New ternary $EuPt_2Al_3$ and $EuIr_2Al_4$ aluminides*

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During phase-analytical investigations of the Eu-Pt-Al and Eu-Ir-Al ternary systems at 873 K, the existence of two new ternary compounds has been established. The structures of both compounds were investigated by X-ray single crystal diffraction.

Both compounds of compositions $Eu_{0.25}T_{0.25}Al_{0.50}$ (T = Pt, Ir) were synthesized in a sealed-fused silica tube which was heated to 1373 K in a programmed muffle furnace for 6 hours and further annealed at 873 K for 240 h, after what good quality $EuPt_2Al_3$ and $EuIr_2Al_4$ single crystals were isolated from samples.

Intensity data of $EuPt_2Al_3$ was collected at room temperature on a STOE StadiVari equipped with a Mo micro focus source and a Pilatus 100K detection system diffractometer and $EuIr_2Al_4$ was measured at room temperature on a STOE IPDS-II (MoKα radiation) diffractometer. Refined data you can see in Table 1 and Table 2.

Table 1. Crystal data and structure refinement for $EuPt_2Al_3$ and $EuIr_2Al_4$

	$EuPt_2Al_3$	$EuIr_2Al_4$
Formula weight / g mol^{-1}	623.1	644.3
Unit cell dimensions / Å; Z (single-crystal data)	a = 4.2032(2), b = 11.5261(8), c = 13.8792(9); Z = 6	a = 7.9181(2), c = 7.7335(4); Z = 4
Unit cell volume / $Å^3$	672.40(7)	484.8619
Calculated density / g cm^{-3}	9.2322	8.8267
Crystal size / μm^3	45×40×55	30×65×40
F(000)/e	1548	1076
θ range for data collection / °	3-33	3-33
Range in hkl	±6,±17, ±21	±12, -10;+12, ±11
Total no. reflections	6375	5728
Independent reflections / R_{int}	1491/0.0507	474/0.053
Reflections with I>3σ(I)	1186/0.0181	407/0.0052
Data/parameters	1491/62	474/19
Goodness-of-fit on F^2	2.01	2.10
R1/wR2 for I>2σ(I))	0.0335/0.0380	0.0235/0.548
R1/wR2 (all data)	0.0435/0.0392	0.0302/0.0560
Largest diff. peak/hole / $eÅ^{-3}$	3.84/-3.25	2.48/-2.04

Table 2. Atomic coordinates and equivalent displacement parameters for $EuPt_2Al_3$ and $EuIr_2Al_4$

Atom	Wyckoff position	*x/a*	*y/b*	*z/c*	$U_{eq.}$
Eu1	*4e*	1/4	0.55652	0.79319	0.0224(2)
Eu2	*2b*	1/4	3/4	0.51384	0.02164(16)
Pt1	*4e*	1/4	0.05623	0.38806	0.02082(17)
Pt2	*4e*	1/4	0.61483	0.09794	0.02091(17)
Pt3	*2a*	1/4	1/4	0.13302	0.02148(13)
Pt4	*2a*	1/4	¼	0.66431	0.02102(12)
Al1	*4e*	1/4	0.05320	0.57082	0.0192(14)
Al2	*4e*	1/4	0.08100	0.01197	0.0257(17)
Al3	*4e*	1/4	0.63130	0.28785	0.0224(15)
Al4	*2b*	1/4	3/4	0.96087	0.0205(10)
Al5	*2a*	1/4	1/4	0.30945	0.022(1)
Al6	*2a*	1/4	1/4	0.84769	0.0217(10)

All atom coordinates for $EuPt_2Al_3$ are standardized.

Atom	Wyckoff position	*x/a*	*y/b*	*z/c*	$U_{eq.}$
Eu	*4c*	1/2	0	0.35712(7)	0.01045(12)
Ir	*8f*	0.64249(3)	0.64249(3)	1/4	0.00638(9)
Al	*16g*	0.1336(2)	0.1652(3)	0.4135(3)	0.0080(5)

The Eu atoms in the $EuPt_2Al_3$ structure fill hexagonal prisms and the aluminum atoms form connected trigonal nets. The $EuIr_2Al_4$ structure can be described as 3*D* 48_2-framework where eight-membered rings are filled by Eu atoms and four-membered rings from Al and Ir atoms are empty (Fig. 1).

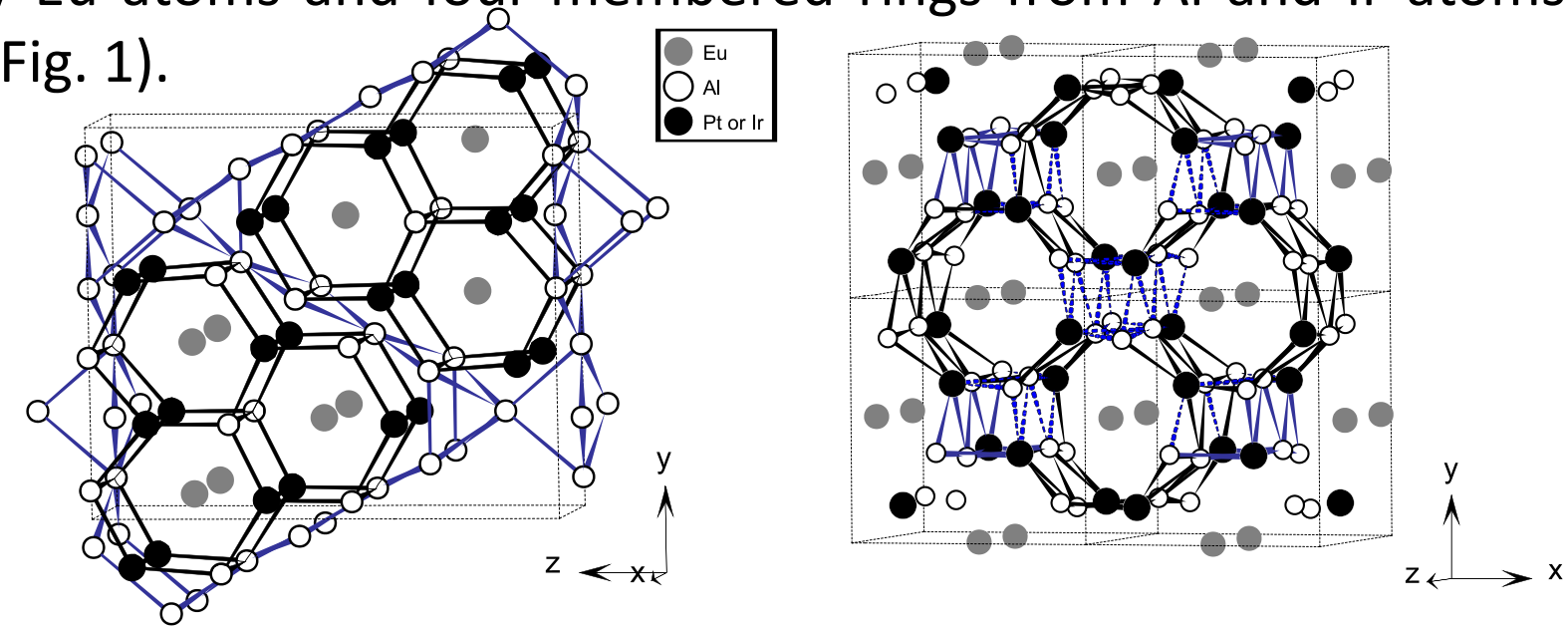

Figure 1. – Prisms and nets in $EuPt_2Al_3$ and $EuIr_2Al_4$ structures

The electronic structure calculations for both phases confirm that the atoms of aluminum and transition metal form atomic nets with much higher values of the electron localization function (ELF) than around the Eu atoms, where the electron localization function is minimal.

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