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Potassium tetrachlorogallate

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Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(Ga–Cl) = 0.002 Å
R factor = 0.047
wR factor = 0.117
Data-to-parameter ratio = 27.9

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

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From a solution of potassium tetrachloroplatinate and gallium trichloride in benzene, potassium tetrachlorogallate, $K[GaCl_4]$, could be crystallized and its structure determined. The crystal structure is isotypic with $Ga[AlCl_4]$. It consists of tetrahedral anions $GaCl_4^-$ and potassium cations which are coordinated by Cl^- in a tricapped trigonal prismatic geometry.

Comment

The structure of $K[GaCl_4]$ consists of K^+ ions and tetrahedral $[GaCl_4]^-$ ions. The two ions are displayed in Fig. 1. Fig. 2 shows the arrangement in the unit cell. The K^+ ion is coordinated by nine Cl^- ions. The coordination polyhedron can be described as a tricapped trigonal prism. The anions show only a very slight distortion, with interatomic distances ranging from 2.1677 (19) to 2.1730 (17) Å. The angles are in the range 106.05 (7) to 113.13 (9)°, thus rather close to the ideal tetrahedral angle. The structure is isotypic with a number of other structures of the composition $M^{I}[M^{III}X_4]$, which have been published earlier. $K[AlCl_4]$ (Mairesse *et al.*, 1978) and $K[FeCl_4]$ (Cerisier *et al.*, 1988) have apparently the same structure. However, they crystallized in space group $P2_1$, thus

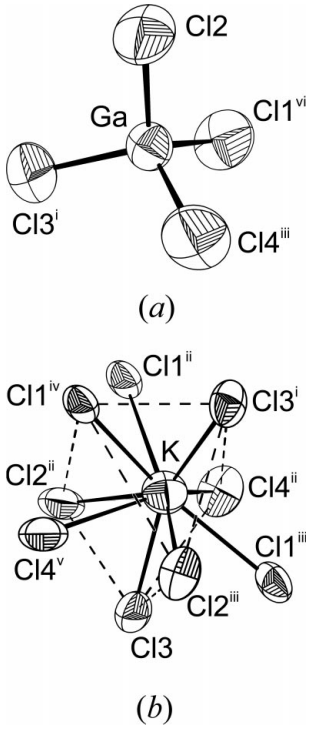

Figure 1
The (*a*) $GaCl_4^-$ anion and (*b*) K^+ cation with surrounding Cl^- ions in the structure of $K[GaCl_4]$. Displacement ellipsoids are drawn at the 70% probability level. Symmetry codes are in Table 1.

lacking the inversion centre. Ga[$AlCl_4$] (Staffel & Meyer, 1987) is reported with the same structure as the title compound.

Experimental

$GaCl_3$ (Aldrich Chemical Company, 99.99%, H_2O < 100 p.p.m.) was used as purchased. $K_2[PtCl_4]$ was synthesized according to a literature procedure (Chernyaev, 1964). Toluene was dried prior to use. Carbon monoxide of 99.9995% purity was used. The synthesis of the starting solution was performed in a glove-box under an inert atmosphere of dry nitrogen (< 1 p.p.m. H_2O). Toluene (2.56 g) was added to the solid mixture of $K_2[PtCl_4]$ (100 mg, 0.241 mmol) and $GaCl_3$ (400 mg, 2.272 mmol). The colour of the solution turned red–brown. After 5–10 min, the liquid separated into two phases, *viz*. a lower dark brown and an upper light brown layer, in an approximate 1:5 ratio by volume. Carbon monoxide was bubbled through the solution (both phases) at room temperature for 2 h. As a by-product, pale yellow crystals of the title compound formed; these were washed twice with toluene.

Crystal data

K[$GaCl_4$]	D_x = 2.373 Mg m^{-3}
M_r = 250.63	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2561 reflections
a = 7.2230 (3) Å	θ = 4.2–27.1°
b = 10.4377 (4) Å	μ = 5.91 mm^{-1}
c = 9.3194 (4) Å	T = 297 K
β = 93.290 (2)°	Irregular, colourless
V = 701.45 (5) Å^3	0.60 × 0.25 × 0.15 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	1537 independent reflections
φ and ω scans	1323 reflections with $I > 2\sigma(I)$
Absorption correction: numerical (Herrendorf & Bärnighausen, 1997)	R_{int} = 0.037
	θ_{max} = 27.1°
T_{min} = 0.304, T_{max} = 0.438	$h = -9 \rightarrow 9$
4148 measured reflections	$k = -12 \rightarrow 13$
	$l = -8 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 2.9803P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.047	
$wR(F^2)$ = 0.117	
S = 1.17	$(\Delta/\sigma)_{max}$ < 0.001
1537 reflections	$\Delta\rho_{max}$ = 0.90 e Å^{-3}
55 parameters	$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Table 1
Selected geometric parameters (Å).

K—Cl3^{i}	3.196 (2)	K—Cl4^{v}	3.727 (3)
K—Cl4^{ii}	3.251 (3)	K—Cl1^{ii}	3.761 (3)
K—Cl3	3.260 (2)	Ga—Cl2	2.1668 (17)
K—Cl2^{iii}	3.304 (3)	Ga—Cl4^{iii}	2.1677 (19)
K—Cl1^{iv}	3.310 (2)	Ga—Cl1^{vi}	2.1679 (15)
K—Cl2^{ii}	3.322 (3)	Ga—Cl3^{i}	2.1730 (17)
K—Cl1^{iii}	3.572 (3)		

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

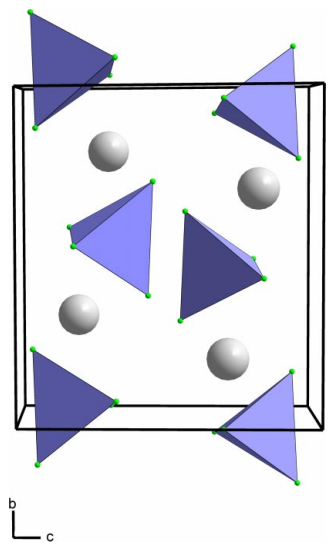

Figure 2
The unit cell of K[$GaCl_4$], viewed along *a*.

Data collection: *KappaCCD Software* (Nonius, 1997); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *maXus* (Mackay *et al.*, 1998).

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