Capturing ammonium nitrate in a synthetic uranium oxide hydrate phase: revealing the role of ammonium ions and anion inclusions

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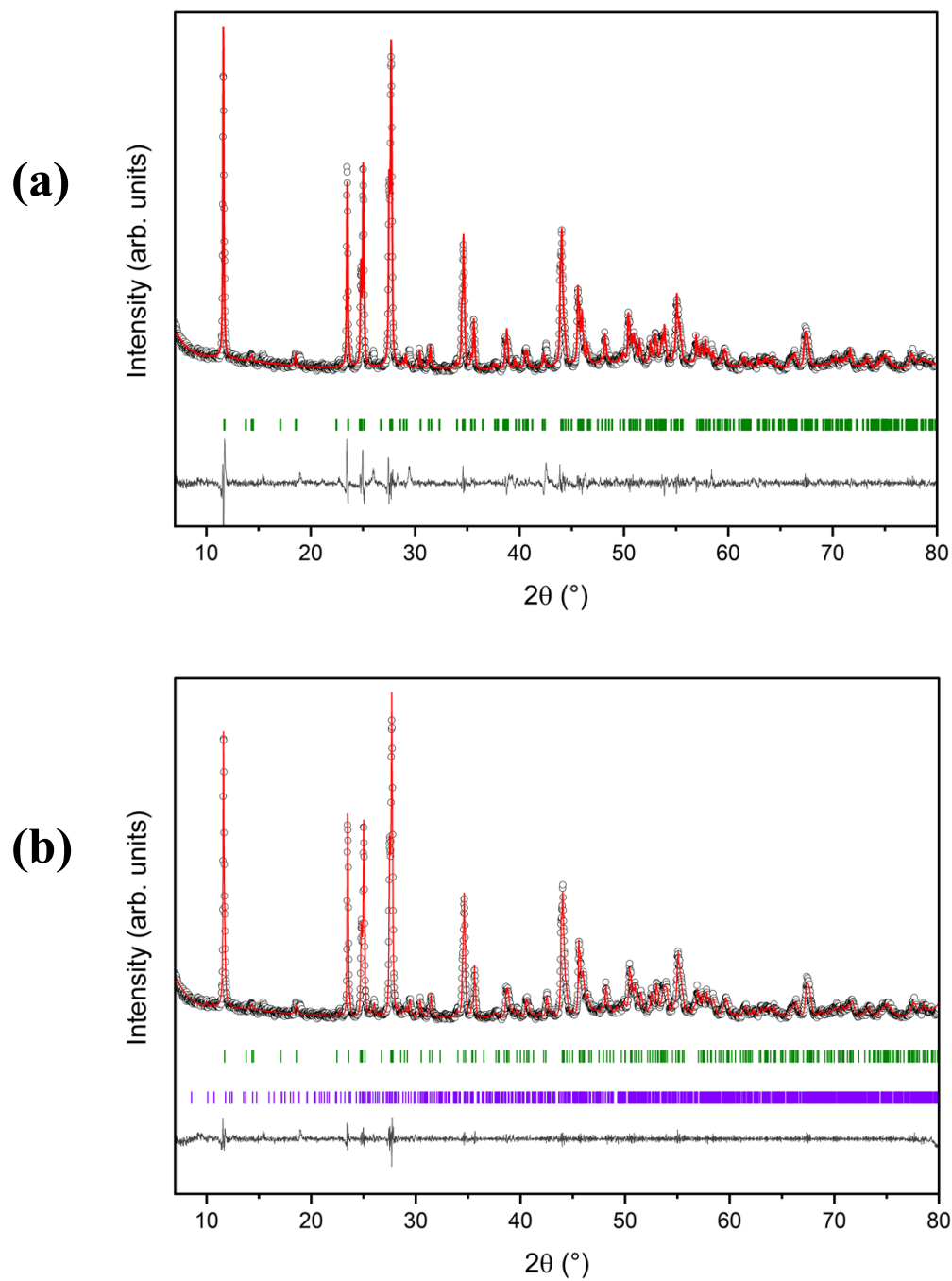* Corresponding author: *Email: yzx@ansto.gov.au* (Y. Zhang)

Figure S1. Le Bail fitting of PXRD data for compound **U-N1**: for **U-N1** (a), **U-N1** and meta-schoepite (b).
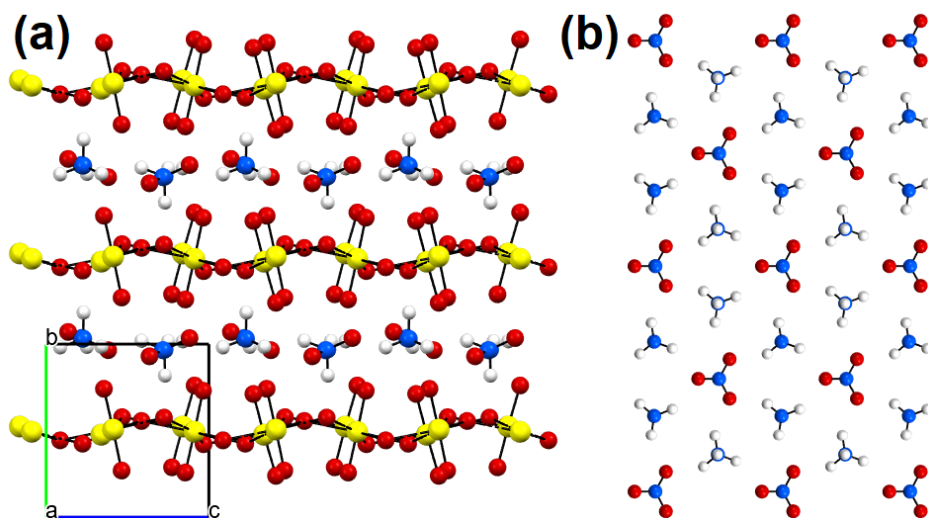
Figure S2. A ball-stick crystal packing view of compound **U-N1** along the *a*-axis (a) and the interlayer cation and anion arrangement (b).
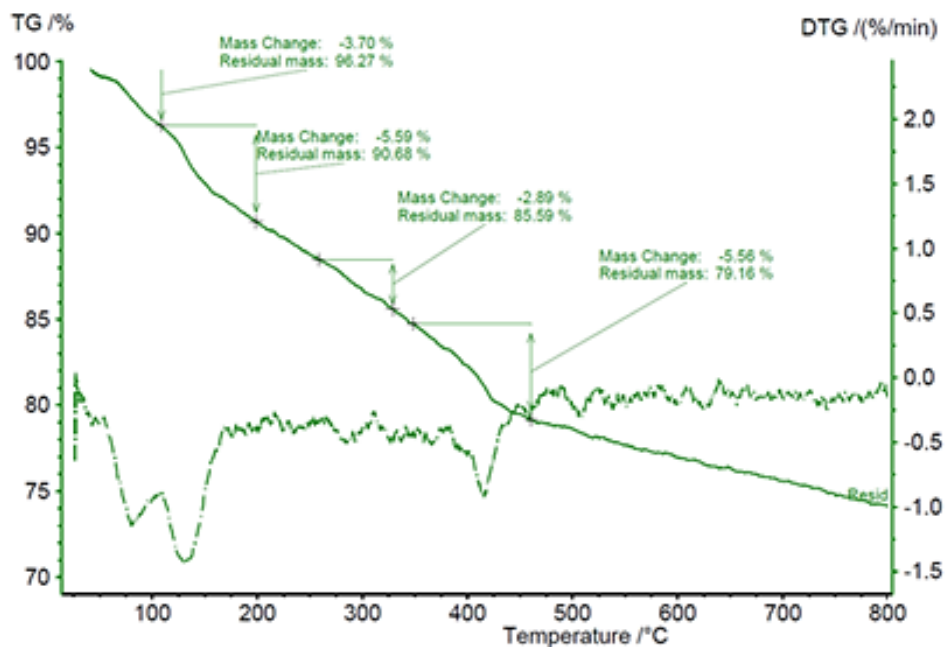

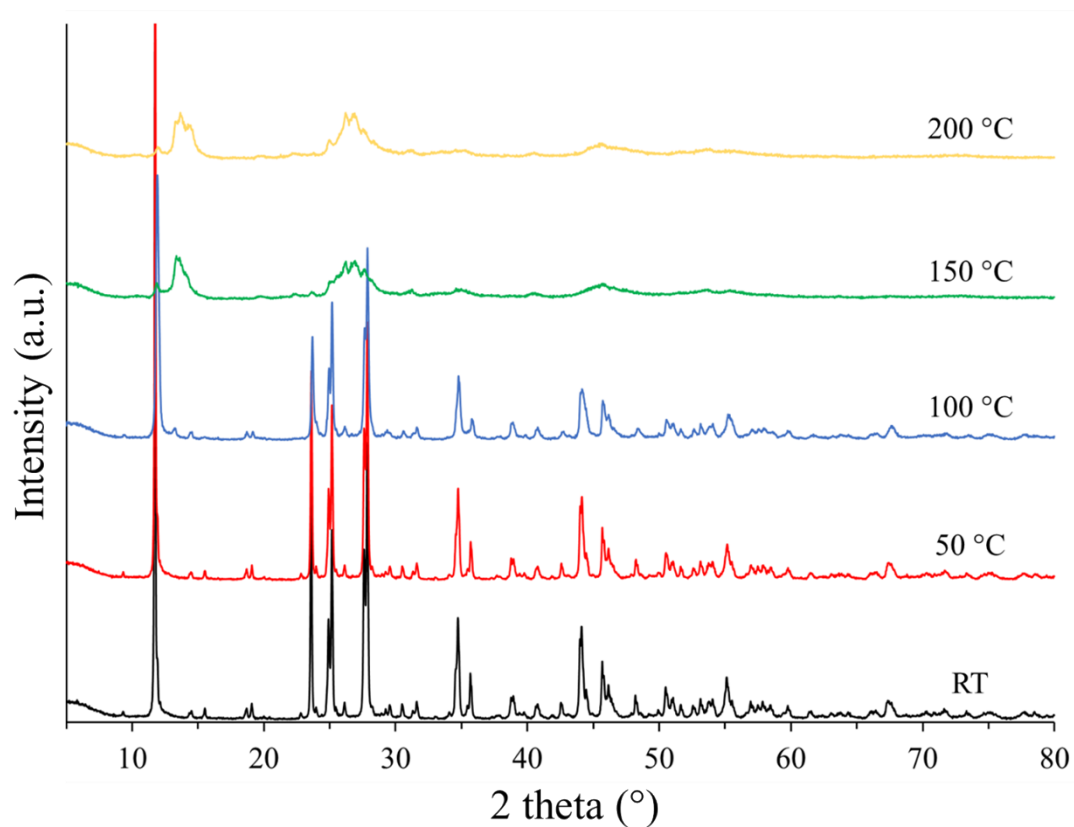**Figure S3**. Thermal analysis results for compound **U-N1**.

Figure S4. PXRD patterns of compound **U–N1** at room temperature (black) and after heating to 50°C (red), 100°C (blue), 150°C (green) and 200°C (yellow).

Table S1. Average EDS values for multiple point analyses and the U : N : O ratio for **U-N1**.

Atom% U	Atom% N	Atom% O	U : N : O ratio
16.5	17.0	66.5	1 : 1 : 4

Table S2. Analysis of Potential Hydrogen Bonds in **U-N1**.

Donor–H···Acceptor	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (º)
N2–H2A···O2	1.11	2.11	2.9004(7)	125
N2–H2A···O9	1.11	2.24	3.1665(8)	139'
N2–H2B···O8	1.12	2.27	3.1475(8)	133
N2–H2B···O1	1.12	2.02	2.8388(7)	127'
N2–H2C···O3	1.12	1.81	2.9281(7)	180
N2–H2D···O6	1.11	2.50	3.1478(8)	116
N2–H2D···O7	1.11	2.40	2.8704(7)	104'
N2–H2D···O8	1.11	2.10	3.1061(8)	150"

Table S3. Calculated bond valence sums (BVS) for cations and anions in compound **U-N1**.

	U1	U2	
CN	7	7	$\sum$
O1	1.63		**1.63**
O2	1.60		**1.60**
O3	0.66, 0.65	0.67×2	**1.98**
O4	0.44, 0.33	0.51×2	**1.28 (OH)**
O5	0.45	0.32	**0.77 (OH)**
O6		1.60	**1.60**
O7		1.54	**1.54**
$\sum$	**5.76**	**5.81**	