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**Key indicators**

Single-crystal X-ray study  
 T = 130 K  
 Mean  $\sigma(C-C)$  = 0.007 Å  
 R factor = 0.045  
 wR factor = 0.098  
 Data-to-parameter ratio = 15.5

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

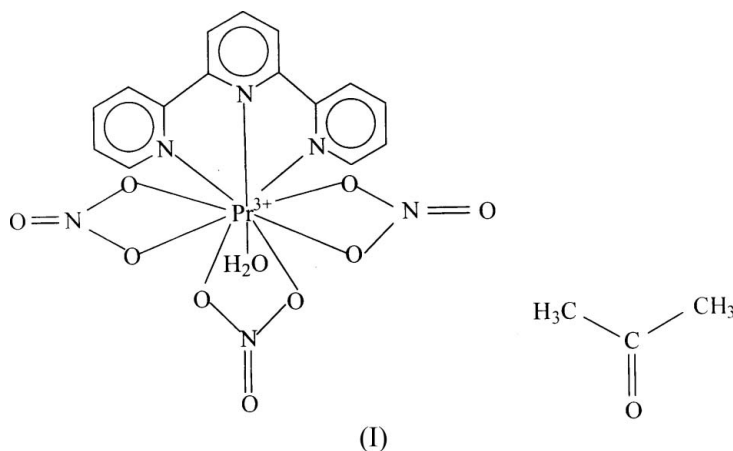
**Aquatris(nitrato- $\kappa^2O,O'$ )(2,2':6,2''-terpyridine)-  
 praseodymium(III) acetone solvate**

The Pr atom in the title complex,  $[Pr(NO_3)_3(C_{15}H_{11}N_3)(H_2O)] \cdot C_3H_6O$ , is ten-coordinated and the arrangement can be described as a distorted bicapped square antiprism.

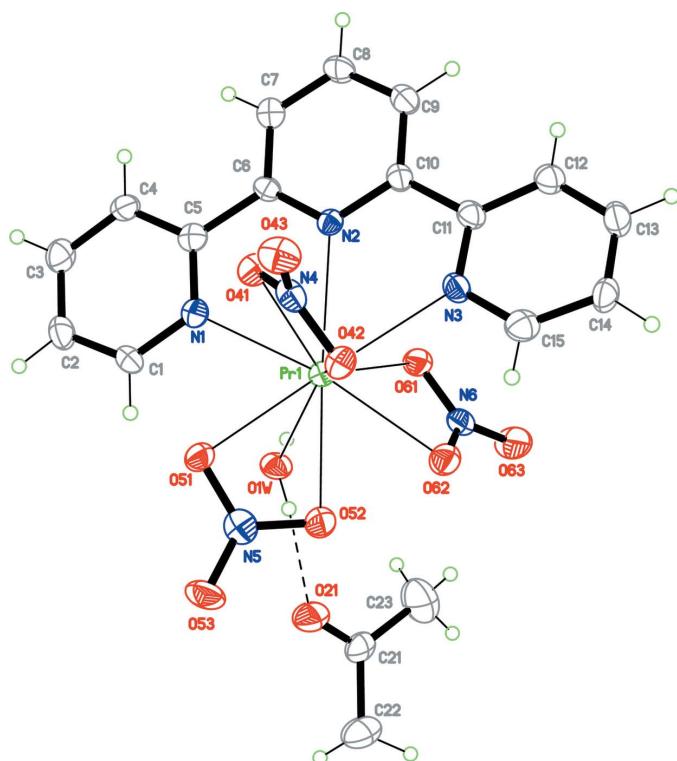
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**Comment**

The reprocessing of spent nuclear fuel includes the extraction and subsequent separation of trivalent actinides from trivalent lanthanides. A search for ligands suitable for the selective separation of elements from nitric acid solutions into the organic phase has been carried out (Chan *et al.*, 1996, 1997; Drew *et al.*, 1998). 2,2'-6,2''-Terpyridine (terpy) and its derivatives are among such ligands (Byers *et al.*, 1996; Drew *et al.*, 2000). The title compound,  $[Pr(NO_3)_3(terpy)(H_2O)] \cdot (CH_3)_2CO$ , (I), is a new complex with Pr, which represents the beginning of the lanthanide series.



The crystal structure of (I) (Fig. 1) consists of neutral  $[Pr(NO_3)_3(terpy)(H_2O)]$  complexes and acetone molecules, which are linked *via* hydrogen bonds (Table 2). In the  $[Pr(NO_3)_3(terpy)(H_2O)]$  complex, the Pr atom is coordinated by the tridentate terpy molecule, three bidentate nitrate ions and a water molecule. The mean Pr–ligand distances have the following values: Pr–N = 2.616 (4), Pr–O<sub>aqua</sub> = 2.513 (3) and Pr–O<sub>nitro</sub> = 2.572 (3) Å. The coordination number of the Pr<sup>3+</sup> cation is 10, and the polyhedron is described as a distorted bicapped square antiprism. The bicapped square antiprism is characterized as the most stable stereochemistry for ten-coordinate compounds (Kepert, 1982). In most of the previously published terpy adducts of lanthanide nitrates with the same composition of the coordination sphere for the metal atoms, for example  $[Nd(NO_3)_3(terpy)(H_2O)]$  and  $[Er(NO_3)_3(terpy)(H_2O)]$  (Drew *et al.*, 2000), and  $[Eu(NO_3)_3(terpy)(H_2O)]$  and  $[Tb(NO_3)_3(terpy)(H_2O)]$



**Figure 1**  
The molecular structure of (I), showing 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

(Cotton *et al.*, 2003), the coordination polyhedron is described as a sphenocorona, with the water molecule at the apical vertex, as seen in Fig. 2.

## Experimental

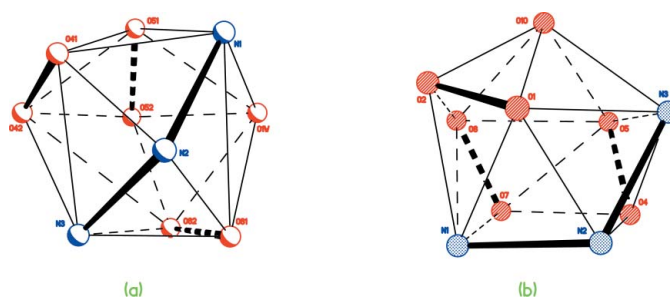
NaNO<sub>3</sub> (20 mg) was added to a solution (1 ml) containing Pr(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O (0.05 mol) and 2,2'-6,2''-terpyridine (0.025 mol). Heating the solution to 323 K resulted in precipitation of compound (I). Green crystals of (I) were obtained from an acetone solution.

### Crystal data

[Pr(NO <sub>3</sub> ) <sub>3</sub> (C <sub>15</sub> H <sub>11</sub> N <sub>3</sub> )(H <sub>2</sub> O)]·C <sub>3</sub> H <sub>6</sub> O	$D_x = 1.838 \text{ Mg m}^{-3}$
$M_r = 636.30$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 16338 reflections
$a = 9.7282 (6) \text{ \AA}$	$\theta = 2-27.5^\circ$
$b = 15.7656 (10) \text{ \AA}$	$\mu = 2.19 \text{ mm}^{-1}$
$c = 15.1477 (10) \text{ \AA}$	$T = 130 (2) \text{ K}$
$\beta = 98.183 (6)^\circ$	Plate, green
$V = 2299.6 (3) \text{ \AA}^3$	$0.44 \times 0.19 \times 0.03 \text{ mm}$
$Z = 4$	

### Data collection

Nonius KappaCCD area-detector diffractometer	5204 independent reflections
$\varphi$ and $\omega$ scans	3727 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (MULABS; Blessing, 1995)	$R_{\text{int}} = 0.099$
$T_{\text{min}} = 0.619$ , $T_{\text{max}} = 0.925$	$\theta_{\text{max}} = 27.5^\circ$
16338 measured reflections	$h = -12 \rightarrow 10$
	$k = -20 \rightarrow 19$
	$l = -19 \rightarrow 16$



**Figure 2**  
The coordination polyhedron of Pr in (a) (I) and (b) [Eu(NO<sub>3</sub>)<sub>3</sub>(terpy)(H<sub>2</sub>O)] (Cotton *et al.*, 2003).

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.045$   
 $wR(F^2) = 0.098$   
 $S = 0.98$   
 5204 reflections  
 335 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0334P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 1.12 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -1.48 \text{ e \AA}^{-3}$

**Table 1**

Selected bond lengths ( $\text{\AA}$ ).

Pr1—O1W	2.513 (3)	Pr1—N1	2.598 (4)
Pr1—O62	2.530 (3)	Pr1—O61	2.605 (3)
Pr1—O52	2.537 (3)	Pr1—N3	2.614 (4)
Pr1—O41	2.558 (3)	Pr1—O42	2.632 (3)
Pr1—O51	2.569 (3)	Pr1—N2	2.640 (4)

**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1 $\cdots$ O43 <sup>i</sup>	0.99 (6)	1.94 (6)	2.825 (5)	148 (5)
O1W—H2 $\cdots$ O21	0.80 (6)	1.90 (6)	2.694 (5)	168 (6)

Symmetry code: (i)  $x, -y + \frac{1}{2}, z + \frac{1}{2}$ .

The H atoms of the water molecule were located in a difference Fourier map and refined isotropically. All H atoms on C atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 or 0.96  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2-1.5U_{\text{eq}}(\text{C})$ . A rotating-group model was used for the methyl group. The highest peak and deepest hole are 0.97 and 0.88  $\text{\AA}$ , respectively, from the Pr atom.

Data collection: COLLECT (Nonius, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997); data reduction: SCALEPACK (Otwinowski & Minor, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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