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Triamminetrichloroindium(III), $[InCl_3(NH_3)_3]$

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(In–N) = 0.004 Å
R factor = 0.028
wR factor = 0.073
Data-to-parameter ratio = 18.1

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

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The triammoniate of indium(III) chloride has been obtained as single crystals from the reaction of indium metal and ammonium chloride in a sealed Monel metal container. It crystallizes as a salt with $[In(NH_3)_4Cl_2]^+$ and $[In(NH_3)_2Cl_4]^-$ ions, both of which lie on inversion centers.

Comment

The triammoniate of indium(III) chloride, $In(NH_3)_3Cl_3$, crystallizes as a salt containing the complex ions $[In(NH_3)_4Cl_2]^+$ and $[In(NH_3)_2Cl_4]^-$. Both the cations and anions are distorted octahedra. In the cations, In^{3+} is surrounded equatorially by four ammine ligands, with In—N distances around 2.25 Å, and axially by two chloride ligands, at distances of 2.51 Å. In the anions, In^{3+} is surrounded equatorially by four chloride ligands, with In—Cl distances around 2.53 Å, and axially by two ammine ligands, at distances of 2.23 Å (precise bond lengths are given in Table 1). The complex cations and anions are arranged in a pseudo-body-centered fashion. The crystal structure of the analogous complex $Al(NH_3)_3Cl_3$ was first determined by Jacobs & Nöcker (1992, 1993) and was recently redetermined by Bremm & Meyer (2001).

Experimental

Ammonium chloride, NH_4Cl, and indium metal were sealed under inert conditions (argon dry-box) in 1:1 to 3:1 molar ratios in Monel metal ($Cu_{32}Ni_{68}$) containers which were jacketed with silica ampoules. The reaction mixtures were heated for 4–7 d at temperatures between 673 and 773 K. The ampoules were opened in a dry-box. Colourless single crystals of $In(NH_3)_3Cl_3$ were thus obtained.

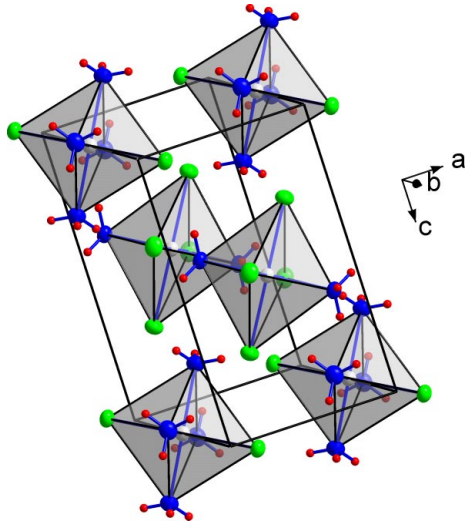

Figure 1
The unit cell of $In(NH_3)_3Cl_3$.

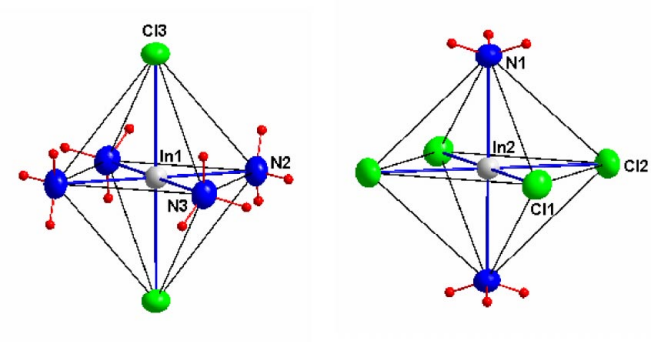

Figure 2
The $[In(NH_3)_4Cl_2]^+$ and $[In(NH_3)_2Cl_4]^-$ ions in $In(NH_3)_3Cl_3$. Displacement ellipsoids are drawn at the 50% probability level.

Crystal data

$[In(NH_3)_4Cl_2]^+\cdot[In(NH_3)_2Cl_4]^-$	$Z = 1$
$M_r = 544.54$	$D_x = 2.327$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 5.8652$ (15) Å	Cell parameters from 1719 reflections
$b = 6.8130$ (18) Å	$\theta = 1.9$–$26°$
$c = 9.794$ (2) Å	$\mu = 3.98$ mm^{-1}
$\alpha = 86.14$ (3)°	$T = 293$ (2) K
$\beta = 86.68$ (3)°	Irregular, colourless
$\gamma = 85.26$ (3)°	0.25 × 0.15 × 0.10 mm
$V = 388.59$ (17) Å^3	

Data collection

Stoe IPDS diffractometer	$R_{int} = 0.023$
φ scans	$\theta_{max} = 26.0°$
Absorption correction: none	$h = -6 \rightarrow 7$
1719 measured reflections	$k = -8 \rightarrow 7$
1234 independent reflections	$l = -12 \rightarrow 12$
1049 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0559P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.028$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.073$	$\Delta\rho_{max} = 0.81$ e Å^{-3}
$S = 0.96$	$\Delta\rho_{min} = -0.75$ e Å^{-3}
1234 reflections	Extinction correction: *SHELXL*97
68 parameters	Extinction coefficient: 0.023 (3)
H-atom parameters constrained	

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl2^{i}	0.89	2.61	3.415 (4)	150
N1—H1B···Cl2^{ii}	0.89	2.74	3.470 (4)	141
N1—H1C···Cl3^{ii}	0.89	2.52	3.349 (4)	156
N2—H2A···Cl2^{i}	0.89	2.72	3.476 (5)	144
N2—H2B···Cl1^{ii}	0.89	2.85	3.659 (5)	151
N2—H2C···Cl3^{iii}	0.89	2.73	3.376 (5)	131
N3—H3A···Cl1^{iv}	0.89	2.82	3.484 (5)	132
N3—H3B···Cl2	0.89	2.74	3.602 (4)	163
N3—H3C···Cl1^{v}	0.89	2.69	3.504 (5)	153

Symmetry codes: (i) $1+x, y, z$; (ii) $1-x, 1-y, 1-z$; (iii) $x, y, 1+z$; (iv) $-x, 1-y, 1-z$; (v) $-x, -y, 1-z$.

Atomic parameters were obtained for the H atoms using the HFIX 133 instruction in *SHELXL*97 (Sheldrick, 1997). Interatomic distances and angles for the hydrogen bonding were generated using the HTAB instruction.

Data collection: *IPDS Software* (Stoe & Cie, 1996–1997); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; 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: *SHELXL*97.

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References

Brandenburg, K. (2001). *DIAMOND*. Version 2.1e. Crystal Impact GbR, Bonn, Germany.
Bremm, S. & Meyer, G. (2001). *Z. Anorg. Allg. Chem.* **627**, 407–410.
Jacobs, H. & Nöcker, B. (1992). *Z. Anorg. Allg. Chem.* **614**, 25–29.
Jacobs, H. & Nöcker, B. (1993). *Z. Anorg. Allg. Chem.* **619**, 73–76.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Stoe & Cie (1996–1997). *IPDS Software*. Stoe & Cie, Darmstadt, Germany.