Electronic Supplementary Material (ESI) for Dalton Transactions. This journal is © The Royal Society of Chemistry 2016

Supplementary Data



Fig. S1. C-H...O(C) intra- and intermolecular bonding in crystalline L (shown in blue and red, respectively). Hydrogen atoms not involved in H-bonding are omitted for clarity.



Fig. S2. C-H...O(C) intra- and intermolecular bonding in crystalline complex **1** (shown in blue and red, respectively). Hydrogen atoms not involved in H-bonding are omitted for clarity.



Fig. S3. C–H...O(C) intra- and intermolecular bonding in crystalline isostructural complexes **3**, **4** (shown in blue and red, respectively). Hydrogen atoms and solvate molecules not involved in H-bonding are omitted for clarity. For **3** and **4** the values of bond lengths are divided by slash.



Fig. S4. C–H...O(C) and O–H...O(P) intra- and intermolecular bonding in crystalline complex **5** (shown in blue and red, respectively). Hydrogen atoms not involved in H-bonding are omitted for clarity.

| Compound | v(N=O) | $v_{as}(NO_2)$ | v _s (NO ₂) | δ (out-of- plane) | γ (bending in plane) |
|----------|---------------------------|----------------|-----------------------------------|-------------------------|----------------------------|
| 1 | 1518, 1483 | 1308,1282 | 1039,1032 | 812 | 748 |
| 3 | 1458br | 1313,1295sh | 1031 | 820 | 732 |
| 4 | 1503,1468 | 1300 | 1031 | 818 | 730 |
| 6 | 1518sh, 1494 | 1310 | 1030 | 815 | 747 |
| 4 6 | 1503,1468 1518sh, 1494 | 1300 1310 | 1031 1030 | 818 815 | 730 747 |

Table S1. Selected IR data (v, δ and γ , cm⁻¹) and assignments^a for complexes 1, 3–6^b

^a K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, *Part B, Applications in Coordination, Organometallic, and Bioinorganic Chemistry*, Wiley, New York, 6th Edition, 2009, 424 pp.

^b Spectral data for coordinated nitrate ions in complexes **4** and **5** are identical.

Table S2. Extraction of *f*-block elements by ligandes L and L' (0.01 M solutions in CHCl₃) from 3.75 M HNO₃; the initial concentration of lanthanide and uranyl nitrates in the aqueous phase is $2.5 \cdot 10^{-4}$ M.

| Distribution ratios (D _M) | | | | | | | |
|---------------------------------------|--|---|--|---|--|--|--|
| U(VI) | La(III) | Nd(III) | Ho(III) | Yb(III) | | | |
| | | | | | | | |
| 37.2 ± 1.5 | 0.58 ± 0.01 | 0.65 ± 0.01 | 0.69 ± 0.01 | 1.05 ± 0.01 | | | |
| 6.4 ± 0.2 | | 0.18 ± 0.01 | 0.20 ± 0.01 | | | | |
| | U(VI) 37.2 ± 1.5 6.4 ± 0.2 | $\begin{array}{c} & \text{Dis} \\ U(\text{VI}) & \text{La(III)} \\ 37.2 \pm 1.5 & 0.58 \pm 0.01 \\ 6.4 \pm 0.2 \end{array}$ | Distribution ratios (IU(VI)La(III)Nd(III) 37.2 ± 1.5 0.58 ± 0.01 0.65 ± 0.01 6.4 ± 0.2 0.18 ± 0.01 | Distribution ratios (D_M)U(VI)La(III)Nd(III)Ho(III)37.2 ± 1.50.58 ± 0.010.65 ± 0.010.69 ± 0.016.4 ± 0.20.18 ± 0.010.20 ± 0.01 | | | |



Fig. S6. ¹³C NMR spectrum of L (0.02 M solution in CD₃CN).



Fig. S7. ¹H NMR spectrum of complex 1 (saturated solution, ~ 0.003 M, in CDCl₃).



Fig. S8. ¹³C NMR spectrum of complex 1 (saturated solution, ~ 0.003 M, in CD₃CN).





Fig. S11. ¹H NMR spectrum of complex 6 (0.01 M, in CD₃CN).



Fig. S12. ¹³C NMR spectrum of complex 6 (0.01 M, in CD₃CN).