

The First Organically Templated Tetravalent Uranium Phosphates with Dimer-Structured Topologies

Yu-Lun Lai,^a Ray-Kuang Chiang,^b Kwang-Hwa Lii,^c and Sue-Lein Wang^{a,*}

^aDepartment of Chemistry, National Tsing Hua University, Hsinchu 30013, Taiwan

^bDepartment of Chemical Engineering, Far East College, Tainan, 74448, Taiwan

^cDepartment of Chemistry, National Central University, Chungli 32054, Taiwan

Table S1. Fluorine tests, ICP-AES and EA analyses

Figure S1. ORTEP of (C₄H₁₆N₃)[U₂F₃(PO₄)₂(HPO₄)] (1)

Figure S2. ORTEP of (C₆H₂₁N₃)[U₂F₄(PO₄)(HPO₄)₂] (2)

Figure S3. ORTEP of (C₄H₁₆N₃)₂[U₂F₁₀(HPO₄)₂] (3)

Figure S4. ORTEP of (C₆H₁₆N₂)₂(UF₇)(H₂PO₄) (4)

Figure S5. Experimental (top) and simulated (bottom) X-ray powder patterns for (C₄H₁₆N₃)[U₂F₃(PO₄)₂(HPO₄)] (1)

Figure S6. Experimental (top) and simulated (bottom) X-ray powder patterns for (C₆H₂₁N₃)[U₂F₄(PO₄)(HPO₄)₂] (2)

Figure S7. Experimental (top) and simulated (bottom) X-ray powder patterns for (C₆H₁₆N₂)₂(UF₇)(H₂PO₄) (4)

Figure S8. Infinite chains of U⁶⁺ and U⁴⁺.

Table S1. Fluorine tests, ICP-AES and EA analyses

	1	2	3	4
%U found (calcd.) ^a	34.43 (34.58)	44.15 (44.47)	48.05 (48.17)	51.12 (51.45)
%P found (calcd.) ^a	4.51 (4.49)	5.64 (5.78)	9.21 (9.40)	9.94 (10.04)
%F found (calcd.) ^b	18.95 (19.32)	17.46(17.75)	7.32(7.69)	5.69 (6.16)
%C found (calcd.)	20.67(20.94)	8.86(8.97)	7.18(7.29)	5.03(5.19)
%N found (calcd.)	8.01(8.14)	7.68(7.85)	5.41(5.69)	4.48(4.54)
%H found (calcd.)	3.15(3.22)	3.11(3.20)	2.15(2.34)	1.69(1.85)

a. ICP-AES results

b. Fluoride test were measured by ion chromatography.

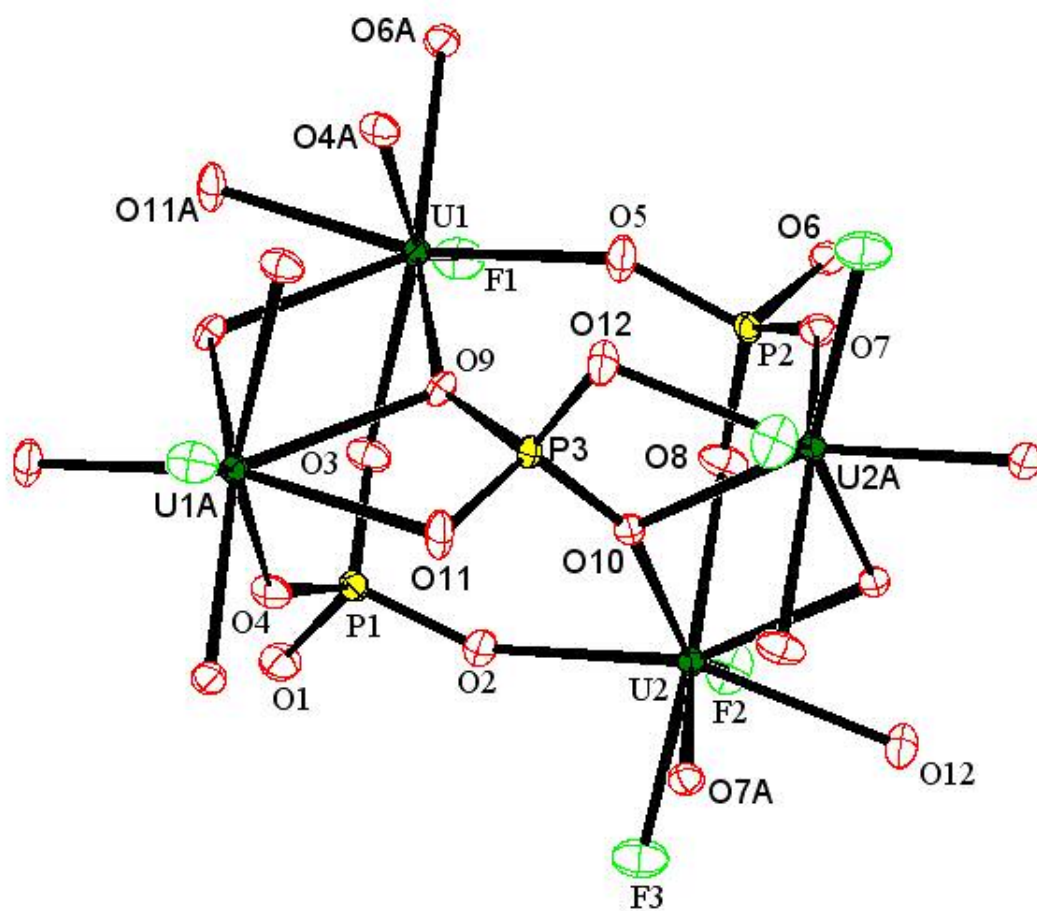
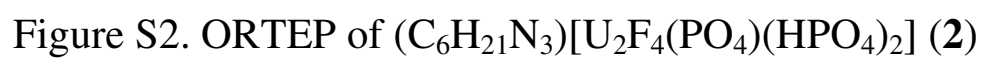


Figure S1. ORTEP of $(\text{C}_4\text{H}_{16}\text{N}_3)[\text{U}_2\text{F}_3(\text{PO}_4)_2(\text{HPO}_4)]$ (**1**)



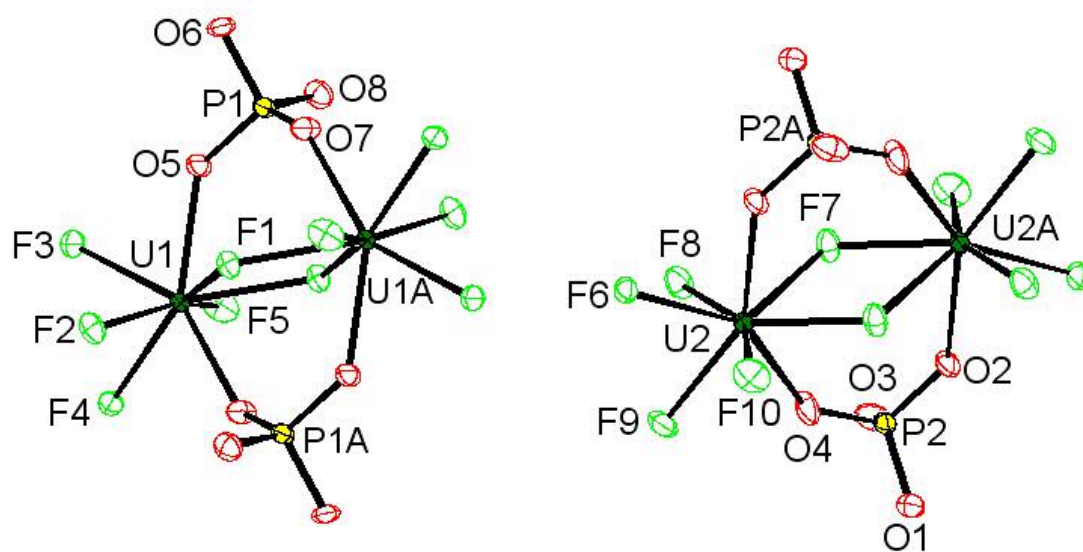


Figure S3. ORTEP of $(C_4H_{16}N_3)_2[U_2F_{10}(HPO_4)_2]$ (**3**)

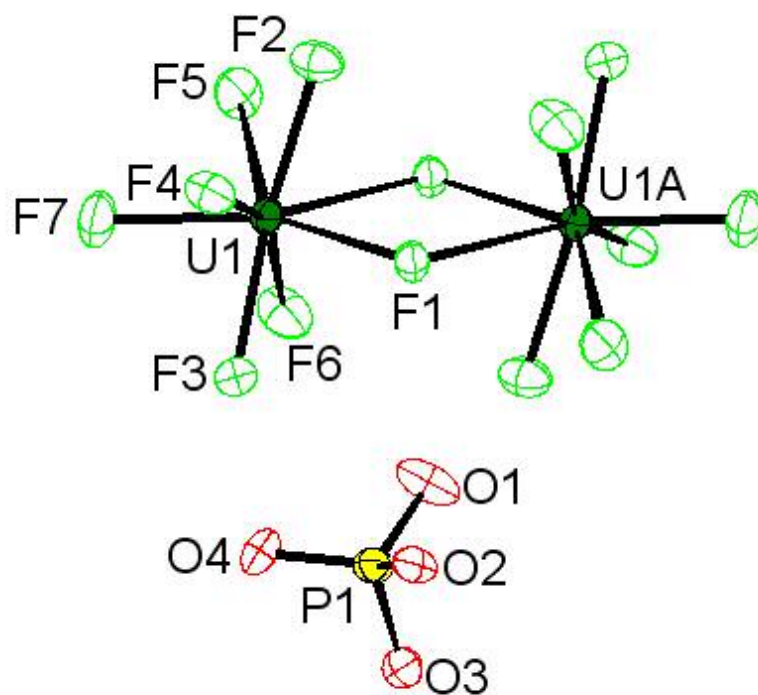


Figure S4. ORTEP of $(\text{C}_6\text{H}_{16}\text{N}_2)_2[(\text{H}_2\text{PO}_4)\text{UF}_7]$ (**4**)

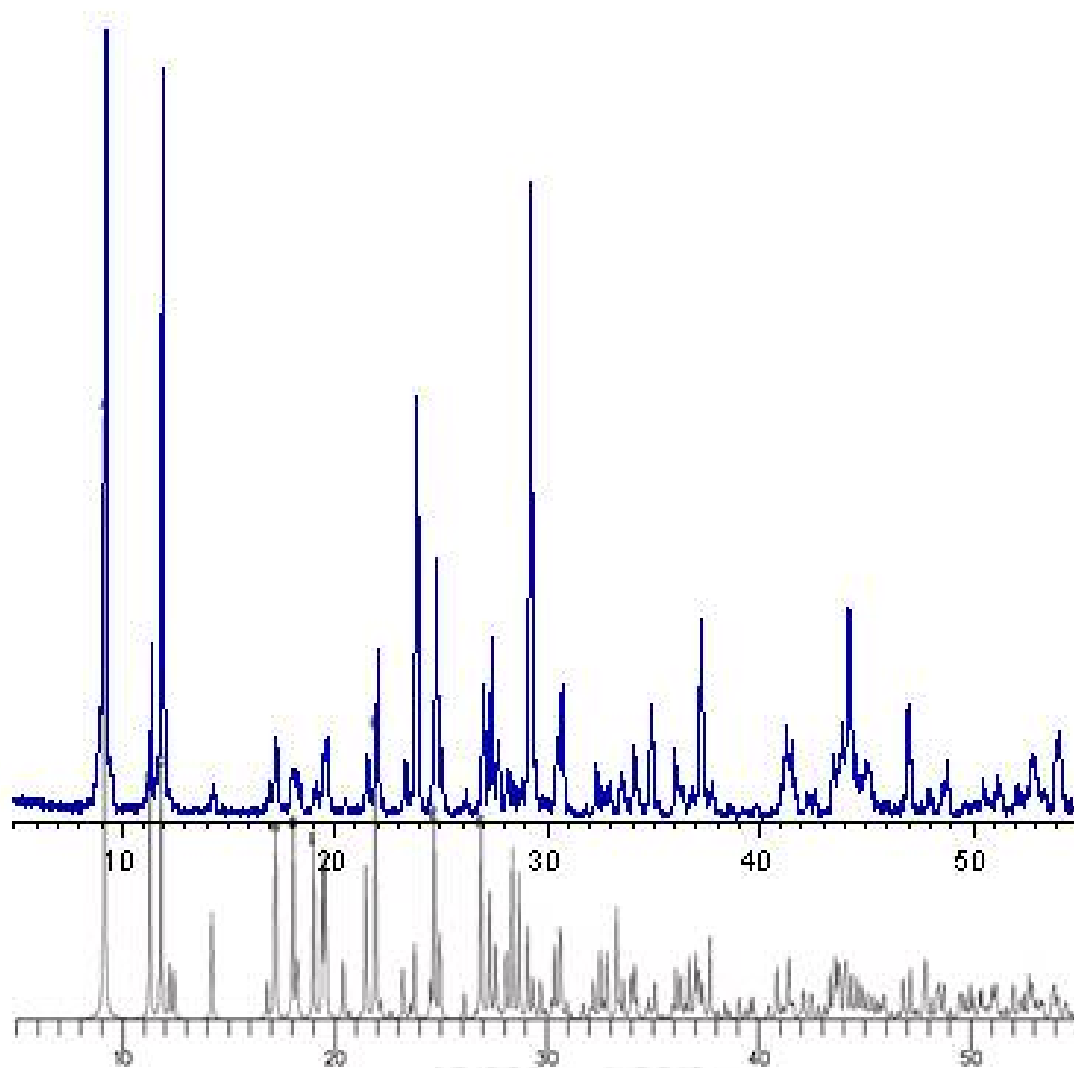


Figure S5. Experimental (top) and simulated (bottom) X-ray powder patterns for $(\text{C}_4\text{H}_{16}\text{N}_3)[\text{U}_2\text{F}_3(\text{PO}_4)_2(\text{HPO}_4)]$ (**1**)

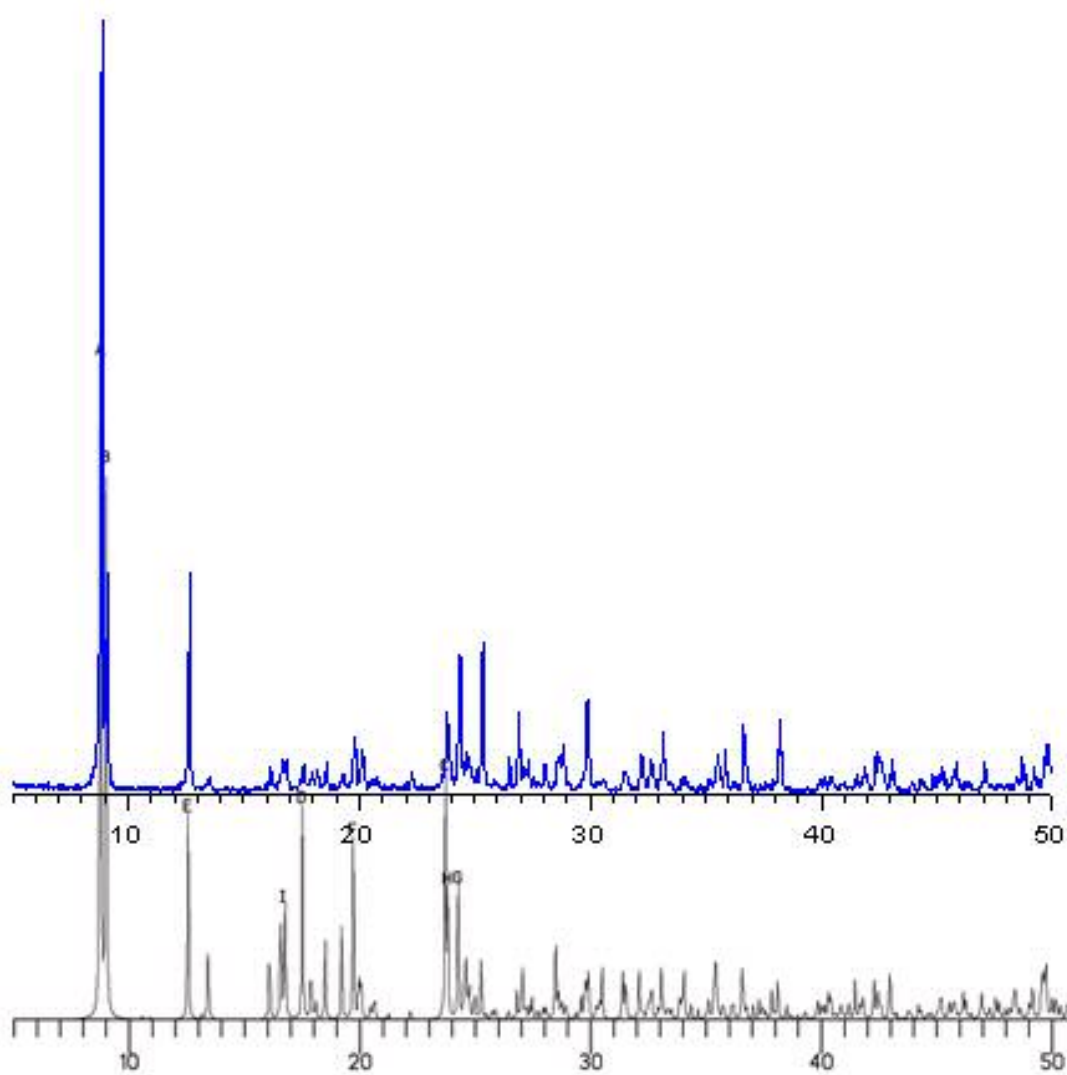


Figure S6. Experimental (top) and simulated (bottom) X-ray powder patterns for $(\text{C}_6\text{H}_{21}\text{N}_3)[\text{U}_2\text{F}_4(\text{PO}_4)(\text{HPO}_4)_2]$ (**2**)

Figure S7. Experimental (top) and simulated (bottom) X-ray powder patterns for $(\text{C}_6\text{H}_{16}\text{N}_2)_2[(\text{H}_2\text{PO}_4)\text{UF}_7]$ (**4**)

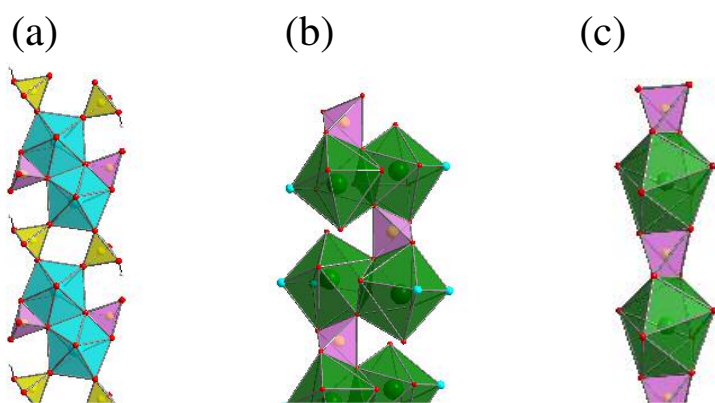


Figure S8. (a) 1D chain structure of U^{6+} $((\text{H}_3\text{A})[\text{UO}_2(\text{PO}_4)(\text{HPO}_4)])$ with $\text{A} = \text{dien}$ or tren) prepared from the same reactions as **1** and **2** by increasing the concentration of amine templates; (b) and (c) showing the similar connection skeleton of the chain B in **1** and the $\infty[\text{UPO}_4]$ chain in $\text{CaU}(\text{PO}_4)_2$