Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

The role of extracellular DNA in uranium precipitation and biomineralisation.

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Control	2 mM	1 mM	0.5 mM	0.25 mM	Assignment*
1700 $_{sh}$	1700 $_{sh}$	17000 $_{sh}$	1700 $_{sh}$	1700 $_{sh}$	ν (C-NH_2) bases; Guanine/ Adenine
1649 $_{m}$	1647 $_{m}$	1647 $_{m}$	1649 $_{m}$	1649 $_{m}$	ν (C=O)
1606 $_{w}$	1605 $_{w}$	1605 $_{w}$	1606 $_{w}$	1606 $_{w}$	-
1579 $_{vw}$	1578 $_{vw}$	1578 $_{vw}$	1579 $_{vw}$	1579 $_{vw}$	Adenine/Cytosine
1529 $_{w}$	1525 $_{w}$	1529 $_{w}$	1529 $_{w}$	1529 $_{w}$	δ (NH)/ ν (C=O), Cytosine/Guanine
1486 $_{m}$	1490 $_{m}$	1490 $_{m}$	1490 $_{m}$	1490 $_{m}$	C-NH_2 scissoring
1419 $_{w}$	1419 $_{w}$	1419 $_{w}$	1419 $_{w}$	1419 $_{w}$	-
1369 $_{m}$	1365 $_{m}$	1367 $_{m}$	1367 $_{m}$	1367 $_{m}$	ν (C=NH) nitrogenous bases
1230 $_{s}$	1206 $_{s}$	1218 $_{s}$	1218 $_{s}$	1218 $_{s}$	ν_{as} (PO_2)
1063 $_{vs}$	1061 $_{vs}$	1062/1057 $_{vs}$	1062/1057 $_{vs}$	1062/1055	ν_s (PO_2), ν (C-OH, C-0-C, C-C)
965 $_{s}$	976 $_{s}$	973 $_{s}$	970 $_{s}$	969 $_{s}$	ν (P-O)
	918 $_{s}$	919 $_{s}$	918 $_{s}$	920 $_{s}$	ν (U–O_{ligand})

sh= shoulder vw= very weak w= weak m= medium s= strong vs= very strong

* Functional group assignment is based on (Cecal et al., 2012), (Alex and Dupuis, 1989), (Parikh and Chorover, 2006), (Kamnev et al., 1999), (Lumetta et al., 1999) and (Kazy et al., 2009)

Table S1. Peak assignment for the FTIR spectra of 1 mg mL-1 eDNA binding to uranium (pH 5) at increasing concentrations.

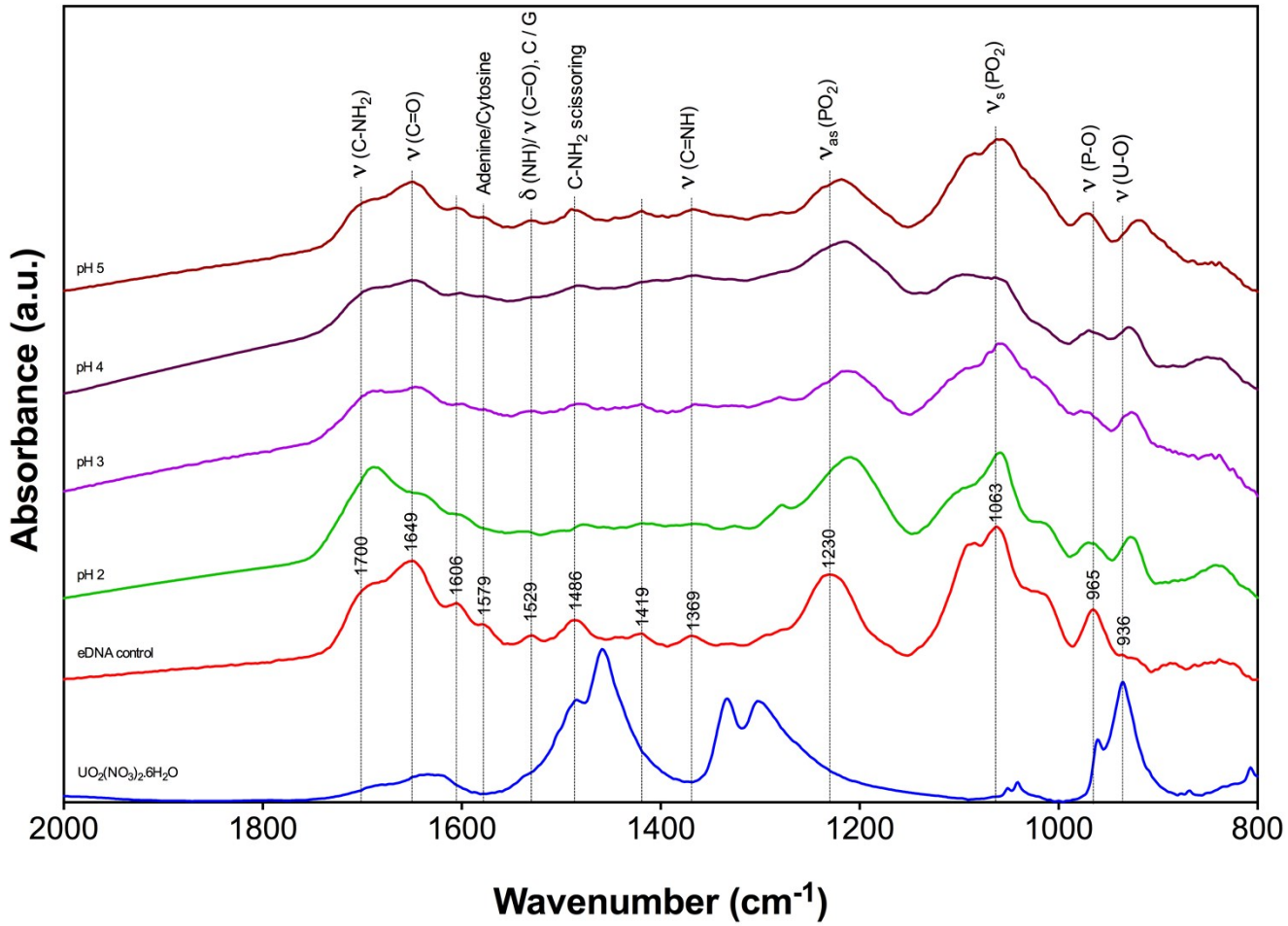


Figure S1. FTIR spectra of 0.5 mM uranium binding to 1 mg mL^{-1} eDNA at increasing pH, eDNA control and uranyl nitrate hexahydrate spectra within the region 2000 – 800 cm^{-1}.

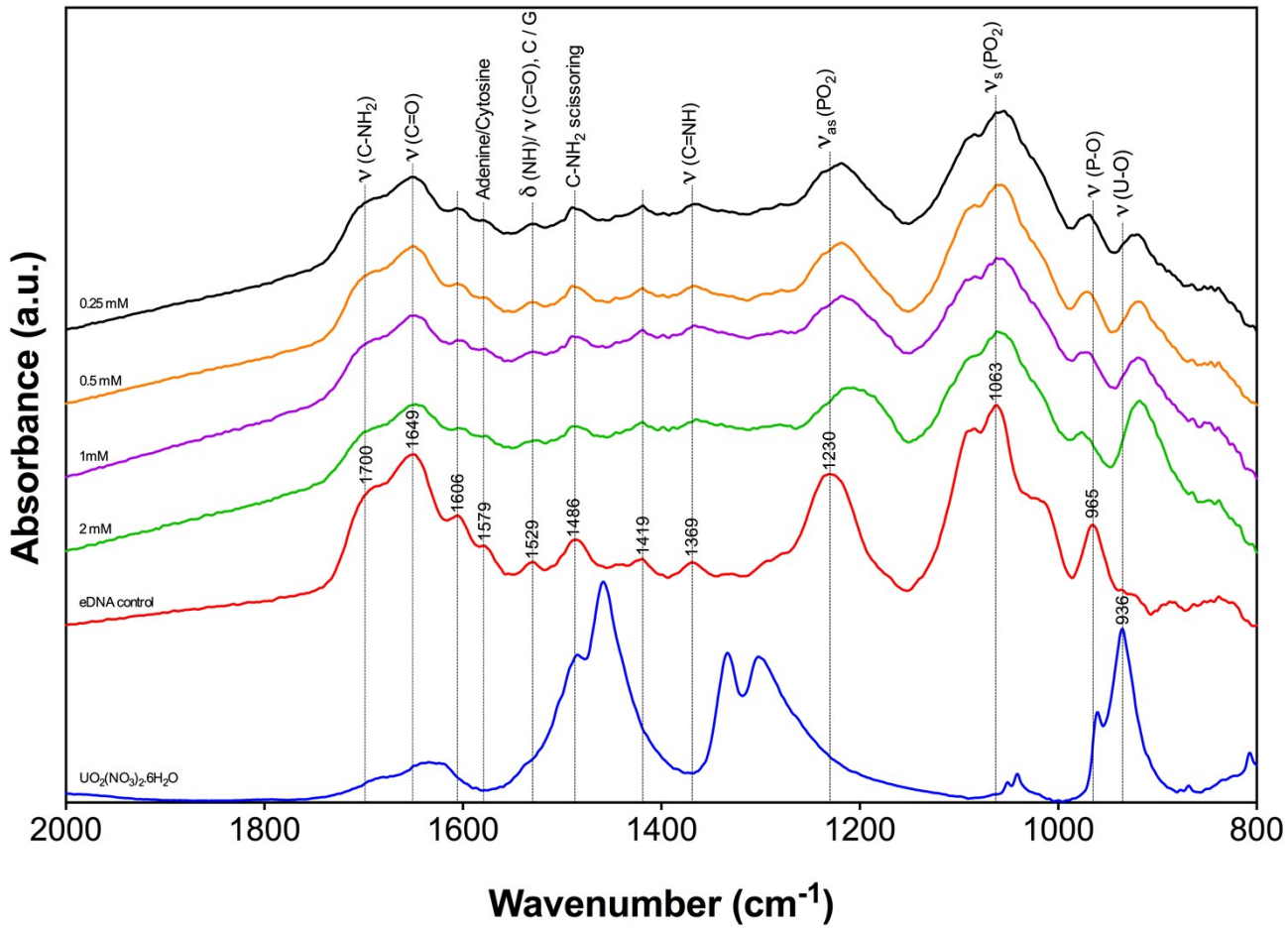


Figure S2. FTIR spectra of 1 mg mL^{-1} eDNA binding to increasing concentrations of uranium (pH 5), , eDNA control and uranyl nitrate hexahydrate spectra within the region 2000 – 800 cm^{-1}

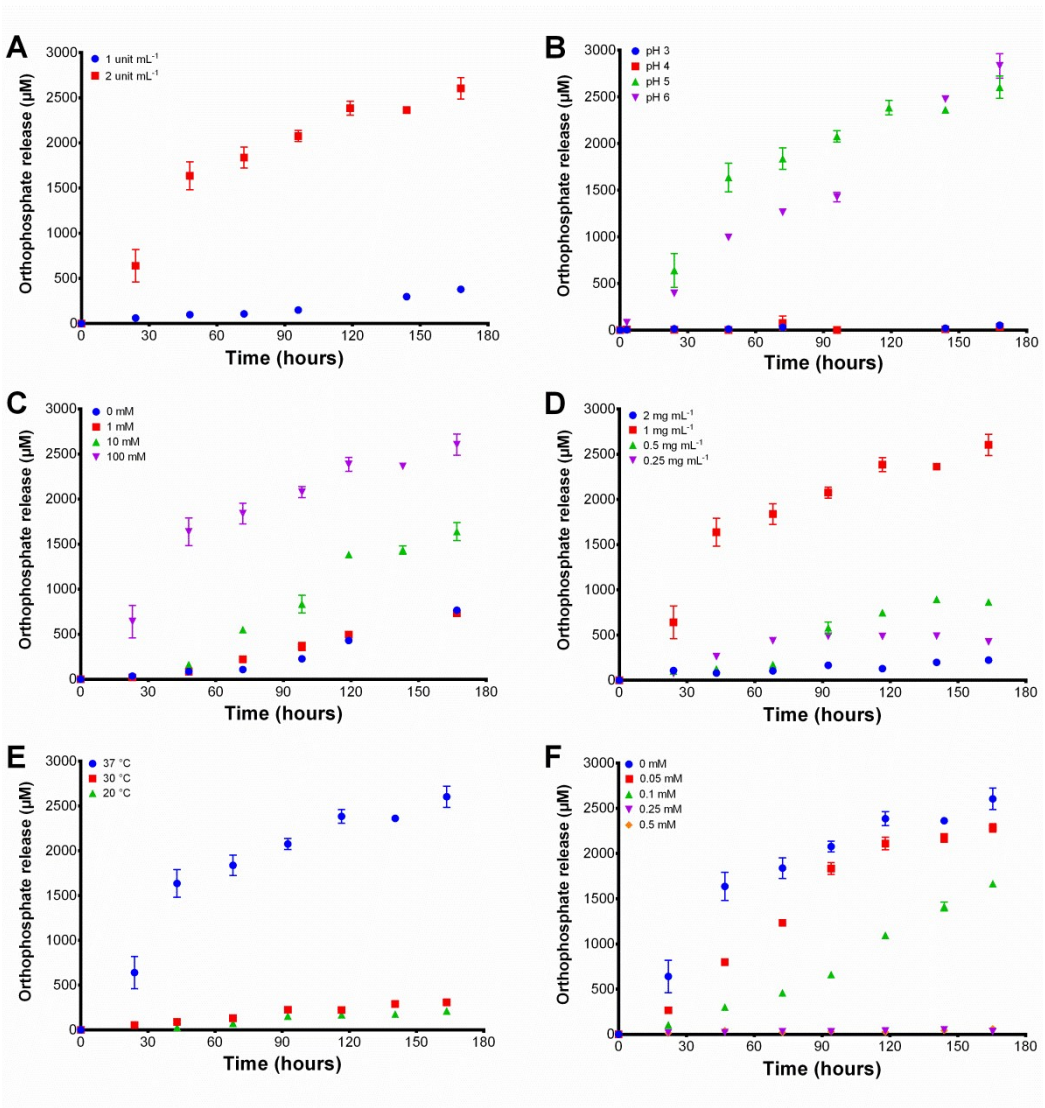


Figure S3. Orthophosphate release from eDNA as a function of [A] varying acid phosphatase concentrations, [B] varying pH, [C] varying ionic strength, [D] varying DNA concentration, [E] varying temperature and [F] varying uranium concentration.

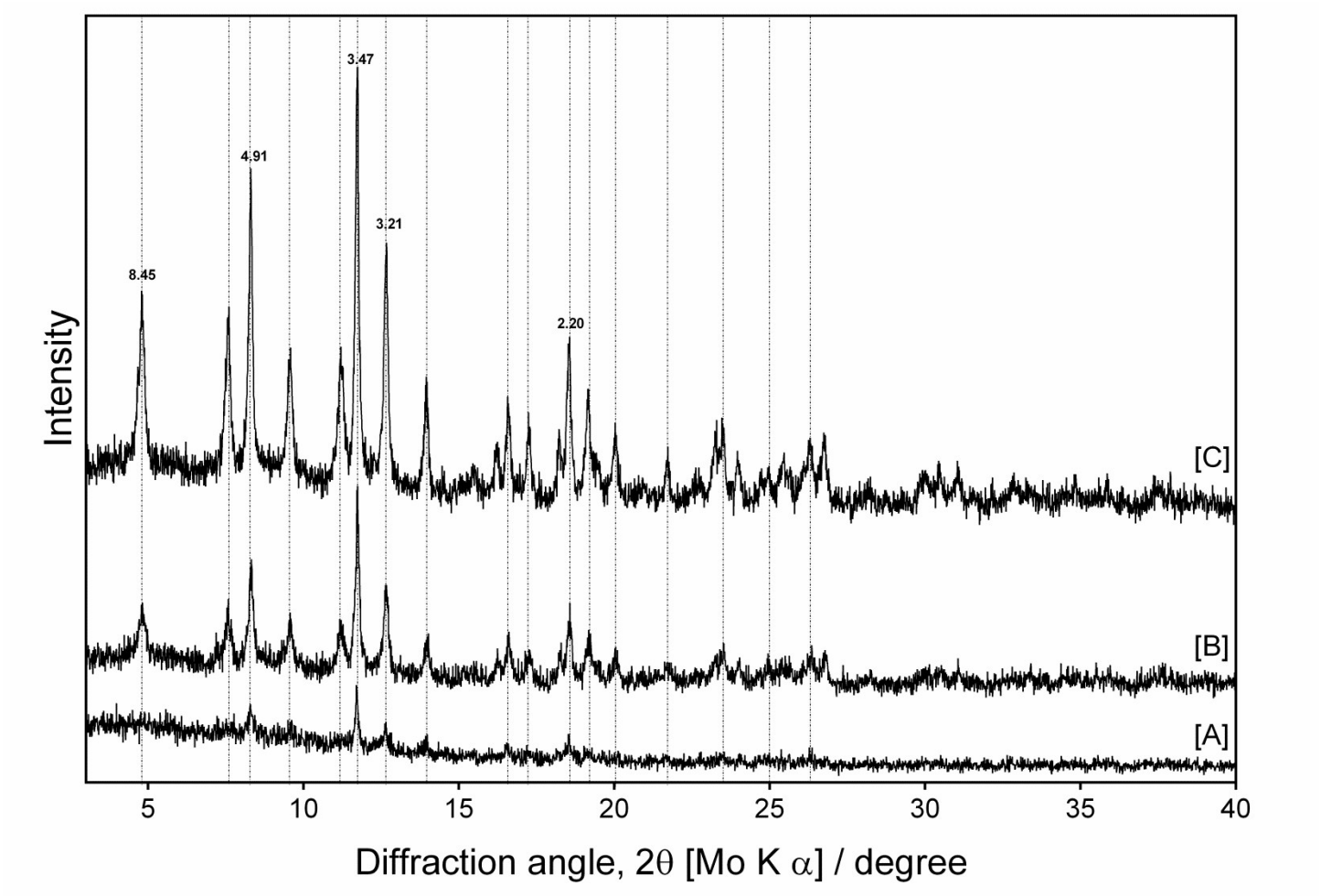


Figure S4. XRD patterns of the minerals formed at molar ratios of [A] 7.5 : 1, [B] 3.8 : 1 and [C] 1.8 : 1 aPO_4 : uranium (pH 5).

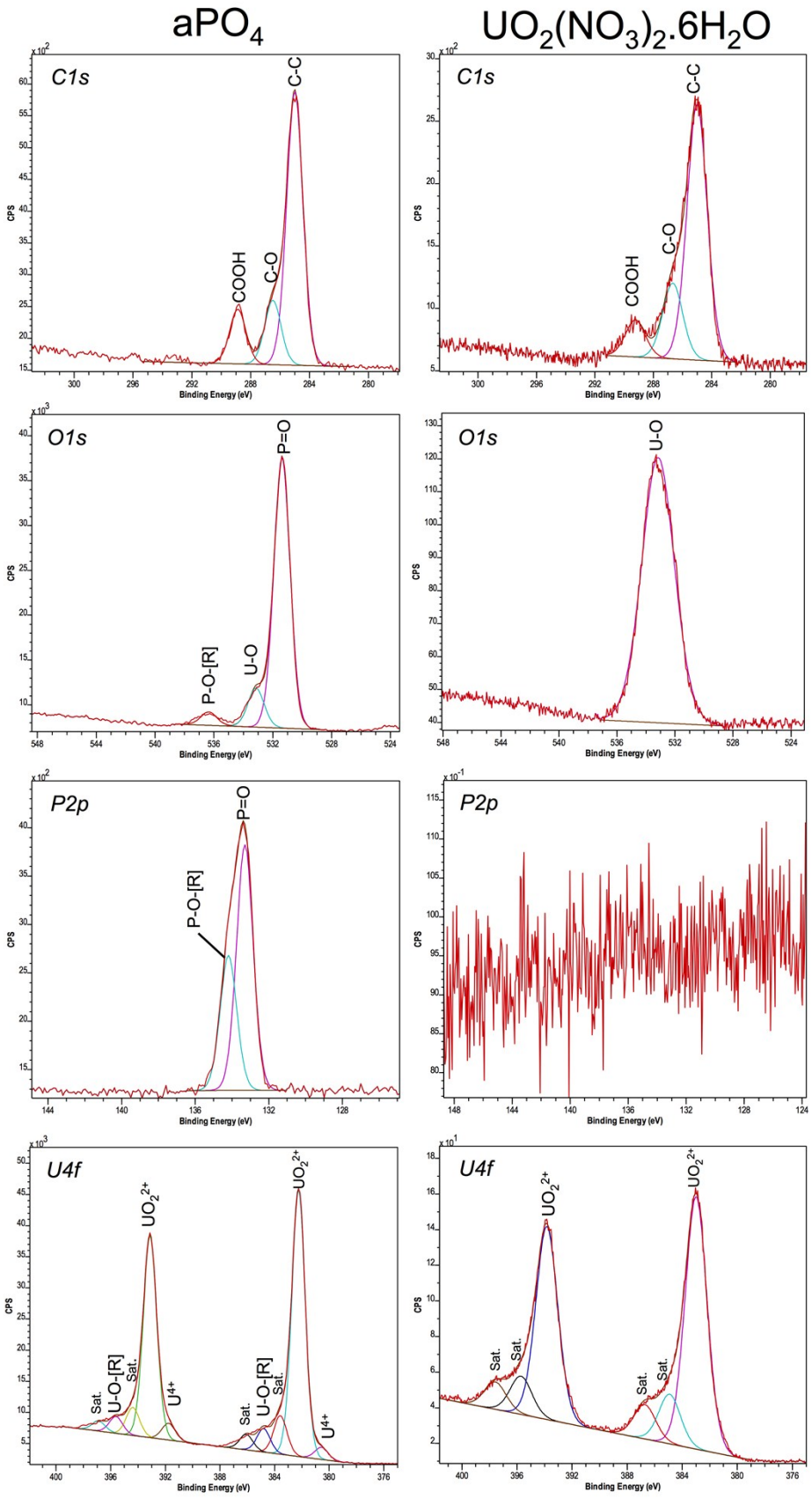
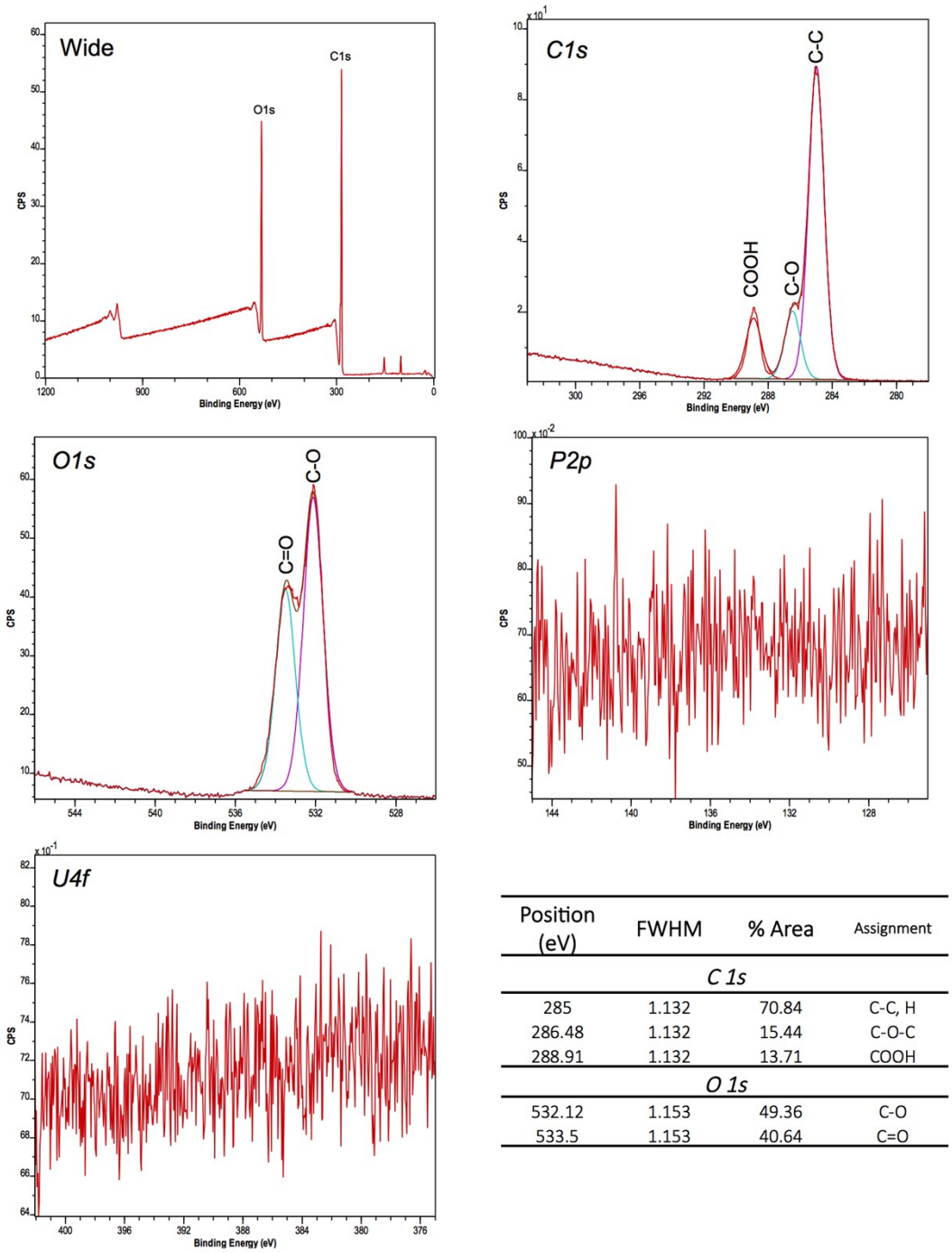


Figure S5. XPS spectrum of uranium minerals synthesised using aPO_4 at a molar ratio of 1.8 : 1 $H_2PO_4^-$: $(UO_2)_3(OH)_5^+$ and of $UO_2(NO_3)_2.6H_2O$ (control solid).



Position (eV)	FWHM	% Area	Assignment
	C 1s		
285	1.132	70.84	C-C, H
286.48	1.132	15.44	C-O-C
288.91	1.132	13.71	COOH
	O 1s		
532.12	1.153	49.36	C-O
533.5	1.153	40.64	C=O

Figure S6. XPS spectra of carbon tape used in this experimental study.

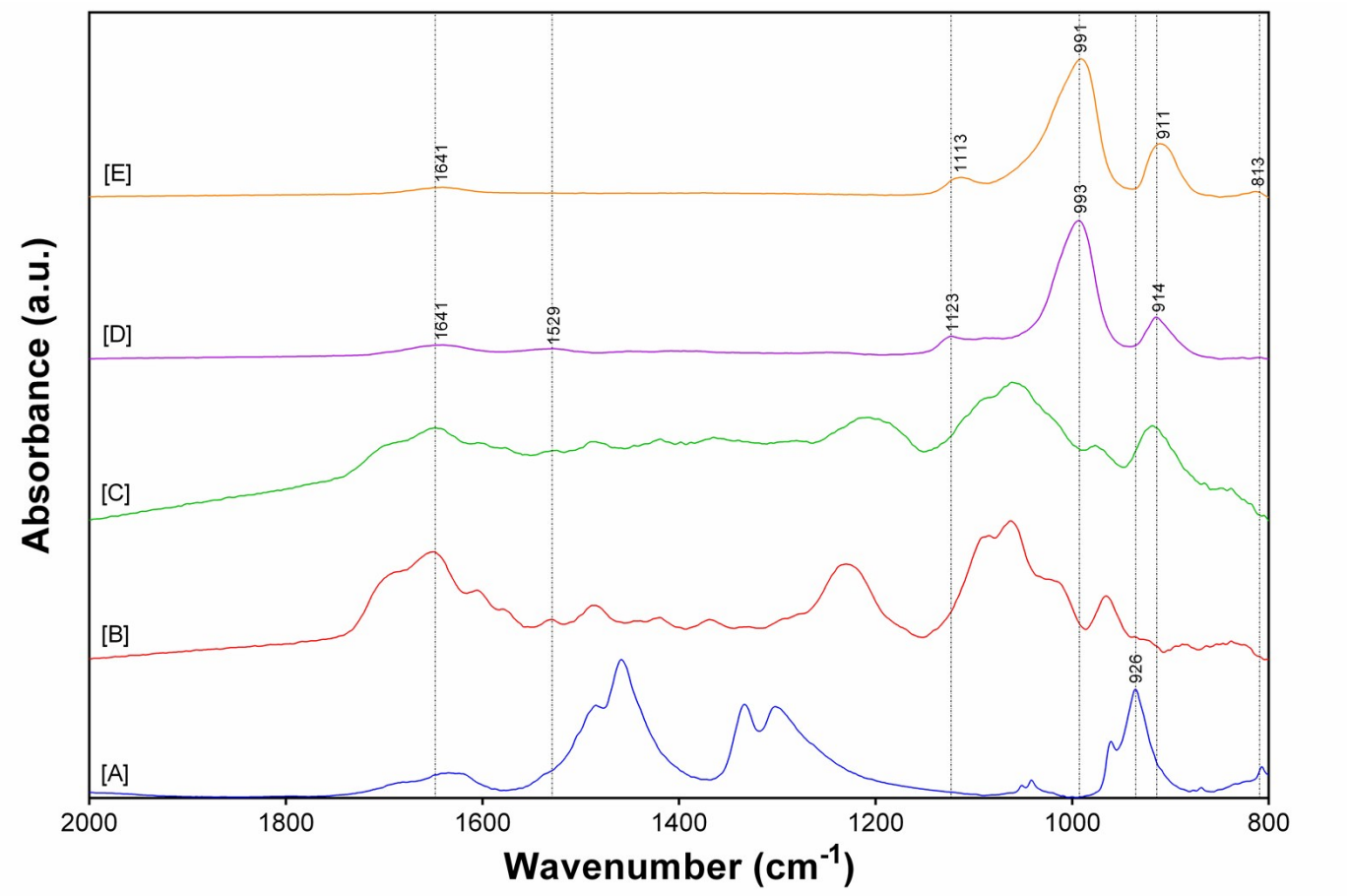


Figure S7. FT-IR spectra of minerals formed from the interaction of ePO_4 with uranium at a molar ratio of 1.8 : 1 $H_2PO_4^-$: $(UO_2)_3(OH)_5^+$ [D] in comparison with the same reaction using aPO_4 [E] within the region 2000 – 800 cm^{-1}. Reference spectra of uranyl nitrate hexahydrate [A], lyophilised DNA [B] and eDNA-U precipitate formed at a similar molar ratio of phosphate to uranium [C].

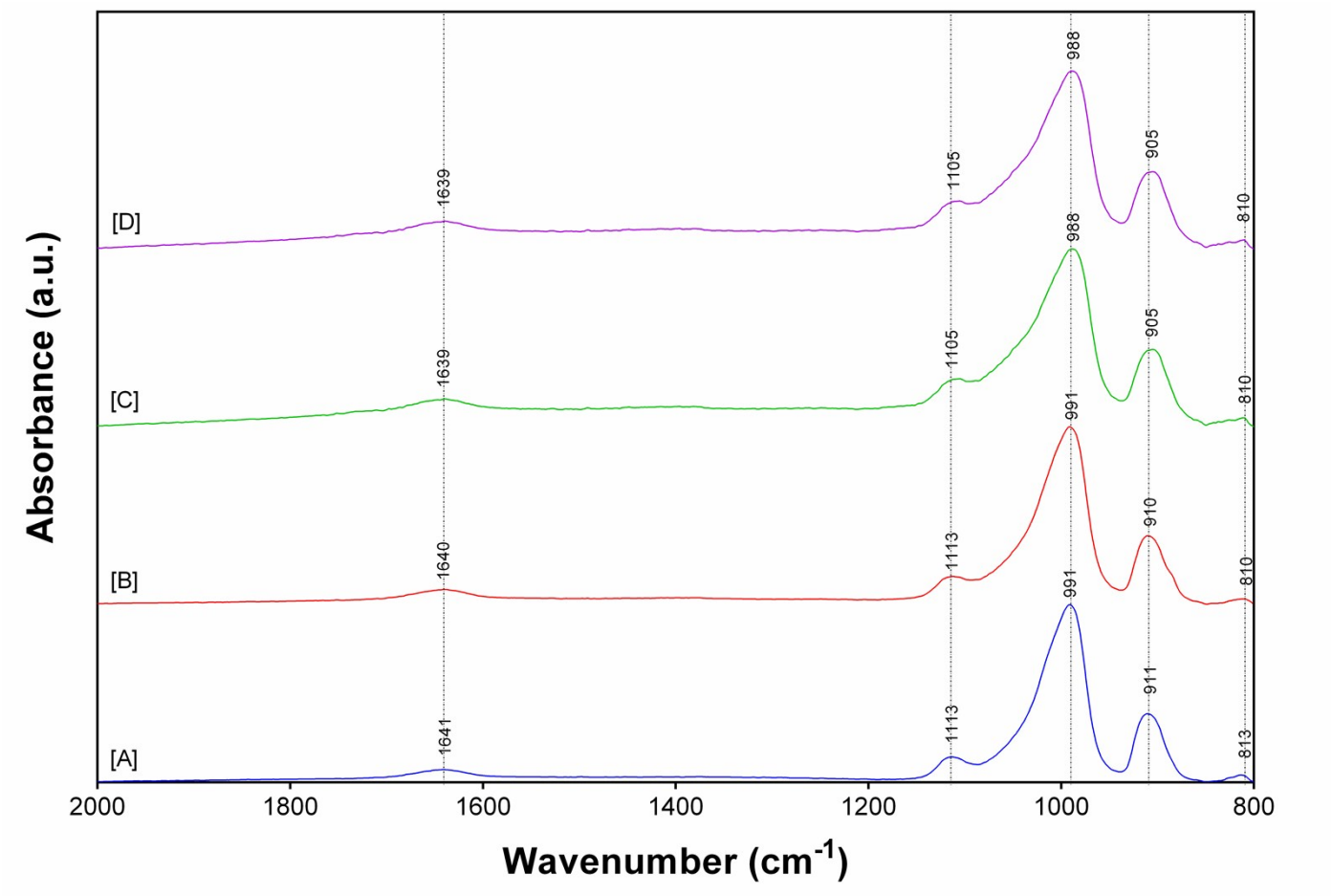


Figure S8. FT-IR spectra of minerals formed from the interaction of ePO_4 with uranium at increasing molar ratios; 1.8 : 1 [A], 3.8 : 1 [B], 7.5 : 1 [C] and 15 : 1 [D] $H_2PO_4^-$: $(UO_2)_3(OH)_5^+$ within the region 2000 – 800 cm^{-1}.

Assignment*			ν (C=O)	δ (N-H)	ν (PO_2)/ ν_{as} (P-O)	ν_s (P-O)	ν (U–O_{ligand})	
1.8:1	**ePO_4**	**σ (cm^{-1})**	**1641**	**1528**	**1123**	**993**	**914**	**-**
		I (a.u.)	0.153	0.113	0.248	1.5	0.453	-
	aPO_4	**σ (cm^{-1})**	**1641**	**-**	**1113**	**991**	**911**	**813**
		I (a.u.)	0.108	-	0.216	1.5	0.58	0.063
3.8:1	**ePO_4**	**σ (cm^{-1})**	**1641**	**1530**	**1118**	**990**	**904**	**-**
		I (a.u.)	0.185	0.12	0.3	1.5	0.578	-
	aPO_4	**σ (cm^{-1})**	**1640**	**-**	**1113**	**991**	**910**	**810**
		I (a.u.)	0.128	-	0.238	1.5	0.58	0.048
7.5:1	**ePO_4**	**σ (cm^{-1})**	**1641**	**1529**	**1119**	**991**	**907**	**-**
		I (a.u.)	0.362	0.259	0.478	1.5	0.644	-
	aPO_4	**σ (cm^{-1})**	**1639**	**-**	**1105**	**988**	**905**	**810**
		I (a.u.)	0.235	-	0.405	1.5	0.651	0.076
15:1	**ePO_4**	**σ (cm^{-1})**	**1641**	**1529**	**1122**	**992**	**912**	**-**
		I (a.u.)	0.441	0.348	0.56	1.5	0.691	-
	aPO_4	**σ (cm^{-1})**	**1639**	**-**	**1105**	**988**	**905**	**810**
		I (a.u.)	0.235	-	0.405	1.5	0.651	0.076

* Functional group assignment has been identified and based on (Baker et al., 2014), (Akyuz et al., 2008), (Garidel et al., 2000) and (Kazy et al., 2009).

Table S2. Infrared adsorption bands of uranium minerals synthesised using ePO_4 and aPO_4 at varying molar ratios.