bonds are 2·12 and 2·17 Å (Klassen & Hoppe, 1976), but here the O atoms are further coordinated to alkali-metal ions. This is also the case in the oxoaurates Li_5AuO_4, $Li_6Au_2O_6$ and $KAuO_2$, where powder data lead to Au—O distances of 2·03, 2·08 and 2·08 Å respectively (Wasel-Nielen & Hoppe, 1970), but these structures were not refined and no e.s.d.'s are given; in addition, Li_5AuO_4 has averaged Li/Au sites and so is not directly comparable.

The Au atom is weakly coordinated by four further O atoms: Au···O(1^c) 2·81, Au···O(2^a) 2·90, Au···O(1^f) 3·19, Au···O(2^g) 3·05 Å [symmetry transformations: (*a*) and (*c*), see Fig. 1; (*f*) $\frac{1}{4} - x, -\frac{1}{4} + y, -\frac{1}{4} + z$; (*g*) $x, y, -1 + z$]. These five atoms lie in a plane (r.m.s. deviation 0·07 Å) at 85° to the AuO_4 bonding plane, O(1^c) and O(2^a) lying above, O(1^f) and O(2^g) below the latter plane.

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Rare-Earth (and Yttrium)—Iridium and —Platinum Compounds with the Fe_3C Structure Type

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Abstract. Sm_3Ir, orthorhombic, *Pnma*, $Z = 4$, $a = 7{\cdot}273\ (4)$, $b = 9{\cdot}584\ (5)$, $c = 6{\cdot}397\ (4)$ Å, $D_x = 9{\cdot}58$ Mg m^{-3}, μ(Ag $K\alpha$) = 37·5 mm^{-1}; Y_3Pt, same type, $a = 7{\cdot}101\ (4)$, $b = 9{\cdot}584\ (7)$, $c = 6{\cdot}454\ (6)$ Å, $D_x = 6{\cdot}98$ Mg m^{-3}, μ(Mo $K\alpha$) = 73·8 mm^{-1}. The structures belong to the Fe_3C structure type. New compounds found to be isotypic are: La_3Ir, Pr_3Ir, Nd_3Ir, Sm_3Ir, Gd_3Ir, Tb_3Ir, Dy_3Ir, Ho_3Ir, Er_3Ir, Tm_3Ir, Lu_3Ir and Y_3Ir; and Gd_3Pt, Tb_3Pt, Dy_3Pt, Ho_3Pt, Er_3Pt, Tm_3Pt, Lu_3Pt and Y_3Pt.

Introduction. In the course of a review of the crystal structures of alloys containing rare-earth elements (and Y) and late transition elements (Parthé & Moreau, 1977; Le Roy, Moreau, Paccard & Parthé, 1978) it became evident that structural studies of rare-earth (*R*) rich alloys formed in the systems *R*–Ir and *R*–Pt were by no means complete. The only information found on such compounds was for La–Ir (Dmitrieva, Vorobev, Varekha, Domashev & Gusynin, 1974), Ce–Ir (Dmitrieva *et al.*, 1973), Yb–Ir (Iandelli & Palenzona, 1976), Nd–Pt, Er–Pt (Moffatt, 1978) and Yb–Pt (Iandelli & Palenzona, 1975). We report here the results of our investigations on other compounds belonging to these systems.

The alloys were made from commercially available elements of high purity by conventional arc-melting techniques. X-ray photographs from powdered samples were obtained on a Guinier camera with Cu $K\alpha$ radiation and were calibrated with Si powder. Small single crystals of Sm_3Ir (130 × 35 × 25 μm) and Y_3Pt (100 × 50 × 40 μm) were isolated by mechanical fragmentation. Intensities were measured with graphite-monochromated Ag $K\alpha$ (Sm_3Ir) and Mo $K\alpha$ (Y_3Pt) radiation on a computer-controlled Philips PW 1100 four-circle diffractometer in the θ–2θ scan mode.

Data collection for Sm_3Ir (Y_3Pt) was carried out to a limit of 0·71 (0·66) $Å^{-1}$ in $\sin\theta/\lambda$, yielding 467 (561)

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independent reflections, of which 397 (412) with $I > 3\sigma_I$ plus 33 (80) with $I < 3\sigma_I$ but where $|F_c| > |F_o|$ were used in the structure refinement. The *CAMEL JOCKEY* program (Flack, 1977) was used to correct for absorption in Sm_3Ir ($\mu R = 0{\cdot}7$). For Y_3Pt a spherical absorption correction was applied ($\mu R = 2{\cdot}4$). Examination of the systematic absences ($0kl$: $k + l = 2n + 1$ and $hk0$: $h = 2n + 1$) indicated that $Pn2_1a$ and *Pnma* were possible space groups. The structure was solved from stereochemical reasoning. Relativistic Hartree–Fock scattering factors (Cromer & Mann, 1968) were used in a least-squares refinement of the atomic parameters with unit weights. The results are given in Table 1. All computer programs were those of the XRAY system (1976). The final $R = \sum|\Delta F|/\sum|F_o| = 4{\cdot}5\%$ for Sm_3Ir and $8{\cdot}3\%$ for Y_3Pt.* The isotypism of La_3Ir, Pr_3Ir, Nd_3Ir, Sm_3Ir, Gd_3Ir, Tb_3Ir, Dy_3Ir, Ho_3Ir, Er_3Ir, Tm_3Ir, Lu_3Ir, Y_3Ir, Gd_3Pt, Tb_3Pt, Dy_3Pt, Ho_3Pt, Er_3Pt, Tm_3Pt, Lu_3Pt and Y_3Pt was established by comparing observed and calculated powder diffraction intensities with the *LAZY PULVERIX* program (Yvon, Jeitschko & Parthé, 1977). The lattice parameters reported in Table 2 were obtained with *PARAM* (XRAY system, 1976).

Table 1. *Positional and thermal parameters for* Sm_3Ir *and* Y_3Pt *with the* Fe_3C *structure type* (*space group Pnma*)

The e.s.d.'s are given in parentheses. The Debye–Waller factor is defined as $\exp[-2\pi^2 \times 10^{-2}\,U\,(2\sin\theta/\lambda)^2]$.

	Equipoint	x	y	z	U (Å^2)
Sm_3Ir					
Sm(1)	4(c)	0·0351 (3)	$\frac{1}{4}$	0·1351 (4)	1·66 (5)
Sm(2)	8(d)	0·1762 (2)	0·0630 (2)	0·6701 (3)	1·66 (4)
Ir	4(c)	0·3823 (3)	$\frac{1}{4}$	0·9447 (3)	2·04 (4)
Y_3Pt					
Y(1)	4(c)	0·0299 (7)	$\frac{1}{4}$	0·1312 (7)	1·36 (9)
Y(2)	8(d)	0·1796 (5)	0·0619 (3)	0·6785 (5)	1·41 (7)
Pt	4(c)	0·3904 (3)	$\frac{1}{4}$	0·9522 (3)	1·76 (6)

Table 2. *Lattice constants of* R_3Ir *and* R_3Pt *compounds with the* Fe_3C *structure type* (*space group Pnma*)

E.s.d.'s are given in parentheses; V = volume of the unit cell, n = number of atoms in the unit cell.

	a (Å)	b (Å)	c (Å)	$(V/n)^{1/2}$
La_3Ir	7·453 (6)	10·103 (9)	6·650 (6)	3·151
Pr_3Ir	7·329 (3)	9·844 (7)	6·518 (3)	3·086
Nd_3Ir	7·307 (4)	9·758 (8)	6·469 (4)	3·066
Sm_3Ir	7·273 (4)	9·584 (5)	6·397 (4)	3·032
Gd_3Ir	7·247 (3)	9·448 (4)	6·382 (3)	3·011
Tb_3Ir	7·217 (2)	9·318 (5)	6·361 (2)	2·990
Dy_3Ir	7·187 (2)	9·237 (6)	6·344 (2)	2·975
Ho_3Ir	7·186 (2)	9·139 (2)	6·326 (1)	2·961
Er_3Ir	7·162 (3)	9·076 (4)	6·306 (2)	2·948
Tm_3Ir	7·133 (3)	8·990 (4)	6·285 (2)	2·931
Lu_3Ir	7·101 (4)	8·884 (6)	6·247 (3)	2·910
Y_3Ir	7·237 (2)	9·297 (6)	6·400 (1)	2·997
Gd_3Pt	7·125 (6)	9·631 (9)	6·460 (8)	3·026
Tb_3Pt	7·077 (4)	9·541 (7)	6·444 (4)	3·007
Dy_3Pt	7·049 (3)	9·485 (5)	6·417 (3)	2·993
Ho_3Pt	7·019 (2)	9·436 (6)	6·394 (3)	2·980
Er_3Pt	7·008 (3)	9·373 (9)	6·374 (4)	2·969
Tm_3Pt	6·981 (4)	9·314 (9)	6·349 (4)	2·955
Lu_3Pt	6·926 (4)	9·225 (9)	6·293 (5)	2·929
Y_3Pt	7·101 (4)	9·584 (7)	6·454 (6)	3·017

Discussion. From previous studies of chemically related compounds it could be expected that the structures of the new R_3Ir and R_3Pt compounds might be built up of characteristic construction elements, *i.e.* trigonal prisms of rare-earth atoms which are centered by transition-metal atoms. Three structure types with composition R_3T are known which belong to this category:

Fe_3C, *Pnma*, *oP*16 which has been found with R_3Co, R_3Ni, R_3Rh and Yb_3Pd (Parthé & Moreau, 1977);

Sc_3Co, *Pnma*, *oP*32 which so far is known only with Sc_3Co (Chabot & Parthé, 1978);

Re_3B, *Cmcm*, *oC*16 which was reported, for example, with Pu_3Co (Larson, Cromer & Roof, 1963) and Zr_3Co (Kripjakevič, Markiv & Burnasova, 1970).

It has already been shown that all three structure types are geometrically related and can be derived by periodic unit-cell twinning of close-packed element structures with different stackings (Chabot & Parthé, 1978). The isotypism of the compounds under investigation with the Fe_3C structure type was expected once the lattice constants had been determined. The structure type could be verified by the intensity calculations and subsequent structure refinements.

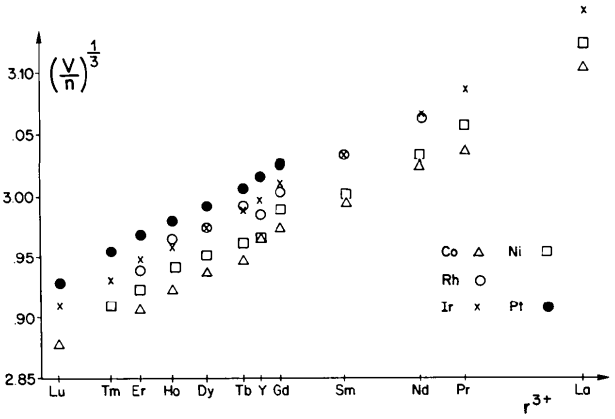

Fig. 1. $(V/n)^{1/3}$ *versus* r^{3+} plot for R_3T compounds with the Fe_3C structure type.

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* Lists of structure factors for Sm_3Ir and Y_3Pt have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34284 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2 shows a variation of the lattice constants which is essentially a consequence of the normal lanthanide contraction. To represent this variation graphically in a series of isostructural rare-earth intermetallic compounds, one may simply plot cell dimensions *versus* trivalent ionic radii of the rare-earth atoms. A linear trend is likewise obtained if the quantity $(V/n)^{1/3}$, *i.e.* the cube root of the ratio of the unit-cell volume to the total number of atoms, is plotted against the rare-earth trivalent ionic radius (Parthé, 1967). A plot of this kind is shown in Fig. 1. Small deviations from linearity can be seen for Co, Ni and Rh compounds. It remains to be clarified whether these deviations are due to imprecisely measured lattice parameters (determined by different authors and reviewed by Parthé & Moreau, 1977) or whether they indicate a non-stoichiometric composition. For Nd_3Rh, at least, Raman (1972) reported that the composition is closer to Nd_4Rh. Presumably there are vacancies at the Fe and C sites in this compound.

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Bariumhexaoxoditellurat(IV,VI): Sauerstoffkoordinationszahl Fünf am vierwertigen Tellur

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Abstract. $BaTe_2O_6$, orthorhombic, $a = 5{\cdot}569$ (2), $b = 12{\cdot}796$ (4), $c = 7{\cdot}320$ (3) Å, *Cmcm*, $Z = 4$, $D_x = 6{\cdot}219$ (4), $D_o = 6{\cdot}19$ (3) Mg m^{-3}. $BaTe_2O_6$ has been prepared from BaO–TeO_2 melts in the presence of air at 973 K. In this structure, which has been refined to $R = 0{\cdot}058$, octahedral $Te^{VI}O_6$ [$d_{Te-O} = 1{\cdot}902$ (4) and 1·924 (3) Å] and pyramidal $Te^{IV}O_5$ groups [$d_{Te-O} = 1{\cdot}830$ (9) and 2·126 (4) Å] are connected by common corners, forming Te_2O_6 layers.

Einleitung. Im Rahmen von Untersuchungen über Oxotellurate(IV) fanden wir im System Ba–Te–O die Verbindung $BaTe_2O_6$, deren Zusammensetzung durch chemische Analyse bestimmt wurde: Barium (gravimetrisch als Sulfat) 27,9 (3), berechnet 28,1%; Tellur (gravimetrisch als Element) 52,1 (1), berechnet 52,2%. Die Gitterkonstanten der Verbindung wurden aus Weissenberg- und Präzessionsaufnahmen bestimmt und nach Zählrohr-Guinier-Aufnahmen (Huber System 600, Cu $K\alpha_1$-Strahlung, Quarzmonochromator) mit Silicium (a = 5,4305 Å) als externem Standard verfeinert. Die Filmaufnahmen zeigten die Auslöschungen hkl nur mit $h + k = 2n$ vorhanden, $h0l$ nur mit $h = 2n$ und $l = 2n$ vorhanden. Danach kamen die Raumgruppe *Cmcm* und ihre nichtzentrosymmetrischen Untergruppen *Cmc*2_1 und *C*2*cm* in Betracht. Reflex-

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