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Trisodium yttrium(III) hexachloride

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(Y–Cl) = 0.001 Å
R factor = 0.027
wR factor = 0.059
Data-to-parameter ratio = 25.7

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

Colourless single crystals of Na_3YCl_6, crystallizing in the cryolite structure type and isotypic with Na_3GdCl_6-II and Na_3MCl_6 (M = Sc, Dy–Lu), were prepared from a flux of YCl_3, NaCN and NaN_3; the trivalent yttrium is octahedrally coordinated by chlorine atoms with an average Y—Cl distance of 2.62 Å. The Y atom and one Na atom lie on centres of symmetry.

Comment

Unlike Na_3GdCl_6-I ($LiSbF_6$ type) (Meyer, 1984), Na_3HoCl_6 (Böcker *et al.*, 2001) and Na_3ErCl_6 (Meyer *et al.*, 1987) which are accessible by metallothermic reduction of the corresponding chlorides with sodium metal, single crystals of Na_3YCl_6 were prepared from fluxes of YCl_3, NaCN and NaN_3. Na_3YCl_6 crystallizes with the cryolite structure type (Fig. 1) and is isotypic with Na_3GdCl_6-II (Meyer, 1984) and also Na_3MCl_6 (M = Sc, Dy–Lu; Meyer *et al.*, 1987). The Y atom and

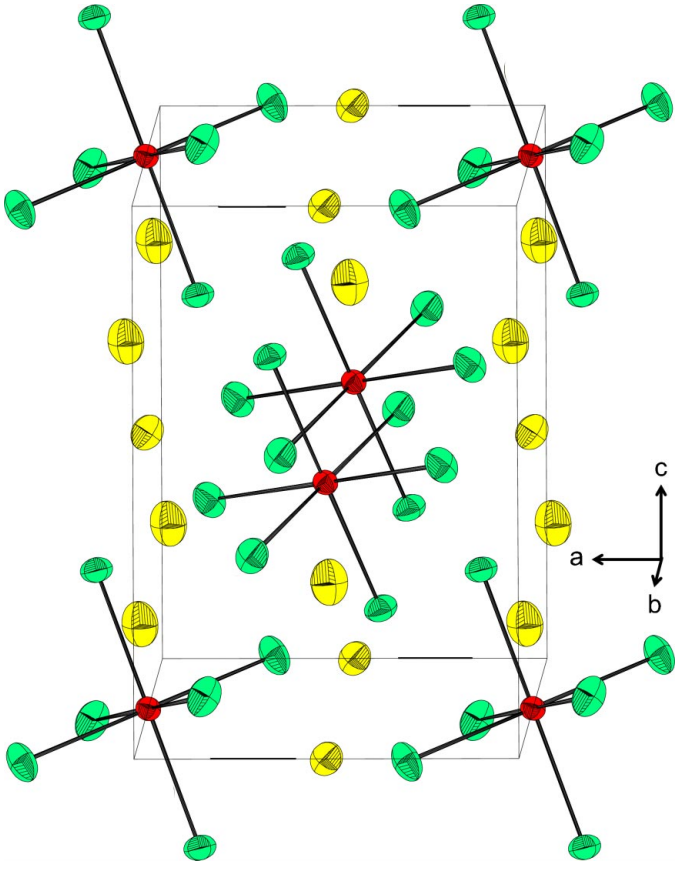

Figure 1
Displacement ellipsoid plot of the crystal structure of Na_3YCl_6, viewed approximately along [010], with ellipsoids drawn at the 50% probability level; Y atoms are red, Cl atoms green, and Na atoms yellow.

one Na atom lie on centres of symmetry. The average Y—Cl distance (2.62 Å) is 0.09 Å smaller than the sum of the corresponding effective ionic radii (Shannon, 1976) and thus suggests that a rigid-body correction of the octahedral entities according to the procedure of Schomaker & Trueblood (1968) is appropriate. The corresponding librational analysis is unsatisfactory (R = 0.131) and yields corrected Y—Cl distances that are enlarged by only 0.01 Å. The attempt to correct the interatomic distances librationally by considering the Na—Cl polyhedra is even worse. We mention, however, that the same effect of apparently too short metal–chlorine bonds is seen also for the above Na_3GdCl_6 (0.08 Å), Na_3HoCl_6 (0.08 Å) and Na_3ErCl_6 (0.09 Å).

Experimental

Single crystals of Na_3YCl_6 were synthesized using a flux route (Liao & Dronskowski, 2004) by sealing YCl_3, NaCN and NaN_3 (2:1:1 ratio) in a tantalum ampoule, heating it to 973 K and cooling it slowly (6 K min^{-1}) over a period of a week.

Crystal data

Na_3YCl_6
M_r = 370.58
Monoclinic, $P2_1/n$
a = 6.856 (1) Å
b = 7.255 (1) Å
c = 10.144 (1) Å
β = 90.87 (1)°
V = 504.51 (12) Å^3
Z = 2
D_x = 2.439 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6796 reflections
θ = 3.5–28.3°
μ = 7.42 mm^{-1}
T = 293 (2) K
Block, colourless
0.13 × 0.09 × 0.04 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.498, T_{max} = 0.743
6796 measured reflections
1258 independent reflections
1055 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 28.3°
$h = -9 \rightarrow 9$
$k = -9 \rightarrow 9$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.059
S = 1.02
1258 reflections
49 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Y—Cl3^{i}	2.6120 (8)	Na1—Cl2^{ii}	3.1923 (18)
Y—Cl2^{i}	2.6226 (8)	Na1—Cl3^{v}	3.3091 (18)
Y—Cl1^{i}	2.6362 (8)	Na2—Cl3^{vi}	2.7218 (8)
Na1—Cl3^{ii}	2.8247 (17)	Na2—Cl2^{vii}	2.7786 (8)
Na1—Cl1^{iii}	2.8433 (16)	Na2—Cl1^{viii}	2.8588 (8)
Na1—Cl2^{iv}	2.8517 (17)		
Cl3^{i}—Y—Cl3	180.0	Cl3—Y—Cl1^{i}	88.22 (3)
Cl3^{i}—Y—Cl2^{i}	88.72 (3)	Cl2^{i}—Y—Cl1^{i}	88.33 (3)
Cl3—Y—Cl2^{i}	91.28 (3)	Cl2—Y—Cl1^{i}	91.67 (3)
Cl2^{i}—Y—Cl2	180.0	Cl1^{i}—Y—Cl1	180.0
Cl3^{i}—Y—Cl1^{i}	91.78 (3)		

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

The structure of Na_3YCl_6 was refined using the coordinates of Na_3HoCl_6 (Böcker *et al.*, 2001) as starting parameters. All atoms were refined with anisotropic displacement parameters.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

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