

$\text{Sr}_3\text{MgPtO}_6$ 

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## Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean  $\sigma(\text{Mg}-\text{O}) = 0.004\text{ \AA}$

$R$  factor = 0.024

$wR$  factor = 0.049

Data-to-parameter ratio = 24.5

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

Single crystals of the mixed alkaline earth platinate, tristrontium magnesium platinum hexaoxide,  $\text{Sr}_3\text{MgPtO}_6$ , were grown from a KOH flux at 1273 K. The compound adopts the rhombohedral  $\text{K}_4\text{CdCl}_6$  structure type, featuring chains of face-shared, distorted  $\text{MgO}_6$  trigonal prisms (Mg site symmetry 32) and  $\text{PtO}_6$  octahedra (Pt site symmetry  $\bar{3}$ ) surrounded by columns of  $\text{Sr}^{2+}$  ions (Sr site symmetry 2).

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## Comment

The structure of  $\text{Sr}_3\text{MgPtO}_6$  was determined in 1997 (Núñez *et al.*, 1997) by powder X-ray diffraction on a polycrystalline sample prepared by conventional sintering techniques, and was shown to adopt the  $\text{K}_4\text{CdCl}_6$  structure type (Bergerhoff & Schmitz-Dumont, 1956). This structure type features two crystallographically and chemically distinct  $\text{K}^+$  positions and consists of chains along [001] of face-shared, distorted  $\text{KCl}_6$  trigonal prisms and  $\text{CdCl}_6$  octahedra. The polyhedral chains are surrounded by spiral columns of  $\text{K}^+$  ions. To date, a large and compositionally diverse group of oxides adopting this structure type has been reported, typically as polycrystalline materials [reviewed in Stitzer *et al.* (2001)]. High-temperature flux growth from molten KOH has proven to be an effective oxide crystal growth medium. Single crystals of  $\text{Sr}_3\text{MgPtO}_6$  were readily grown from molten KOH at 1273 K, using

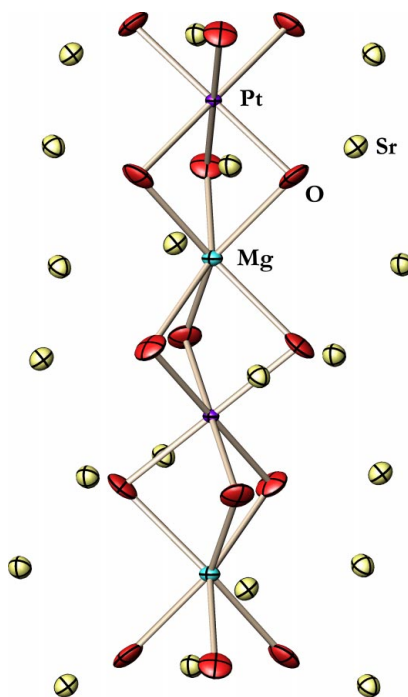
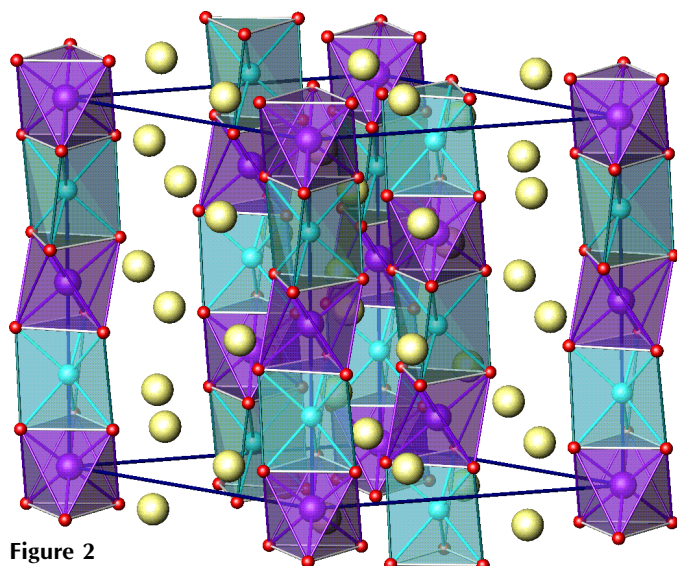


Figure 1

Fragment of the face-shared polyhedral chains in  $\text{Sr}_3\text{MgPtO}_6$ . Displacement ellipsoids are drawn at the 90% probability level.



**Figure 2**  
Polyhedral view of the unit cell of  $\text{Sr}_3\text{MgPtO}_6$ , viewed approximately along  $[110]$ .

$(\text{NH}_4)_2\text{PtCl}_6$  as the platinum source.  $\text{Sr}_3\text{MgPtO}_6$  represents an Mg-substituted form of the  $\text{K}_4\text{CdCl}_6$ -type oxide  $\text{Sr}_4\text{PtO}_6$  (Randall & Katz, 1959), with Mg ordered in the trigonal prism site (site-symmetry 32, Wyckoff symbol 6a) and  $\text{Pt}^{4+}$  in a rhombohedrally elongated octahedral site (site symmetry  $\bar{3}$ , Wyckoff symbol 6b). Fig. 1 illustrates the local coordination of these metal centers. The  $\text{Sr}^{2+}$  ion resides in an irregular eight-coordinate site (Wyckoff symbol 18e) of site symmetry 2. Fig. 2 shows a view of the polyhedral chains and  $\text{Sr}^{2+}$  columns. Bond lengths and angles from the present single-crystal determination of  $\text{Sr}_3\text{MgPtO}_6$  are very close to those derived from powder data [Mg—O = 2.172 (16) Å, Pt—O = 2.011 (16) Å and Sr—O = 2.498 (17)–2.742 (17) Å]. Refinement of the site occupancies for Mg and Pt showed no significant deviation from whole occupancy, indicating a stoichiometric compound, and no Sr/Mg mixing on the trigonal prism site.

## Experimental

The  $(\text{NH}_4)_2\text{PtCl}_6$  precursor was prepared according to a published method (Kaufman, 1967). Subsequently,  $\text{SrCO}_3$  (Alfa, 99.95%),  $\text{MgCO}_3$  (Alfa, 99.8%), and  $(\text{NH}_4)_2\text{PtCl}_6$  (stoichiometric amounts, ca 1 g total reagent mass) and KOH (Fisher, reagent grade; ~10 times by mass the total reagent amount) were loaded into a covered alumina crucible. The mixture was heated at 1273 K for 2 h, cooled to 1023 K at a rate of 1 K h<sup>-1</sup>, at which point the furnace was shut off and allowed to cool to room temperature radiatively. The KOH matrix was dissolved with distilled water, leaving plentiful transparent brown crystals with a rhombohedral habit.

### Crystal data

$\text{Sr}_3\text{MgPtO}_6$   
 $M_r = 578.26$   
Trigonal,  $R\bar{3}c$   
 $a = 9.6432$  (4) Å  
 $c = 11.1112$  (6) Å  
 $V = 894.82$  (7) Å<sup>3</sup>  
 $Z = 6$   
 $D_x = 6.439$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
Cell parameters from 1132 reflections  
 $\theta = 4.2$ – $36.3^\circ$   
 $\mu = 50.13$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
Rhombohedron, brown  
 $0.11 \times 0.05 \times 0.04$  mm

### Data collection

Bruker SMART APEX CCD diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan (SADABS; Bruker, 1999)  
 $T_{\min} = 0.073$ ,  $T_{\max} = 0.239$   
2412 measured reflections

490 independent reflections  
431 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.037$   
 $\theta_{\max} = 36.3^\circ$   
 $h = -16 \rightarrow 7$   
 $k = -11 \rightarrow 16$   
 $l = -18 \rightarrow 8$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.024$   
 $wR(F^2) = 0.049$   
 $S = 1.01$   
490 reflections  
20 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0227P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 2.32$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -3.12$  e Å<sup>-3</sup>  
Extinction correction: SHELXL97  
Extinction coefficient: 0.00118 (8)

**Table 1**

Selected geometric parameters (Å).

Sr—O	2.472 (3)	Mg—O	2.177 (3)
Sr—O <sup>i</sup>	2.637 (3)	Mg—Pt	2.77780 (15)
Sr—O <sup>ii</sup>	2.663 (3)	Pt—O	2.031 (3)
Sr—O <sup>iii</sup>	2.731 (3)		

Symmetry codes: (i)  $\frac{1}{3} - x + y, y - \frac{1}{3}, \frac{1}{6} + z$ ; (ii)  $\frac{2}{3} - x + y, \frac{1}{3} - x, \frac{1}{3} + z$ ; (iii)  $\frac{2}{3} + y, \frac{1}{3} - x + y, \frac{1}{3} - z$ .

Systematic absences in the dataset confirmed a  $c$ -glide operation, indicating the space groups  $R3c$  and  $R\bar{3}c$ . Preliminary powder X-ray diffraction showed the compound to be isostructural with  $\text{K}_4\text{CdCl}_6$  (space group  $R\bar{3}c$ ); therefore, the expected centrosymmetric space group was chosen and confirmed by the structure solution. The largest difference peak and hole were located less than 0.8 Å from the Pt atom.

Data collection: SMART-NT (Bruker, 1999); cell refinement: SAINT-Plus-NT (Bruker, 1999); data reduction: SAINT-Plus-NT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ATOMS (Dowty, 2001); software used to prepare material for publication: SHELXTL (Bruker, 1997).

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