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Supporting Information

Effects of ionic liquid media on the cation selectivity of uranyl structural units in five new compounds produced using the ionothermal technique

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Tables 21-25: Bond valence sums of compounds 1-5.

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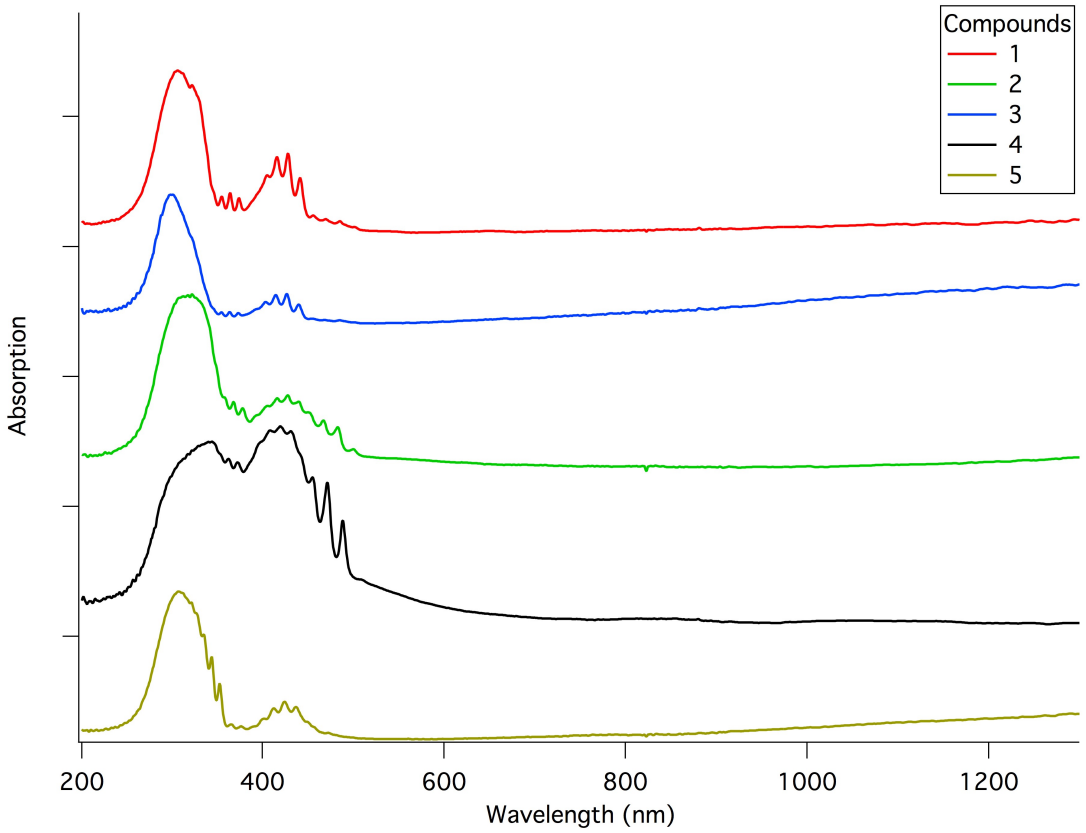

Figure S2: ATR-FTIR spectra of compounds 1-5.

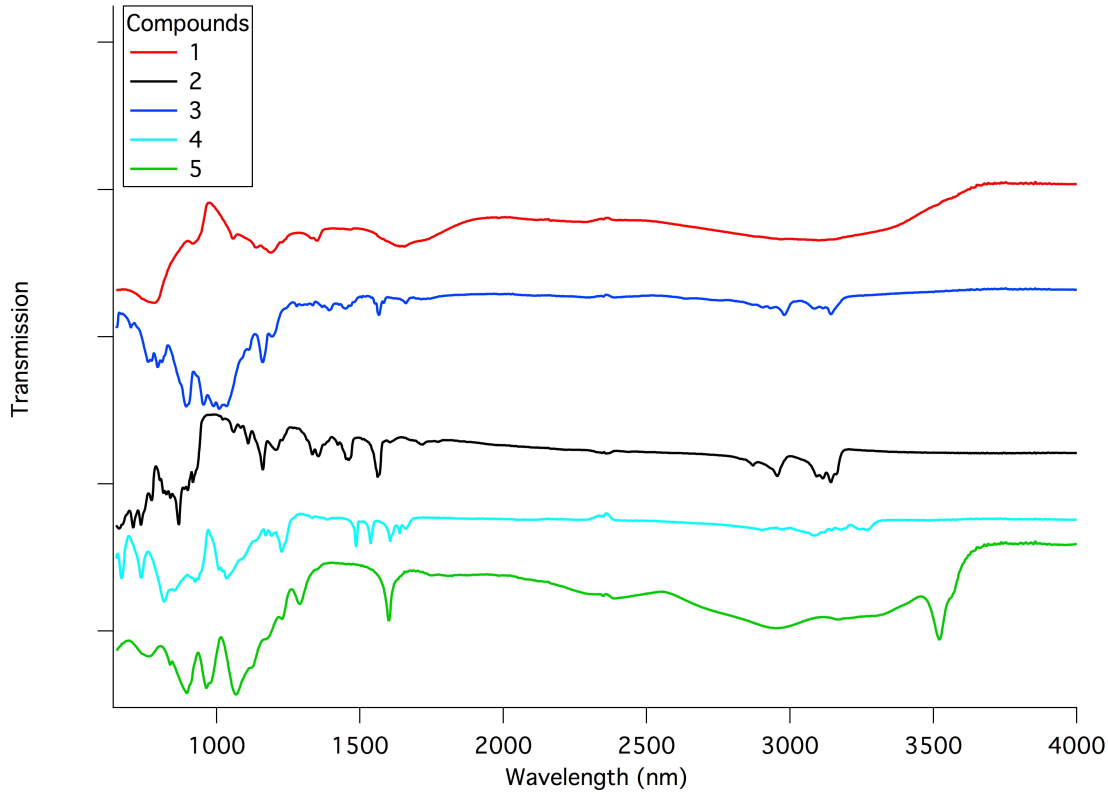

Figure S3: Raman spectra of compounds 1-5.

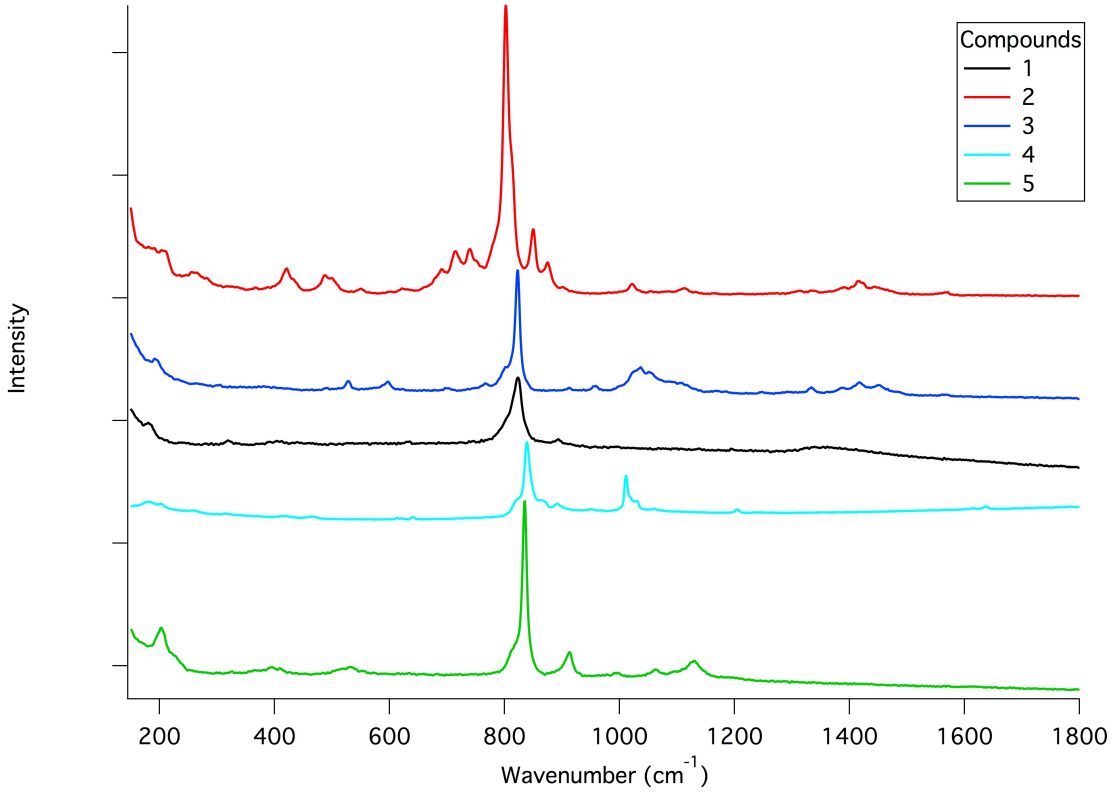

Figure S4: EDAX spectrum of compound 1.

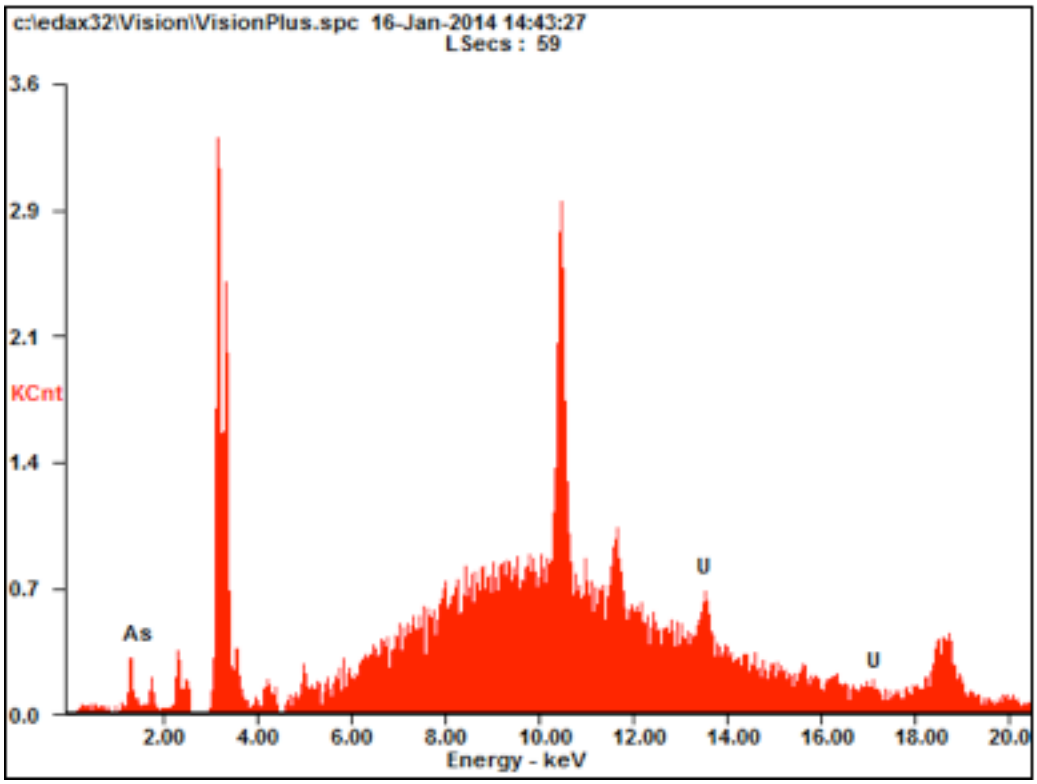

Figure 5: EDAX spectrum of compound 2.

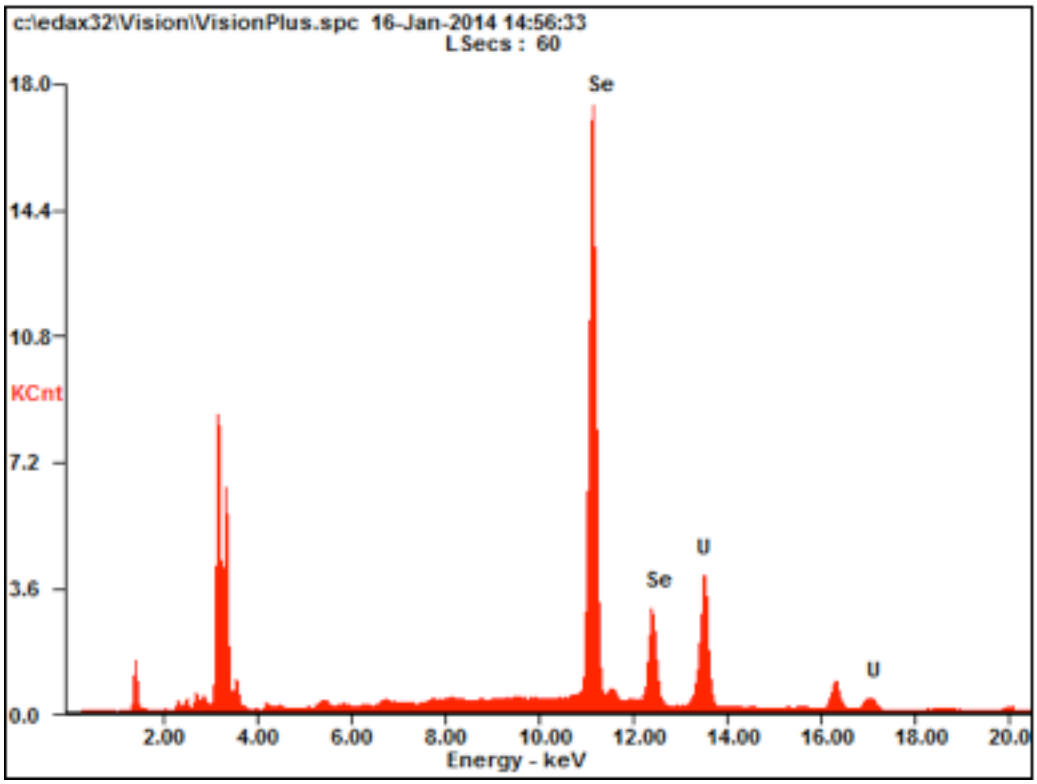

Figure S6: EDAX spectrum of compound 3.

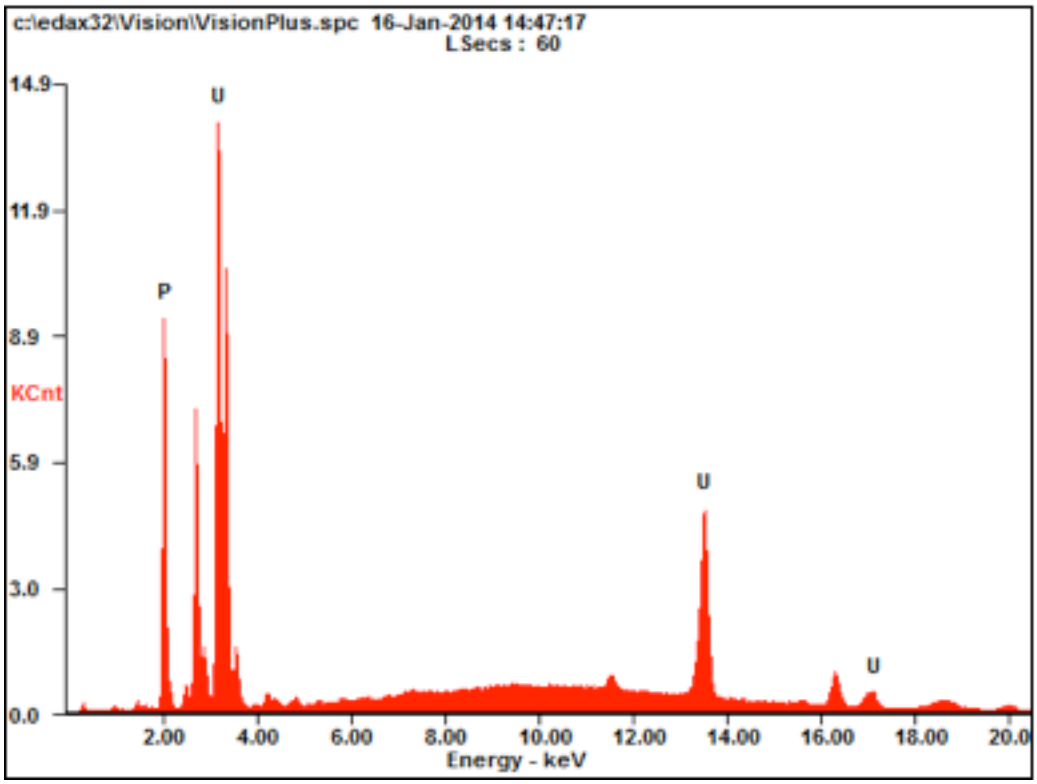

Figure S7: EDAX spectrum of compound 4.

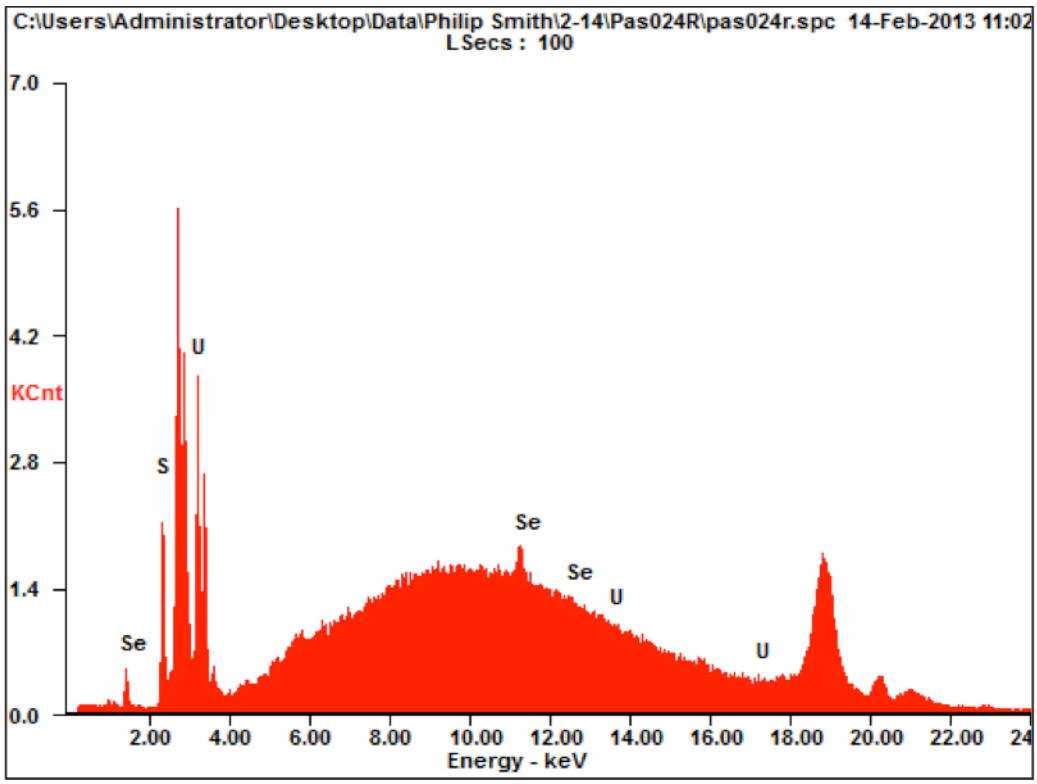

Figure S8: EDAX spectrum of compound 5.

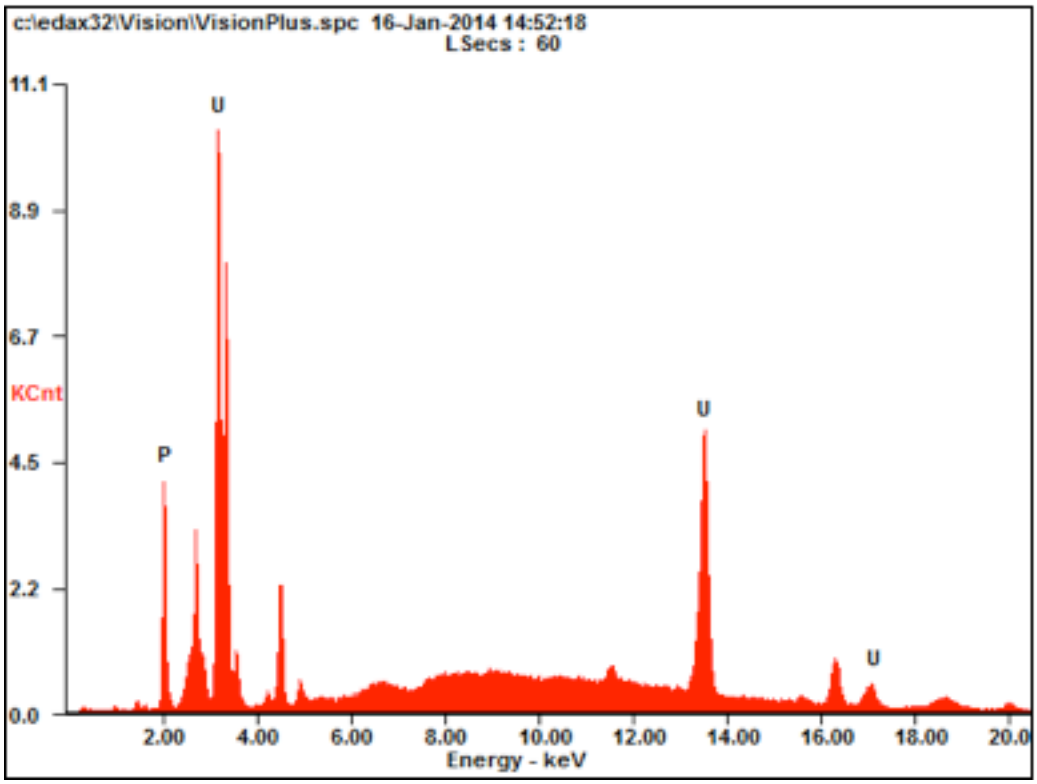

Table 1. Crystal data and structure refinement for C1.

Identification code	p1	
Empirical formula	C4 As N2 O6 U	
Formula weight	485.01	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.170(3) Å	α= 73.511(4) °.
	b = 7.181(3) Å	β= 73.892(4) °.
	c = 9.831(4) Å	γ = 89.122(4) °.
Volume	465.2(3) $Å^3$	
Z	2	
Density (calculated)	3.463 Mg/m^3	
Absorption coefficient	20.980 mm^{-1}	
F(000)	422	
Crystal size	0.08 x 0.04 x 0.02 mm^3	
Theta range for data collection	2.25 to 27.59°.	
Index ranges	-9<=h<=9, -9<=k<=9, -12<=l<=12	
Reflections collected	5568	
Independent reflections	2139 [R(int) = 0.0471]	
Completeness to theta = 27.59∞	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6810	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2139 / 0 / 67	
Goodness-of-fit on F^2	1.013	
Final R indices [I>2sigma(I)]	R1 = 0.0319, wR2 = 0.0627	
R indices (all data)	R1 = 0.0412, wR2 = 0.0659	
Largest diff. peak and hole	1.281 and -1.913 e. $Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
U(1)	7063(1)	2211(1)	1011(1)	6(1)
As(1)	7533(1)	7480(1)	79(1)	6(1)
O(1)	7821(7)	3105(7)	-970(6)	10(1)
O(2)	7333(7)	5249(7)	1270(6)	8(1)
O(3)	9814(8)	8092(7)	-1053(6)	10(1)
O(4)	6145(7)	7486(7)	-1067(6)	9(1)
O(5)	6255(7)	1392(7)	2994(6)	8(1)
O(6)	6803(8)	9069(8)	1031(6)	10(1)
N(1)	1290(9)	7181(9)	4727(7)	11(1)
N(2)	-1445(9)	7199(9)	6309(7)	10(1)
C(1)	355(12)	6606(12)	6152(9)	13(2)
C(2)	48(12)	8160(12)	3927(9)	14(2)
C(3)	-1687(12)	8164(12)	4949(9)	17(2)
C(4)	3366(13)	6944(13)	4077(10)	19(2)

Table 3. Bond lengths [Å] and angles [°] for C1.

U(1)-O(5)	1.793(5)
U(1)-O(1)	1.793(5)
U(1)-O(3)#1	2.257(5)
U(1)-O(6)#2	2.261(5)
U(1)-O(2)	2.283(5)
U(1)-O(4)#3	2.294(5)
As(1)-O(6)	1.663(5)
As(1)-O(2)	1.675(5)
As(1)-O(3)	1.685(5)
As(1)-O(4)	1.697(5)
O(3)-U(1)#1	2.257(5)
O(4)-U(1)#3	2.294(5)
O(6)-U(1)#4	2.261(5)
N(1)-C(1)	1.320(10)
N(1)-C(2)	1.400(10)
N(1)-C(4)	1.476(11)
N(2)-C(1)	1.334(10)
N(2)-C(3)	1.378(10)
C(2)-C(3)	1.365(11)

O(5)-U(1)-O(1)	178.0(2)
O(5)-U(1)-O(3)#1	90.4(2)
O(1)-U(1)-O(3)#1	90.8(2)
O(5)-U(1)-O(6)#2	88.0(2)
O(1)-U(1)-O(6)#2	93.6(2)
O(3)#1-U(1)-O(6)#2	90.21(19)
O(5)-U(1)-O(2)	85.7(2)
O(1)-U(1)-O(2)	92.7(2)
O(3)#1-U(1)-O(2)	87.64(18)
O(6)#2-U(1)-O(2)	173.36(18)
O(5)-U(1)-O(4)#3	87.4(2)
O(1)-U(1)-O(4)#3	91.3(2)
O(3)#1-U(1)-O(4)#3	177.72(19)
O(6)#2-U(1)-O(4)#3	90.35(18)

O(2)-U(1)-O(4)#3	91.56(18)
O(6)-As(1)-O(2)	108.9(3)
O(6)-As(1)-O(3)	111.5(3)
O(2)-As(1)-O(3)	111.9(3)
O(6)-As(1)-O(4)	110.8(3)
O(2)-As(1)-O(4)	108.9(2)
O(3)-As(1)-O(4)	104.7(3)
As(1)-O(2)-U(1)	132.3(3)
As(1)-O(3)-U(1)#1	140.4(3)
As(1)-O(4)-U(1)#3	137.3(3)
As(1)-O(6)-U(1)#4	145.2(3)
C(1)-N(1)-C(2)	109.7(7)
C(1)-N(1)-C(4)	125.3(7)
C(2)-N(1)-C(4)	124.9(7)
C(1)-N(2)-C(3)	110.4(7)
N(1)-C(1)-N(2)	107.5(7)
C(3)-C(2)-N(1)	106.1(7)
C(2)-C(3)-N(2)	106.3(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z #2 x,y-1,z #3 -x+1,-y+1,-z

#4 x,y+1,z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C1. 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}
U(1)	7(1)	6(1)	7(1)	-2(1)	-2(1)	1(1)
As(1)	7(1)	4(1)	9(1)	-2(1)	-3(1)	1(1)

Table 5. Crystal data and structure refinement for C2.

Identification code	pnmax	
Empirical formula	C16 N4 O23 Se5 U4	
Formula weight	1963.12	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pnma	
Unit cell dimensions	a = 18.860(2) Å	α= 90°.
	b = 18.010(2) Å	β= 90°.
	c = 11.1408(13) Å	γ = 90°.
Volume	3784.3(8) $Å^3$	
Z	4	
Density (calculated)	3.446 Mg/m^3	
Absorption coefficient	21.960 mm^{-1}	
F(000)	3384	
Crystal size	0.09 x 0.07 x 0.05 mm^3	
Theta range for data collection	2.12 to 27.54°.	
Index ranges	-24<=h<=24, -23<=k<=23, -14<=l<=14	
Reflections collected	42673	
Independent reflections	4507 [R(int) = 0.0898]	
Completeness to theta = 27.54∞	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.4216	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4507 / 0 / 137	
Goodness-of-fit on F^2	1.149	
Final R indices [I>2sigma(I)]	R1 = 0.0499, wR2 = 0.1046	
R indices (all data)	R1 = 0.0680, wR2 = 0.1103	
Largest diff. peak and hole	5.895 and -2.083 e. $Å^{-3}$	

Table 6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
U(1)	2110(1)	542(1)	5519(1)	17(1)
U(2)	1868(1)	2500	7412(1)	15(1)
U(3)	1669(1)	2500	11214(1)	15(1)
Se(1)	2029(1)	2500	4433(2)	16(1)
Se(2)	3135(1)	-561(1)	7391(1)	22(1)
Se(3)	1834(1)	905(1)	8950(1)	20(1)
O(1)	1874(5)	1121(5)	7441(8)	20(2)
O(2)	1776(5)	1835(5)	5482(8)	18(2)
O(3)	1950(5)	1816(5)	9350(8)	19(2)
O(4)	1429(7)	2500	3373(11)	18(3)
O(5)	2615(5)	501(5)	9218(8)	23(2)
O(6)	2788(7)	2500	7240(13)	25(3)
O(7)	758(7)	2500	10872(12)	20(3)
O(8)	2317(5)	-427(5)	6781(8)	23(2)
O(9)	951(7)	2500	7554(13)	26(3)
O(10)	3021(5)	777(6)	5622(9)	30(2)
O(11)	2586(7)	2500	11618(12)	23(3)
O(12)	3476(5)	-1233(5)	6524(9)	24(2)
O(13)	1220(5)	260(6)	5394(9)	29(2)
O(14)	2892(6)	-1039(6)	8621(9)	30(2)
N(1)	787(11)	-1475(12)	7002(19)	73(6)
N(2)	585(12)	-1440(12)	5070(20)	81(6)
C(1)	1086(13)	-1435(13)	5870(20)	66(6)
C(2)	57(14)	1518(15)	4300(20)	73(7)
C(3)	1110(17)	-1376(18)	8240(30)	103(10)
C(4)	721(18)	-1448(19)	3830(30)	106(10)
C(5)	5039(19)	-1490(20)	8100(30)	116(12)
C(6)	-281(18)	879(19)	6760(30)	107(10)
C(7)	4630(30)	1110(30)	6760(40)	178(19)
C(8)	4930(30)	420(30)	6260(40)	170(18)

Table 7. Bond lengths [Å] and angles [°] for C2.

U(1)-O(13)	1.760(10)
U(1)-O(10)	1.772(10)
U(1)-O(8)	2.275(10)
U(1)-O(14)#1	2.296(10)
U(1)-O(2)	2.412(9)
U(1)-O(1)	2.423(9)
U(1)-O(5)#1	2.429(10)
U(1)-Se(2)	3.4687(14)
U(2)-O(9)	1.737(14)
U(2)-O(6)	1.745(14)
U(2)-O(2)#2	2.467(9)
U(2)-O(2)	2.467(9)
U(2)-O(1)#2	2.483(9)
U(2)-O(1)	2.483(9)
U(2)-O(3)	2.491(9)
U(2)-O(3)#2	2.491(9)
U(2)-Se(1)	3.3323(19)
U(2)-Se(3)	3.3463(13)
U(2)-Se(3)#2	3.3464(13)
U(3)-O(7)	1.759(13)
U(3)-O(11)	1.788(14)
U(3)-O(12)#3	2.325(10)
U(3)-O(12)#4	2.325(10)
U(3)-O(4)#5	2.448(13)
U(3)-O(3)	2.472(9)
U(3)-O(3)#2	2.472(9)
Se(1)-O(4)	1.635(13)
Se(1)-O(2)#2	1.740(9)
Se(1)-O(2)	1.740(9)
Se(2)-O(12)	1.676(10)
Se(2)-O(14)	1.683(10)
Se(2)-O(8)	1.703(10)
Se(3)-O(5)	1.670(10)
Se(3)-O(3)	1.714(9)

Se(3)-O(1)	1.728(9)
O(4)-U(3)#6	2.448(13)
O(5)-U(1)#4	2.429(10)
O(12)-U(3)#1	2.325(10)
O(14)-U(1)#4	2.296(10)
N(1)-C(1)	1.39(3)
N(1)-C(5)#7	1.41(4)
N(1)-C(3)	1.52(3)
N(2)-C(1)	1.30(3)
N(2)-C(4)	1.40(4)
N(2)-C(2)#8	1.41(3)
C(2)-C(5)#1	1.35(4)
C(2)-N(2)#8	1.41(3)
C(4)-C(6)#8	1.48(4)
C(5)-C(2)#4	1.35(4)
C(5)-N(1)#9	1.41(4)
C(6)-C(4)#8	1.48(4)
C(6)-C(7)#7	1.71(5)
C(7)-C(8)	1.47(6)
C(7)-C(6)#9	1.71(5)

O(13)-U(1)-O(10)	176.9(5)
O(13)-U(1)-O(8)	89.4(4)
O(10)-U(1)-O(8)	88.7(4)
O(13)-U(1)-O(14)#1	92.2(4)
O(10)-U(1)-O(14)#1	88.2(4)
O(8)-U(1)-O(14)#1	150.3(4)
O(13)-U(1)-O(2)	91.7(4)
O(10)-U(1)-O(2)	91.4(4)
O(8)-U(1)-O(2)	142.7(3)
O(14)#1-U(1)-O(2)	66.9(3)
O(13)-U(1)-O(1)	91.1(4)
O(10)-U(1)-O(1)	91.0(4)
O(8)-U(1)-O(1)	79.4(3)
O(14)#1-U(1)-O(1)	130.2(3)
O(2)-U(1)-O(1)	63.4(3)

O(13)-U(1)-O(5)#1	86.2(4)
O(10)-U(1)-O(5)#1	90.9(4)
O(8)-U(1)-O(5)#1	74.8(3)
O(14)#1-U(1)-O(5)#1	75.7(3)
O(2)-U(1)-O(5)#1	142.4(3)
O(1)-U(1)-O(5)#1	154.1(3)
O(13)-U(1)-Se(2)	114.4(3)
O(10)-U(1)-Se(2)	63.8(3)
O(8)-U(1)-Se(2)	25.0(2)
O(14)#1-U(1)-Se(2)	141.1(3)
O(2)-U(1)-Se(2)	135.1(2)
O(1)-U(1)-Se(2)	79.5(2)
O(5)#1-U(1)-Se(2)	78.2(2)
O(9)-U(2)-O(6)	178.9(7)
O(9)-U(2)-O(2)#2	90.5(5)
O(6)-U(2)-O(2)#2	88.5(5)
O(9)-U(2)-O(2)	90.5(5)
O(6)-U(2)-O(2)	88.5(5)
O(2)#2-U(2)-O(2)	58.1(4)
O(9)-U(2)-O(1)#2	90.2(2)
O(6)-U(2)-O(1)#2	89.8(2)
O(2)#2-U(2)-O(1)#2	61.7(3)
O(2)-U(2)-O(1)#2	119.8(3)
O(9)-U(2)-O(1)	90.2(2)
O(6)-U(2)-O(1)	89.8(2)
O(2)#2-U(2)-O(1)	119.8(3)
O(2)-U(2)-O(1)	61.7(3)
O(1)#2-U(2)-O(1)	178.4(4)
O(9)-U(2)-O(3)	89.0(5)
O(6)-U(2)-O(3)	91.9(5)
O(2)#2-U(2)-O(3)	179.2(3)
O(2)-U(2)-O(3)	121.3(3)
O(1)#2-U(2)-O(3)	118.9(3)
O(1)-U(2)-O(3)	59.6(3)
O(9)-U(2)-O(3)#2	89.0(5)
O(6)-U(2)-O(3)#2	91.9(5)

O(2)#2-U(2)-O(3)#2	121.3(3)
O(2)-U(2)-O(3)#2	179.2(3)
O(1)#2-U(2)-O(3)#2	59.6(3)
O(1)-U(2)-O(3)#2	118.9(3)
O(3)-U(2)-O(3)#2	59.3(4)
O(9)-U(2)-Se(1)	100.4(5)
O(6)-U(2)-Se(1)	78.5(5)
O(2)#2-U(2)-Se(1)	30.5(2)
O(2)-U(2)-Se(1)	30.5(2)
O(1)#2-U(2)-Se(1)	90.7(2)
O(1)-U(2)-Se(1)	90.7(2)
O(3)-U(2)-Se(1)	149.1(2)
O(3)#2-U(2)-Se(1)	149.1(2)
O(9)-U(2)-Se(3)	86.2(2)
O(6)-U(2)-Se(3)	94.3(2)
O(2)#2-U(2)-Se(3)	149.5(2)
O(2)-U(2)-Se(3)	91.6(2)
O(1)#2-U(2)-Se(3)	148.4(2)
O(1)-U(2)-Se(3)	30.1(2)
O(3)-U(2)-Se(3)	29.8(2)
O(3)#2-U(2)-Se(3)	89.0(2)
Se(1)-U(2)-Se(3)	120.80(2)
O(9)-U(2)-Se(3)#2	86.2(2)
O(6)-U(2)-Se(3)#2	94.3(2)
O(2)#2-U(2)-Se(3)#2	91.6(2)
O(2)-U(2)-Se(3)#2	149.5(2)
O(1)#2-U(2)-Se(3)#2	30.1(2)
O(1)-U(2)-Se(3)#2	148.4(2)
O(3)-U(2)-Se(3)#2	89.0(2)
O(3)#2-U(2)-Se(3)#2	29.8(2)
Se(1)-U(2)-Se(3)#2	120.80(2)
Se(3)-U(2)-Se(3)#2	118.31(5)
O(7)-U(3)-O(11)	177.9(6)
O(7)-U(3)-O(12)#3	85.3(3)
O(11)-U(3)-O(12)#3	94.4(3)
O(7)-U(3)-O(12)#4	85.3(3)

O(11)-U(3)-O(12)#4	94.4(3)
O(12)#3-U(3)-O(12)#4	158.2(5)
O(7)-U(3)-O(4)#5	91.8(5)
O(11)-U(3)-O(4)#5	86.1(5)
O(12)#3-U(3)-O(4)#5	80.3(2)
O(12)#4-U(3)-O(4)#5	80.3(2)
O(7)-U(3)-O(3)	91.6(4)
O(11)-U(3)-O(3)	90.2(4)
O(12)#3-U(3)-O(3)	129.8(3)
O(12)#4-U(3)-O(3)	70.2(3)
O(4)#5-U(3)-O(3)	149.9(2)
O(7)-U(3)-O(3)#2	91.6(4)
O(11)-U(3)-O(3)#2	90.2(4)
O(12)#3-U(3)-O(3)#2	70.2(3)
O(12)#4-U(3)-O(3)#2	129.8(3)
O(4)#5-U(3)-O(3)#2	149.9(2)
O(3)-U(3)-O(3)#2	59.8(4)
O(4)-Se(1)-O(2)#2	107.2(4)
O(4)-Se(1)-O(2)	107.2(4)
O(2)#2-Se(1)-O(2)	87.0(6)
O(4)-Se(1)-U(2)	131.0(5)
O(2)#2-Se(1)-U(2)	46.1(3)
O(2)-Se(1)-U(2)	46.1(3)
O(12)-Se(2)-O(14)	101.8(5)
O(12)-Se(2)-O(8)	102.7(5)
O(14)-Se(2)-O(8)	98.7(5)
O(12)-Se(2)-U(1)	106.3(3)
O(14)-Se(2)-U(1)	129.2(4)
O(8)-Se(2)-U(1)	34.3(3)
O(5)-Se(3)-O(3)	104.9(5)
O(5)-Se(3)-O(1)	103.5(4)
O(3)-Se(3)-O(1)	91.8(4)
O(5)-Se(3)-U(2)	116.6(3)
O(3)-Se(3)-U(2)	46.3(3)
O(1)-Se(3)-U(2)	46.1(3)
Se(3)-O(1)-U(1)	140.5(5)

Se(3)-O(1)-U(2)	103.8(4)
U(1)-O(1)-U(2)	114.8(4)
Se(1)-O(2)-U(1)	127.2(4)
Se(1)-O(2)-U(2)	103.4(4)
U(1)-O(2)-U(2)	115.8(3)
Se(3)-O(3)-U(3)	131.9(5)
Se(3)-O(3)-U(2)	103.9(4)
U(3)-O(3)-U(2)	117.9(4)
Se(1)-O(4)-U(3)#6	125.6(7)
Se(3)-O(5)-U(1)#4	129.2(5)
Se(2)-O(8)-U(1)	120.7(5)
Se(2)-O(12)-U(3)#1	138.5(5)
Se(2)-O(14)-U(1)#4	123.4(5)
C(1)-N(1)-C(5)#7	109(2)
C(1)-N(1)-C(3)	131(2)
C(5)#7-N(1)-C(3)	118(2)
C(1)-N(2)-C(4)	123(3)
C(1)-N(2)-C(2)#8	106(2)
C(4)-N(2)-C(2)#8	130(3)
N(2)-C(1)-N(1)	109(2)
C(5)#1-C(2)-N(2)#8	112(3)
N(2)-C(4)-C(6)#8	109(3)
C(2)#4-C(5)-N(1)#9	102(3)
C(4)#8-C(6)-C(7)#7	102(3)
C(8)-C(7)-C(6)#9	97(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y,z-1/2 #2 x,-y+1/2,z #3 -x+1/2,y+1/2,z+1/2

#4 -x+1/2,-y,z+1/2 #5 x,y,z+1 #6 x,y,z-1

#7 x-1/2,y,-z+3/2 #8 -x,-y,-z+1 #9 x+1/2,y,-z+3/2

Table 8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C2. 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}
U(1)	29(1)	14(1)	7(1)	0(1)	-1(1)	4(1)
U(2)	26(1)	12(1)	8(1)	0	0(1)	0
U(3)	22(1)	15(1)	8(1)	0	0(1)	0
Se(1)	22(1)	16(1)	9(1)	0	-1(1)	0
Se(2)	38(1)	15(1)	11(1)	-1(1)	-6(1)	3(1)
Se(3)	37(1)	12(1)	9(1)	2(1)	0(1)	-2(1)

Table 9. Crystal data and structure refinement for C3.

Identification code	p21n	
Empirical formula	C20 N4 O22 P4 U3	
Formula weight	1486.21	
Temperature	174(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 9.954(7) Å	α= 90°.
	b = 10.264(7) Å	β= 101.758(10)°.
	c = 19.566(14) Å	γ = 90°.
Volume	1957(2) $Å^3$	
Z	2	
Density (calculated)	2.522 Mg/m^3	
Absorption coefficient	12.628 mm^{-1}	
F(000)	1320	
Crystal size	0.06 x 0.05 x 0.04 mm^3	
Theta range for data collection	2.13 to 27.34°.	
Index ranges	-12<=h<=12, -13<=k<=13, -25<=l<=25	
Reflections collected	22325	
Independent reflections	4427 [R(int) = 0.1369]	
Completeness to theta = 27.34°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.603 and 0.473	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4427 / 1 / 181	
Goodness-of-fit on F^2	0.979	
Final R indices [I>2sigma(I)]	R1 = 0.0497, wR2 = 0.1014	
R indices (all data)	R1 = 0.1448, wR2 = 0.1326	
Largest diff. peak and hole	3.486 and -1.624 e.$Å^{-3}$	

Table 10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for C3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
U(1)	5000	5000	0	19(1)
U(2)	8283(1)	5050(1)	2542(1)	22(1)
P(1)	6467(4)	7389(4)	1272(2)	24(1)
P(2)	6980(5)	2702(4)	1210(2)	33(1)
O(1)	5752(12)	3398(9)	794(6)	39(3)
O(2)	5315(11)	6514(9)	890(5)	27(3)
O(3)	7605(11)	6639(10)	1729(6)	32(3)
O(4)	6703(10)	5217(10)	-113(5)	31(3)
O(5)	6571(10)	4729(9)	2629(6)	35(3)
O(6)	5867(11)	8436(9)	1682(5)	27(3)
O(7)	6545(12)	1593(11)	1614(6)	42(3)
O(8)	9992(10)	5342(9)	2450(5)	32(3)
O(9)	2803(12)	11915(10)	-723(6)	36(3)
O(10)	7993(12)	3596(10)	1644(6)	40(3)
O(11)	7680(15)	2130(12)	622(7)	57(4)
N(1)	14112(16)	2032(14)	3856(8)	50(4)
N(2)	13366(15)	3432(13)	3029(8)	43(4)
C(1)	3753(18)	11038(18)	-203(9)	45(5)
C(2)	12250(20)	3167(18)	3319(10)	50(5)
C(3)	14525(17)	2810(16)	3350(9)	38(4)
C(4)	12720(20)	2268(19)	3808(11)	56(5)
C(5)	13300(20)	4414(19)	2408(11)	60(6)
C(6)	15080(20)	1163(19)	4294(10)	57(6)
C(7)	3120(20)	10970(20)	452(11)	65(6)
C(8)	12920(30)	3580(20)	1805(14)	96(9)
C(10)	8840(40)	1520(40)	749(19)	153(14)
C(9)	10010(40)	1160(40)	1200(20)	220(20)

Table 11. Bond lengths [Å] and angles [°] for C3.

U(1)-O(4)	1.768(10)
U(1)-O(4)#1	1.768(10)
U(1)-O(1)	2.281(11)
U(1)-O(1)#1	2.281(11)
U(1)-O(2)	2.308(9)
U(1)-O(2)#1	2.308(9)
U(2)-O(8)	1.772(10)
U(2)-O(5)	1.777(10)
U(2)-O(7)#2	2.269(11)
U(2)-O(10)	2.278(11)
U(2)-O(3)	2.283(10)
U(2)-O(6)#3	2.289(10)
P(1)-O(3)	1.504(11)
P(1)-O(2)	1.526(11)
P(1)-O(6)	1.533(11)
P(1)-O(9)#4	1.584(12)
P(2)-O(10)	1.494(12)
P(2)-O(7)	1.499(12)
P(2)-O(1)	1.504(12)
P(2)-O(11)	1.575(14)
O(6)-U(2)#2	2.289(10)
O(7)-U(2)#3	2.269(11)
O(9)-C(1)	1.53(2)
O(9)-P(1)#4	1.584(12)
O(11)-C(10)	1.29(4)
N(1)-C(4)	1.39(2)
N(1)-C(3)	1.40(2)
N(1)-C(6)	1.46(2)
N(2)-C(3)	1.36(2)
N(2)-C(2)	1.37(2)
N(2)-C(5)	1.57(2)
C(1)-C(7)	1.54(2)
C(2)-C(4)	1.34(2)
C(5)-C(8)	1.44(3)

C(10)-C(9)	1.36(3)
O(4)-U(1)-O(4)#1	179.999(1)
O(4)-U(1)-O(1)	89.2(4)
O(4)#1-U(1)-O(1)	90.8(4)
O(4)-U(1)-O(1)#1	90.8(4)
O(4)#1-U(1)-O(1)#1	89.2(4)
O(1)-U(1)-O(1)#1	179.999(1)
O(4)-U(1)-O(2)	91.4(4)
O(4)#1-U(1)-O(2)	88.6(4)
O(1)-U(1)-O(2)	89.8(4)
O(1)#1-U(1)-O(2)	90.2(4)
O(4)-U(1)-O(2)#1	88.6(4)
O(4)#1-U(1)-O(2)#1	91.4(4)
O(1)-U(1)-O(2)#1	90.2(4)
O(1)#1-U(1)-O(2)#1	89.8(4)
O(2)-U(1)-O(2)#1	179.999(1)
O(8)-U(2)-O(5)	179.0(5)
O(8)-U(2)-O(7)#2	91.4(4)
O(5)-U(2)-O(7)#2	89.5(4)
O(8)-U(2)-O(10)	90.3(5)
O(5)-U(2)-O(10)	88.8(4)
O(7)#2-U(2)-O(10)	175.7(4)
O(8)-U(2)-O(3)	87.8(4)
O(5)-U(2)-O(3)	92.6(4)
O(7)#2-U(2)-O(3)	88.6(4)
O(10)-U(2)-O(3)	87.6(4)
O(8)-U(2)-O(6)#3	87.5(4)
O(5)-U(2)-O(6)#3	92.0(4)
O(7)#2-U(2)-O(6)#3	93.4(4)
O(10)-U(2)-O(6)#3	90.5(4)
O(3)-U(2)-O(6)#3	175.0(4)
O(3)-P(1)-O(2)	112.9(6)
O(3)-P(1)-O(6)	112.0(7)
O(2)-P(1)-O(6)	109.5(6)
O(3)-P(1)-O(9)#4	103.9(7)

O(2)-P(1)-O(9)#4	109.6(7)
O(6)-P(1)-O(9)#4	108.7(6)
O(10)-P(2)-O(7)	113.6(7)
O(10)-P(2)-O(1)	113.3(7)
O(7)-P(2)-O(1)	110.9(7)
O(10)-P(2)-O(11)	107.3(8)
O(7)-P(2)-O(11)	108.7(7)
O(1)-P(2)-O(11)	102.3(8)
P(2)-O(1)-U(1)	146.0(7)
P(1)-O(2)-U(1)	137.6(7)
P(1)-O(3)-U(2)	149.3(7)
P(1)-O(6)-U(2)#2	136.3(6)
P(2)-O(7)-U(2)#3	157.9(8)
C(1)-O(9)-P(1)#4	114.1(10)
P(2)-O(10)-U(2)	143.7(8)
C(10)-O(11)-P(2)	123(2)
C(4)-N(1)-C(3)	106.6(16)
C(4)-N(1)-C(6)	132.7(17)
C(3)-N(1)-C(6)	120.7(17)
C(3)-N(2)-C(2)	113.5(16)
C(3)-N(2)-C(5)	124.1(15)
C(2)-N(2)-C(5)	122.3(15)
O(9)-C(1)-C(7)	106.0(14)
C(4)-C(2)-N(2)	103.7(17)
N(2)-C(3)-N(1)	104.6(16)
C(2)-C(4)-N(1)	111.4(18)
C(8)-C(5)-N(2)	102.6(17)
O(11)-C(10)-C(9)	150(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x+3/2,y+1/2,-z+1/2 #3 -x+3/2,y-1/2,-z+1/2

#4 -x+1,-y+2,-z

Table 12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C3. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
U(1)	22(1)	15(1)	16(1)	-1(1)	-3(1)	0(1)
U(2)	24(1)	18(1)	22(1)	1(1)	-2(1)	0(1)
P(1)	28(3)	16(2)	22(3)	-1(2)	-7(2)	2(2)
P(2)	50(3)	18(2)	25(3)	0(2)	-9(2)	0(2)
O(1)	59(9)	12(6)	43(9)	2(5)	2(7)	-6(6)
O(2)	35(7)	22(6)	22(7)	-17(5)	2(5)	0(5)
O(3)	31(7)	30(6)	31(8)	10(5)	-4(6)	9(5)
O(4)	28(6)	33(7)	32(6)	-14(5)	4(5)	-6(5)
O(5)	25(6)	29(7)	50(7)	7(5)	2(5)	5(5)
O(6)	35(7)	26(6)	17(6)	5(5)	2(5)	-5(5)
O(7)	53(9)	40(7)	27(7)	13(6)	-2(6)	10(6)
O(8)	22(6)	31(7)	43(7)	15(5)	3(5)	1(5)
O(9)	40(8)	30(7)	38(8)	7(6)	9(6)	6(5)
O(10)	53(9)	33(7)	29(8)	-12(6)	-5(6)	10(6)
O(11)	70(11)	59(9)	40(9)	-15(7)	7(8)	9(8)

Table 13. Crystal data and structure refinement for C4.

Identification code	pccn	
Empirical formula	C10 N2 O16 Se3 U2	
Formula weight	1117.06	
Temperature	373(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pccn	
Unit cell dimensions	a = 9.987(7) Å	α= 90°.
	b = 10.251(7) Å	β= 90°.
	c = 20.957(14) Å	γ = 90°.
Volume	2146(2) $Å^3$	
Z	4	
Density (calculated)	3.458 Mg/m^3	
Absorption coefficient	20.248 mm^{-1}	
F(000)	1952	
Crystal size	0.1 x 0.1 x 0.1 mm^3	
Theta range for data collection	1.94 to 27.58°.	
Index ranges	-12<=h<=12, -13<=k<=13, -27<=l<=27	
Reflections collected	23233	
Independent reflections	2479 [R(int) = 0.1201]	
Completeness to theta = 27.58∞	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7454 and 0.6113	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2479 / 0 / 120	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0647, wR2 = 0.1623	
R indices (all data)	R1 = 0.0941, wR2 = 0.1784	
Largest diff. peak and hole	2.718 and -4.545 e. $Å^{-3}$	

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
U(1)	558(1)	4447(1)	3027(1)	19(1)
Se(1)	2500	7500	2548(1)	24(1)
Se(2)	-880(3)	5954(2)	1581(1)	48(1)
O(1)	-10(20)	5158(19)	1181(8)	53(5)
O(2)	1590(15)	6623(14)	2988(6)	40(4)
O(3)	-1590(15)	3377(14)	2902(7)	40(4)
O(4)	-672(13)	5730(13)	2299(8)	38(4)
O(5)	-191(13)	5103(14)	3716(6)	28(3)
O(6)	-2364(14)	5640(18)	1446(7)	49(5)
O(7)	1317(13)	3753(13)	2346(5)	29(3)
O(8)	-622(19)	7413(14)	1441(7)	50(5)
N(1)	2500	2500	1219(15)	53(8)
C(1)	-2500	7500	60(20)	68(11)
C(2)	1400(30)	2760(30)	919(13)	60(7)
N(2)	-2500	2500	4259(18)	74(10)
C(3)	1320(30)	2780(30)	238(14)	66(8)
C(4)	-2400(40)	3570(40)	4501(18)	95(12)
C(5)	-2630(40)	3600(50)	210(20)	114(14)
C(6)	-2500	2500	480(20)	83(14)

Table 15. Bond lengths [Å] and angles [°] for C4.

U(1)-O(5)	1.759(13)
U(1)-O(7)	1.765(12)
U(1)-O(6)#1	2.353(14)
U(1)-O(4)	2.361(13)
U(1)-O(8)#2	2.365(14)
U(1)-O(3)	2.423(14)
U(1)-O(2)	2.458(14)
Se(1)-O(2)	1.577(13)
Se(1)-O(2)#3	1.577(13)
Se(1)-O(3)#1	1.589(13)
Se(1)-O(3)#4	1.589(13)
Se(2)-O(1)	1.457(17)
Se(2)-O(4)	1.535(16)
Se(2)-O(6)	1.542(14)
Se(2)-O(8)	1.545(14)
O(3)-Se(1)#2	1.589(13)
O(6)-U(1)#5	2.353(14)
O(8)-U(1)#4	2.365(14)
N(1)-C(2)#6	1.29(3)
N(1)-C(2)	1.29(3)
C(1)-C(3)#7	1.36(4)
C(1)-C(3)#8	1.36(4)
C(2)-C(3)	1.43(4)
N(2)-C(4)#9	1.21(4)
N(2)-C(4)	1.21(4)
C(3)-C(1)#8	1.36(4)
C(4)-C(5)#10	1.48(5)
C(5)-C(6)	1.27(5)
C(5)-C(4)#11	1.48(5)
C(6)-C(5)#9	1.27(5)
O(5)-U(1)-O(7)	178.6(6)
O(5)-U(1)-O(6)#1	90.3(6)
O(7)-U(1)-O(6)#1	89.2(5)

O(5)-U(1)-O(4)	95.5(6)
O(7)-U(1)-O(4)	85.7(6)
O(6)#1-U(1)-O(4)	141.6(6)
O(5)-U(1)-O(8)#2	87.8(6)
O(7)-U(1)-O(8)#2	90.8(6)
O(6)#1-U(1)-O(8)#2	73.8(6)
O(4)-U(1)-O(8)#2	144.1(6)
O(5)-U(1)-O(3)	83.4(5)
O(7)-U(1)-O(3)	96.3(6)
O(6)#1-U(1)-O(3)	144.5(6)
O(4)-U(1)-O(3)	73.8(5)
O(8)#2-U(1)-O(3)	71.1(6)
O(5)-U(1)-O(2)	81.9(6)
O(7)-U(1)-O(2)	99.1(6)
O(6)#1-U(1)-O(2)	71.4(6)
O(4)-U(1)-O(2)	72.0(5)
O(8)#2-U(1)-O(2)	143.5(6)
O(3)-U(1)-O(2)	141.1(5)
O(2)-Se(1)-O(2)#3	108.4(10)
O(2)-Se(1)-O(3)#1	110.8(8)
O(2)#3-Se(1)-O(3)#1	109.9(8)
O(2)-Se(1)-O(3)#4	109.9(8)
O(2)#3-Se(1)-O(3)#4	110.8(8)
O(3)#1-Se(1)-O(3)#4	107.2(11)
O(1)-Se(2)-O(4)	113.6(9)
O(1)-Se(2)-O(6)	110.5(10)
O(4)-Se(2)-O(6)	106.2(8)
O(1)-Se(2)-O(8)	109.4(10)
O(4)-Se(2)-O(8)	108.0(8)
O(6)-Se(2)-O(8)	109.1(10)
Se(1)-O(2)-U(1)	141.1(8)
Se(1)#2-O(3)-U(1)	145.8(8)
Se(2)-O(4)-U(1)	141.9(9)
Se(2)-O(6)-U(1)#5	140.3(8)
Se(2)-O(8)-U(1)#4	140.2(8)
C(2)#6-N(1)-C(2)	122(3)

C(3)#7-C(1)-C(3)#8	126(4)
N(1)-C(2)-C(3)	123(3)
C(4)#9-N(2)-C(4)	130(5)
C(1)#8-C(3)-C(2)	114(3)
N(2)-C(4)-C(5)#10	116(4)
C(6)-C(5)-C(4)#11	115(5)
C(5)-C(6)-C(5)#9	127(6)

Symmetry transformations used to generate equivalent atoms:

#1 x+1/2,-y+1,-z+1/2 #2 -x,y-1/2,-z+1/2 #3 -x+1/2,-y+3/2,z

#4 -x,y+1/2,-z+1/2 #5 x-1/2,-y+1,-z+1/2 #6 -x+1/2,-y+1/2,z

#7 x-1/2,y+1/2,-z #8 -x,-y+1,-z #9 -x-1/2,-y+1/2,z

#10 -x-1/2,y,z+1/2 #11 -x-1/2,y,z-1/2

Table 16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C4. 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}
U(1)	22(1)	18(1)	17(1)	-1(1)	0(1)	2(1)
Se(1)	22(1)	18(1)	31(1)	0	0	-1(1)
Se(2)	47(1)	40(1)	55(2)	1(1)	1(1)	1(1)
O(1)	64(11)	61(11)	36(9)	-2(8)	7(8)	25(10)
O(2)	47(9)	42(8)	32(7)	0(7)	6(7)	-24(8)
O(3)	38(8)	39(8)	43(8)	-14(7)	0(7)	-19(7)
O(4)	30(7)	25(7)	58(10)	20(7)	-11(7)	6(6)
O(5)	24(7)	34(7)	28(7)	-11(6)	6(5)	-9(6)
O(6)	29(8)	87(13)	32(8)	-6(8)	7(6)	-29(8)
O(7)	32(7)	38(8)	16(6)	-1(5)	-4(5)	13(6)
O(8)	91(14)	29(8)	31(8)	-2(7)	-1(9)	-26(9)

Table 17. Crystal data and structure refinement for C5.

Identification code	p21n	
Empirical formula	C4 N2 O31 P4 U5	
Formula weight	1886.09	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.5152(9) Å	α= 90°.
	b = 33.144(3) Å	β= 93.2110(10) °.
	c = 9.6569(10) Å	γ = 90°.
Volume	3040.7(5) $Å^3$	
Z	4	
Density (calculated)	4.120 Mg/m^3	
Absorption coefficient	26.866 mm^{-1}	
F(000)	3224	
Crystal size	0.1 x 0.08 x 0.06 mm^3	
Theta range for data collection	1.23 to 27.53°.	
Index ranges	-12<=h<=12, -43<=k<=43, -12<=l<=12	
Reflections collected	30943	
Independent reflections	6967 [R(int) = 0.0958]	
Completeness to theta = 27.53∞	99.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6967 / 0 / 230	
Goodness-of-fit on F^2	1.015	
Final R indices [I>2sigma(I)]	R1 = 0.0450, wR2 = 0.1036	
R indices (all data)	R1 = 0.0684, wR2 = 0.1163	
Largest diff. peak and hole	2.930 and -2.577 e. $Å^{-3}$	

Table 18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
U(1)	805(1)	2402(1)	6634(1)	12(1)
U(2)	1815(1)	2406(1)	2667(1)	11(1)
U(3)	5494(1)	74(1)	7998(1)	13(1)
U(4)	9492(1)	76(1)	6954(1)	12(1)
U(5)	6440(1)	1305(1)	4429(1)	16(1)
P(1)	7116(3)	202(1)	4587(3)	10(1)
P(2)	4282(3)	2217(1)	4949(3)	11(1)
P(3)	7850(3)	212(1)	10387(3)	15(1)
P(4)	-1681(3)	2307(1)	4329(3)	12(1)
O(1)	-2410(9)	2592(2)	3313(8)	14(2)
O(2)	6161(9)	-102(3)	3844(8)	18(2)
O(3)	6991(9)	178(3)	6179(8)	15(2)
O(4)	8830(10)	-52(3)	11266(9)	21(2)
O(5)	4358(9)	2369(3)	3449(8)	17(2)
O(6)	8020(9)	169(3)	8828(8)	18(2)
O(7)	-1719(9)	2470(3)	5839(9)	16(2)
O(8)	-56(9)	2303(3)	4150(8)	15(2)
O(9)	5031(10)	2510(3)	5939(9)	18(2)
O(10)	2654(9)	2238(3)	5126(8)	14(2)
O(11)	8681(10)	75(3)	4484(9)	22(2)
O(12)	4803(9)	1796(3)	5121(8)	21(2)
O(13)	6317(10)	88(3)	10520(9)	22(2)
O(14)	5215(10)	590(3)	8165(9)	25(2)
O(15)	9787(9)	595(3)	6815(9)	23(2)
O(16)	1831(9)	2923(3)	3087(9)	22(2)
O(17)	9189(9)	-447(3)	7066(9)	22(2)
O(18)	485(9)	1893(3)	6985(8)	21(2)
O(19)	6854(9)	614(3)	4050(8)	21(2)
O(20)	5823(10)	-448(3)	7846(9)	28(2)
O(21)	1779(9)	1880(3)	2305(8)	20(2)

O(22)	1121(9)	2913(3)	6199(8)	20(2)
O(23)	5721(10)	1342(3)	2747(9)	26(2)
O(24)	8080(10)	659(3)	10804(9)	30(2)
O(25)	7121(10)	1243(3)	6150(10)	30(2)
O(26)	-2292(9)	1894(3)	4212(9)	22(2)
O(27)	8769(10)	1179(3)	3320(10)	29(2)
O(28)	4269(11)	945(3)	5040(10)	32(2)
O(29)	8755(11)	1716(3)	1022(11)	43(3)
O(30)	1675(14)	1247(4)	4730(13)	65(4)
O(31)	7919(17)	1184(5)	8992(16)	93(5)
N(1)	2529(15)	1190(4)	9547(14)	43(4)
C(1)	2330(20)	1224(6)	8170(20)	60(5)
N(2)	3550(20)	1440(6)	7815(19)	81(6)
C(2)	3770(20)	1379(6)	70(20)	61(6)
C(3)	-600(20)	3493(6)	3920(20)	59(5)
C(4)	8510(20)	-994(7)	9580(20)	79(7)

Table 19. Bond lengths [Å] and angles [°] for C5.

U(1)-O(18)	1.750(9)
U(1)-O(22)	1.773(9)
U(1)-O(1)#1	2.282(8)
U(1)-O(10)	2.408(8)
U(1)-O(5)#2	2.412(8)
U(1)-O(7)	2.490(9)
U(1)-O(8)	2.512(8)
U(1)-P(4)	3.171(3)
U(1)-U(2)	4.0012(7)
U(1)-U(2)#2	4.0298(7)
U(2)-O(16)	1.759(9)
U(2)-O(21)	1.779(9)
U(2)-O(9)#3	2.330(9)
U(2)-O(7)#4	2.346(9)
U(2)-O(8)	2.372(8)
U(2)-O(5)	2.498(9)
U(2)-O(10)	2.524(8)
U(2)-P(2)	3.190(3)
U(2)-U(1)#4	4.0298(7)
U(3)-O(14)	1.741(10)
U(3)-O(20)	1.763(10)
U(3)-O(2)#5	2.310(8)
U(3)-O(3)	2.348(8)
U(3)-O(13)#6	2.362(9)
U(3)-O(6)	2.511(8)
U(3)-O(13)	2.516(9)
U(3)-P(3)	3.159(3)
U(3)-U(4)	3.9902(7)
U(3)-U(3)#6	4.0595(9)
U(4)-O(15)	1.748(9)
U(4)-O(17)	1.761(9)
U(4)-O(4)#7	2.281(9)
U(4)-O(11)#8	2.339(9)
U(4)-O(6)	2.370(8)

U(4)-O(11)	2.465(9)
U(4)-O(3)	2.478(8)
U(4)-P(1)	3.152(3)
U(4)-U(4)#8	3.9794(9)
U(5)-O(23)	1.731(9)
U(5)-O(25)	1.762(9)
U(5)-O(26)#9	2.310(9)
U(5)-O(19)	2.357(9)
U(5)-O(12)	2.376(9)
U(5)-O(28)	2.485(10)
U(5)-O(27)	2.549(10)
P(1)-O(19)	1.474(9)
P(1)-O(2)	1.512(9)
P(1)-O(3)	1.551(8)
P(1)-O(11)	1.557(10)
P(2)-O(12)	1.487(9)
P(2)-O(9)	1.512(9)
P(2)-O(5)	1.539(9)
P(2)-O(10)	1.569(9)
P(3)-O(4)	1.506(9)
P(3)-O(13)	1.528(10)
P(3)-O(6)	1.529(8)
P(3)-O(24)	1.548(11)
P(4)-O(26)	1.491(10)
P(4)-O(1)	1.502(9)
P(4)-O(7)	1.557(9)
P(4)-O(8)	1.566(9)
O(1)-U(1)#3	2.282(8)
O(2)-U(3)#5	2.310(8)
O(4)-U(4)#7	2.281(9)
O(5)-U(1)#4	2.412(8)
O(7)-U(2)#2	2.346(9)
O(9)-U(2)#1	2.330(9)
O(11)-U(4)#8	2.339(9)
O(13)-U(3)#6	2.362(9)
O(26)-U(5)#10	2.310(9)

N(1)-C(1)	1.33(2)
N(1)-C(2)#11	1.41(2)
N(1)-C(4)#6	1.48(3)
C(1)-N(2)	1.42(2)
N(2)-C(3)#1	1.32(2)
C(2)-C(3)#4	1.36(3)
C(2)-N(1)#12	1.41(2)
C(3)-N(2)#3	1.32(2)
C(3)-C(2)#2	1.36(3)
C(4)-N(1)#6	1.48(3)

O(18)-U(1)-O(22)	177.5(4)
O(18)-U(1)-O(1)#1	90.1(3)
O(22)-U(1)-O(1)#1	91.8(3)
O(18)-U(1)-O(10)	92.4(3)
O(22)-U(1)-O(10)	86.1(3)
O(1)#1-U(1)-O(10)	83.8(3)
O(18)-U(1)-O(5)#2	92.8(3)
O(22)-U(1)-O(5)#2	89.0(3)
O(1)#1-U(1)-O(5)#2	85.0(3)
O(10)-U(1)-O(5)#2	167.6(3)
O(18)-U(1)-O(7)	88.4(3)
O(22)-U(1)-O(7)	90.8(3)
O(1)#1-U(1)-O(7)	152.2(3)
O(10)-U(1)-O(7)	124.0(3)
O(5)#2-U(1)-O(7)	67.4(3)
O(18)-U(1)-O(8)	90.5(3)
O(22)-U(1)-O(8)	87.1(3)
O(1)#1-U(1)-O(8)	150.4(3)
O(10)-U(1)-O(8)	66.6(3)
O(5)#2-U(1)-O(8)	124.5(3)
O(7)-U(1)-O(8)	57.3(3)
O(18)-U(1)-P(4)	84.8(3)
O(22)-U(1)-P(4)	93.3(3)
O(1)#1-U(1)-P(4)	174.8(2)
O(10)-U(1)-P(4)	95.45(19)

O(5)#2-U(1)-P(4)	96.2(2)
O(7)-U(1)-P(4)	28.8(2)
O(8)-U(1)-P(4)	29.1(2)
O(18)-U(1)-U(2)	104.0(3)
O(22)-U(1)-U(2)	73.6(3)
O(1)#1-U(1)-U(2)	118.1(2)
O(10)-U(1)-U(2)	36.77(18)
O(5)#2-U(1)-U(2)	150.8(2)
O(7)-U(1)-U(2)	89.09(19)
O(8)-U(1)-U(2)	33.85(19)
P(4)-U(1)-U(2)	62.50(6)
O(18)-U(1)-U(2)#2	85.8(3)
O(22)-U(1)-U(2)#2	94.7(3)
O(1)#1-U(1)-U(2)#2	119.8(2)
O(10)-U(1)-U(2)#2	156.32(18)
O(5)#2-U(1)-U(2)#2	35.5(2)
O(7)-U(1)-U(2)#2	32.46(19)
O(8)-U(1)-U(2)#2	89.75(19)
P(4)-U(1)-U(2)#2	60.87(6)
U(2)-U(1)-U(2)#2	121.109(15)
O(16)-U(2)-O(21)	177.9(4)
O(16)-U(2)-O(9)#3	92.6(4)
O(21)-U(2)-O(9)#3	88.3(3)
O(16)-U(2)-O(7)#4	90.3(4)
O(21)-U(2)-O(7)#4	91.7(3)
O(9)#3-U(2)-O(7)#4	83.1(3)
O(16)-U(2)-O(8)	89.9(4)
O(21)-U(2)-O(8)	88.3(3)
O(9)#3-U(2)-O(8)	84.7(3)
O(7)#4-U(2)-O(8)	167.9(3)
O(16)-U(2)-O(5)	89.0(3)
O(21)-U(2)-O(5)	91.1(3)
O(9)#3-U(2)-O(5)	151.3(3)
O(7)#4-U(2)-O(5)	68.2(3)
O(8)-U(2)-O(5)	123.9(3)
O(16)-U(2)-O(10)	90.0(3)

O(21)-U(2)-O(10)	88.3(3)
O(9)#3-U(2)-O(10)	151.6(3)
O(7)#4-U(2)-O(10)	125.2(3)
O(8)-U(2)-O(10)	67.0(3)
O(5)-U(2)-O(10)	56.9(3)
O(16)-U(2)-P(2)	92.0(3)
O(21)-U(2)-P(2)	87.1(3)
O(9)#3-U(2)-P(2)	175.3(2)
O(7)#4-U(2)-P(2)	96.2(2)
O(8)-U(2)-P(2)	95.9(2)
O(5)-U(2)-P(2)	28.2(2)
O(10)-U(2)-P(2)	28.98(19)
O(16)-U(2)-U(1)	77.4(3)
O(21)-U(2)-U(1)	100.5(3)
O(9)#3-U(2)-U(1)	118.8(2)
O(7)#4-U(2)-U(1)	154.9(2)
O(8)-U(2)-U(1)	36.2(2)
O(5)-U(2)-U(1)	89.47(19)
O(10)-U(2)-U(1)	34.83(19)
P(2)-U(2)-U(1)	62.93(6)
O(16)-U(2)-U(1)#4	84.7(3)
O(21)-U(2)-U(1)#4	96.5(3)
O(9)#3-U(2)-U(1)#4	117.6(2)
O(7)#4-U(2)-U(1)#4	34.7(2)
O(8)-U(2)-U(1)#4	157.2(2)
O(5)-U(2)-U(1)#4	34.14(19)
O(10)-U(2)-U(1)#4	90.85(19)
P(2)-U(2)-U(1)#4	62.30(6)
U(1)-U(2)-U(1)#4	121.179(15)
O(14)-U(3)-O(20)	178.5(4)
O(14)-U(3)-O(2)#5	86.0(4)
O(20)-U(3)-O(2)#5	95.3(4)
O(14)-U(3)-O(3)	91.5(4)
O(20)-U(3)-O(3)	87.9(4)
O(2)#5-U(3)-O(3)	80.4(3)
O(14)-U(3)-O(13)#6	92.6(4)

O(20)-U(3)-O(13)#6	88.1(4)
O(2)#5-U(3)-O(13)#6	89.3(3)
O(3)-U(3)-O(13)#6	168.6(3)
O(14)-U(3)-O(6)	89.7(4)
O(20)-U(3)-O(6)	88.8(4)
O(2)#5-U(3)-O(6)	147.1(3)
O(3)-U(3)-O(6)	67.1(3)
O(13)#6-U(3)-O(6)	123.6(3)
O(14)-U(3)-O(13)	86.2(3)
O(20)-U(3)-O(13)	92.9(4)
O(2)#5-U(3)-O(13)	155.0(3)
O(3)-U(3)-O(13)	123.5(3)
O(13)#6-U(3)-O(13)	67.4(4)
O(6)-U(3)-O(13)	56.5(3)
O(14)-U(3)-P(3)	84.0(3)
O(20)-U(3)-P(3)	94.6(3)
O(2)#5-U(3)-P(3)	169.0(2)
O(3)-U(3)-P(3)	95.1(2)
O(13)#6-U(3)-P(3)	95.9(2)
O(6)-U(3)-P(3)	28.48(19)
O(13)-U(3)-P(3)	28.5(2)
O(14)-U(3)-U(4)	100.0(3)
O(20)-U(3)-U(4)	78.8(3)
O(2)#5-U(3)-U(4)	115.1(2)
O(3)-U(3)-U(4)	35.28(19)
O(13)#6-U(3)-U(4)	153.1(2)
O(6)-U(3)-U(4)	34.02(18)
O(13)-U(3)-U(4)	89.7(2)
P(3)-U(3)-U(4)	62.39(6)
O(14)-U(3)-U(3)#6	89.2(3)
O(20)-U(3)-U(3)#6	90.7(3)
O(2)#5-U(3)-U(3)#6	123.6(2)
O(3)-U(3)-U(3)#6	155.89(19)
O(13)#6-U(3)-U(3)#6	34.9(2)
O(6)-U(3)-U(3)#6	88.84(18)
O(13)-U(3)-U(3)#6	32.5(2)

P(3)-U(3)-U(3)#6	60.96(6)
U(4)-U(3)-U(3)#6	121.063(17)
O(15)-U(4)-O(17)	179.1(4)
O(15)-U(4)-O(4)#7	89.1(4)
O(17)-U(4)-O(4)#7	91.7(4)
O(15)-U(4)-O(11)#8	92.1(4)
O(17)-U(4)-O(11)#8	87.5(4)
O(4)#7-U(4)-O(11)#8	85.9(3)
O(15)-U(4)-O(6)	92.0(4)
O(17)-U(4)-O(6)	88.6(4)
O(4)#7-U(4)-O(6)	81.2(3)
O(11)#8-U(4)-O(6)	166.4(3)
O(15)-U(4)-O(11)	88.3(3)
O(17)-U(4)-O(11)	90.8(3)
O(4)#7-U(4)-O(11)	153.8(3)
O(11)#8-U(4)-O(11)	68.1(4)
O(6)-U(4)-O(11)	124.9(3)
O(15)-U(4)-O(3)	90.0(3)
O(17)-U(4)-O(3)	89.7(4)
O(4)#7-U(4)-O(3)	148.5(3)
O(11)#8-U(4)-O(3)	125.7(3)
O(6)-U(4)-O(3)	67.3(3)
O(11)-U(4)-O(3)	57.6(3)
O(15)-U(4)-P(1)	85.7(3)
O(17)-U(4)-P(1)	93.5(3)
O(4)#7-U(4)-P(1)	174.1(2)
O(11)#8-U(4)-P(1)	97.1(2)
O(6)-U(4)-P(1)	96.1(2)
O(11)-U(4)-P(1)	29.0(2)
O(3)-U(4)-P(1)	28.96(19)
O(15)-U(4)-U(4)#8	90.2(3)
O(17)-U(4)-U(4)#8	89.0(3)
O(4)#7-U(4)-U(4)#8	120.9(2)
O(11)#8-U(4)-U(4)#8	35.1(2)
O(6)-U(4)-U(4)#8	157.8(2)
O(11)-U(4)-U(4)#8	33.1(2)

O(3)-U(4)-U(4)#8	90.63(18)
P(1)-U(4)-U(4)#8	62.06(6)
O(15)-U(4)-U(3)	100.4(3)
O(17)-U(4)-U(3)	79.7(3)
O(4)#7-U(4)-U(3)	116.5(2)
O(11)#8-U(4)-U(3)	154.2(2)
O(6)-U(4)-U(3)	36.3(2)
O(11)-U(4)-U(3)	89.6(2)
O(3)-U(4)-U(3)	33.18(18)
P(1)-U(4)-U(3)	61.85(6)
U(4)#8-U(4)-U(3)	121.661(17)
O(23)-U(5)-O(25)	177.0(5)
O(23)-U(5)-O(26)#9	92.1(4)
O(25)-U(5)-O(26)#9	91.0(4)
O(23)-U(5)-O(19)	89.1(4)
O(25)-U(5)-O(19)	88.8(4)
O(26)#9-U(5)-O(19)	135.6(3)
O(23)-U(5)-O(12)	89.1(4)
O(25)-U(5)-O(12)	91.5(4)
O(26)#9-U(5)-O(12)	78.4(3)
O(19)-U(5)-O(12)	145.9(3)
O(23)-U(5)-O(28)	88.1(4)
O(25)-U(5)-O(28)	89.3(4)
O(26)#9-U(5)-O(28)	150.7(3)
O(19)-U(5)-O(28)	73.7(3)
O(12)-U(5)-O(28)	72.3(3)
O(23)-U(5)-O(27)	85.7(4)
O(25)-U(5)-O(27)	95.4(4)
O(26)#9-U(5)-O(27)	68.3(3)
O(19)-U(5)-O(27)	67.6(3)
O(12)-U(5)-O(27)	146.0(3)
O(28)-U(5)-O(27)	140.8(3)
O(19)-P(1)-O(2)	111.4(5)
O(19)-P(1)-O(3)	112.1(5)
O(2)-P(1)-O(3)	110.9(5)
O(19)-P(1)-O(11)	111.9(5)

O(2)-P(1)-O(11)	109.9(5)
O(3)-P(1)-O(11)	100.1(5)
O(19)-P(1)-U(4)	118.6(4)
O(2)-P(1)-U(4)	130.1(4)
O(3)-P(1)-U(4)	50.6(3)
O(11)-P(1)-U(4)	50.2(3)
O(12)-P(2)-O(9)	112.9(5)
O(12)-P(2)-O(5)	112.3(5)
O(9)-P(2)-O(5)	109.9(5)
O(12)-P(2)-O(10)	110.8(5)
O(9)-P(2)-O(10)	109.6(5)
O(5)-P(2)-O(10)	100.8(5)
O(12)-P(2)-U(2)	119.3(4)
O(9)-P(2)-U(2)	127.8(4)
O(5)-P(2)-U(2)	50.0(3)
O(10)-P(2)-U(2)	51.2(3)
O(4)-P(3)-O(13)	111.1(5)
O(4)-P(3)-O(6)	113.9(5)
O(13)-P(3)-O(6)	102.2(5)
O(4)-P(3)-O(24)	109.6(5)
O(13)-P(3)-O(24)	110.9(5)
O(6)-P(3)-O(24)	108.9(5)
O(4)-P(3)-U(3)	136.0(4)
O(13)-P(3)-U(3)	51.7(3)
O(6)-P(3)-U(3)	51.5(3)
O(24)-P(3)-U(3)	114.4(4)
O(26)-P(4)-O(1)	111.3(5)
O(26)-P(4)-O(7)	111.1(5)
O(1)-P(4)-O(7)	111.1(5)
O(26)-P(4)-O(8)	111.5(5)
O(1)-P(4)-O(8)	110.9(5)
O(7)-P(4)-O(8)	100.5(5)
O(26)-P(4)-U(1)	114.6(4)
O(1)-P(4)-U(1)	134.0(4)
O(7)-P(4)-U(1)	50.5(3)
O(8)-P(4)-U(1)	51.4(3)

P(4)-O(1)-U(1)#3	140.1(5)
P(1)-O(2)-U(3)#5	134.7(5)
P(1)-O(3)-U(3)	146.4(5)
P(1)-O(3)-U(4)	100.4(4)
U(3)-O(3)-U(4)	111.5(3)
P(3)-O(4)-U(4)#7	146.1(6)
P(2)-O(5)-U(1)#4	147.8(5)
P(2)-O(5)-U(2)	101.8(4)
U(1)#4-O(5)-U(2)	110.3(3)
P(3)-O(6)-U(4)	149.7(5)
P(3)-O(6)-U(3)	100.0(4)
U(4)-O(6)-U(3)	109.6(3)
P(4)-O(7)-U(2)#2	144.2(5)
P(4)-O(7)-U(1)	100.6(4)
U(2)#2-O(7)-U(1)	112.8(3)
P(4)-O(8)-U(2)	147.6(5)
P(4)-O(8)-U(1)	99.5(4)
U(2)-O(8)-U(1)	110.0(3)
P(2)-O(9)-U(2)#1	145.9(5)
P(2)-O(10)-U(1)	146.6(5)
P(2)-O(10)-U(2)	99.8(4)
U(1)-O(10)-U(2)	108.4(3)
P(1)-O(11)-U(4)#8	147.3(5)
P(1)-O(11)-U(4)	100.8(4)
U(4)#8-O(11)-U(4)	111.9(4)
P(2)-O(12)-U(5)	146.3(5)
P(3)-O(13)-U(3)#6	147.6(5)
P(3)-O(13)-U(3)	99.8(4)
U(3)#6-O(13)-U(3)	112.6(4)
P(1)-O(19)-U(5)	150.5(5)
P(4)-O(26)-U(5)#10	166.8(6)
C(1)-N(1)-C(2)#11	113.0(16)
C(1)-N(1)-C(4)#6	122.6(17)
C(2)#11-N(1)-C(4)#6	124.3(16)
N(1)-C(1)-N(2)	102.2(17)
C(3)#1-N(2)-C(1)	111.2(18)

C(3)#4-C(2)-N(1)#12 104.1(17)
N(2)#3-C(3)-C(2)#2 109(2)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+1/2,z+1/2 #2 x-1/2,-y+1/2,z+1/2
#3 x-1/2,-y+1/2,z-1/2 #4 x+1/2,-y+1/2,z-1/2
#5 -x+1,-y,-z+1 #6 -x+1,-y,-z+2 #7 -x+2,-y,-z+2
#8 -x+2,-y,-z+1 #9 x+1,y,z #10 x-1,y,z #11 x,y,z+1
#12 x,y,z-1

Table 20. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for C5. 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}
U(1)	10(1)	18(1)	7(1)	-1(1)	0(1)	1(1)
U(2)	9(1)	18(1)	8(1)	1(1)	0(1)	0(1)
U(3)	9(1)	21(1)	8(1)	0(1)	0(1)	-1(1)
U(4)	9(1)	20(1)	7(1)	0(1)	0(1)	1(1)
U(5)	17(1)	16(1)	14(1)	0(1)	0(1)	2(1)
P(1)	9(2)	16(2)	6(1)	-4(1)	-1(1)	1(1)
P(2)	9(2)	17(2)	8(1)	0(1)	0(1)	0(1)
P(3)	9(2)	31(2)	6(1)	1(1)	1(1)	1(1)
P(4)	9(2)	18(2)	9(1)	0(1)	0(1)	0(1)

Table 21: Bond valence sums (V.U.) for Compound 1

U1	5.83
As1	5.06
O1	1.64
O2	1.91
O3	1.91
O4	1.82
O5	1.64
O6	1.98

Table 22: Bond valence sums (V.U.) for Compound 2

U1	6.21
U2	6.06
U3	6.64
Se1	4.58
Se2	4.01
Se3	4.28
O1	2.12
O2	2.14
O3	2.29
O4	2.05
O5	1.91
O6	1.84
O7	1.76
O8	2.54
O9	2.00
O10	1.83
O11	1.91
O12	1.96
O13	1.73
O14	1.80

Table 23: Bond valence sums (V.U.) for Compound 3

U1	6.24
U2	6.27
P1	4.81
P2	5.01
O1	1.98
O2	1.87
O3	1.97
O4	1.79

O5	1.87
O6	2.01
O7	1.81
O8	1.81
O9	2.01
O10	2.30

Table 24: Bond valence sums (V.U.) for Compound 4

U1	6.34
Se1	5.49
Se2	6.54
O1	1.93
O2	1.86
O3	1.85
O4	1.85
O5	2.11
O6	1.83
O7	2.08

Table 25: Bond valence sums (V.U.) for Compound 5

U1	5.91
U2	5.89
U3	6.03
U4	6.12
U5	6.05
P1	4.99
P2	4.95
P3	4.92
P4	4.92
O1	1.95
O2	1.88
O3	2.13
O4	1.93
O5	2.09
O6	2.15
O7	2.11
O8	2.03
O9	1.85
O10	1.98
O11	2.14
O12	1.89
O13	2.16

O14	1.81
O15	1.79
O16	1.75
O17	1.74
O18	1.78
O19	1.96
O20	1.74
O21	1.68
O22	1.70
O23	1.85
O24	1.16
O25	1.74
O26	1.95
O27	0.37
O28	0.42
O29	No bonds
O30	No bonds
O31	No bonds