Supporting Information

Ionothermal effects on low-dimensionality uranyl compounds using task specific ionic liquids.

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Figure S1: UV-vis-NIR spectrum of **1**.

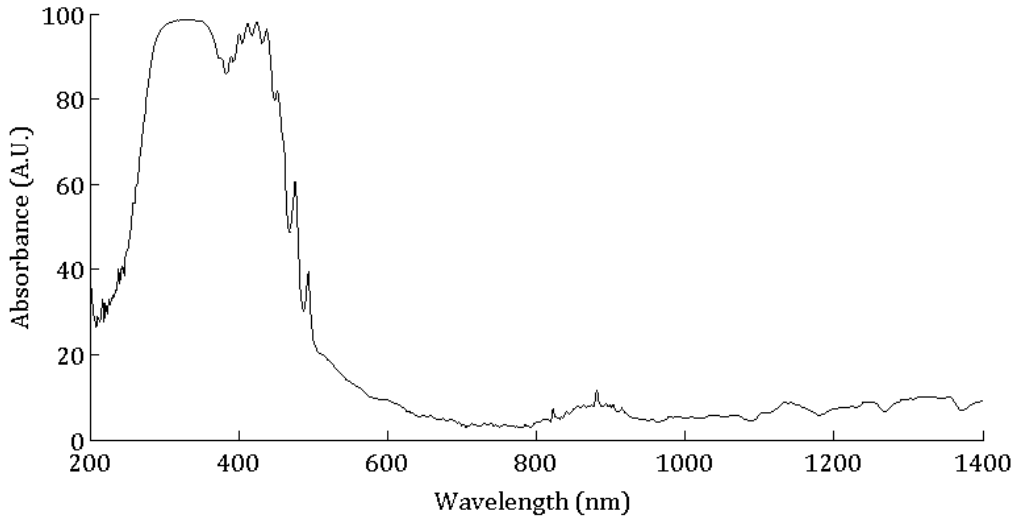

Figure S2: UV-vis-NIR spectrum of **2**.

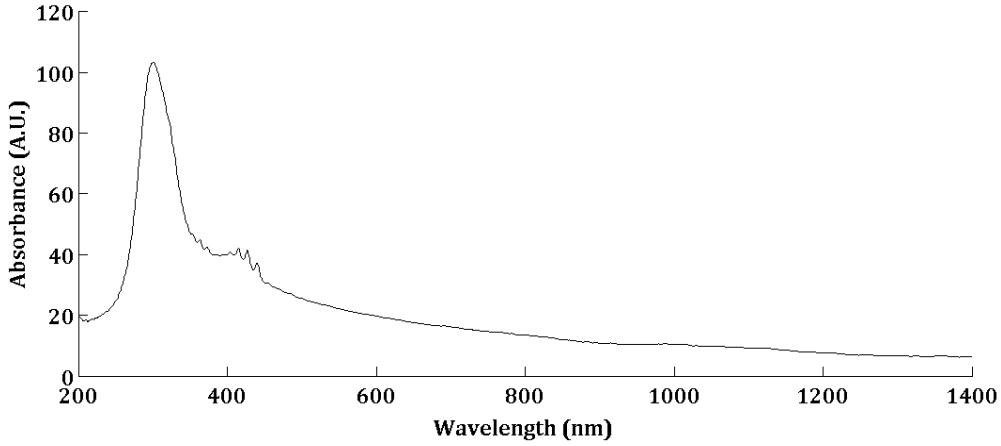

Figure S3: ATR-FTIR spectrum of **1**.

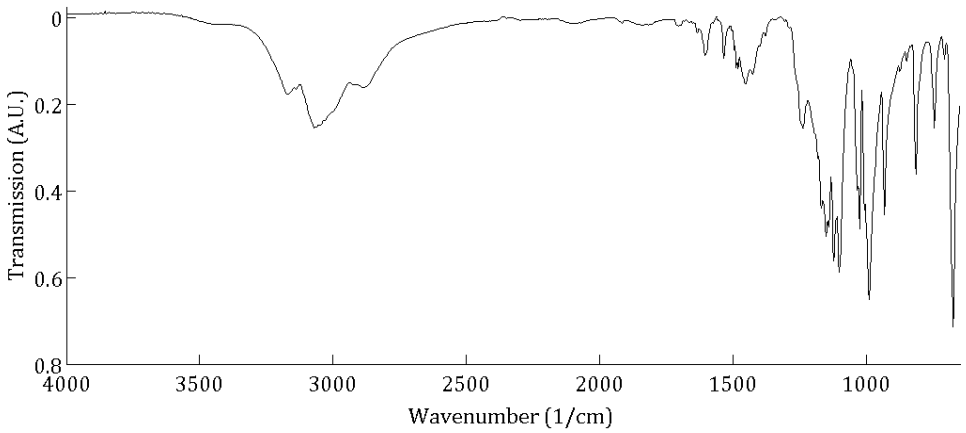

Figure S4: ATR-FTIR spectrum of **2**.

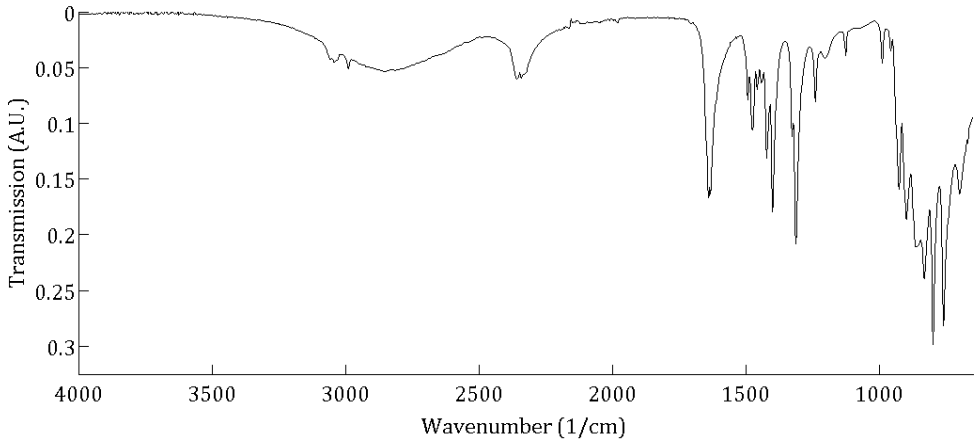

Figure S5: EDAX spectrum of **1** showing 83:17% ratio for S:U respectively, confirming the 4:1 ratio determined crystallographically.

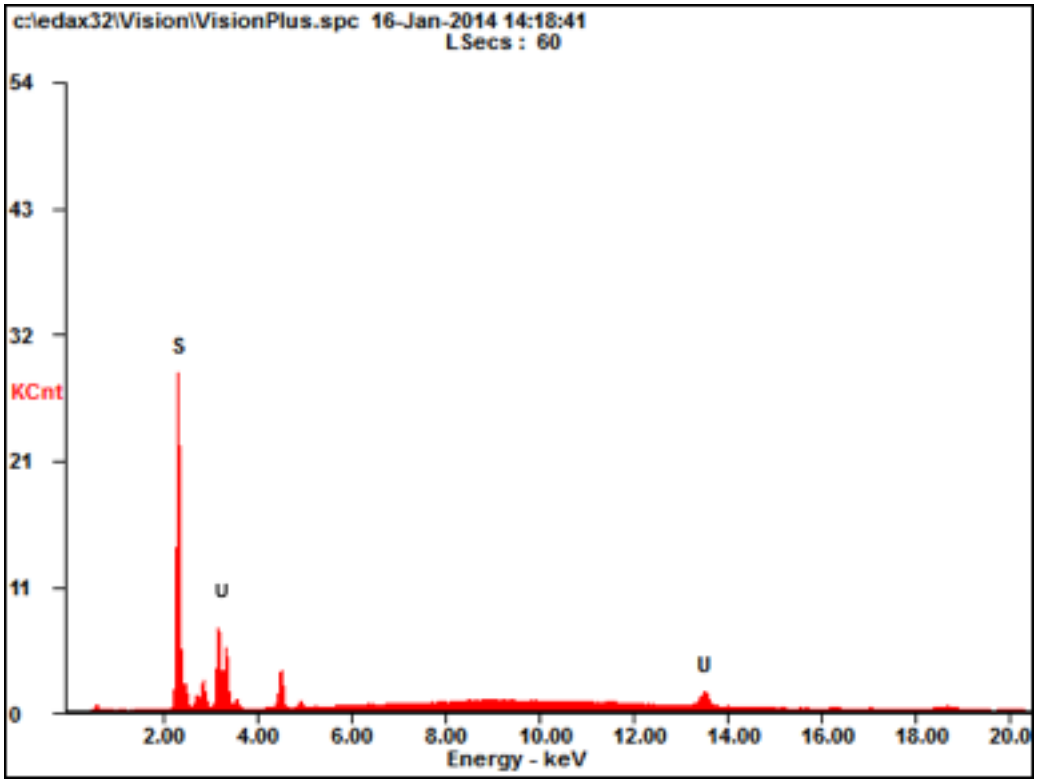

Figure S6: EDAX spectrum of **2** showing a 52:48% ratio for As:U respectively, confirming the crystallographically determined elemental ratio.

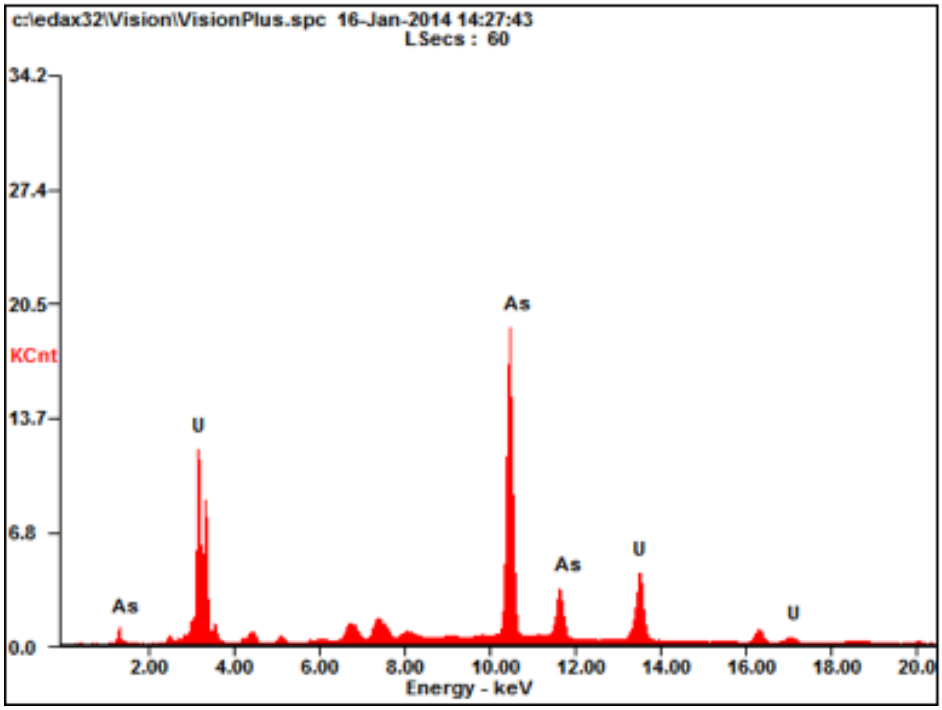

Figure S7a: Thermal Ellipsoid plot of the asymmetric unit of **1**, showing H-bond interactions between pyridinium and sulfonate moieties.

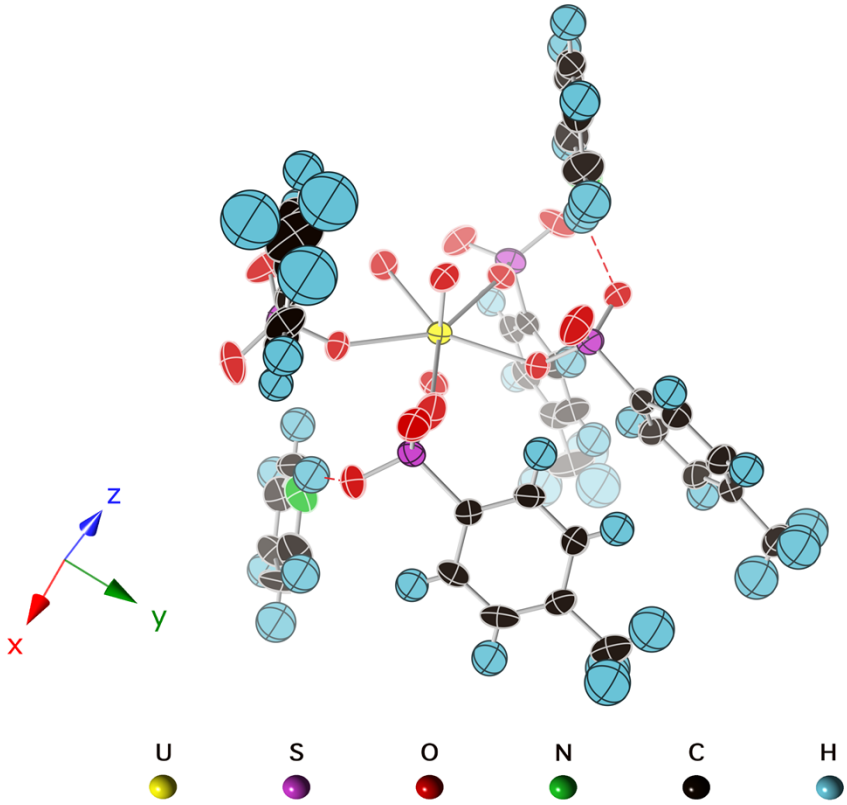

Figure S7b: Alternate Thermal Ellipsoid plot of the asymmetric unit of **1**, excluding those hydrogens not participating in H-bond interactions between the pyridinium and sulfonate moieties.

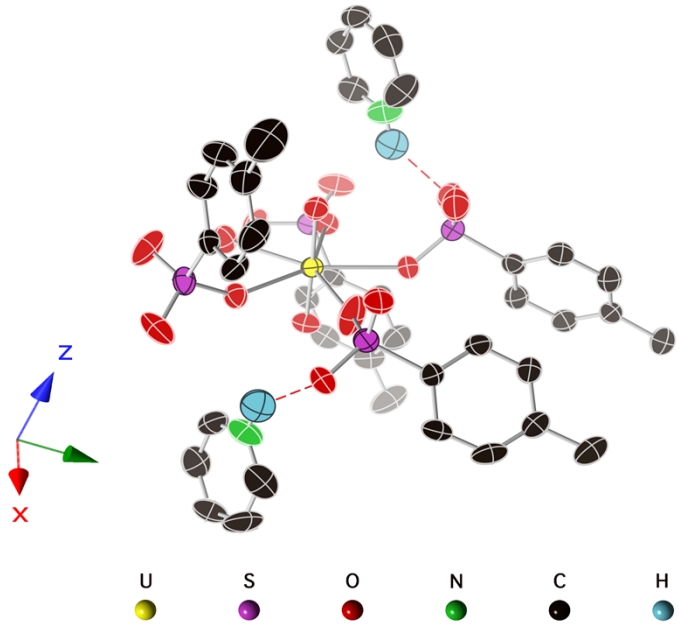

Figure S8a,b: Mixed Polyhedra - Ball and Stick plot of the asymmetric unit of **1**, showing p-touenesulfonate arrangement round the uranyl center; hydrogens are excluded for clarity.

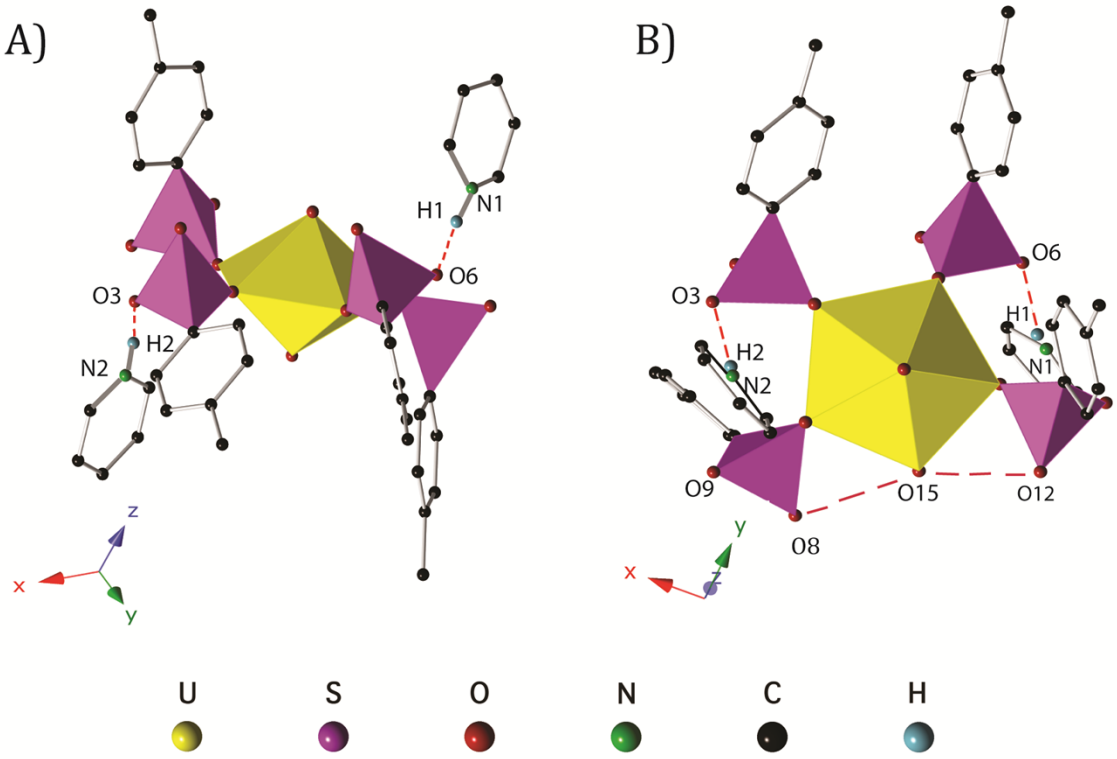

Figure S9: Mixed Ball and Stick - Polyhedra plot of **1** showing H-bonding interactions between monomers as extended along the y-axis.

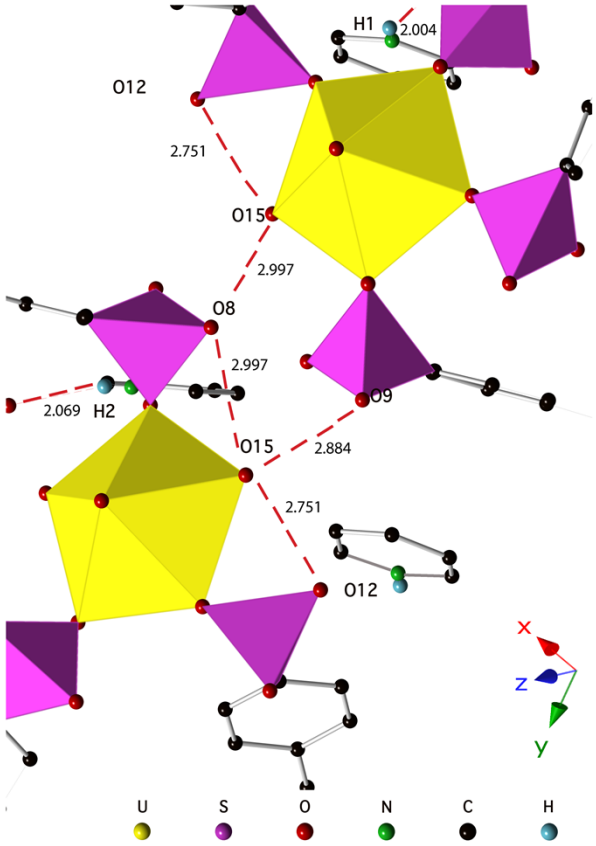

Figure S10: Thermal Ellipsoid plot of the asymmetric unit of **2**.

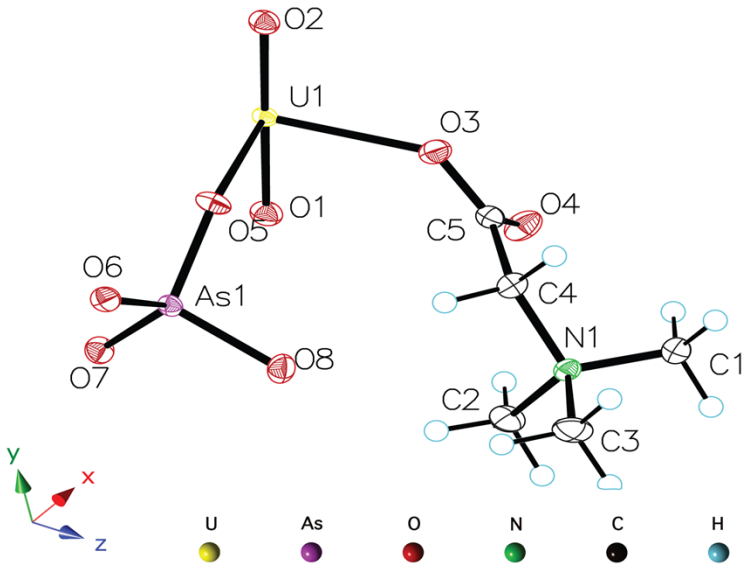

Figure S11: Polyhedra plot of **2** along the z-axis, emphasizing the 2D-zigzag chain topology.

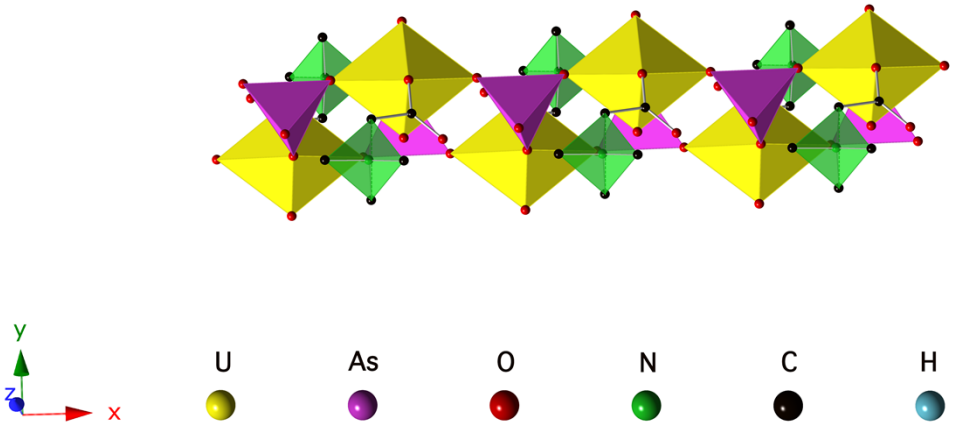

Figure S12: Mixed Ball and Stick - Polyhedra plot of **2**, emphasizing H-bond interaction between the betaine and arsenate moieties.

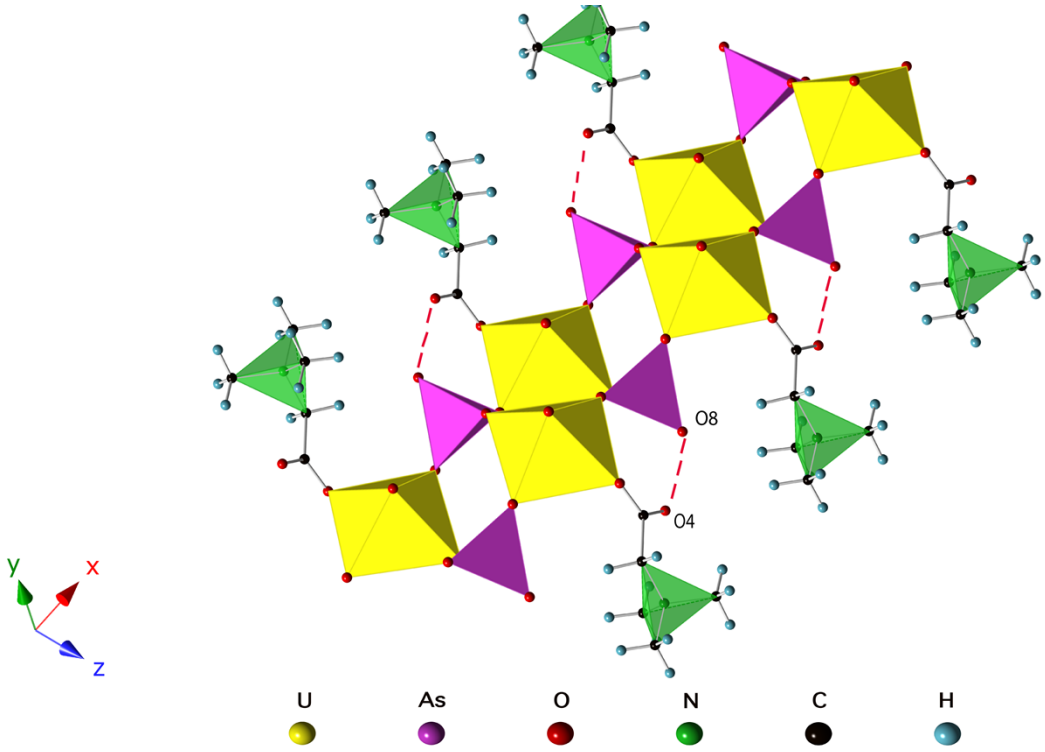

Figure S13: Thermal Ellipsoid plot of **2**, emphasizing H-bond interaction between the betaine and arsenate moieties

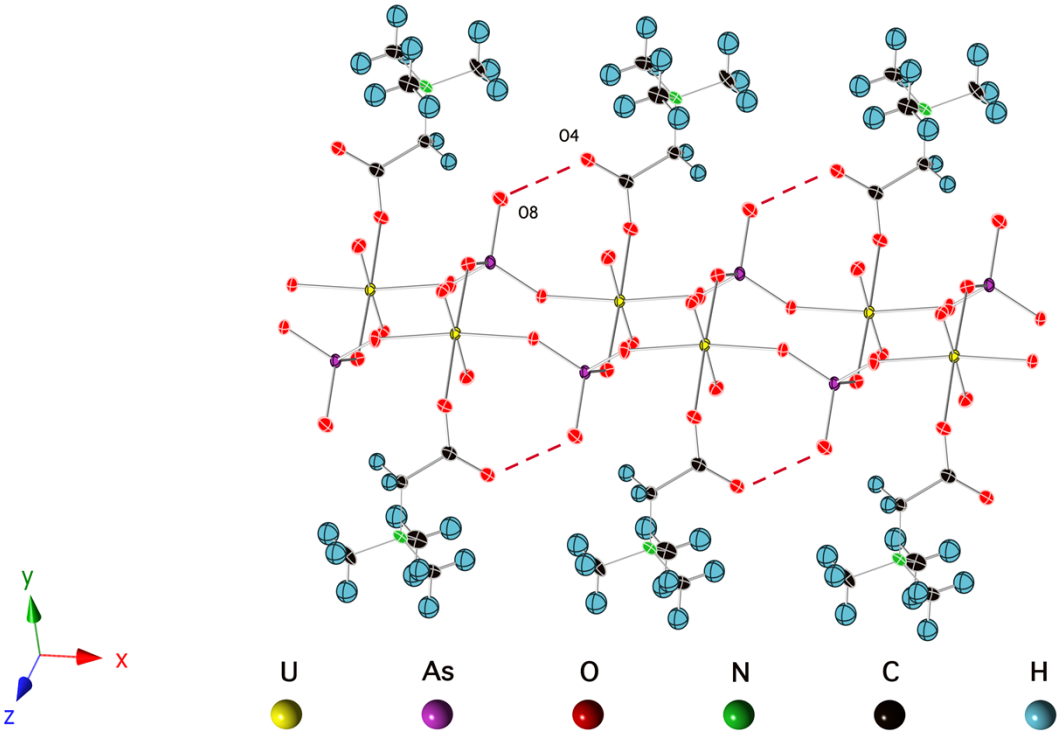

Figure S14: Alternate view of figure **S13**.

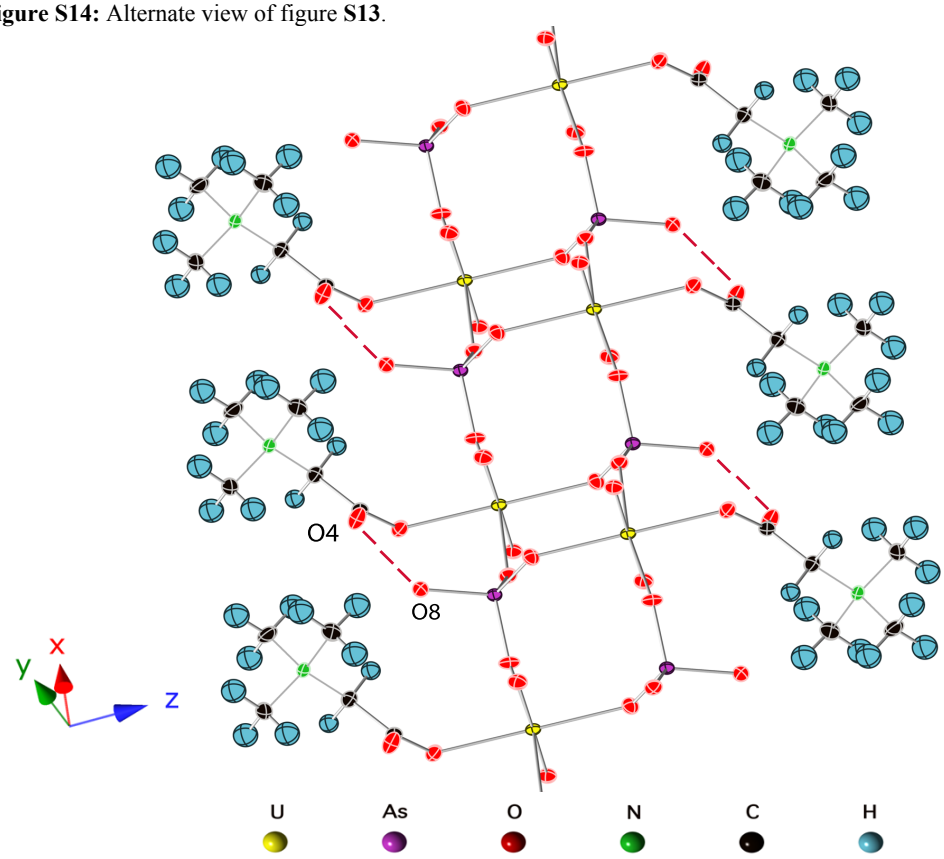

Figure S15: Packing diagram of **2** along the x-axis, using a mixed Ball and Stick - Polyhedra plot.

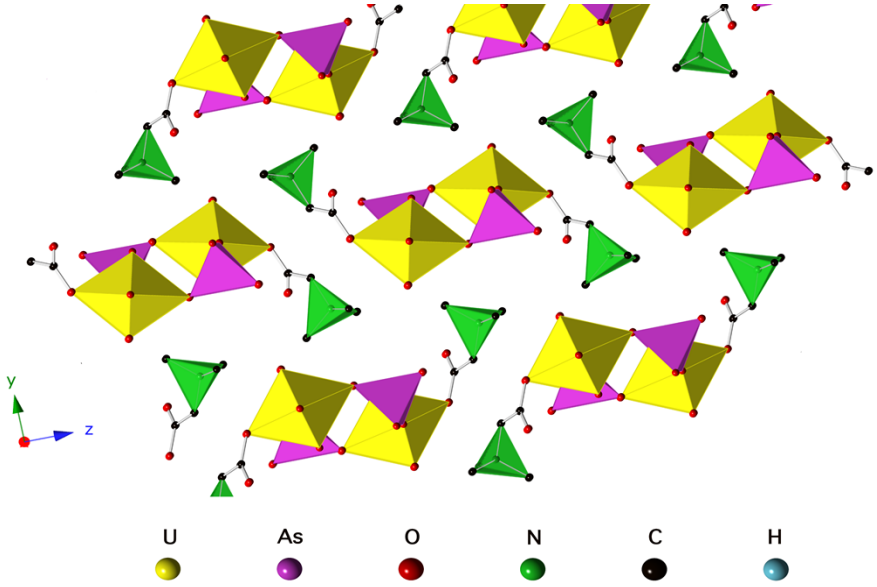

Table 1. Crystal data and structure refinement for **1**

Crystal data

CCDC: 985929

$C_{38}H_{42}N_2O_{15}S_4U$	Z = 4
M_r = 1133.00	F(000) = 2232
Monoclinic, $P2_1/c$	D_x = 1.739g cm^{-3}
Hall symbol: -P2yc	Mo Kα radiation, λ = 0.71073 Å
a = 12.3917(15) Å	Cell parameters from 9165 reflections
b = 36.745(4) Å	μ = 4.020 mm^{-1}
c = 10.2457(12) Å	T = 200K
β = 112.1900(13)°	Rectangular prism, dark yellow
V = 4319.7(9) Å	0.095 x 0.13 x 0.142 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	φ and π scans
Radiation source: microfocus sealed tube	Absorption correction: multi-scan SADABS V2012 (Bruker, 2012) was used
Graphite monochromator	wR2(int) = 0.2078 before and 0.2042 after correction
$Resolution_{max}$ = 0.80 Å	θ_{min} = 1.78, θ_{max} =26.37°
Completeness = 100%	T_{min} = 0.599, T_{max} = 0.701
46962 Measured reflections	h = -15 → 15
8837 Independent reflections	k = -45 → 45
6990 reflections with I >2σ(I)	l = -12 →12
R_{int} = 0.0715	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.0328	All H-atom treated by refinement constrained
$wR(F^2)$ = 0.0734	w=1/[σ2(Fo2)+(0.0231P)2+3.0883P] where P=(Fo2+2Fc2)/3
S = 1.023	$(\Delta/\sigma)_{max}$ < 0.001
8837 Reflections	$\Delta\rho_{max}$ = 0.507 e Å−3
545 Parameters	$\Delta\rho_{min}$ = -0.632 e Å−3
0 Restraints	Extinction correction: none
Primary atom site location: intrinsic phasing	

Table 2. Atomic coordinates and equivalent isotropic displacement parameters (Å ^{2}) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	X	Y	Z	U(eq)
U1	0.99664(2)	0.59887(2)	0.21632(2)	0.02797(6)
S1	0.32109(9)	0.61799(3)	0.35716(12)	0.0349(3)
S2	0.99483(11)	0.67672(3)	0.42449(13)	0.0401(3)
S3	0.13319(11)	0.51049(3)	0.20266(12)	0.0404(3)
S4	0.68034(10)	0.61781(4)	0.06321(13)	0.0408(3)
O4	0.0033(2)	0.65950(8)	0.2982(3)	0.0375(7)
O13	0.9765(3)	0.61496(9)	0.0481(3)	0.0434(8)
O3	0.3707(3)	0.59831(8)	0.2714(3)	0.0452(8)
O10	0.7993(2)	0.61529(8)	0.1746(3)	0.0380(7)
O2	0.3672(2)	0.60776(9)	0.5028(4)	0.0575(10)
O7	0.0995(3)	0.54926(8)	0.1738(3)	0.0403(7)
O14	0.0108(3)	0.58150(8)	0.3815(3)	0.0405(7)
O6	0.8737(3)	0.67809(9)	0.4108(4)	0.0636(11)
O11	0.5987(3)	0.63060(11)	0.1218(4)	0.0589(10)
O15	0.8584(3)	0.54863(9)	0.1005(4)	0.0506(9)
O12	0.6471(3)	0.58370(9)	0.9873(4)	0.0562(10)
O5	0.0728(4)	0.66071(9)	0.5520(4)	0.0662(11)
O9	0.2117(3)	0.50088(10)	0.1353(4)	0.0631(11)
O8	0.0318(3)	0.48771(10)	0.1686(4)	0.0702(12)
O1	0.1932(3)	0.61668(10)	0.2956(5)	0.0735(13)
C32	0.6874(4)	0.65044(12)	0.9409(4)	0.0349(10)
C18	0.0375(4)	0.72219(12)	0.4235(5)	0.0353(10)
C21	0.0923(4)	0.79556(12)	0.4195(5)	0.0409(11)
C11	0.3539(4)	0.66479(12)	0.3501(4)	0.0318(10)
N1	0.7654(4)	0.62019(12)	0.4831(5)	0.0574(12)
C13	0.3379(4)	0.7257313)	0.4191(5)	0.0453(12)
C37	0.6178(4)	0.64680(14)	0.8001(5)	0.0424(12)
C12	0.3129(4)	0.6893313)	0.4218(5)	0.0430(12)
C16	0.4214(4)	0.67675(14)	0.2759(5)	0.0437(12)
C25	0.2119(4)	0.50703(11)	0.3867(5)	0.0348(11)
N2	0.2653(5)	0.57948(14)	0.9829(4)	0.0577(13)
C23	0.1102(5)	0.73894(14)	0.5428(5)	0.0439(12)
C33	0.7609(4)	0.68049(14)	0.9862(6)	0.0461(13)
C35	0.6923(5)	0.70288(17)	0.7479(6)	0.0522(14)
C36	0.6204(4)	0.67315(16)	0.7063(6)	0.0491(13)
C22	0.1370(5)	0.77539(14)	0.5409(6)	0.0454(13)
C2	0.6351(5)	0.58289(15)	0.5298(7)	0.0504(14)
C26	0.1607(5)	0.49202(15)	0.4721(6)	0.0481(13)

C1	0.6630(5)	0.60407(16)	0.4400(6)	0.0549(15)
C34	0.7618(5)	0.70598(16)	0.8899(6)	0.0568(15)
C28	0.3395(6)	0.49842(15)	0.6723(6)	0.0588(16)
C3	0.7139(5)	0.57784(15)	0.6624(6)	0.0518(14)
C15	0.4446(5)	0.71353(16)	0.2767(6)	0.0503(14)
C20	0.0188(5)	0.77873(15)	0.2981(6)	0.0469(13)
C14	0.4048(4)	0.73841(14)	0.3468(6)	0.0444(13)
C19	0.9916(4)	0.74212(14)	0.2988(5)	0.0441(13)
C30	0.3257(5)	0.51826(14)	0.4421(6)	0.0464(13)
C10	0.1667(5)	0.56727(15)	0.8888(7)	0.0541(15)
C24	0.1275(6)	0.83482(14)	0.4166(7)	0.0648(18)
C29	0.3887(5)	0.51434(15)	0.5861(6)	0.0573(16)
C9	0.1457(5)	0.57084(17)	0.7507(6)	0.0586(16)
C27	0.2237(6)	0.48767(17)	0.6134(6)	0.0602(16)
C6	0.3457(5)	0.59509(18)	0.9451(7)	0.0641(18)
C17	0.4283(5)	0.77858(16)	0.3427(7)	0.0672(18)
C4	0.8209(6)	0.59467(17)	0.7061(7)	0.0629(17)
C8	0.2249(6)	0.58666(18)	0.7084(6)	0.0603(16)
C5	0.8433(5)	0.61648(19)	0.6132(8)	0.0721(19)
C7	0.3267(6)	0.59870(19)	0.8073(8)	0.073(2)
C38	0.6944(6)	0.7320(2)	0.6442(7)	0.085(2)
C31	0.4103(7)	0.4934(2)	0.8297(7)	0.098(3)

Table 3. Bond lengths [Å] and angles [°] for **1**.

Bond	Length (Å)	Bonds	Angle (°)
U1-O13	1.748(3)	O13-U1-O14	177.26(15)
U1-O14	1.755(3)	O13-U1-O1	89.4517)
U1-O1	2.351(4)	O14-U1-O1	93.14(17)
U1-O7	2.357(3)	O13-U1-O7	88.00(14)
U1-O4	2.371(3)	O14-U1-O7	91.90(14)
U1-O10	2.396(3)	O1-U1-O7	73.58(13)
U1-O15	2.493(3)	O13-U1-O4	90.22(14)
S1-O2	1.432(4)	O14-U1-O4	91.33(13)
S1-O3	1.442(4)	O1-U1-O4	73.93(12)
S1-O1	1.469(4)	O7-U1-O4	147.48(11)
S1-C11	1.775(5)	O13-U1-O10	89.00(14)
S2-O5	1.426(4)	O14-U1-O10	89.26(14)
S2-O6	1.455(4)	O1-U1-O10	147.48(14)
S2-O4	1.480(3)	O7-U1-O10	138.46(11)
S2-C18	1.758(5)	O4-U1-O10	73.9311)

S3-O9	1.434(4)	O13-U1-O15	87.95(15)
S3-O8	1.439(4)	O14-U1-O15	89.44(14)
S3-O7	1.483(3)	O1-U1-O15	143.76(13)
S3-C25	1.770(5)	O7-U1-O15	70.20(11)
S4-O11	1.437(4)	O4-U1-O15	142.19(11)
S4-O12	1.450(4)	O10-U1-O15	68.29(11)
S4-O10	1.487(3)	O13-U1-O14	177.35(15)
S4-C32	1.760(5)	O13-U1-O1	89.34(17)
C32-C37	1.380(6)	O14-U1-O1	93.21(17)
C32-C33	1.391(7)	O13-U1-O7	88.06(14)
C18-C19	1.369(7)	O14-U1-O7	91.98(14)
C18-C23	1.382(7)	O1-U1-O7	73.64(13)
C21-C22	1.373(7)	O13-U1-O4	90.10(14)
C21-C20	1.377(7)	O14-U1-O4	91.29(13)
C21-C24	1.515(7)	O1-U1-O4	73.89(12)
C11-C12	1.376(7)	O7-U1-O4	147.50(11)
C11-C16	1.396(7)	O13-U1-O10	88.90(14)
N1-C1	1.320(7)	O14-U1-O10	89.32(14)
N1-C5	1.325(8)	O1-U1-O10	147.69(14)
C13-C12	1.375(7)	O7-U1-O10	138.51(11)
C13-C14	1.388(7)	O4-U1-O10	73.85(11)
C37-C36	1.370(7)	O13-U1-O15	88.04(15)
C16-C15	1.378(7)	O14-U1-O15	89.48(14)
C25-C30	1.371(7)	O1-U1-O15	143.82(13)
C25-C26	1.375(7)	O7-U1-O15	70.21(11)
N2-C10	1.319(7)	O4-U1-O15	142.16(11)
N2-C6	1.323(8)	O10-U1-O15	68.33(11)
C23-C22	1.381(7)	O2-S1-O1	112.3(3)
C33-C34	1.368(7)	O2-S1-C11	106.8(2)
C35-C36	1.377(8)	O1-S1-C11	104.0(2)
C35-C34	1.387(7)	O2-S1-O3	114.412)
C35-C38	1.515(8)	O3-S1-O1	111.2(2)
C2-C1	1.348(8)	O3-S1-C11	107.7(2)
C2-C3	1.353(8)	O5-S2-O4	112.2(2)
C26-C27	1.372(8)	O5-S2-C18	108.0(2)
C28-C29	1.378(8)	O4-S2-C18	105.31(2)
C28-C27	1.387(8)	O5-S2-O6	114.8(3)
C28-C31	1.524(8)	O6-S2-O4	110.0(2)
C3-C4	1.375(8)	O6-S2-C18	105.9(2)
C15-C14	1.368(8)	O9-S3-O7	109.4(2)
C20-C19	1.386(7)	O9-S3-C25	107.1(2)
C14-C17	1.507(7)	O7-S3-C25	106.38(2)
C30-C29	1.389(7)	O9-S3-O8	115.4(3)

C10-C9	1.342(8)	O8-S3-O7	110.9(2)
C9-C8	1.345(8)	O8-S3-C25	107.2(2)
C6-C7	1.354(9)	O11-S4-O12	113.9(2)
C4-C5	1.352(9)	O11-S4-O10	110.5(2)
C8-C7	1.361(9)	O12-S4-O10	110.8(2)
		O11-S4-C32	107.9(2)
		O12-S4-C32	106.7(2)
		O10-S4-C32	106.7(2)
		S1-O1-U1	165.2(2)
		S2-O4-U1	134.97(18)
		S3-O7-U1	146.87(19)
		S4-O10-U1	143.30(18)
		C1-N1-C5	122.0(5)
		C10-N2-C6	121.6(5)
		C37-C32-S4	119.9(4)
		C19-C18-C23	119.4(4)
		C23-C18-S2	120.0(4)
		C22-C21-C24	120.9(5)
		C12-C11-C16	120.2(4)
		C16-C11-S1	121.4(4)
		C12-C13-C14	121.5(5)
		C11-C12-C13	119.7(5)
		C30-C25-C26	120.5(5)
		C26-C25-S3	120.3(4)
		C18-C23-C22	119.8(5)
		C36-C35-C34	117.7(5)
		C34-C35-C38	120.7(6)
		C21-C22-C23	121.3(5)
		C27-C26-C25	120.2(5)
		C33-C34-C35	121.9(6)
		C29-C28-C31	120.7(6)
		C2-C3-C4	120.5(6)
		C21-C20-C19	120.8(5)
		C15-C14-C17	122.2(5)
		C18-C19-C20	120.3(5)
		N2-C10-C9	119.8(5)
		C8-C9-C10	120.5(6)
		N2-C6-C7	119.7(6)
		C9-C8-C7	119.0(6)
		C6-C7-C8	119.5(6)
		C37-C32-C33	119.9(4)
		C33-C32-S4	120.2(3)
		C19-C18-S2	120.4(4)

C22-C21-C20	118.5(4)
C20-C21-C24	120.6(5)
C12-C11-S1	118.4(4)
C36-C37-C32	119.7(5)
C15-C16-C11	118.2(5)
C30-C25-S3	119.2(4)
C34-C33-C32	119.1(5)
C36-C35-C38	121.5(5)
C37-C36-C35	121.6(5)
C1-C2-C3	119.3(6)
N1-C1-C2	119.9(6)
C29-C28-C27	118.6(5)
C27-C28-C31	120.8(6)
C14-C15-C16	122.9(5)
C15-C14-C13	117.5(5)
C13-C14-C17	120.3(5)
C25-C30-C29	119.1(5)
C28-C29-C30	121.2(5)
C26-C27-C28	120.5(6)
C5-C4-C3	117.9(6)
N1-C5-C4	120.4(6)

Symmetry codes:

(I) x, -y+1/2, z-1/2; (II) x, -y+1/2, z+1/2

Table 4. Anisotropic displacement parameters ($Å^2$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	0.02546(9)	0.03191(9)	0.02485(9)	-0.00024(7)	0.00757(6)	-0.00266(7)
S1	0.0269(6)	0.0400(7)	0.0375(7)	-0.0044(5)	0.0118(5)	-0.0035(5)
S2	0.0480(8)	0.0344(7)	0.0421(7)	-0.0040(6)	0.0219(6)	-0.0077(6)
S3	0.0493(8)	0.0330(7)	0.0309(7)	-0.0019(5)	0.0061(6)	0.0016(6)
S4	0.0251(6)	0.0556(8)	0.0386(7)	-0.0008(6)	0.0087(5)	-0.0056(6)
O4	0.0401(18)	0.0357(18)	0.0369(18)	-0.0077(14)	0.0148(16)	-0.0041215)
O13	0.046(2)	0.0510(19)	0.0369(19)	0.0047(17)	0.0200(17)	0.0028(17)
O3	0.049(2)	0.0484(19)	0.0390(19)	-0.0082(16)	0.0176(18)	0.0056(17)
O10	0.0250(16)	0.0491(19)	0.0364(19)	-0.0040(16)	0.0077(14)	-0.0040(15)
O2	0.090(3)	0.047(2)	0.042(2)	0.0050(18)	0.033(2)	-0.0017(19)
O7	0.0474(19)	0.0318(17)	0.0395(18)	0.0026(15)	0.0140(17)	0.0055(15)
O14	0.052(2)	0.0381(19)	0.0265(18)	0.0039(15)	0.0096(16)	-0.0037 (17)
O6	0.060(3)	0.051(2)	0.103(3)	-0.014(2)	0.057(3)	-0.0190(19)

O11	0.0298(18)	0.097(3)	0.056(3)	0.011(2)	0.0225(19)	0.0062(18)
O15	0.044(2)	0.049(2)	0.056(2)	-0.0194(18)	0.0161(18)	-0.0111(17)
O12	0.047(2)	0.054(2)	0.049(2)	-0.0001(19)	-0.0029(19)	-0.0168(19)
O5	0.106(3)	0.042(2)	0.040(2)	0.0019(18)	0.016(2)	-0.006(2)
O9	0.081(3)	0.070(3)	0.038(2)	0.004(2)	0.022(2)	0.034(2)
O8	0.074(3)	0.054(3)	0.051(2)	0.0072(18)	-0.013(2)	-0.032(2)
O1	0.0273(19)	0.049(2)	0.135(4)	-0.023(3)	0.020(2)	-0.0097(17)
C32	0.031(3)	0.043(3)	0.032(2)	-0.002(2)	0.013(2)	0.005(2)
C18	0.036(3)	0.037(2)	0.037(3)	-0.004(2)	0.018(2)	-0.001(2)
C21	0.046(3)	0.036(3)	0.049(3)	-0.007(2)	0.028(3)	-0.003(2)
C11	0.026(2)	0.038(2)	0.026(2)	-0.0022(19)	0.0025(19)	-0.0038(19)
N1	0.058(3)	0.059(3)	0.066(3)	0.022(3)	0.034(3)	0.006(2)
C13	0.048(3)	0.039(3)	0.052(3)	-0.010(3)	0.022(3)	-0.008(2)
C37	0.029(3)	0.056(3)	0.037(3)	-0.009(2)	0.007(2)	0.001(2)
C12	0.042(3)	0.049(3)	0.042(3)	-0.002(2)	0.021(2)	-0.010(2)
C16	0.042(3)	0.059(3)	0.035(3)	0.001(2)	0.020(2)	-0.001(3)
C25	0.041(3)	0.029(2)	0.029(2)	-0.0014(19)	0.007(2)	0.0023(19)
N2	0.067(3)	0.074(4)	0.029(2)	0.006(2)	0.015(2)	0.017(3)
C23	0.052(3)	0.046(3)	0.032(3)	0.004(2)	0.014(2)	-0.001(2)
C33	0.036(3)	0.054(3)	0.039(3)	0.000(2)	0.003(2)	-0.005(2)
C35	0.037(3)	0.068(4)	0.046(3)	0.014(3)	0.010(3)	0.007(3)
C36	0.034(3)	0.073(4)	0.035(3)	0.002(3)	0.005(2)	0.012(3)
C22	0.048(3)	0.044(3)	0.041(3)	-0.012(2)	0.012(2)	-0.014(2)
C2	0.041(3)	0.046(3)	0.065(4)	0.002(3)	0.022(3)	0.000(3)
C26	0.043(3)	0.061(4)	0.040(3)	-0.010(3)	0.016(2)	-0.010(3)
C1	0.049(3)	0.067(4)	0.039(3)	0.006(3)	0.008(3)	0.005(3)
C34	0.052(4)	0.058(4)	0.053(3)	0.008(3)	0.011(3)	-0.013(3)
C28	0.079(4)	0.047(3)	0.035(3)	0.009(3)	0.004(3)	-0.002(3)
C3	0.061(4)	0.044(3)	0.060(4)	0.017(3)	0.034(3)	0.014(3)
C15	0.039(3)	0.064(3)	0.053(4)	0.013(3)	0.019(3)	-0.013(3)
C20	0.063(4)	0.039(3)	0.043(3)	0.006(2)	0.024(3)	0.001(3)
C14	0.039(3)	0.041(3)	0.051(3)	0.002(2)	0.014(2)	-0.008(2)
C19	0.049(3)	0.043(3)	0.037(3)	-0.007(2)	0.013(2)	-0.011(2)
C30	0.050(3)	0.043(3)	0.038(3)	0.005(2)	0.008(2)	-0.013(3)
C10	0.054(4)	0.054(4)	0.062(4)	0.003(3)	0.030(3)	-0.012(3)
C24	0.096(5)	0.036(3)	0.073(4)	-0.012(3)	0.046(4)	-0.018(3)
C29	0.049(3)	0.056(4)	0.049(3)	0.005(3)	-0.002(3)	-0.014(3)
C9	0.051(3)	0.066(4)	0.049(3)	-0.015(3)	0.006(3)	-0.008(3)
C27	0.083(4)	0.068(4)	0.037(3)	0.002(3)	0.029(3)	-0.006(3)
C6	0.037(3)	0.090(5)	0.055(4)	-0.024(3)	0.005(3)	-0.007(3)
C17	0.066(4)	0.054(3)	0.082(5)	0.007(3)	0.031(4)	-0.017(3)
C4	0.059(4)	0.073(4)	0.040(3)	-0.002(3)	-0.002(3)	0.016(3)
C8	0.069(4)	0.080(4)	0.036(3)	0.002(3)	0.025(3)	0.004(3)

C5	0.041(3)	0.072(5)	0.091(5)	0.006(4)	0.011(3)	-0.011(3)
C7	0.060(4)	0.100(6)	0.077(5)	0.006(4)	0.043(4)	-0.023(4)
C38	0.066(5)	0.099(6)	0.067(5)	0.040(4)	0.002(4)	-0.009(4)
C31	0.127(7)	0.092(6)	0.038(4)	0.015(4)	-0.010(4)	-0.026(5)

Table 5. Crystal data and structure refinement for **2**

Crystal data

CCDC: 985928

$AsC_5H_{12}NO_8U$	Z = 4
M_r = 521.11	F(000) = 948
Monoclinic, $P2_1/c$	D_x = 2.993 g cm^{-3}
Hall symbol: -P2yc	Mo Kα radiation, λ = 0.71073 Å
a = 7.167(2) Å	Cell parameters from 105 reflections
b = 14.704(3) Å	μ = 16.740 mm^{-1}
c = 11.157(3) Å	T = 125.0K
β = 96.747(4) °	Rectangular prisms, greenish yellow
V = 1167.6(4) Å	0.065 x 0.010 x 0.003 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	φ and π scans
Radiation source: microfocus sealed tube	Absorption correction: multi-scan SADABS V2012 (Bruker, 2012) was used
Graphite monochromator	wR2(int) = 0.1359 before and 0.0369 after correction
$Resolution_{max}$ = 0.80 Å	θ_{min} = 2.30, θ_{max} = 26.37°
Completeness = 100.0%	T_{min} = 0.4701, T_{max} = 0.7458
11720 Measured reflections	h = -8 → 8
2385 Independent reflections	k = -18 → 18
2204 reflections with I >2σ(I)	l = -13 →13
R_{int} = 0.0276	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.0166	All H-atom treated by refinement constrained
$wR(F^2)$ = 0.0381	w=1/[σ2(Fo2)+(0.0135P)2+3.57P] where P=(Fo2+2Fc2)/3
S = 1.080	$(\Delta/\sigma)_{max}$ < 0.001
2385 Reflections	$\Delta\rho_{max}$ = 0.855 e Å−3
148 Parameters	$\Delta\rho_{min}$ = -0.726 e Å−3
0 Restraints	Extinction correction: none
Primary atom site location: intrinsic phasing	

Table 6. Atomic coordinates and equivalent isotropic displacement parameters (Å ^{2}) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	X	Y	Z	U(eq)
U1	0.22260(2)	0.05023(2)	0.84301(2)	0.00954(5)
As1	0.72008(5)	0.98117(3)	0.83527(3)	0.01061(8)
O1	0.2342(4)	0.93187(18)	0.8789(2)	0.0167(6)
O2	0.2159(3)	0.16788(18)	0.8048(2)	0.0147(6)
O3	0.1605(4)	0.00969(19)	0.6402(2)	0.0171(6)
O4	0.0147(4)	0.8752(2)	0.6131(3)	0.0215(6)
O5	0.5295(4)	0.04719(18)	0.8147(2)	0.0158(6)
O6	0.9078(4)	0.04918(18)	0.8396(2)	0.0146(6)
O7	0.7232(4)	0.91431(19)	0.9565(2)	0.0156(6)
O8	0.7076(4)	0.9135(2)	0.7087(2)	0.0191(6)
N1	0.3069(4)	0.8084(2)	0.4787(3)	0.0138(7)
C1	0.1384(6)	0.7874(3)	0.3900(4)	0.0212(9)
C2	0.3207(6)	0.7418(3)	0.5816(4)	0.0231(9)
C3	0.4820(6)	0.7986(3)	0.4172(4)	0.0229(9)
C4	0.3006(5)	0.9045(3)	0.5239(3)	0.0156(8)
C5	0.1427(5)	0.9289(3)	0.5980(3)	0.0157(8)

Table 7. Bond lengths [Å] and angles [°] for **2**.

Bond	Length (Å)	Bonds	Angle (°)
U1-O1	1.786(3)	O1-U1-O3	88.11(11)
U1-O2	1.781(3)	O1-U1-O5	89.52(11)
U1-O3	2.331(3)	O1-U1-O6	90.98(11)
U1-O5	2.259(3)	O1-U1-O7	90.27(11)
U1-O6	2.252(3)	O2-U1-O1	178.49(12)
U1-O7	2.286(3)	O2-U1-O3	91.10(11)
As1-O5	1.670(3)	O2-U1-O5	89.15(10)
As1-O6	1.673(3)	O2-U1-O6	90.22(10)
As1-O7	1.670(3)	O2-U1-O7	90.55(11)
As1-O8	1.721(3)	O3-U1-O5	86.41(10)
O3-C5	1.279(5)	O6-U1-O3	84.57(10)
O4-C5	1.237(5)	O6-U1-O5	170.94(10)
O6-U1	2.252(3)	O7-U1-O3	177.92(9)
N1-C1	1.500(5)	O7-U1-O5	94.88(10)
N1-C2	1.503(5)	O7-U1-O6	94.16(9)
N1-C3	1.507(5)	O5-As1-O6	107.38(13)
N1-C4	1.502(5)	O5-As1-O7	112.74(13)

C4-C5	1.520(5)	O5-As1-O8	105.10(13)
		O6-As1-O7	113.21(13)
		O6-As1-O8	109.48(13)
		O7-As1-O8	108.59(14)
		C5-O3-U1	126.5(2)
		As1-O5-U1	141.89(15)
		As1-O6-U1	143.66(15)
		As1-O7-U1	130.01(15)
		C2-N1-C1	110.2(3)
		C3-N1-C1	109.2(3)
		C3-N1-C2	107.6(3)
		C4-N1-C1	111.2(3)
		C4-N1-C2	111.0(3)
		C4-N1-C3	107.6(3)
		N1-C4-C5	117.2(3)
		O3-C5-C4	111.8(3)
		O4-C5-O3	125.9(4)
		O4-C5-C4	122.4(3)

Symmetry codes:

(I) x-1, y, z; (II) -x+1, -y+1, -z+1; (III) x+1, y, z

Table 8. Anisotropic displacement parameters (Å ^{2}) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U1	0.00739(7)	0.00879(8)	0.01242(8)	0.00057(5)	0.00108(5)	0.00030(5)
As1	0.00737(17)	0.01298(19)	0.01144(18)	-0.00021(14)	0.00097(13)	0.00067(14)
O1	0.0172(14)	0.0132(14)	0.0194(14)	0.0025(11)	0.0005(11)	0.0009(11)
O2	0.0139(13)	0.0124(14)	0.0176(13)	0.0016(11)	0.0007(10)	0.0001(11)
O3	0.0196(15)	0.0151(14)	0.0170(14)	-0.0018(11)	0.0034(11)	0.0028(11)
O4	0.0209(15)	0.0214(15)	0.0237(15)	-0.0068(12)	0.0092(12)	-0.0023(13)
O5	0.0103(13)	0.0151(14)	0.0221(14)	0.0043(11)	0.0022(11)	0.0034(11)
O6	0.0096(13)	0.0158(14)	0.0185(14)	-0.0015(11)	0.0020(10)	-0.0008(11)
O7	0.0185(14)	0.0145(13)	0.0134(13)	0.0021(11)	0.0011(10)	-0.0010(11)
O8	0.0162(14)	0.0249(15)	0.0156(14)	-0.0073(12)	-0.0009(11)	0.0002(12)
N1	0.0168(16)	0.0148(16)	0.0101(14)	-0.0011(13)	0.0029(12)	0.0042(13)
C1	0.027(2)	0.019(2)	0.0162(19)	-0.0032(16)	-0.0026(17)	0.0061(18)
C2	0.037(3)	0.016(2)	0.016(2)	0.0071(16)	0.0017(18)	0.0070(18)
C3	0.021(2)	0.027(2)	0.022(2)	0.0011(18)	0.0091(17)	0.0104(18)
C4	0.0171(19)	0.014(2)	0.0158(18)	-0.0015(15)	0.0032(15)	-0.0001(16)
C5	0.018(2)	0.015(2)	0.0140(19)	0.0004(15)	-0.0002(15)	0.0050(16)