10 \rightarrow 10$
764 measured reflections	$l = -9 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0117P)^2 + 19.6603P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.016$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.045$	$\Delta\rho_{max} = 0.95$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -1.32$ e Å^{-3}
55 reflections	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
5 parameters	Extinction coefficient: 0.0038 (5)
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
Ce	0.0000	0.0000	0.0000	0.0098 (4)
Zn	0.2500	0.2500	0.2500	0.0153 (4)
Mg	0.5000	0.5000	0.5000	0.0112 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ce	0.0098 (4)	0.0098 (4)	0.0098 (4)	0.000	0.000	0.000
Zn	0.0153 (4)	0.0153 (4)	0.0153 (4)	0.000	0.000	0.000
Mg	0.0112 (11)	0.0112 (11)	0.0112 (11)	0.000	0.000	0.000

Geometric parameters (Å, °)

Ce—Zn^i	3.04659 (17)	Zn—Ce^{xi}	3.04659 (17)
Ce—Zn	3.04659 (17)	Zn—Ce^{xii}	3.04659 (17)
Ce—Zn^{ii}	3.04659 (17)	Zn—Mg^v	3.04659 (17)
Ce—Zn^{iii}	3.04659 (17)	Zn—Mg^{iii}	3.04659 (17)
Ce—Zn^{iv}	3.04659 (17)	Mg—Zn^{xiii}	3.04659 (17)
Ce—Zn^v	3.04659 (17)	Mg—Zn^{xiv}	3.04659 (17)
Ce—Zn^{vi}	3.04659 (17)	Mg—Zn^{xv}	3.04659 (17)
Ce—Zn^{vii}	3.04659 (17)	Mg—Zn^{xvi}	3.04659 (17)
Ce—Mg^{iv}	3.5179 (2)	Mg—Zn^{xii}	3.04659 (17)
Ce—Mg^{viii}	3.5179 (2)	Mg—Zn^{xi}	3.04659 (17)
Ce—Mg^v	3.5179 (2)	Mg—Zn^x	3.04659 (17)
Ce—Mg^{ix}	3.5179 (2)	Mg—Ce^{xvii}	3.5179 (2)
Zn—Mg	3.04659 (17)	Mg—Ce^{xviii}	3.5179 (2)
Zn—Mg^{iv}	3.04659 (17)	Mg—Ce^{xii}	3.5179 (2)
Zn—Ce^x	3.04659 (17)	Mg—Ce^x	3.5179 (2)
Zn^i—Ce—Zn	180.0	Ce^{xi}—Zn—Ce^{xii}	109.5
Zn^i—Ce—Zn^{ii}	109.5	Mg—Zn—Mg^v	109.5
Zn—Ce—Zn^{ii}	70.5	Ce—Zn—Mg^v	70.5
Zn^i—Ce—Zn^{iii}	70.5	Mg^{iv}—Zn—Mg^v	109.5
Zn—Ce—Zn^{iii}	109.5	Ce^x—Zn—Mg^v	180.0
Zn^{ii}—Ce—Zn^{iii}	70.5	Ce^{xi}—Zn—Mg^v	70.5
Zn^i—Ce—Zn^{iv}	70.5	Ce^{xii}—Zn—Mg^v	70.5
Zn—Ce—Zn^{iv}	109.5	Mg—Zn—Mg^{iii}	109.5
Zn^{ii}—Ce—Zn^{iv}	180.0	Ce—Zn—Mg^{iii}	70.5
Zn^{iii}—Ce—Zn^{iv}	109.5	Mg^{iv}—Zn—Mg^{iii}	109.5
Zn^i—Ce—Zn^v	70.5	Ce^x—Zn—Mg^{iii}	70.5
Zn—Ce—Zn^v	109.5	Ce^{xi}—Zn—Mg^{iii}	180.0
Zn^{ii}—Ce—Zn^v	70.5	Ce^{xii}—Zn—Mg^{iii}	70.5
Zn^{iii}—Ce—Zn^v	109.5	Mg^v—Zn—Mg^{iii}	109.5
Zn^{iv}—Ce—Zn^v	109.5	Zn^{xiii}—Mg—Zn	180.0
Zn^i—Ce—Zn^{vi}	109.5	Zn^{xiii}—Mg—Zn^{xiv}	109.5
Zn—Ce—Zn^{vi}	70.5	Zn—Mg—Zn^{xiv}	70.5

Zn^{ii}—Ce—Zn^{vi}	109.5	Zn^{xiii}—Mg—Zn^{xv}	109.5
Zn^{iii}—Ce—Zn^{vi}	70.5	Zn—Mg—Zn^{xv}	70.5
Zn^{iv}—Ce—Zn^{vi}	70.5	Zn^{xiv}—Mg—Zn^{xv}	109.5
Zn^{v}—Ce—Zn^{vi}	180.0	Zn^{xiii}—Mg—Zn^{xvi}	109.5
Zn^{i}—Ce—Zn^{vii}	109.5	Zn—Mg—Zn^{xvi}	70.5
Zn—Ce—Zn^{vii}	70.5	Zn^{xiv}—Mg—Zn^{xvi}	109.5
Zn^{ii}—Ce—Zn^{vii}	109.5	Zn^{xv}—Mg—Zn^{xvi}	109.5
Zn^{iii}—Ce—Zn^{vii}	180.0	Zn^{xiii}—Mg—Zn^{xii}	70.5
Zn^{iv}—Ce—Zn^{vii}	70.5	Zn—Mg—Zn^{xii}	109.5
Zn^{v}—Ce—Zn^{vii}	70.5	Zn^{xiv}—Mg—Zn^{xii}	180.0
Zn^{vi}—Ce—Zn^{vii}	109.5	Zn^{xv}—Mg—Zn^{xii}	70.5
Zn^{i}—Ce—Mg^{iv}	125.3	Zn^{xvi}—Mg—Zn^{xii}	70.5
Zn—Ce—Mg^{iv}	54.7	Zn^{xiii}—Mg—Zn^{xi}	70.5
Zn^{ii}—Ce—Mg^{iv}	125.3	Zn—Mg—Zn^{xi}	109.5
Zn^{iii}—Ce—Mg^{iv}	125.3	Zn^{xiv}—Mg—Zn^{xi}	70.5
Zn^{iv}—Ce—Mg^{iv}	54.7	Zn^{xv}—Mg—Zn^{xi}	180.0
Zn^{v}—Ce—Mg^{iv}	125.3	Zn^{xvi}—Mg—Zn^{xi}	70.5
Zn^{vi}—Ce—Mg^{iv}	54.7	Zn^{xii}—Mg—Zn^{xi}	109.5
Zn^{vii}—Ce—Mg^{iv}	54.7	Zn^{xiii}—Mg—Zn^{x}	70.5
Zn^{i}—Ce—Mg^{viii}	54.7	Zn—Mg—Zn^{x}	109.5
Zn—Ce—Mg^{viii}	125.3	Zn^{xiv}—Mg—Zn^{x}	70.5
Zn^{ii}—Ce—Mg^{viii}	125.3	Zn^{xv}—Mg—Zn^{x}	70.5
Zn^{iii}—Ce—Mg^{viii}	54.7	Zn^{xvi}—Mg—Zn^{x}	180.0
Zn^{iv}—Ce—Mg^{viii}	54.7	Zn^{xii}—Mg—Zn^{x}	109.5
Zn^{v}—Ce—Mg^{viii}	125.3	Zn^{xi}—Mg—Zn^{x}	109.5
Zn^{vi}—Ce—Mg^{viii}	54.7	Zn^{xiii}—Mg—Ce^{xvii}	54.7
Zn^{vii}—Ce—Mg^{viii}	125.3	Zn—Mg—Ce^{xvii}	125.3
Mg^{iv}—Ce—Mg^{viii}	90.0	Zn^{xiv}—Mg—Ce^{xvii}	125.3
Zn^{i}—Ce—Mg^{v}	125.3	Zn^{xv}—Mg—Ce^{xvii}	125.3
Zn—Ce—Mg^{v}	54.7	Zn^{xvi}—Mg—Ce^{xvii}	54.7
Zn^{ii}—Ce—Mg^{v}	54.7	Zn^{xii}—Mg—Ce^{xvii}	54.7
Zn^{iii}—Ce—Mg^{v}	125.3	Zn^{xi}—Mg—Ce^{xvii}	54.7
Zn^{iv}—Ce—Mg^{v}	125.3	Zn^{x}—Mg—Ce^{xvii}	125.3
Zn^{v}—Ce—Mg^{v}	54.7	Zn^{xiii}—Mg—Ce^{xviii}	54.7
Zn^{vi}—Ce—Mg^{v}	125.3	Zn—Mg—Ce^{xviii}	125.3
Zn^{vii}—Ce—Mg^{v}	54.7	Zn^{xiv}—Mg—Ce^{xviii}	54.7
Mg^{iv}—Ce—Mg^{v}	90.0	Zn^{xv}—Mg—Ce^{xviii}	125.3
Mg^{viii}—Ce—Mg^{v}	180.0	Zn^{xvi}—Mg—Ce^{xviii}	125.3
Zn^{i}—Ce—Mg^{ix}	54.7	Zn^{xii}—Mg—Ce^{xviii}	125.3
Zn—Ce—Mg^{ix}	125.3	Zn^{xi}—Mg—Ce^{xviii}	54.7
Zn^{ii}—Ce—Mg^{ix}	125.3	Zn^{x}—Mg—Ce^{xviii}	54.7

$\mathrm{Zn^{iii}}$—Ce—$\mathrm{Mg^{ix}}$	125.3	$\mathrm{Ce^{xvii}}$—Mg—$\mathrm{Ce^{xviii}}$	90.0
$\mathrm{Zn^{iv}}$—Ce—$\mathrm{Mg^{ix}}$	54.7	$\mathrm{Zn^{xiii}}$—Mg—$\mathrm{Ce^{xii}}$	125.3
$\mathrm{Zn^{v}}$—Ce—$\mathrm{Mg^{ix}}$	54.7	Zn—Mg—$\mathrm{Ce^{xii}}$	54.7
$\mathrm{Zn^{vi}}$—Ce—$\mathrm{Mg^{ix}}$	125.3	$\mathrm{Zn^{xiv}}$—Mg—$\mathrm{Ce^{xii}}$	125.3
$\mathrm{Zn^{vii}}$—Ce—$\mathrm{Mg^{ix}}$	54.7	$\mathrm{Zn^{xv}}$—Mg—$\mathrm{Ce^{xii}}$	54.7
$\mathrm{Mg^{iv}}$—Ce—$\mathrm{Mg^{ix}}$	90.0	$\mathrm{Zn^{xvi}}$—Mg—$\mathrm{Ce^{xii}}$	54.7
$\mathrm{Mg^{viii}}$—Ce—$\mathrm{Mg^{ix}}$	90.0	$\mathrm{Zn^{xii}}$—Mg—$\mathrm{Ce^{xii}}$	54.7
$\mathrm{Mg^{v}}$—Ce—$\mathrm{Mg^{ix}}$	90.0	$\mathrm{Zn^{xi}}$—Mg—$\mathrm{Ce^{xii}}$	125.3
Mg—Zn—Ce	180.0	$\mathrm{Zn^{x}}$—Mg—$\mathrm{Ce^{xii}}$	125.3
Mg—Zn—$\mathrm{Mg^{iv}}$	109.5	$\mathrm{Ce^{xvii}}$—Mg—$\mathrm{Ce^{xii}}$	90.0
Ce—Zn—$\mathrm{Mg^{iv}}$	70.5	$\mathrm{Ce^{xviii}}$—Mg—$\mathrm{Ce^{xii}}$	180.0
Mg—Zn—$\mathrm{Ce^{x}}$	70.5	$\mathrm{Zn^{xiii}}$—Mg—$\mathrm{Ce^{x}}$	125.3
Ce—Zn—$\mathrm{Ce^{x}}$	109.5	Zn—Mg—$\mathrm{Ce^{x}}$	54.7
$\mathrm{Mg^{iv}}$—Zn—$\mathrm{Ce^{x}}$	70.5	$\mathrm{Zn^{xiv}}$—Mg—$\mathrm{Ce^{x}}$	54.7
Mg—Zn—$\mathrm{Ce^{xi}}$	70.5	$\mathrm{Zn^{xv}}$—Mg—$\mathrm{Ce^{x}}$	54.7
Ce—Zn—$\mathrm{Ce^{xi}}$	109.5	$\mathrm{Zn^{xvi}}$—Mg—$\mathrm{Ce^{x}}$	125.3
$\mathrm{Mg^{iv}}$—Zn—$\mathrm{Ce^{xi}}$	70.5	$\mathrm{Zn^{xii}}$—Mg—$\mathrm{Ce^{x}}$	125.3
$\mathrm{Ce^{x}}$—Zn—$\mathrm{Ce^{xi}}$	109.5	$\mathrm{Zn^{xi}}$—Mg—$\mathrm{Ce^{x}}$	125.3
Mg—Zn—$\mathrm{Ce^{xii}}$	70.5	$\mathrm{Zn^{x}}$—Mg—$\mathrm{Ce^{x}}$	54.7
Ce—Zn—$\mathrm{Ce^{xii}}$	109.5	$\mathrm{Ce^{xvii}}$—Mg—$\mathrm{Ce^{x}}$	180.0
$\mathrm{Mg^{iv}}$—Zn—$\mathrm{Ce^{xii}}$	180.0	$\mathrm{Ce^{xviii}}$—Mg—$\mathrm{Ce^{x}}$	90.0
$\mathrm{Ce^{x}}$—Zn—$\mathrm{Ce^{xii}}$	109.5	$\mathrm{Ce^{xii}}$—Mg—$\mathrm{Ce^{x}}$	90.0

Symmetry codes: (i) −x, −y, −z; (ii) −x+1/2, −y+1/2, −z; (iii) x−1/2, y, z−1/2; (iv) x−1/2, y−1/2, z; (v) x, y−1/2, z−1/2; (vi) −x, −y+1/2, −z+1/2; (vii) −x+1/2, −y, −z+1/2; (viii) x−1, y−1/2, z−1/2; (ix) x−1/2, y−1, z−1/2; (x) x, y+1/2, z+1/2; (xi) x+1/2, y, z+1/2; (xii) x+1/2, y+1/2, z; (xiii) −x+1, −y+1, −z+1; (xiv) −x+1/2, −y+1/2, −z+1; (xv) −x+1/2, −y+1, −z+1/2; (xvi) −x+1, −y+1/2, −z+1/2; (xvii) x+1, y+1/2, z+1/2; (xviii) x+1/2, y+1/2, z+1.

Fig. 1