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# YMgGa

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Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(Mg–Mg) = 0.007 Å; $R$ factor = 0.035; $wR$ factor = 0.088; data-to-parameter ratio = 25.6.

The crystal structure of YMgGa, yttrium magnesium gallide, is isotypic with LaMgGa and crystallizes in the hexagonal ZrNiAl type structure. It consists of a three-dimensional network of Mg and Ga atoms, in which Y atoms fill channels. There are two crystallographically independent Ga sites. One Ga atom (Ga1) has three Mg atoms as near neighbours and six Y atoms at a slightly longer distance, giving rise to a [3 + 6] coordination. Another Ga atom (Ga2) is also nine-coordinate but has six near Mg neighbours and three Y at a somewhat longer distance in a [6 + 3] coordination. The Mg atom is tetrahedrally coordinated by four Ga atoms and has two additional Mg neighbours at a slightly longer distance. The site symmetries for Y, Ga1, Ga2 and Mg are $m2m$, $\overline{6}$, $\overline{6}2m$ and $m2m$, respectively. The crystal used was an inversion twin.

## Related literature

For structure refinement of LaMgGa and for the unit-cell parameters of YMgGa, see: Kraft *et al.* (2003). The crystal structure of YMgGa is related to the $Fe_2P$ type structure (Rundqvist & Jellinek, 1959). For structural investigations of Mg and binaries in the Y–Mg–Ga system, see: Smith *et al.* (1969); Owen *et al.* (1935); Smith *et al.* (1965); Schob & Parthé, (1965). For Mg alloys and hydrogen-absorbing properties of Mg compounds, see: Sakintuna *et al.* (2007); Zlotea *et al.* (2006); Sahlberg & Andersson (2007).

## Experimental

*Crystal data*

| | |
|---|---|
| YMgGa | $a$ = 7.2689 (10) Å |
| $M_r$ = 182.94 | $c$ = 4.4205 (9) Å |
| Hexagonal, $P\overline{6}2m$ | $V$ = 202.27 (6) Å$^3$ |
| $Z$ = 3 | $T$ = 293 (2) K |
| Ag $K\alpha$ radiation | 0.09 × 0.07 × 0.05 mm |
| $\mu$ = 16.83 mm$^{-1}$ | |

*Data collection*

| | |
|---|---|
| Bruker APEX diffractometer | 4365 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001) | 333 independent reflections |
| $T_{min}$ = 0.276, $T_{max}$ = 0.431 | 324 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.087 |

*Refinement*

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.035 | $\Delta\rho_{max}$ = 1.65 e Å$^{-3}$ |
| $wR(F^2)$ = 0.088 | $\Delta\rho_{min}$ = −1.78 e Å$^{-3}$ |
| $S$ = 1.15 | Absolute structure: Flack (1983), 136 Friedel pairs |
| 333 reflections | Flack parameter: 0.43 (5) |
| 13 parameters | |

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Ga1—Mg1 | 2.803 (3) | Ga2—Y1$^{ii}$ | 3.1033 (12) |
| Ga1—Y1$^{i}$ | 3.0936 (4) | Mg1—Mg1$^{iii}$ | 3.076 (7) |
| Ga2—Mg1 | 2.835 (3) | Mg1—Y1$^{i}$ | 3.255 (3) |

Symmetry codes: (i) $x, y, z+1$; (ii) $-x+y, -x+2, z$; (iii) $-x+y-1, -x+1, z$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Crystal Impact, 2006); software used to prepare material for publication: *SHELXTL* and *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2155).

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# supplementary materials

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# YMgGa

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## Comment

The potential use of magnesium alloys as storage materials for hydrogen has led to a large number of investigations on different magnesium alloys (Sakintuna *et al.*, 2007). The studies of compounds in the systems Mg—Y, Mg—Ga and Mg—Y—Zn have shown some very interesting hydrogen absorbing properties, such as hydrogen induced nanowhisker formation and improved hydrogen absorption/desorption properties, as compared to pure Mg (Zlotea *et al.*, 2006; Sahlberg & Andersson, 2007). Recently we have grown single crystals of YMgGa, and determined its crystal structure. The existence of this phase and the unit-cell parameters were previously reported (Kraft *et al.*, 2003), but no crystal structure refinement has been published.

In the title compound Mg and Ga atoms form a network with distorted channels which are occupied by Y atoms. YMgGa crystallizes in the hexagonal ZrNiAl type structure which is related to the $Fe_2P$ type structure (Rundqvist & Jellinek, 1959). The two Fe sites are then occupied with Mg and Y atoms, and the two distinct Ga atoms are located at the corresponding P positions. The Mg—Ga distances, 2.803 (3) and 2.835 (3) Å, respectively, are in agreement with the binary Mg—Ga compounds (Smith *et al.*, 1969). However, the Mg—Mg distance is 3.076 (7) Å, which is significantly shorter than in metallic magnesium, 3.20 Å (Owen *et al.*, 1935). The strong Mg—Ga and Mg—Mg interactions lead to a three-dimensional network which is shown in Figure 1. The Y—Mg (3.255 (3) Å) and Y—Ga (3.0936 (4) Å and 3.1033 (12) Å) distances are likewise in agreement with the binary compounds (Smith *et al.*, 1965; Schob & Parthé, 1965).

The coordination around Ga can be described as a slightly distorted capped trigonal prism. Ga1 is surrounded by 3 Mg atoms at 2.803 (3) Å and by 6 Y atoms at 3.0936 (4) Å in a [3 + 6] coordination. The Mg atoms form a triangle and the Y atoms are situated in the corners of a trigonal prism. Ga2 has a [6 + 3] coordination by 6 Mg at 2.835 (3) Å forming a trigonal prism that is capped by 3 Y at 3.1033 (12) Å. The Mg atom is tetrahedrally coordinated by 4 Ga atoms at 2.803 (3) and 2.835 (3) Å, and has 2 additional Mg neighbours at 3.076 (7) Å. The Y atom has 5 Ga neighbours in a pyramidal coordination and 6 additional Mg atoms forming a trigonal prism. The different coordination polyhedra around each atom are displayed in Figure 2.

## Experimental

YMgGa single crystals were obtained by heating appropriate amounts of the elements (Mg 99.95%, Y 99.9%, Ga 99.998%) inside an argon filled sealed tantalum tube in a high-frequency induction furnace at 1373 K. The sample was then heat-treated at 573 K for seven d to improve crystal growth. Large single crystals were removed from the surface of the sample and cut into smaller pieces. Bulk samples were characterized by X-ray powder diffraction.

## Refinement

The highest peak in the final Fourier map is located is 1.05 Å, and the deepest hole 1.51 Å from Y1. The measured crystal was an inversion twin with an approximate twin ratio of 1:1 (Flack parameter 0.43 (5).

**Figures**

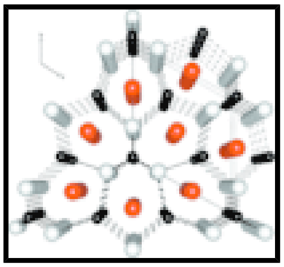

Fig. 1. The packing of the crystal structure of YMgGa, viewed down the *c* axis. The dotted lines show the Mg—Ga network and the channels filled by Y atoms. The Mg, Ga and Y atoms are gray, black and red, respectively.

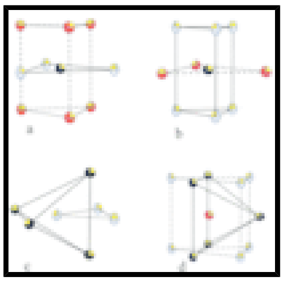

Fig. 2. The coordination polyhedra of YMgGa, displayed with ellipsoids at the 90% probability level. a) represents the coordination around Ga1, b) around Ga2, c) around Mg and d) around Y.

## Yttrium magnesium gallide

### *Crystal data*

| | |
|---|---|
| YMgGa | $Z = 3$ |
| $M_r = 182.94$ | $F_{000} = 246$ |
| Hexagonal, $P\overline{6}2m$ | $D_x = 4.505$ Mg m$^{-3}$ |
| Hall symbol: P -6 -2 | Ag $K\alpha$ radiation<br>$\lambda = 0.56085$ Å |
| $a = 7.2689$ (10) Å | Cell parameters from 801 reflections |
| $b = 7.2689$ (10) Å | $\theta = 3.6–22.4°$ |
| $c = 4.4205$ (9) Å | $\mu = 16.83$ mm$^{-1}$ |
| $\alpha = 90°$ | $T = 293$ (2) K |
| $\beta = 90°$ | Block, grey |
| $\gamma = 120°$ | 0.09 × 0.07 × 0.05 mm |
| $V = 202.27$ (6) Å$^3$ | |

### *Data collection*

| | |
|---|---|
| Bruker Apex1<br>diffractometer | 333 independent reflections |
| Radiation source: fine-focus sealed tube | 324 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.087$ |
| $T = 293(2)$ K | $\theta_{max} = 26.3°$ |
| ω–scans | $\theta_{min} = 2.6°$ |
| Absorption correction: multi-scan<br>(SADABS; Sheldrick, 2001) | $h = -11\rightarrow11$ |
| $T_{min} = 0.276$, $T_{max} = 0.431$ | $k = -11\rightarrow11$ |
| 4365 measured reflections | $l = -6\rightarrow6$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | $w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.5229P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.035$ | $(\Delta/\sigma)_{max} = 0.001$ |
| $wR(F^2) = 0.088$ | $\Delta\rho_{max} = 1.65$ e Å$^{-3}$ |
| $S = 1.15$ | $\Delta\rho_{min} = -1.78$ e Å$^{-3}$ |
| 333 reflections | Extinction correction: none |
| 13 parameters | Absolute structure: Flack (1983), 136 Friedel pairs |
| Primary atom site location: structure-invariant direct methods | Flack parameter: 0.43 (5) |

*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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Y1 | 0.57308 (15) | 1.0000 | 0.5000 | 0.0116 (2) |
| Ga1 | 0.3333 | 0.6667 | 1.0000 | 0.0104 (3) |
| Ga2 | 0.0000 | 1.0000 | 0.5000 | 0.0125 (4) |
| Mg1 | 0.2443 (5) | 1.0000 | 1.0000 | 0.0109 (7) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Y1 | 0.0118 (3) | 0.0103 (4) | 0.0121 (4) | 0.0052 (2) | 0.000 | 0.000 |
| Ga1 | 0.0101 (4) | 0.0101 (4) | 0.0112 (6) | 0.0050 (2) | 0.000 | 0.000 |
| Ga2 | 0.0138 (6) | 0.0138 (6) | 0.0100 (9) | 0.0069 (3) | 0.000 | 0.000 |
| Mg1 | 0.0088 (14) | 0.0102 (19) | 0.0141 (17) | 0.0051 (9) | 0.000 | 0.000 |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Y1—Ga1$^{i}$ | 3.0936 (4) | Ga1—Y1$^{xii}$ | 3.0936 (4) |
| Y1—Ga1$^{ii}$ | 3.0936 (4) | Ga2—Mg1$^{xiii}$ | 2.835 (3) |
| Y1—Ga1$^{iii}$ | 3.0936 (4) | Ga2—Mg1 | 2.835 (3) |

| | | | |
|---|---|---|---|
| Y1—Ga1 | 3.0936 (4) | Ga2—Mg1$^{xiv}$ | 2.835 (3) |
| Y1—Ga2$^{iv}$ | 3.1033 (12) | Ga2—Mg1$^{xv}$ | 2.835 (3) |
| Y1—Mg1$^{ii}$ | 3.255 (3) | Ga2—Mg1$^{ii}$ | 2.835 (3) |
| Y1—Mg1 | 3.255 (3) | Ga2—Mg1$^{xvi}$ | 2.835 (3) |
| Y1—Mg1$^{v}$ | 3.4869 (8) | Ga2—Y1$^{xvii}$ | 3.1033 (12) |
| Y1—Mg1$^{vi}$ | 3.4868 (8) | Ga2—Y1$^{ix}$ | 3.1033 (12) |
| Y1—Mg1$^{vii}$ | 3.4868 (8) | Ga2—Y1$^{xviii}$ | 3.1033 (12) |
| Y1—Mg1$^{viii}$ | 3.4868 (8) | Mg1—Ga1$^{i}$ | 2.803 (3) |
| Y1—Y1$^{v}$ | 3.7491 (7) | Mg1—Ga2$^{x}$ | 2.835 (2) |
| Ga1—Mg1 | 2.803 (3) | Mg1—Mg1$^{xvi}$ | 3.076 (7) |
| Ga1—Mg1$^{ix}$ | 2.803 (3) | Mg1—Mg1$^{xiv}$ | 3.076 (7) |
| Ga1—Mg1$^{vii}$ | 2.803 (3) | Mg1—Y1$^{x}$ | 3.255 (3) |
| Ga1—Y1$^{x}$ | 3.0936 (4) | Mg1—Y1$^{ix}$ | 3.4869 (8) |
| Ga1—Y1$^{ix}$ | 3.0936 (4) | Mg1—Y1$^{xix}$ | 3.4869 (8) |
| Ga1—Y1$^{xi}$ | 3.0936 (4) | Mg1—Y1$^{xi}$ | 3.4868 (8) |
| Ga1—Y1$^{vii}$ | 3.0936 (4) | Mg1—Y1$^{xvii}$ | 3.4868 (8) |

| | | | |
|---|---|---|---|
| Ga1$^{i}$—Y1—Ga1$^{ii}$ | 160.23 (4) | Mg1$^{xiii}$—Ga2—Mg1 | 143.50 (5) |
| Ga1$^{i}$—Y1—Ga1$^{iii}$ | 91.197 (16) | Mg1$^{xiii}$—Ga2—Mg1$^{xiv}$ | 143.50 (5) |
| Ga1$^{ii}$—Y1—Ga1$^{iii}$ | 85.420 (15) | Mg1—Ga2—Mg1$^{xiv}$ | 65.69 (10) |
| Ga1$^{i}$—Y1—Ga1 | 85.420 (15) | Mg1$^{xiii}$—Ga2—Mg1$^{xv}$ | 65.69 (10) |
| Ga1$^{ii}$—Y1—Ga1 | 91.197 (16) | Mg1—Ga2—Mg1$^{xv}$ | 143.50 (5) |
| Ga1$^{iii}$—Y1—Ga1 | 160.23 (4) | Mg1$^{xiv}$—Ga2—Mg1$^{xv}$ | 102.44 (13) |
| Ga1$^{i}$—Y1—Ga2$^{iv}$ | 99.89 (2) | Mg1$^{xiii}$—Ga2—Mg1$^{ii}$ | 65.69 (10) |
| Ga1$^{ii}$—Y1—Ga2$^{iv}$ | 99.89 (2) | Mg1—Ga2—Mg1$^{ii}$ | 102.44 (13) |
| Ga1$^{iii}$—Y1—Ga2$^{iv}$ | 99.89 (2) | Mg1$^{xiv}$—Ga2—Mg1$^{ii}$ | 143.50 (5) |
| Ga1—Y1—Ga2$^{iv}$ | 99.89 (2) | Mg1$^{xv}$—Ga2—Mg1$^{ii}$ | 65.69 (10) |
| Ga1$^{i}$—Y1—Mg1$^{ii}$ | 111.04 (4) | Mg1$^{xiii}$—Ga2—Mg1$^{xvi}$ | 102.44 (13) |
| Ga1$^{ii}$—Y1—Mg1$^{ii}$ | 52.33 (3) | Mg1—Ga2—Mg1$^{xvi}$ | 65.69 (10) |
| Ga1$^{iii}$—Y1—Mg1$^{ii}$ | 52.33 (3) | Mg1$^{xiv}$—Ga2—Mg1$^{xvi}$ | 65.69 (10) |
| Ga1—Y1—Mg1$^{ii}$ | 111.04 (4) | Mg1$^{xv}$—Ga2—Mg1$^{xvi}$ | 143.50 (5) |
| Ga2$^{iv}$—Y1—Mg1$^{ii}$ | 137.24 (5) | Mg1$^{ii}$—Ga2—Mg1$^{xvi}$ | 143.50 (5) |
| Ga1$^{i}$—Y1—Mg1 | 52.33 (3) | Mg1$^{xiii}$—Ga2—Y1$^{xvii}$ | 128.78 (6) |
| Ga1$^{ii}$—Y1—Mg1 | 111.04 (4) | Mg1—Ga2—Y1$^{xvii}$ | 71.75 (3) |
| Ga1$^{iii}$—Y1—Mg1 | 111.04 (4) | Mg1$^{xiv}$—Ga2—Y1$^{xvii}$ | 71.75 (3) |
| Ga1—Y1—Mg1 | 52.33 (3) | Mg1$^{xv}$—Ga2—Y1$^{xvii}$ | 71.75 (3) |
| Ga2$^{iv}$—Y1—Mg1 | 137.24 (5) | Mg1$^{ii}$—Ga2—Y1$^{xvii}$ | 71.75 (3) |
| Mg1$^{ii}$—Y1—Mg1 | 85.53 (10) | Mg1$^{xvi}$—Ga2—Y1$^{xvii}$ | 128.78 (6) |
| Ga1$^{i}$—Y1—Mg1$^{v}$ | 49.99 (5) | Mg1$^{xiii}$—Ga2—Y1$^{ix}$ | 71.75 (3) |
| Ga1$^{ii}$—Y1—Mg1$^{v}$ | 149.44 (7) | Mg1—Ga2—Y1$^{ix}$ | 71.75 (3) |
| Ga1$^{iii}$—Y1—Mg1$^{v}$ | 105.24 (5) | Mg1$^{xiv}$—Ga2—Y1$^{ix}$ | 128.78 (6) |

| | | | |
|---|---|---|---|
| Ga1—Y1—Mg1$^{v}$ | 87.44 (4) | Mg1$^{xv}$—Ga2—Y1$^{ix}$ | 128.78 (6) |
| Ga2$^{iv}$—Y1—Mg1$^{v}$ | 50.55 (5) | Mg1$^{ii}$—Ga2—Y1$^{ix}$ | 71.75 (3) |
| Mg1$^{ii}$—Y1—Mg1$^{v}$ | 153.75 (6) | Mg1$^{xvi}$—Ga2—Y1$^{ix}$ | 71.75 (3) |
| Mg1—Y1—Mg1$^{v}$ | 92.07 (7) | Y1$^{xvii}$—Ga2—Y1$^{ix}$ | 120.0 |
| Ga1$^{i}$—Y1—Mg1$^{vi}$ | 149.44 (7) | Mg1$^{xiii}$—Ga2—Y1$^{xviii}$ | 71.75 (3) |
| Ga1$^{ii}$—Y1—Mg1$^{vi}$ | 49.99 (5) | Mg1—Ga2—Y1$^{xviii}$ | 128.78 (6) |
| Ga1$^{iii}$—Y1—Mg1$^{vi}$ | 87.44 (4) | Mg1$^{xiv}$—Ga2—Y1$^{xviii}$ | 71.75 (3) |
| Ga1—Y1—Mg1$^{vi}$ | 105.24 (5) | Mg1$^{xv}$—Ga2—Y1$^{xviii}$ | 71.75 (3) |
| Ga2$^{iv}$—Y1—Mg1$^{vi}$ | 50.55 (5) | Mg1$^{ii}$—Ga2—Y1$^{xviii}$ | 128.78 (6) |
| Mg1$^{ii}$—Y1—Mg1$^{vi}$ | 92.07 (7) | Mg1$^{xvi}$—Ga2—Y1$^{xviii}$ | 71.75 (3) |
| Mg1—Y1—Mg1$^{vi}$ | 153.75 (6) | Y1$^{xvii}$—Ga2—Y1$^{xviii}$ | 120.0 |
| Mg1$^{v}$—Y1—Mg1$^{vi}$ | 101.11 (10) | Y1$^{ix}$—Ga2—Y1$^{xviii}$ | 120.0 |
| Ga1$^{i}$—Y1—Mg1$^{vii}$ | 87.44 (4) | Ga1—Mg1—Ga1$^{i}$ | 96.93 (12) |
| Ga1$^{ii}$—Y1—Mg1$^{vii}$ | 105.24 (5) | Ga1—Mg1—Ga2 | 114.538 (6) |
| Ga1$^{iii}$—Y1—Mg1$^{vii}$ | 149.44 (7) | Ga1$^{i}$—Mg1—Ga2 | 114.538 (6) |
| Ga1—Y1—Mg1$^{vii}$ | 49.99 (5) | Ga1—Mg1—Ga2$^{x}$ | 114.538 (6) |
| Ga2$^{iv}$—Y1—Mg1$^{vii}$ | 50.55 (5) | Ga1$^{i}$—Mg1—Ga2$^{x}$ | 114.538 (6) |
| Mg1$^{ii}$—Y1—Mg1$^{vii}$ | 153.75 (6) | Ga2—Mg1—Ga2$^{x}$ | 102.44 (12) |
| Mg1—Y1—Mg1$^{vii}$ | 92.07 (7) | Ga1—Mg1—Mg1$^{xvi}$ | 101.54 (6) |
| Mg1$^{v}$—Y1—Mg1$^{vii}$ | 52.34 (12) | Ga1$^{i}$—Mg1—Mg1$^{xvi}$ | 161.54 (6) |
| Mg1$^{vi}$—Y1—Mg1$^{vii}$ | 78.67 (2) | Ga2—Mg1—Mg1$^{xvi}$ | 57.15 (5) |
| Ga1$^{i}$—Y1—Mg1$^{viii}$ | 105.24 (5) | Ga2$^{x}$—Mg1—Mg1$^{xvi}$ | 57.15 (5) |
| Ga1$^{ii}$—Y1—Mg1$^{viii}$ | 87.44 (4) | Ga1—Mg1—Mg1$^{xiv}$ | 161.54 (6) |
| Ga1$^{iii}$—Y1—Mg1$^{viii}$ | 49.99 (5) | Ga1$^{i}$—Mg1—Mg1$^{xiv}$ | 101.54 (6) |
| Ga1—Y1—Mg1$^{viii}$ | 149.44 (7) | Ga2—Mg1—Mg1$^{xiv}$ | 57.15 (5) |
| Ga2$^{iv}$—Y1—Mg1$^{viii}$ | 50.55 (5) | Ga2$^{x}$—Mg1—Mg1$^{xiv}$ | 57.15 (5) |
| Mg1$^{ii}$—Y1—Mg1$^{viii}$ | 92.07 (7) | Mg1$^{xvi}$—Mg1—Mg1$^{xiv}$ | 60.0 |
| Mg1—Y1—Mg1$^{viii}$ | 153.75 (6) | Ga1—Mg1—Y1$^{x}$ | 60.87 (6) |
| Mg1$^{v}$—Y1—Mg1$^{viii}$ | 78.67 (2) | Ga1$^{i}$—Mg1—Y1$^{x}$ | 60.87 (6) |
| Mg1$^{vi}$—Y1—Mg1$^{viii}$ | 52.34 (12) | Ga2—Mg1—Y1$^{x}$ | 171.54 (11) |
| Mg1$^{vii}$—Y1—Mg1$^{viii}$ | 101.11 (10) | Ga2$^{x}$—Mg1—Y1$^{x}$ | 86.01 (3) |
| Ga1$^{i}$—Y1—Y1$^{v}$ | 52.703 (6) | Mg1$^{xvi}$—Mg1—Y1$^{x}$ | 129.48 (4) |
| Ga1$^{ii}$—Y1—Y1$^{v}$ | 134.380 (9) | Mg1$^{xiv}$—Mg1—Y1$^{x}$ | 129.48 (4) |
| Ga1$^{iii}$—Y1—Y1$^{v}$ | 52.703 (6) | Ga1—Mg1—Y1 | 60.87 (6) |
| Ga1—Y1—Y1$^{v}$ | 134.380 (9) | Ga1$^{i}$—Mg1—Y1 | 60.87 (6) |
| Ga2$^{iv}$—Y1—Y1$^{v}$ | 74.21 (3) | Ga2—Mg1—Y1 | 86.01 (3) |
| Mg1$^{ii}$—Y1—Y1$^{v}$ | 101.53 (2) | Ga2$^{x}$—Mg1—Y1 | 171.54 (11) |
| Mg1—Y1—Y1$^{v}$ | 101.53 (2) | Mg1$^{xvi}$—Mg1—Y1 | 129.48 (4) |
| Mg1$^{v}$—Y1—Y1$^{v}$ | 53.32 (5) | Mg1$^{xiv}$—Mg1—Y1 | 129.48 (4) |
| Mg1$^{vi}$—Y1—Y1$^{v}$ | 104.56 (7) | Y1$^{x}$—Mg1—Y1 | 85.53 (10) |
| Mg1$^{vii}$—Y1—Y1$^{v}$ | 104.56 (7) | Ga1—Mg1—Y1$^{ix}$ | 57.70 (2) |

| | | | |
|---|---|---|---|
| Mg1$^{viii}$—Y1—Y1$^{v}$ | 53.32 (5) | Ga1$^{i}$—Mg1—Y1$^{ix}$ | 128.28 (9) |
| Mg1—Ga1—Mg1$^{ix}$ | 120.0 | Ga2—Mg1—Y1$^{ix}$ | 57.70 (3) |
| Mg1—Ga1—Mg1$^{vii}$ | 120.000 (1) | Ga2$^{x}$—Mg1—Y1$^{ix}$ | 117.00 (8) |
| Mg1$^{ix}$—Ga1—Mg1$^{vii}$ | 120.0 | Mg1$^{xvi}$—Mg1—Y1$^{ix}$ | 63.83 (6) |
| Mg1—Ga1—Y1$^{x}$ | 66.80 (4) | Mg1$^{xiv}$—Mg1—Y1$^{ix}$ | 109.25 (6) |
| Mg1$^{ix}$—Ga1—Y1$^{x}$ | 134.247 (10) | Y1$^{x}$—Mg1—Y1$^{ix}$ | 118.53 (8) |
| Mg1$^{vii}$—Ga1—Y1$^{x}$ | 72.31 (4) | Y1—Mg1—Y1$^{ix}$ | 67.47 (3) |
| Mg1—Ga1—Y1$^{ix}$ | 72.31 (4) | Ga1—Mg1—Y1$^{xix}$ | 128.28 (9) |
| Mg1$^{ix}$—Ga1—Y1$^{ix}$ | 66.80 (4) | Ga1$^{i}$—Mg1—Y1$^{xix}$ | 57.70 (2) |
| Mg1$^{vii}$—Ga1—Y1$^{ix}$ | 134.247 (10) | Ga2—Mg1—Y1$^{xix}$ | 117.00 (8) |
| Y1$^{x}$—Ga1—Y1$^{ix}$ | 139.045 (6) | Ga2$^{x}$—Mg1—Y1$^{xix}$ | 57.70 (3) |
| Mg1—Ga1—Y1$^{xi}$ | 72.31 (4) | Mg1$^{xvi}$—Mg1—Y1$^{xix}$ | 109.25 (6) |
| Mg1$^{ix}$—Ga1—Y1$^{xi}$ | 66.80 (4) | Mg1$^{xiv}$—Mg1—Y1$^{xix}$ | 63.83 (6) |
| Mg1$^{vii}$—Ga1—Y1$^{xi}$ | 134.247 (10) | Y1$^{x}$—Mg1—Y1$^{xix}$ | 67.47 (3) |
| Y1$^{x}$—Ga1—Y1$^{xi}$ | 74.593 (12) | Y1—Mg1—Y1$^{xix}$ | 118.53 (8) |
| Y1$^{ix}$—Ga1—Y1$^{xi}$ | 91.197 (16) | Y1$^{ix}$—Mg1—Y1$^{xix}$ | 172.63 (13) |
| Mg1—Ga1—Y1 | 66.80 (4) | Ga1—Mg1—Y1$^{xi}$ | 57.70 (2) |
| Mg1$^{ix}$—Ga1—Y1 | 134.247 (10) | Ga1$^{i}$—Mg1—Y1$^{xi}$ | 128.28 (9) |
| Mg1$^{vii}$—Ga1—Y1 | 72.31 (4) | Ga2—Mg1—Y1$^{xi}$ | 117.00 (8) |
| Y1$^{x}$—Ga1—Y1 | 91.197 (16) | Ga2$^{x}$—Mg1—Y1$^{xi}$ | 57.70 (3) |
| Y1$^{ix}$—Ga1—Y1 | 74.593 (12) | Mg1$^{xvi}$—Mg1—Y1$^{xi}$ | 63.83 (6) |
| Y1$^{xi}$—Ga1—Y1 | 139.045 (6) | Mg1$^{xiv}$—Mg1—Y1$^{xi}$ | 109.25 (6) |
| Mg1—Ga1—Y1$^{vii}$ | 134.247 (10) | Y1$^{x}$—Mg1—Y1$^{xi}$ | 67.47 (3) |
| Mg1$^{ix}$—Ga1—Y1$^{vii}$ | 72.31 (4) | Y1—Mg1—Y1$^{xi}$ | 118.53 (8) |
| Mg1$^{vii}$—Ga1—Y1$^{vii}$ | 66.80 (4) | Y1$^{ix}$—Mg1—Y1$^{xi}$ | 78.67 (2) |
| Y1$^{x}$—Ga1—Y1$^{vii}$ | 139.045 (6) | Y1$^{xix}$—Mg1—Y1$^{xi}$ | 100.84 (3) |
| Y1$^{ix}$—Ga1—Y1$^{vii}$ | 74.593 (12) | Ga1—Mg1—Y1$^{xvii}$ | 128.28 (9) |
| Y1$^{xi}$—Ga1—Y1$^{vii}$ | 139.045 (6) | Ga1$^{i}$—Mg1—Y1$^{xvii}$ | 57.70 (2) |
| Y1—Ga1—Y1$^{vii}$ | 74.593 (12) | Ga2—Mg1—Y1$^{xvii}$ | 57.70 (3) |
| Mg1—Ga1—Y1$^{xii}$ | 134.247 (10) | Ga2$^{x}$—Mg1—Y1$^{xvii}$ | 117.00 (8) |
| Mg1$^{ix}$—Ga1—Y1$^{xii}$ | 72.31 (4) | Mg1$^{xvi}$—Mg1—Y1$^{xvii}$ | 109.25 (6) |
| Mg1$^{vii}$—Ga1—Y1$^{xii}$ | 66.80 (4) | Mg1$^{xiv}$—Mg1—Y1$^{xvii}$ | 63.83 (6) |
| Y1$^{x}$—Ga1—Y1$^{xii}$ | 74.593 (12) | Y1$^{x}$—Mg1—Y1$^{xvii}$ | 118.53 (8) |
| Y1$^{ix}$—Ga1—Y1$^{xii}$ | 139.045 (6) | Y1—Mg1—Y1$^{xvii}$ | 67.47 (3) |
| Y1$^{xi}$—Ga1—Y1$^{xii}$ | 74.593 (12) | Y1$^{ix}$—Mg1—Y1$^{xvii}$ | 100.84 (3) |
| Y1—Ga1—Y1$^{xii}$ | 139.045 (6) | Y1$^{xix}$—Mg1—Y1$^{xvii}$ | 78.67 (2) |
| Y1$^{vii}$—Ga1—Y1$^{xii}$ | 91.197 (16) | Y1$^{xi}$—Mg1—Y1$^{xvii}$ | 172.63 (13) |

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

Fig. 1

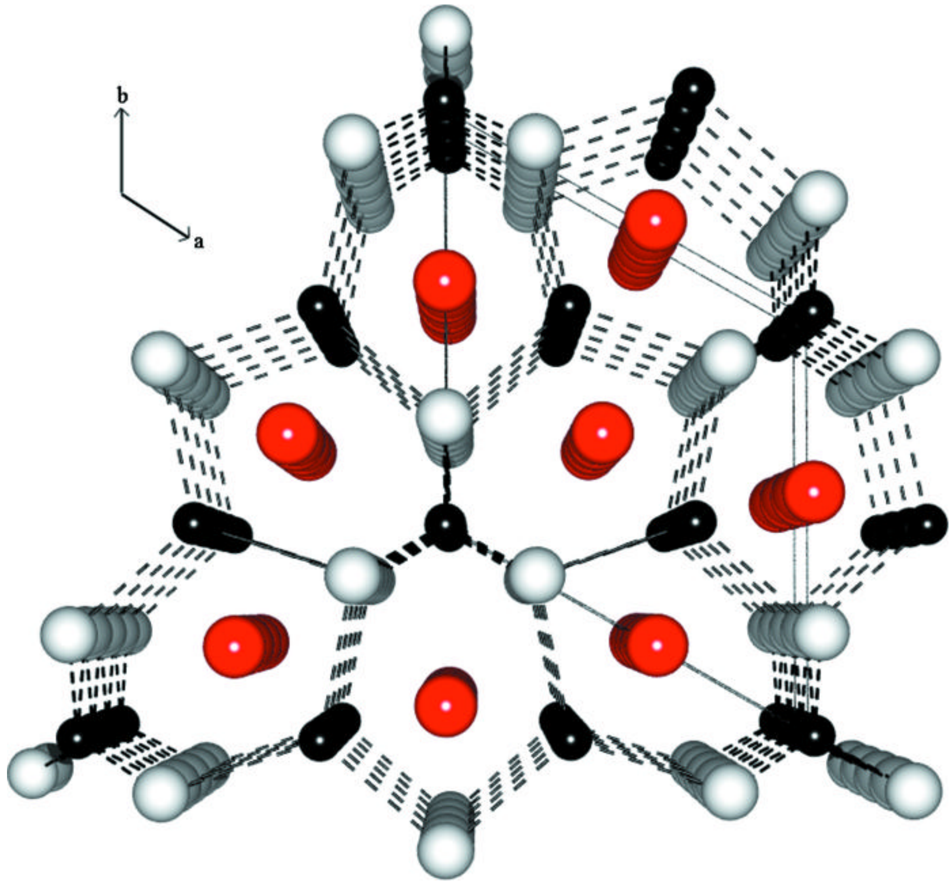

Fig. 2