

Supplementary Materials

Neptunyl(VI) Nitrate Coordination Polymer with Bis(2-pyrrolidone) Linkers Highlighting Crystallographic Analogy and Solubility Difference in Actinyl(VI) Nitrates

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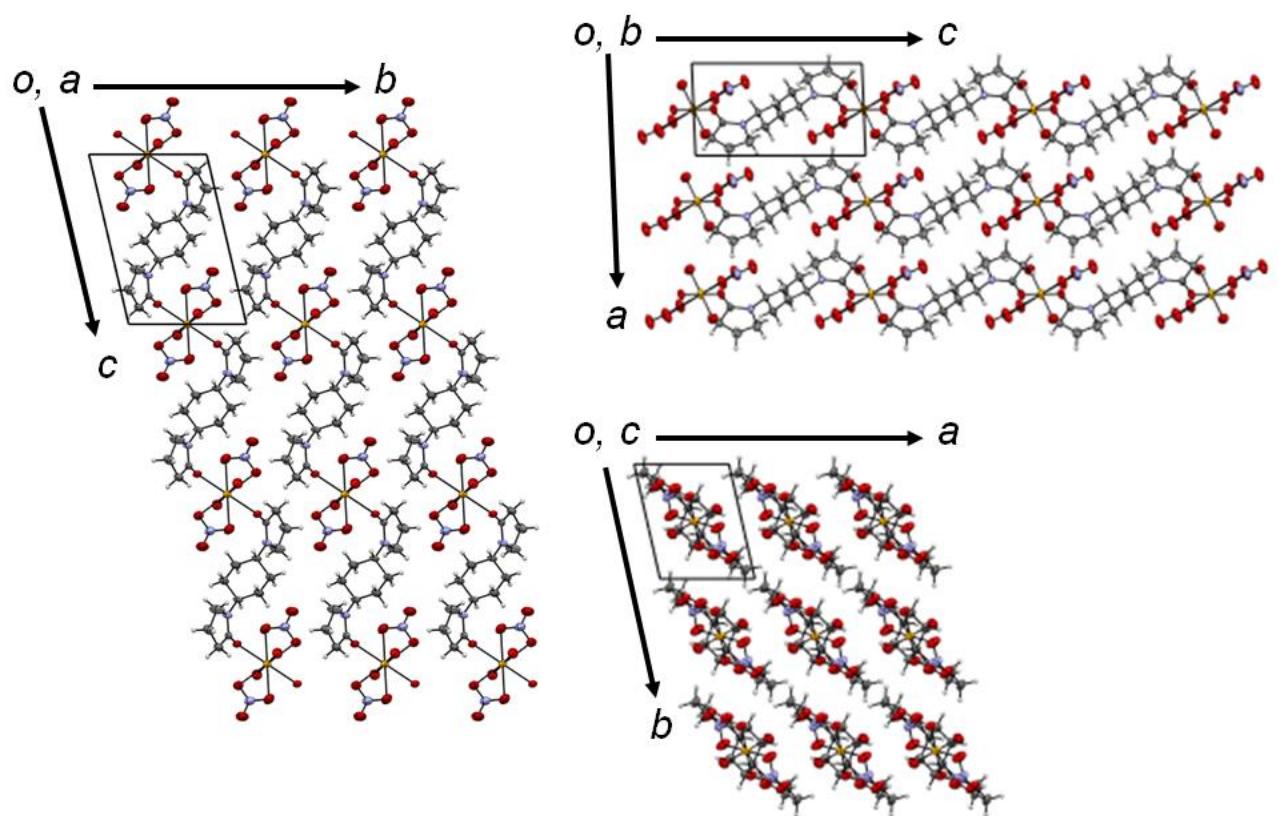


Figure S1. Packing diagram of $[NpO_2(NO_3)_2(L1)]_n$.

Table S1. Logarithmic Stability Constants ($\log \beta$) of Typical Actinyl(VI) Complexes ($(AnO_2(L)_n)^{m+}$; An = U, Np, Pu; L = CO_3^{2-} , CH_3COO^- , F^- , Cl^- , NO_3^- , SO_4^{2-}), in Aqueous Systems at 298 K and Zero Ionic Strength^[S1, S2]

L	$AnO_2^{2+}:L$	stoichiometry $\log \beta$		
		An = U	Np	Pu
CO_3^{2-}	1:1	9.94	9.86	9.50
	1:2	16.61	16.52	14.70
	1:3	21.84	19.90	18.00
CH_3COO^-	1:1	3.06	2.92	2.76
	1:2	5.57	5.14	4.47
	1:3	6.97	6.91	5.93
F^-	1:1	5.16	4.57	4.56
	1:2	8.83	7.60	7.25
	1:3	10.90		
	1:4	11.84		
Cl^-	1:1	0.17	0.40	0.23
	1:2	-1.10		-1.15
NO_3^-	1:1	-0.19		
SO_4^{2-}	1:1	3.15	3.28	3.38
	1:2	4.14	4.70	4.40
	1:3	3.02		

References.

- [S1] *NIST Critically Selected Stability Constants of Metal Complexes Database*, ed. by R. M. Smith, A. E. Martell, R. J. Motekaitis, **2004**.
- [S2] *Second Update on the Chemical Thermodynamics of Uranium, Neptunium, Plutonium, Americium and Technetium*, ed. by I. Grenthe, X. Gaona, A. V. Plyasunov, L. Rao, W. H. Runde, B. Grambow, R. J. M. Konings, A. L. Smith, E. E. Moore, OECD Nuclear Energy Agency, Data Bank, Paris, France, **2020**.