Crystal structure of terbium chromium aluminium, $Tb_6Cr_{4+x}Al_{43-x}$ (x=1.6), erbium chromium aluminium, $Er_6Cr_{4+x}Al_{43-x}$ (x=1.96), holmium chromium aluminium, $Ho_6Cr_{4+x}Al_{43-x}$ (x=1.6), and lutetium chromium aluminium, $Lu_6Cr_{4+x}Al_{43-x}$ (x=2.76)

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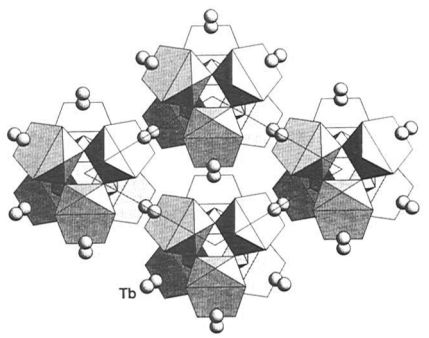
Source of material: Synthesis from elements by arc melting and annealing at 773 K in evacuated quartz tubes.
The compounds crystallize in the $Yb_6Cr_{4+x}Al_{43-x}$ (x = 1.76) structure type with mixed Cr/Al occupation of the 8*h* site (see ref. 1).

1. Structure of $Tb_6Cr_{4+x}Al_{43-x}$ (x = 1.6)

Nominal composition $Tb_6Cr_6Al_{41}$.



$Al_{41.4}Cr_{5.6}Tb_6$, hexagonal, $P6_3/mcm$ (No. 193),
a = 10.964(2) Å, c = 17.719(3) Å, V = 1844.7 Å^3, Z = 2
$R(F)$ = 0.087, $R_w(F)$ = 0.060.

Table 1. Parameters used for the X-ray data collection

Crystal:	metallic plate, size 0.016 x 0.048 x 0.060 mm
Wave length:	Mo K_α radiation (0.71073Å)
μ:	139.13 cm^{-1}
Diffractometer:	Philips PW1100
Scan mode:	ω/2θ
$T_{measurement}$:	293 K
$2\theta_{max}$:	64°
$N(hkl)_{unique}$:	453
Criterion for F_o:	$F_o > 4\,\sigma(F_o)$
$N(param)_{refined}$:	52
Program:	XTAL 3.2

Table 2. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	Occ.	x	y	z	U_{iso}
Al(6)	8*h*	0.60(5)	1/3	2/3	0.1282(8)	0.012(4)
Cr(6)	8*h*	0.40(5)	1/3	2/3	0.1282(8)	0.012(4)

Table 3. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Tb	12*k*	0.4677(2)	0	0.0968(1)	0.0090(7)	$2U_{12}$	0.0038(7)	0.0028(5)	−0.0022(9)	0
Cr(1)	6*g*	0.266(1)	0	1/4	0.009(4)	$2U_{12}$	0.009(5)	0.002(2)	0	0
Cr(2)	2*b*	0	0	0	$2U_{12}$	$2U_{12}$	0.005(9)	0.004(3)	0	0
Al(1)	24*l*	0.232(1)	0.394(1)	0.1635(4)	0.011(5)	0.011(5)	0.001(4)	0.001(4)	0.007(4)	0.002(4)
Al(2)	12*k*	0.154(1)	0	0.1165(7)	0.007(5)	$2U_{12}$	−0.003(6)	0.001(3)	0.001(5)	0
Al(3)	12*k*	0.252(2)	0	0.5290(8)	0.006(5)	$2U_{12}$	0.008(7)	0.015(5)	−0.006(6)	0
Al(4)	12*j*	0.150(2)	0.549(2)	1/4	0.025(9)	0.002(8)	0.018(8)	0.007(8)	0	0
Al(5)	12*i*	0.249(1)	2*x*	0	0.019(7)	$2U_{12}$	0.04(1)	0.005(4)	0.009(9)	0
Al(7)	6*g*	0.852(2)	0	1/4	0.010(9)	$2U_{12}$	0.01(1)	0.001(5)	0	0

2. Structure of $Er_6Cr_{4+x}Al_{43-x}$ (x = 1.96)

Nominal composition $Er_6Cr_6Al_{41}$.

$Al_{41.04}Cr_{5.96}Er_6$, hexagonal, *P6₃/mcm* (No. 193),
a = 10.853(2) Å, c = 17.543(7) Å, V = 1789.4 Å^3, Z = 2
$R(F)$ = 0.085, $R_w(F)$ = 0.052.

Table 4. Parameters used for the X-ray data collection

Crystal:	metallic plate, size 0.016 x 0.048 x 0.060 mm
Wave length:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	166.62 cm^{-1}
Diffractometer:	Philips PW1100
Scan mode:	ω/2θ
$T_{measurement}$:	293 K
$2\theta_{max}$:	60°
$N(hkl)_{unique}$:	307
Criterion for F_o:	$F_o > 4\,\sigma(F_o)$
$N(param)_{refined}$:	27
Program:	XTAL 3.2

Table 5. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	Occ.	x	y	z	U_{iso}
Er	12*k*		0.4661(2)	0	0.0966(1)	0.0065(6)
Cr(1)	6*g*		0.262(1)	0	¼	0.006(3)
Cr(2)	2*b*		0	0	0	0.011(6)
Al(1)	24*l*		0.233(1)	0.395(1)	0.1642(6)	0.004(2)
Al(2)	12*k*		0.155(1)	0	0.117(1)	0.006(4)
Al(3)	12*k*		0.255(2)	0	0.5316(8)	0.001(4)
Al(4)	12*j*		0.151(2)	0.549(2)	¼	0.008(4)
Al(5)	12*i*		0.251(1)	2*x*	0	0.019(5)
Al(7)	6*g*		0.853(2)	0	¼	0.001(6)
Al(6)	8*h*	0.51(5)	⅓	⅔	0.1306(8)	0.01(5)
Cr(6)	8*h*	0.49(5)	⅓	⅔	0.1306(8)	0.01(5)

3. Structure of $Ho_6Cr_{4+x}Al_{43-x}$ (x = 1.6)

Nominal composition $Ho_6Cr_6Al_{41}$.

$Al_{41.4}Cr_{5.6}Ho_6$, hexagonal, *P6₃/mcm* (No. 193)
a = 10.962(2) Å, c = 17.715(4) Å, V = 1843.4 Å^3, Z = 2,
$R(F)$ = 0.059, $R_w(F)$ = 0.044.

Table 6. Parameters used for the X-ray data collection

Crystal:	metallic plate, size 0.008 x 0.024 x 0.040
Wave length:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	152.90 cm^{-1}
Diffractometer:	Philips PW1100
Scan mode:	ω/2θ
$T_{measurement}$:	293 K
$2\theta_{max}$:	54°
$N(hkl)_{unique}$:	208
Criterion for F_o^2:	$F_o^2 > 3\,\sigma(F_o^2)$
$N(param)_{refined}$:	28
Program:	XTAL 3.2

Table 7. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	Occ.	x	y	z	U_{iso}
Ho	12*k*		0.4675(2)	0	0.0970(2)	0.0064(7)
Cr(1)	6*g*		0.263(2)	0	¼	0.009(3)
Cr(2)	2*b*		0	0	0	0.006(6)
Al(1)	24*l*		0.234(1)	0.394(1)	0.1644(4)	0.006(3)
Al(2)	12*k*		0.154(2)	0	0.1164(8)	0.006(4)
Al(3)	12*k*		0.257(2)	0	0.5299(7)	0.003(3)
Al(4)	12*j*		0.152(2)	0.551(2)	¼	0.010(4)
Al(5)	12*i*		0.247(1)	2*x*	0	0.024(5)
Al(7)	6*g*		0.849(3)	0	¼	0.004(7)
Al(6)	8*h*	0.60(6)	⅓	⅔	0.1300(7)	0.007(5)
Cr(6)	8*h*	0.40(6)	⅓	⅔	0.1300(7)	0.007(5)

4. Structure of $Lu_6Cr_{4+x}Al_{43-x}$ (x = 2.76)

Nominal composition $Lu_6Cr_6Al_{41}$.

$Al_{40.24}Cr_{6.76}Lu_6$, hexagonal, *P6₃/mcm* (No. 193),
a = 10.851(1) Å, c = 17.322(3) Å, V = 1766.4 Å^3, Z = 2,
$R(F)$ = 0.065, $R_w(F^2)$ = 0.089.

Table 8. Parameters used for the X-ray data collection

Crystal:	metallic plate, size 0.012 x 0.016 x 0.020 mm
Wave length:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	195.95 cm^{-1}
Diffractometer:	Philips PW1100
Scan mode:	ω/2θ
$T_{measurement}$:	293 K
$2\theta_{max}$:	60°
$N(hkl)_{unique}$:	228
Criterion for F_o^2:	$F_o^2 > 3\,\sigma(F_o^2)$
$N(param)_{refined}$:	28
Program:	XTAL 3.2

Table 9. Final atomic coordinates and displacement parameters (in Å^2)

Atom	Site	Occ.	x	y	z	U_{iso}
Lu	12*k*		0.4656(3)	0	0.0973(1)	0.0075(7)
Cr(1)	6*g*		0.261(2)	0	¼	0.011(4)
Cr(2)	2*b*		0	0	0	0.002(6)
Al(1)	24*l*		0.235(2)	0.399(2)	0.1609(6)	0.008(3)
Al(2)	12*k*		0.154(2)	0	0.116(1)	0.008(5)
Al(3)	12*k*		0.255(2)	0	0.5290(9)	0.003(4)
Al(4)	12*j*		0.151(3)	0.546(3)	¼	0.008(5)
Al(5)	12*i*		0.250(1)	2*x*	0	0.014(5)
Al(7)	6*g*		0.847(4)	0	¼	0.01(1)
Al(6)	8*h*	0.31(7)	⅓	⅔	0.1304(8)	0.006(5)
Cr(6)	8*h*	0.69(7)	⅓	⅔	0.1304(8)	0.006(5)

References

1. Yanson, T.I., Manyako, M.B., Bodak, O.I., Zarechnyuk, O.S., Gladyshevskii, R.E., Cerny, R., Yvon, K.: Crystal structure of hexagonal $Yb_6Cr_{4+x}Al_{43-x}$ (x = 1.76). Acta Crystallogr. accepted.