Table 1. *Coordinates and isotropic temperature factors (Å^2) in FeSnF$_6$.6H$_2$O (e.s.d.'s in parentheses)*

	x	y	z	B
Fe	0	0	$\frac{1}{2}$	1·99 (2)*
Sn	0	0	0	1·67 (1)*
F	0·1460 (2)	0·1718 (2)	0·1126 (2)	4·2 (1)*
O	0·1840 (3)	0·1701 (3)	0·3813 (2)	4·8 (1)*
H(1)	0·310 (5)	0·223 (5)	0·411 (4)	6·0
H(2)	0·161 (6)	0·151 (5)	0·271 (4)	6·0

* Equivalent isotropic temperature factor, defined as
$B_{eq} = [4/3]\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$ (Hamilton, 1959).

Table 2. *Selected bond lengths (Å) and angles (°) in FeSnF$_6$.6H$_2$O (e.s.d.'s in parentheses)*

6 × Fe—O	2·116 (2)	O—H(2)	1·14 (4)
6 × Sn—F	1·945 (2)	F···H(1)	1·61 (5)
O—H(1)	1·12 (5)	F···H(2)	1·63 (4)
O—H(1)···F	176 (4)	Fe—O—H(2)	114 (2)
O—H(2)···F	165 (4)	O—Fe—O	89·96 (8)
H(1)—O—H(2)	115 (4)	F—Sn—F	89·21 (8)
Fe—O—H(1)	121 (2)		

Unlike FeSiF$_6$.6H$_2$O, no extra reflection, signifying a lowering of symmetry from $R\bar{3}$, can be seen in FeSnF$_6$.6(H$_2$O).

The structure is built up from isolated Fe(H$_2$O)$_6$ and SnF$_6$ octahedra. The stability of the structure is ensured by hydrogen bonds: H atoms of water molecules point towards fluoride anions of neighbouring octahedra (Fig. 1 and Table 2). The mean Sn—F distance [1·945 (2) Å] is close to the sum of the ionic radii of Sn^{4+} (0·69 Å) and F$^-$ (1·285 Å).
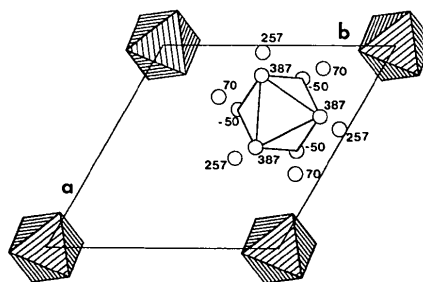
Fig. 1. [0001] projection of FeSnF$_6$.6H$_2$O. SnF$_6$ octahedra (at z = 0) are shaded; heights of the H atoms of the water molecules in the Fe(H$_2$O)$_6$ octahedra (at z = 1/6) are multiplied by 10^3.

References

CALAGE, Y., TORTEVOIS, P. & VARRET, F. (1990). *J. Phys. Chem. Solids*, **51**, 911–913.
CHAPPERT, J., JEHANNO, G. & VARRET, F. (1977). *J. Phys. (Paris)*, **38**, 411–418.
CHEVRIER, G., HARDY, A. & JEHANNO, G. (1981). *Acta Cryst.* A37, 578–584.
HAMILTON, W. C. (1959). *Acta Cryst.* **12**, 609–610.
HAMILTON, W. C. (1962). *Acta Cryst.* **15**, 353–360.
HASSEL, O. (1927). *Z. Phys. Chem.* **126**, 118–126.
JEHANNO, G. & VARRET, F. (1975). *Acta Cryst.* A31, 857–858.
KODERA, E., TORII, A., OSAKI, K. & WATANABE, T. (1972). *J. Phys. Soc. Jpn*, **32**, 863.
PAULING, L. (1930). *Z. Kristallogr.* **72**, 482.
RAY, S., ZALKIN, A. & TEMPLETON, D. H. (1973). *Acta Cryst.* B28, 2741–2747.
SHELDRICK, G. M. (1976). *SHELX76.* Program for crystal structure determination. Univ. of Cambridge, England.
SYOYAMA, S. & OSAKI, K. (1972). *Acta Cryst.* B28, 2616–2627.

Aluminium Trimagnesium Diplatinum

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Abstract. AlMg$_3$Pt$_2$, M_r = 490·10, cubic, $Fd\bar{3}m$, a = 11·802 (1) Å, V = 1643·9 (4) Å^3, Z = 16, D_x = 7·92 Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ = 133·0 mm^{-1}, $F(000)$ = 3280, T = 296 K. The structure was refined to R = 0·017, wR = 0·025 for 78 absorption-corrected reflections. AlMg$_3$Pt$_2$ crystallizes as an ordered ternary variant of the NiTi$_2$ structure.

Experimental. The alloy was synthesized by reaction of a stoichiometric mixture of the elements in a modified Belt-type high-pressure apparatus (Range & Leeb, 1975). This method avoids the vaporization losses of Al and Mg inevitably found in normal-pressure experiments and allows for exact control of composition. From the reaction product obtained at 40 kbar ($\equiv$4 GPa) and 1675 K (BN capsule, reaction time 30 min, subsequent slow cooling to 1275 K and quenching to ambient conditions) a crystal fragment

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(approx. dimensions $0.030 \times 0.040 \times 0.075$ mm) was isolated and used for data collection on an Enraf–Nonius CAD-4 diffractometer (Cu $K\alpha$, $\lambda = 1.5418$ Å, graphite monochromator in incident beam). An EDX analysis made on the same crystal after data collection showed Al, Mg, and Pt to be present in the approximate atomic ratio 1:3:2. The result of the structure analysis finally confirmed the composition $AlMg_3Pt_2$. Lattice parameters were refined from 2θ values of 25 reflections in the range $6.5 \le \theta \le 19.8°$. Intensities were measured for $2 \le \theta \le 65°$; ω–2θ scan technique, scan width $(0.7 + 0.14\tan\theta)°$. Three standard reflections showed only small random fluctuations and indicated no loss of intensity throughout data collection. Merging of the 4270 collected intensities ($\sin\theta_{max}/\lambda = 0.59$ Å^{-1}; $-13 \le h \le 13$, $-13 \le k \le 13$, $-13 \le l \le 13$) gave 88 unique reflections ($R_{int} = 0.088$), of which 78 with $I > 0.8\sigma(I)$ were considered as observed and used for all calculations (program system SDP3·1; Enraf–Nonius, 1988).

The structure was solved by routine direct methods, followed by successive difference-Fourier synthesis. In the least-squares refinement $|F|$ magnitudes were used to refine an overall scale factor, positional parameters and isotropic temperature factors. Refinement of the occupation factors for Mg, Pt, and Al confirmed the stoichiometry $AlMg_3Pt_2$ within two standard deviations. Consequently, the s.o.f.'s were fixed at 100% before applying a numerical correction for the very serious absorption to the original 4270 data [program DIFABS (Walker & Stuart, 1983); correction factors minimum 0.21, maximum 1.00; R_{int} after merging of the corrected data 0.031] and performing the final anisotropic refinement (including an extinction parameter). Final $R = 0.017$, $wR = 0.025$. $w = 4I/[\sigma^2(I) + 0.007I^2]$, $(\Delta/\sigma)_{max} < 0.001$ in final refinement cycle, 11 variables, $E = 1.41 (4) \times 10^{-6}$, $S = 0.49$. Maximum features in the final difference-Fourier synthesis $+0.4$, -0.3 e Å^{-3}. Atomic scattering factors and f', f'' values as set by SDP program. Bond distances and angles were calculated using the program SADIAN (Baur & Wenninger, 1969). Final atomic coordinates and equivalent isotropic temperature factors are given in Table 1, derived bond distances in Table 2.*

The structure of $AlMg_3Pt_2$ is an ordered ternary variant of the $NiTi_2$ structure (Yurko, Barton & Parr, 1959). Ni, Ti(1) and Ti(2) are replaced by Pt, Al and Mg, respectively. The Pt—Al (2.599 Å) and

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* List of structure factors, anisotropic thermal parameters and bond angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53187 (14 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates and equivalent isotropic temperature factors* (Å² × 10⁴)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Al	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	43 (8)
Mg	0.9288 (4)	$\frac{1}{8}$	$\frac{1}{8}$	42 (4)
Pt	0.71438 (3)	0.71438 (3)	0.71438 (3)	24.7 (5)

Table 2. *Interatomic distances* (Å)

Pt—Al	2.599 (1)	(3×)	Al—Pt	2.599 (1)	(6×)
Pt—Mg	2.714 (1)	(2×)	Al—Mg	2.967 (3)	(6×)
Pt—Mg	2.938 (3)	(3×)	Mg—Pt	2.714 (1)	(2×)
Pt—Pt	2.984 (1)	(3×)	Mg—Pt	2.938 (3)	(2×)
			Mg—Al	2.967 (3)	(2×)

mean Pt—Mg (2.826 Å) distances agree well with those found in Pt_8Al_{21} (Range & Christl, 1988) and Mg_2PtSi (Range, Rau & Klement, 1990).

Related literature. No structural details for ternary Al—Mg—Pt compounds could be found in the literature. A similar structure was derived from X-ray powder data for compounds like Nb_3Ni_2Si (Gladyshevskij, Kuz'ma & Kripyakevich, 1963). $NiTi_2$ (Duwez & Taylor, 1950) was claimed to be an oxide with composition Ni_2Ti_4O (Karlsson, 1951). Mueller & Knott (1963) concluded from powder neutron diffraction data that the structure can exist for the composition $NiTi_2$ as well as for Ni_2Ti_4O. In the present study no evidence for the existence of additional interstitial atoms in $AlMg_3Pt_2$ has been found.

References

BAUR, W. H. & WENNINGER, G. (1969). SADIAN. Program for calculation of atomic distances and angles in crystal structures. Univ. of Illinois, USA.

DUWEZ, P. & TAYLOR, J. C. (1950). J. Met. 3, 1173–1176.

Enraf–Nonius (1988). Structure Determination Package. Version 3.1. Enraf–Nonius, Delft, The Netherlands.

GLADYSHEVSKIJ, E. I., KUZ'MA, J. B. & KRIPYAKEVICH, P. I. (1963). Zh. Strukt. Khim. 4, 372–379.

KARLSSON, N. (1951). Nature (London), 168, 558.

MUELLER, M. H. & KNOTT, H. W. (1963). Trans. Metall. Soc. AIME, 227, 674–678.

RANGE, K.-J. & CHRISTL, E. G. (1988). J.Less-Common Met. 136, 277–285.

RANGE, K.-J. & LEEB, R. (1975). Z. Naturforsch. Teil B, 30, 889–895.

RANGE, K.-J., RAU, F. & KLEMENT, U. (1990). Acta Cryst. C46, 1092–1093.

WALKER, N. & STUART, D. (1983). Acta Cryst. A39, 159–163.

YURKO, G. A., BARTON, J. W. & PARR, J. C. (1959). Acta Cryst. 12, 901–912; see Structure Reports, 22, 888.