3D coordination polymers of uranium (IV) terephthalates

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SUPPLEMENTARY INFORMATION

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Table S1: Elemental chemical analyses for $U_2O_2(bdc)_2(DMF)$ and $U_2O_2(bdc)_2(DEF)$ (4).

	N%	C%	H%
Experimental			
$U_2O_2(bdc)_2(DMF)$	1.73	25.02	1.72
$U_2O_2(bdc)_2(DEF)$	1.47	27.16	2.03
Calculated			
$U_2O_2(bdc)_2(DMF)$	1.54	25.08	1.65
$U_2O_2(bdc)_2(DEF)$	1.49	26.89	2.02

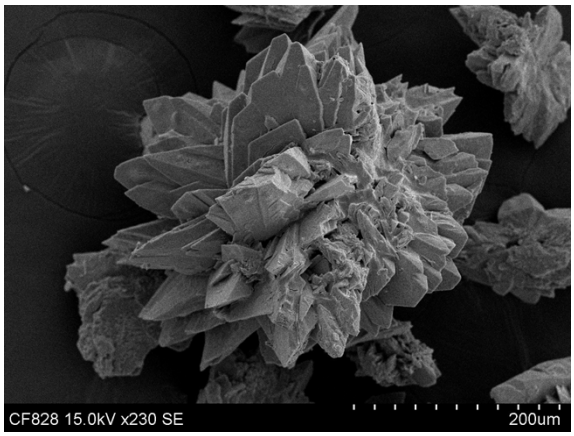

Figure S1a: SEM photographs of the mixture of *T*- *& M*-$U_2Cl_2(bdc)_3(DMF)_4$ (**1&2**)

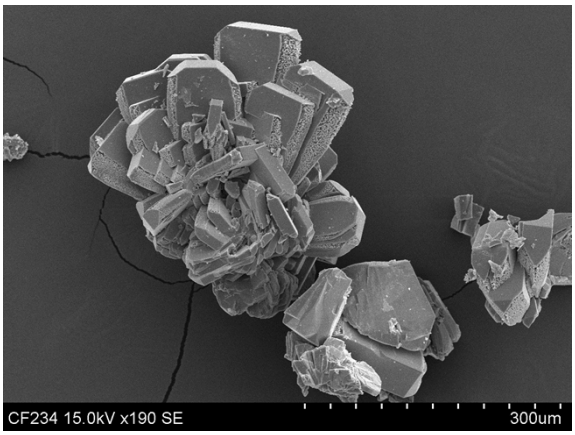

Figure S1b: SEM photographs of $U_2(bdc)_4(DMF)_4$ (**3**).

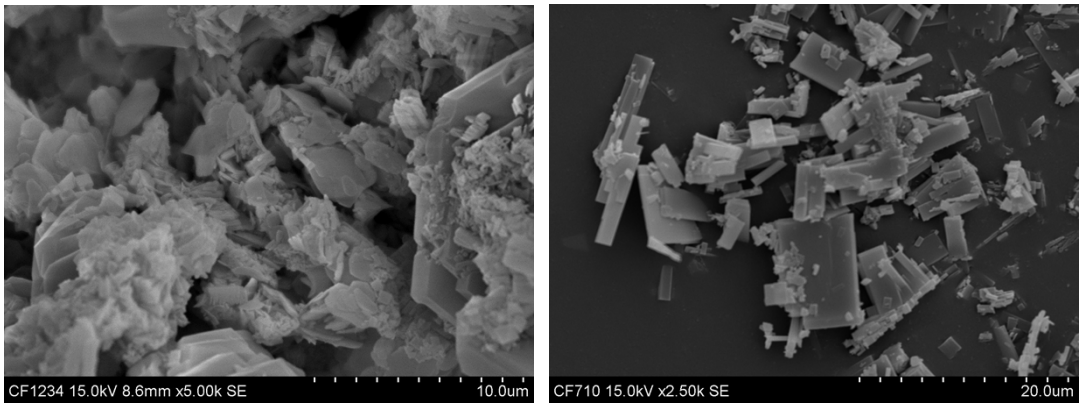

Figure S1c: SEM photographs $U_2O_2(bdc)_2(DMF)$ and $U_2O_2(bdc)_2(DEF)$ (**4**), synthesized in DMF and DEF solvent, respectively.

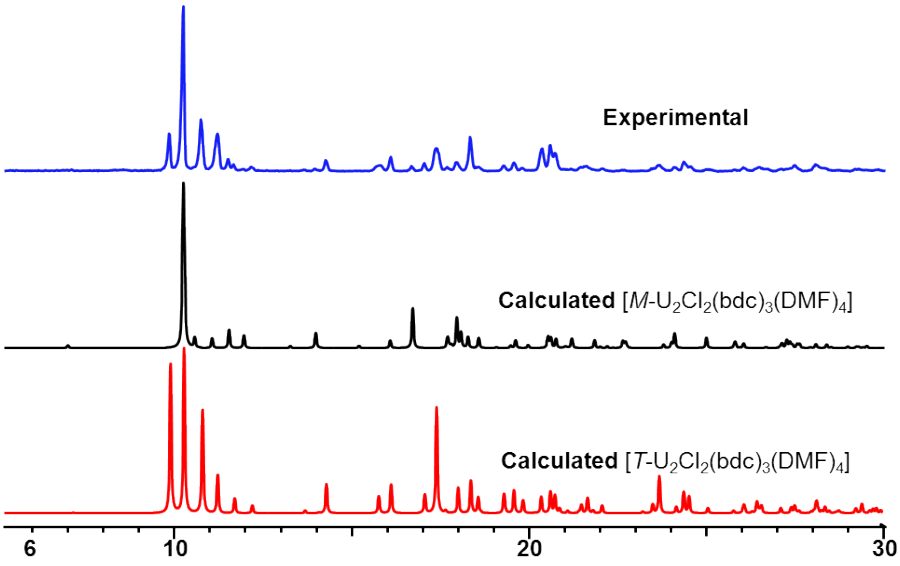

Figure S2a: Comparison between the calculated and experimental (blue line) XRD patterns of *T*-$U_2Cl_2(bdc)_3(DMF)_4$ (**1**) (red line) and *M*-$U_2Cl_2(bdc)_3(DMF)_4$ (**2**) (black line), showing the mixture of the two polytypes – Copper radiation.

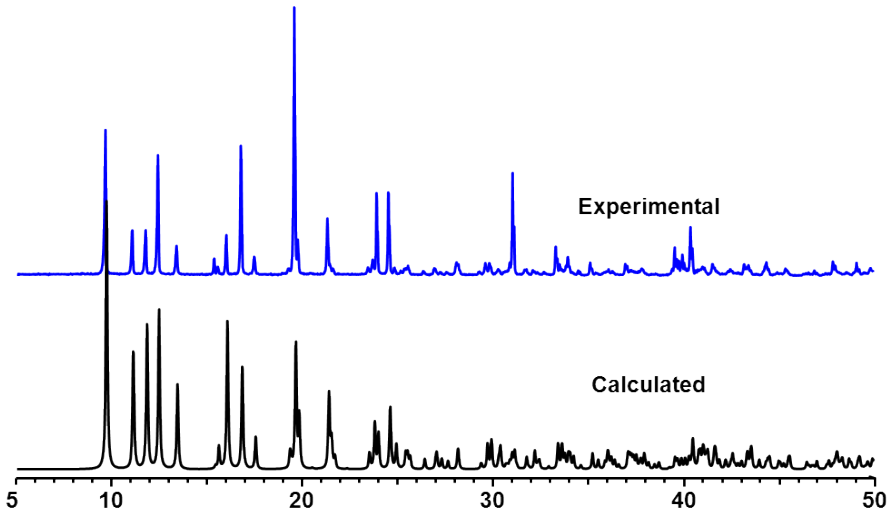

Figure S2b: Comparison between the calculated (black line) and experimental XRD patterns of $U_2(bdc)_4(DMF)_4$ (**3**) (blue line) – Copper radiation.

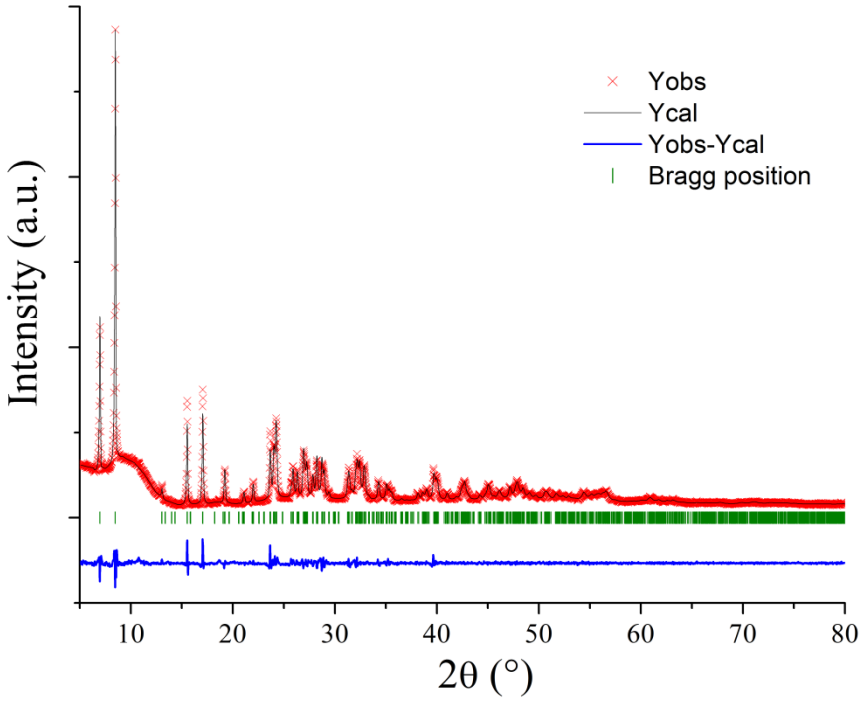

Figure S2c: Observed, calculated and difference PXRD patterns of $U_2O_2(bdc)_2(DEF)$ (**4**) as a fucntions of 2θ°. The vertical bars indicate the Bragg positions. (copper Kα1/α2 radiation).

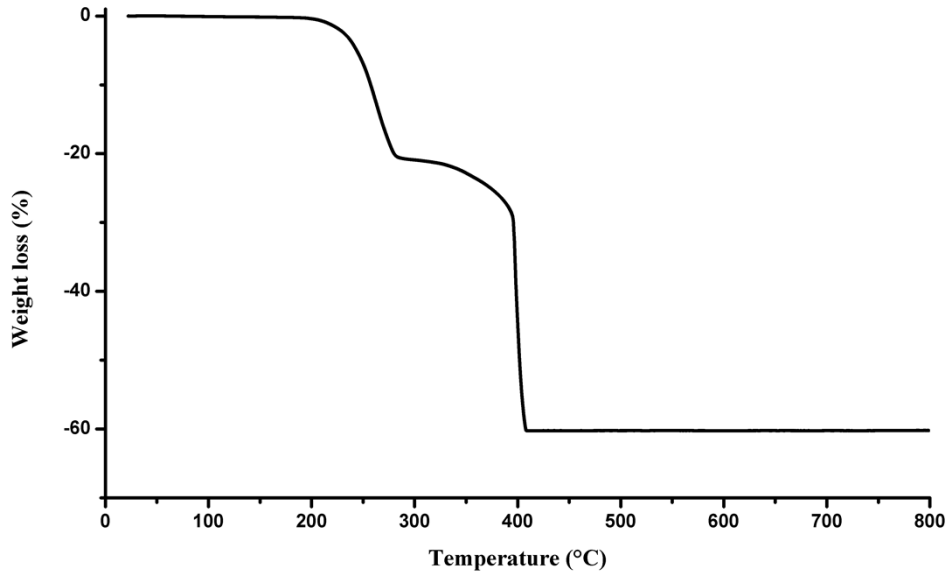

Figure S3a: Thermogravimetric curve of compounds $U_2(bdc)_4(DMF)_4$ (**3**) under air atmosphere (heating rate: 10°C/min).

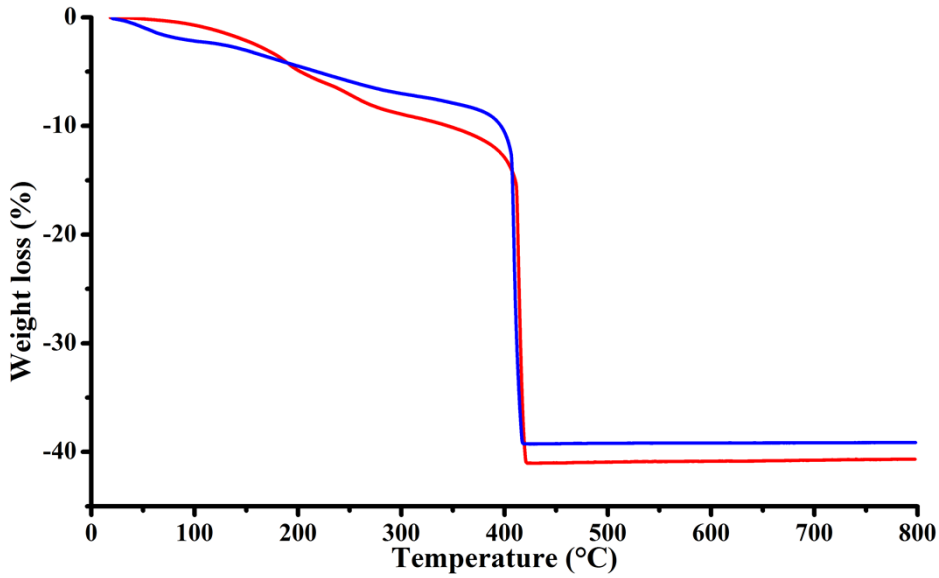

Figure S3b: Thermogravimetric curves of compounds $U_2O_2(bdc)_2(X)$ (**4**), where X = DMF (blue line) and X = DEF (red line) under air atmosphere (heating rate: 10°C/min).

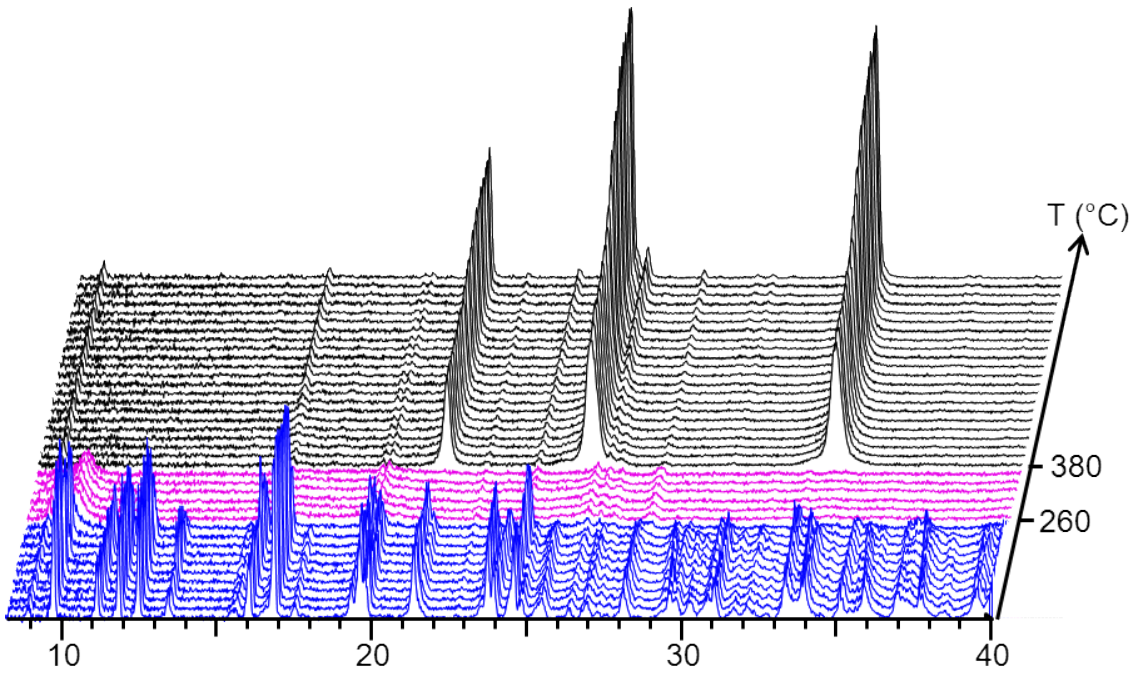

Figure S4a: In situ X-ray diffractograms of $U_2(bdc)_4(DMF)_4$ (**3**) as a function of temperature (copper radiation) under air atmosphere.

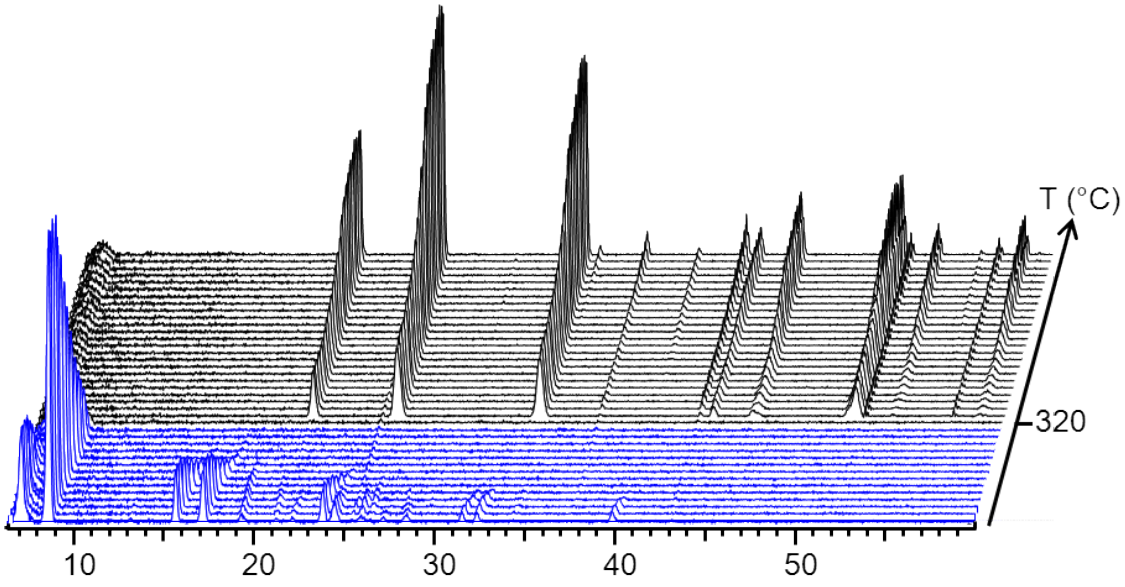

Figure S4b: In situ X-ray diffractograms of $U_2O_2(bdc)_2(DEF)$ (**4**) as a function of temperature (copper radiation) under air atmosphere.

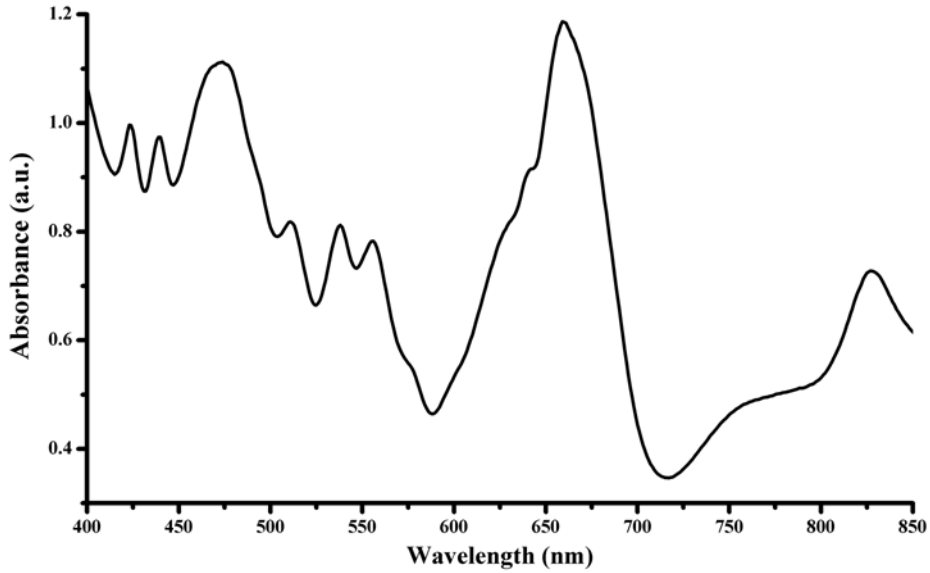

Figure S5a: Solid-state UV/Vis spectrum of $U_2(bdc)_4(DMF)_4$ (**3**)

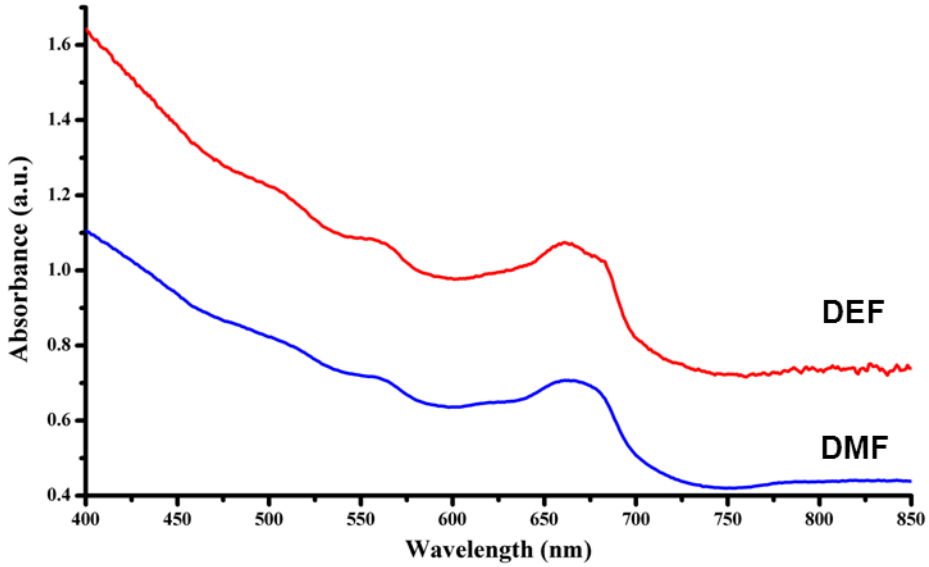

Figure S5b: Solid-state UV/vis spectra of $U_2O_2(bdc)_2(X)$ (**4**) where X= DMF (blue line) and X=DEF (red line).

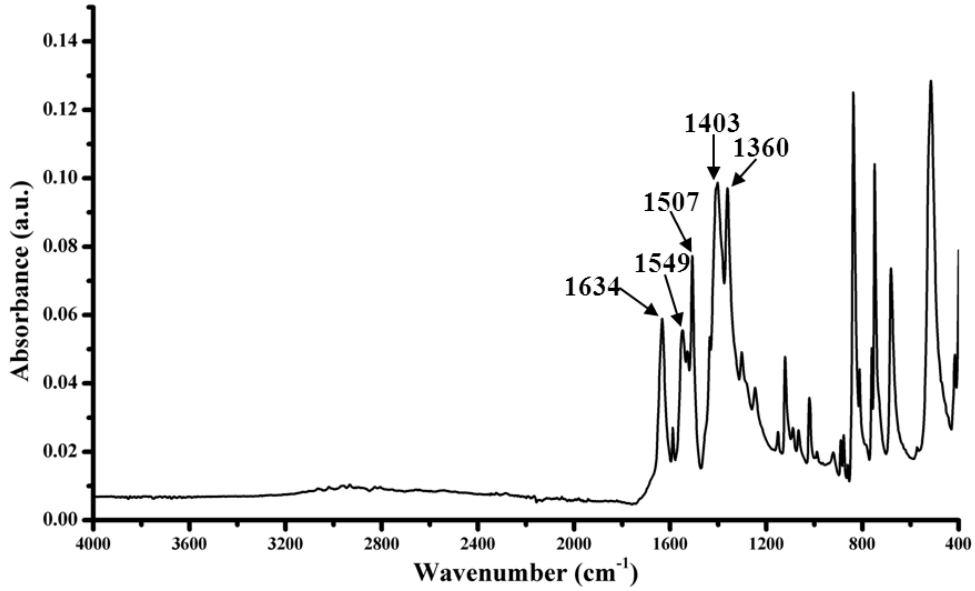

Figure S6a: Solid-state IR spectrum of $U_2(bdc)_4(DMF)_4$ (**3**)

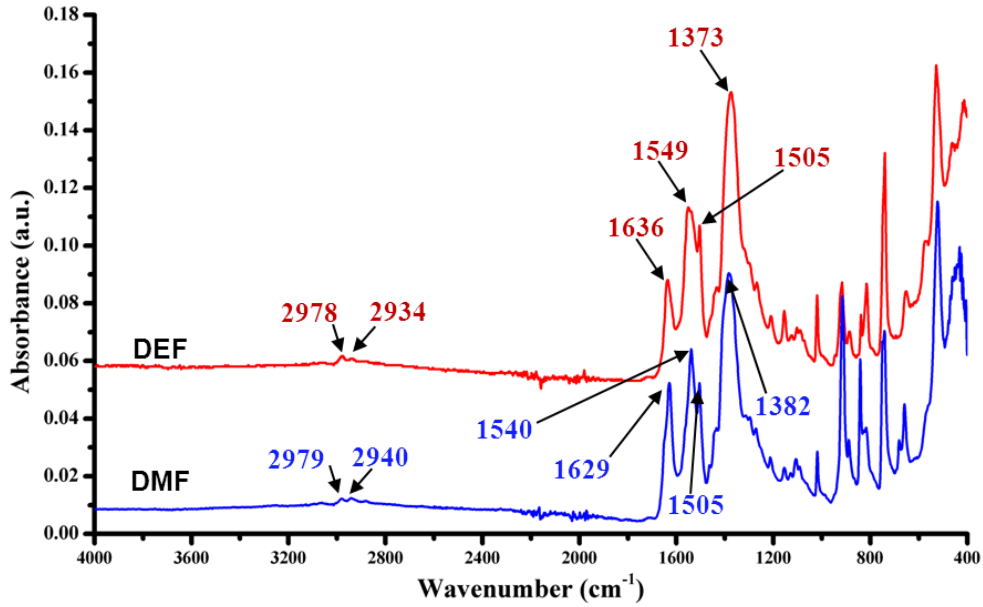

Figure S6b: Solid-state IR spectra of $U_2O_2(bdc)_2(X)$ (**4**) where X= DMF (blue line) and X=DEF (red line).

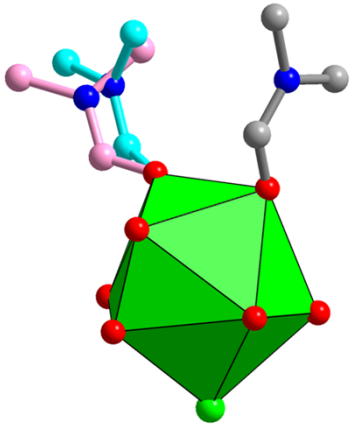

*Figure S7a: Detailed view of two DMF molecules linked to the uranium center in the compound **1**, and showing the disorder of one of the two crystallographically inequivalent DMF molecules.*

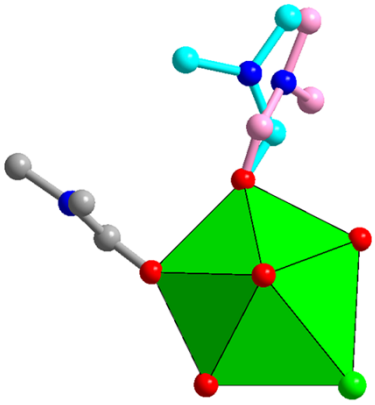

*Figure S7b: Detailed view of two DMF molecules linked to the uranium center in the compound **2**, and showing the disorder of one of the two crystallographically inequivalent DMF molecules.*