fraction (Michel & Raveau, 1982) and then by single-crystal diffractometry (Hazen *et al.*, 1987).

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Tetraaquatrinitratopraseodymium–4,4′-Bipyridine–Water (1/2/1)

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Abstract. $[Pr(NO_3)_3(H_2O)_4].2C_{10}H_8N_2.H_2O$, $M_r = 729{\cdot}4$, orthorhombic, $P2_12_12_1$, $a = 7{\cdot}142\ (3)$, $b = 16{\cdot}119\ (12)$, $c = 24{\cdot}816\ (24)$ Å, $V = 2857\ (6)$ Å^3, $Z = 4$, $D_x = 1{\cdot}695$ g cm^{-3}, $\lambda(\text{Cu } K\alpha) = 1{\cdot}5418$ Å, $\mu = 140$ cm^{-1}, $F(000) = 1452$, $T = 294$ K, $R = 0{\cdot}051$ for 1270 observed reflections. The compound is isostructural with the neodymium analogue [Al-Rasoul & Drew (1987). *Acta Cryst.* C**43**, 2081–2084] apart from having larger [32, 34 (2)°] dihedral angles between the rings of the 4,4′-bpy molecules. The complex contains ten-coordinate Pr with three bidentate nitrate ligands [Pr—O 2·52–2·75 (3) Å] and four aqua ligands [Pr—O 2·46–2·48 (2) Å], and has approximate twofold symmetry. The complex, the 4,4′-bpy molecules, and the lattice water molecule are linked *via* a three-dimensional system of hydrogen bonds.

Experimental. Preparation: Weakley (1982). Intensity data from multi-film Weissenberg photographs (layers 0–4*kl*, *h*0–5*l*), scanned by microdensitometer (SERC Service, Daresbury Laboratory, Warrington, England); crystal dimensions $0{\cdot}17 \times 0{\cdot}17 \times 0{\cdot}45$ and $0{\cdot}15 \times 0{\cdot}15 \times 0{\cdot}39$ mm; merging $R = 0{\cdot}094$ before, 0·068 after absorption correction (transmission factors 0·091 to 0·375); range of indices $0 \le h \le 8$, $0 \le k \le 19$, $0 \le l \le 30$. The data films showed sharp reflections to high angles ($2\theta_{max} = 143°$) but in many festoons the reflections were all weak or absent. The only *systematic* absence appeared to be 0*kl* for *k* odd [the absences in *h*00 and 00*l* were taken to be special cases of the general weakness of *h*0*l* reflections with $(h + l)$ odd], but attempts to solve the structure in space groups $Pbm2$, $Pb2_1m$ and $Pbmm$ were unsuccessful (Weakley, 1984). The similarity of the cell parameters to those of the Nd compound (Al-Rasoul & Drew, 1987) prompted a successful structure solution in $P2_12_12_1$: Pr coordinates from Patterson synthesis, other non-H atoms from difference syntheses (problem of false mirror symmetry from situation of Pr at $z \simeq 0{\cdot}25$); anisotropic thermal parameters for Pr, NO_3, water O atoms; 4,4′-bpy C, N isotropic; H atoms included at calculated positions riding on C atoms; blocked-matrix least-squares refinement (on *F*) converged at $R = 0{\cdot}051$, $wR = 0{\cdot}070$, 250 parameters, 1270 independent data, function minimized $\sum w(\Delta F)^2$; $w = [1 + 0{\cdot}00545F^2]^{-1}$, max. $\Delta/\sigma = 0{\cdot}18$ in last cycle, final $\Delta\rho$ synthesis flat to $\pm 0{\cdot}90$ e Å^{-3}. All calculations by use of *SHELX*76 (Sheldrick, 1976), which incorporated atomic scattering factors taken from *International Tables for X-ray Crystallography* (1974). Atomic coordinates are given in Table 1, and selected dimensions in Table 2.† The labelling of atoms is shown in Fig. 1.

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† Lists of structure factors, anisotropic thermal parameters, remaining bond lengths and angles, and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51462 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Atomic coordinates* ($\times 10^4$) *and isotropic or equivalent isotropic thermal parameters* ($Å^2 \times 10^3$)

	x	y	z	U_{eq}
Pr(1)	2088 (2)	579 (1)	2483 (1)	33 (1)†
N(10)	−629 (34)	881 (12)	1556 (7)	43 (6)†
O(11)	1108 (35)	924 (13)	1488 (7)	75 (8)†
O(12)	−1319 (35)	813 (15)	1998 (8)	81 (9)†
O(13)	−1551 (30)	879 (14)	1125 (6)	72 (8)†
N(20)	2180 (43)	2448 (11)	2452 (14)	57 (8)†
O(21)	717 (34)	2086 (13)	2513 (23)	140 (14)†
O(22)	3528 (36)	1996 (15)	2578 (23)	195 (25)†
O(23)	2100 (30)	3217 (11)	2446 (13)	81 (8)†
N(30)	4708 (44)	946 (14)	3450 (10)	74 (10)†
O(31)	2969 (34)	1004 (17)	3484 (9)	86 (9)†
O(32)	5325 (35)	877 (18)	2968 (9)	94 (12)†
O(33)	5841 (36)	928 (14)	3830 (9)	79 (9)†
N(41)	4907 (38)	1378 (19)	6091 (11)	63 (7)
C(42)	4545 (51)	2142 (22)	6128 (14)	71 (9)
C(43)	4630 (44)	2787 (18)	5722 (11)	57 (7)
C(44)	5054 (41)	2532 (17)	5200 (11)	49 (7)
C(45)	5369 (41)	1714 (18)	5138 (11)	52 (7)
C(46)	5277 (45)	1150 (21)	5575 (13)	67 (8)
C(47)	5102 (36)	3159 (17)	4726 (8)	42 (5)
C(48)	5712 (48)	3899 (21)	4851 (13)	66 (8)
C(49)	5772 (52)	4454 (25)	4389 (13)	79 (9)
N(410)	5200 (36)	4246 (16)	3890 (9)	61 (7)
C(411)	4710 (49)	3445 (23)	3808 (13)	67 (9)
C(412)	4674 (39)	2900 (16)	4232 (10)	49 (7)
N(71)	−944 (36)	−785 (14)	3887 (9)	59 (6)
C(72)	−362 (42)	−1604 (9)	3804 (11)	59 (7)
C(73)	−384 (40)	−2223 (17)	4204 (10)	53 (6)
C(74)	−885 (42)	−1976 (17)	4711 (11)	58 (7)
C(75)	−1419 (39)	−1161 (17)	4813 (9)	50 (6)
C(76)	−1496 (42)	−512 (20)	4381 (11)	63 (7)
C(77)	−900 (36)	−2607 (13)	5165 (8)	39 (5)
C(78)	−1317 (34)	−3403 (13)	5044 (8)	35 (5)
C(79)	−1281 (40)	−3980 (16)	5474 (10)	52 (6)
N(710)	−929 (32)	−3729 (14)	5993 (8)	52 (5)
C(711)	−423 (41)	−2948 (19)	6110 (12)	65 (8)
C(712)	−413 (44)	−2318 (18)	5650 (11)	61 (7)
Aq(1)	4824 (30)	355 (11)	1884 (7)	63 (7)†
Aq(2)	3003 (33)	−691 (13)	2982 (8)	71 (8)†
Aq(3)	944 (36)	−659 (13)	2010 (6)	76 (9)†
Aq(4)	−694 (31)	293 (13)	3056 (8)	65 (8)†
Aq(5)	7057 (31)	2767 (14)	2435 (18)	96 (10)†

† $U_{eq} = \frac{1}{3}\sum_i \sum_j U_{ij} \mathbf{a}_i . \mathbf{a}_j a_i^* a_j^*$.

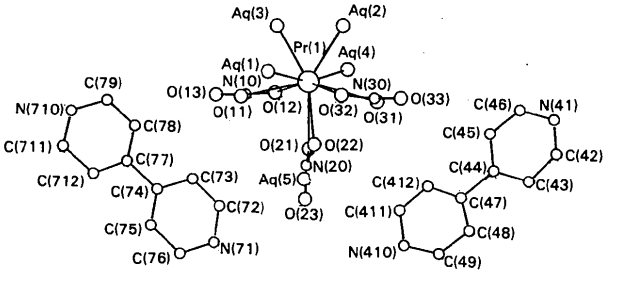

Fig. 1. The asymmetric unit of $[Pr(NO_3)_3(H_2O)_4].2C_{10}H_8N_2.H_2O$. A packing diagram for the Nd isomorph has been published (Al-Rasoul & Drew, 1987).

Table 2. *Selected bond lengths* (Å) *and interbond angles* (°)

Pr(1)–Aq(1)	2·48 (2)	N(10)–O(11)	1·25 (4)
Pr(1)–Aq(2)	2·48 (2)	N(10)–O(12)	1·21 (3)
Pr(1)–Aq(3)	2·46 (2)	N(10)–O(13)	1·26 (3)
Pr(1)–Aq(4)	2·48 (3)	N(20)–O(21)	1·21 (4)
Pr(1)–O(11)	2·63 (2)	N(20)–O(22)	1·25 (4)
Pr(1)–O(12)	2·75 (2)	N(20)–O(23)	1·24 (3)
Pr(1)–O(21)	2·62 (2)	N(30)–O(31)	1·25 (4)
Pr(1)–O(22)	2·52 (3)	N(30)–O(32)	1·28 (3)
Pr(1)–O(31)	2·65 (2)	N(30)–O(33)	1·24 (4)
Pr(1)–O(32)	2·65 (3)		

O(11)–Pr(1)–O(12)	47·2 (7)	O(21)–Pr(1)–Aq(4)	82·4 (10)
O(21)–Pr(1)–O(22)	46·2 (8)	O(31)–Pr(1)–Aq(4)	73·2 (10)
O(31)–Pr(1)–O(32)	47·2 (7)	O(32)–Pr(1)–Aq(4)	117·1 (10)
O(11)–Pr(1)–O(31)	152·8 (8)	Aq(1)–Pr(1)–Aq(2)	88·3 (6)
O(11)–Pr(1)–O(32)	128·4 (8)	Aq(1)–Pr(1)–Aq(3)	81·6 (7)
O(12)–Pr(1)–O(31)	125·6 (7)	Aq(1)–Pr(1)–Aq(4)	160·4 (8)
O(12)–Pr(1)–O(32)	161·0 (8)	Aq(2)–Pr(1)–Aq(3)	69·4 (7)
O(11)–Pr(1)–Aq(1)	71·1 (7)	Aq(2)–Pr(1)–Aq(4)	76·7 (9)
O(12)–Pr(1)–Aq(1)	117·0 (6)	Aq(3)–Pr(1)–Aq(4)	81·7 (9)
O(22)–Pr(1)–Aq(1)	82·2 (10)		

O(12)···Aq(1^{i})	2·87 (3)	N(410)···Aq(1^{iv})	2·63 (3)
O(21)···Aq(5^{i})	2·85 (4)	N(71)···Aq(4)	2·72 (4)
O(22)···Aq(5)	2·82 (4)	N(710)···Aq(2^{v})	2·83 (4)
O(32)···Aq(4^{ii})	3·02 (4)	Aq(2)···Aq(5^{vi})	2·69 (4)
N(41)···Aq(3^{iii})	2·63 (4)		

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

Related literature. Crystal structures of adducts of lanthanide nitrates, 4,4′-bipyridine and water: Bukowska-Strzyzewska & Tosik (1978), Al-Rasoul & Weakley (1982), Weakley (1982, 1984), Al-Rasoul & Drew (1987).

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