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## An $\eta^6$ -Toluene Complex of Neodymium: $[\text{Nd}(\eta^6\text{-C}_6\text{H}_5\text{CH}_3)(\text{AlCl}_4)_3]$

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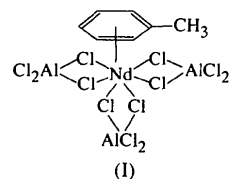
### Abstract

The Nd<sup>III</sup> ion in hexa- $\mu$ -chloro-1:2 $\kappa^2$ Cl;1:3 $\kappa^2$ Cl;1:4 $\kappa^2$ Cl-hexachloro-2 $\kappa^2$ Cl,3 $\kappa^2$ Cl,4 $\kappa^2$ Cl-[1( $\eta^6$ )-toluene]trialuminiumneodymium has distorted pentagonal bipyramidal coordination geometry. Five Cl atoms form the equatorial plane, and the toluene ring and the sixth Cl atom occupy the apical sites. The average Nd—C( $\eta^6$ ) and Nd—Cl distances are 2.926 (5) and 2.857 (1) Å, respectively.

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## Comment

$\eta^6$ -Arene-lanthanoid complexes have special catalytic properties (Hu, Tian, Shen & Liang, 1992). We are interested in the chemical behaviour of such complexes when sterically congested ligands are present. During an attempt to synthesize  $[\text{Nd}(\eta^6\text{-1,3,5-}^t\text{BuC}_6\text{H}_3)(\text{AlCl}_4)_3]$  in toluene solution, the title complex, (I), was isolated instead.



A molecule of (I) (Fig. 1) consists of one Nd atom, one toluene molecule and three aluminium tetrachloride ions. The coordination number of Nd<sup>III</sup> may be regarded as nine provided that toluene is thought to occupy three vertices of the polyhedron. Alternatively, the coordination polyhedron can be viewed as a distorted pentagonal bipyramid. The equatorial plane comprises five Cl atoms (Cl1, Cl2, Cl3, Cl4 and Cl5), with Cl6 and the centroid of the toluene ring occupying the apical positions. This mode of coordination is similar to those of related Ln<sup>III</sup> compounds (Cotton & Schwotzer, 1986; Fan, Shen & Lin, 1989a; Biagini, Lugli & Millini, 1994) with distorted pentagonal bipyramidal coordination. The equatorial Nd—Cl bond lengths are 2.846 (1)–2.902 (1) Å, rather longer than the apical Nd—Cl6 distance of 2.799 (1) Å. Very similar values have been found for the isomorphous and isostructural Sm compound (Fan, Shen & Lin, 1989b).

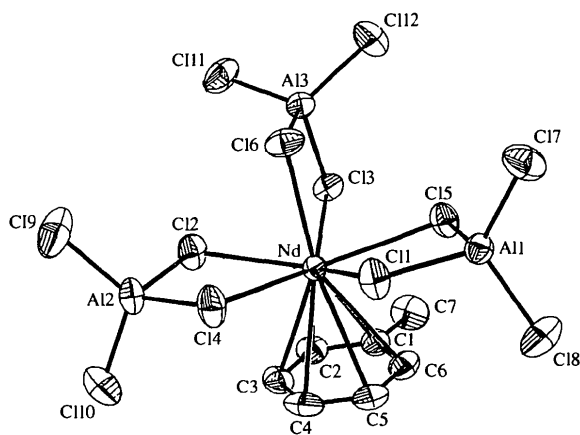


Fig. 1. Molecular structure of (I) showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

## Experimental

The synthesis of the title compound was conducted under argon by Schlenk techniques. Crystals were obtained by reac-

tion of NdCl<sub>3</sub>, 1,3,5-<sup>t</sup>BuC<sub>6</sub>H<sub>3</sub> and AlCl<sub>3</sub> (molar ratio 1:1:3) in toluene for 30 min at 353 K, followed by crystallization at 268 K.

#### Crystal data

[Al<sub>3</sub>NdCl<sub>12</sub>(C<sub>7</sub>H<sub>8</sub>)]

*M<sub>r</sub>* = 742.761

Monoclinic

*P*2<sub>1</sub>/*n*

*a* = 9.728 (3) Å

*b* = 19.856 (11) Å

*c* = 12.939 (4) Å

$\beta$  = 103.75 (3)°

*V* = 2427.7 (14) Å<sup>3</sup>

*Z* = 4

*D<sub>x</sub>* = 2.032 Mg m<sup>-3</sup>

*D<sub>m</sub>* not measured

Mo *K*α radiation

$\lambda$  = 0.71069 Å

Cell parameters from 25 reflections

$\theta$  = 2.62–12.63°

$\mu$  = 3.580 mm<sup>-1</sup>

*T* = 298 K

Needle

0.44 × 0.28 × 0.24 mm

Yellow

#### Data collection

Nicolet R3m/E diffractometer

$\omega$ -2 $\theta$  scans

Absorption correction:

$\psi$  scans (SHELXTL);

Sheldrick, 1984)

*T<sub>min</sub>* = 0.265, *T<sub>max</sub>* = 0.642

5982 measured reflections

5837 independent reflections

4236 reflections with

*I* > 3 $\sigma$ (*I*)

*R<sub>int</sub>* = 0.017

$\theta_{\max}$  = 28.0°

*h* = 0 → 13

*k* = 0 → 27

*l* = 0 → 18

2 standard reflections

every 100 reflections

intensity decay: none

#### Refinement

Refinement on *F*<sup>2</sup>

*R* = 0.039

*wR* = 0.038

*S* = 1.464

4236 reflections

208 parameters

H atoms not refined

*w* = 1/[ $\sigma^2(F) + 0.0002F^2$ ]

( $\Delta/\sigma$ )<sub>max</sub> = 0.051

$\Delta\rho_{\max}$  = 0.46 e Å<sup>-3</sup>

$\Delta\rho_{\min}$  = -1.33 e Å<sup>-3</sup>

(near the Nd atom)

Extinction correction: none

Scattering factors from

SHELXTL

Table 1. Selected geometric parameters (Å, °)

Nd—C11	2.864 (1)	Nd—C1	2.999 (6)
Nd—C12	2.902 (1)	Nd—C2	2.910 (5)
Nd—C13	2.857 (1)	Nd—C3	2.879 (5)
Nd—C14	2.846 (1)	Nd—C4	2.871 (5)
Nd—C15	2.875 (1)	Nd—C5	2.923 (5)
Nd—C16	2.799 (1)	Nd—C6	2.976 (6)
C11—Nd—C14	69.8 (1)	C12—Nd—C14	69.4 (1)
C11—Nd—C15	69.4 (1)	C13—Nd—C15	71.7 (1)
C11—Nd—C16	81.2 (1)	C13—Nd—C16	72.2 (1)
C12—Nd—C13	73.7 (1)		

The main program used was SHELXTL (Sheldrick, 1984). The structure was solved by the Patterson method and refined by least-squares calculations, initially with isotropic and finally with anisotropic displacement parameters for the non-H atoms. H atoms were not observed in difference maps but were placed in the calculated positions and assigned an isotropic displacement parameter *U*<sub>iso</sub> of 0.08 Å<sup>2</sup>.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: MUI314). Services for accessing these data are described at the back of the journal.

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### Piperazine (and Derivatives) Platinum(II) Complexes: *trans*-Bis(*N*-methylpiperazine-*N,N'*)platinum(II) Dichloride Tetrahydrate

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#### Abstract

The title compound, *trans*-[L<sub>2</sub>Pt<sup>II</sup>]<sup>2+</sup>·2Cl<sup>-</sup>·4H<sub>2</sub>O, (*L* = *N*-methylpiperazine), [Pt(C<sub>5</sub>H<sub>12</sub>N<sub>2</sub>)<sub>2</sub>]Cl<sub>2</sub>·4H<sub>2</sub>O, has been synthesized in the course of our work on complexes formed by the Pt<sup>2+</sup> ion with piperazine derivatives. X-ray diffraction analysis showed that two *N*-methylpiperazine molecules bind one Pt<sup>2+</sup> ion in such a way that the two methyl groups lie in opposite directions with respect to the Pt atom. The coordination around the Pt atom is square planar with four N atoms occupying the coordination sites, and the coordination plane is perfectly planar because the Pt atom lies on a centre of symmetry. This type of coordination imposes a boat conformation on the six-membered *N*-methylpiperazine ring. As found in other *N*-methylpiperazine complexes, the molecule has a local mirror plane coincident with the square-planar coordination plane and nearly bisecting the piperazine six-membered ring.