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Review

Organically Templated Uranyl Sulfates and Selenates: Structural Complexity and Crystal Chemical Restrictions for Isotypic Compounds Formation

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Abstract: This paper reviews the state of the art in the structural chemistry of organically templated uranyl sulfates and selenates, which are considered as the most representative groups of U-bearing synthetic compounds. In total, there are 194 compounds known for both groups, the crystal structures of which include 84 various organic molecules. Structural studies and topological analysis clearly indicate complex crystal chemical limitations in terms of the isomorphic substitution implementation, since the existence of isotypic phases has to date been confirmed only for 24 compounds out of 194, which is slightly above 12%. The structural architecture of the entire compound depends on the combination of the organic and oxyanion parts, changes in which are sometimes realized even while maintaining the topology of the U-bearing complex. An increase in the size of the hydrocarbon part and number of charge functional groups of the organic cation leads to the formation of rare and more complex topologies. In addition, the crystal structures of two novel uranyl sulfates and one uranyl selenate, templated by isopropylammonium cations, are reported.

Keywords: uranyl; sulfate; selenate; isopropylamine; crystal structure; structural complexity; X-ray diffraction

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1. Introduction

Crystal chemical studies of uranium compounds began to develop actively in the middle of the last century; however, the most rapid growth of structural research occurred at the turn of the century and continues to this day. Of particular interest from the structural chemistry point of view is the study of hexavalent uranium compounds. The unique structural diversity cannot leave indifferent researchers in the field of crystallography, thereby generating new discovered substances and new published papers every year. Two of the most abundant groups of synthetic U-bearing compounds are uranyl selenates and sulfates, and a significant portion of them are hybrid organic–inorganic compounds. Their study is of genuine interest, since such complexes inherit the properties of both structural components: a solid inorganic uranium-bearing structure and a flexible organic one.

At present, almost 200 organically templated compounds within both named groups are known (Table 1). In this review, we evaluate the possibility of isostructural compounds' existence among uranyl sulfates and selenates, as well as involve a recently developed analytical approach to calculating the structural complexity parameters, which allows the comparison of crystal structures in terms of the information content. In addition, we report on a description of the crystal structures of three novel uranyl compounds, $[C_3H_{10}N]_2[(UO_2)_6(SO_4)_7(H_2O)_2]$ (**1**), $[C_3H_{10}N]_2[(UO_2)_2(SO_4)_3(H_2O)](H_2O)$ (**3**), and $[C_3H_{10}N](H_3O)[(UO_2)_2(SeO_4)_3(H_2O)](H_2SeO_3)$ (**4**), and on the refinement of the previously studied compound $[C_3H_{10}N]_2[(UO_2)_2(SeO_4)_3(H_2O)](H_2O)$ (**2**) to twice-better convergence parameters and interatomic bonds precision, all of which are templated by isopropylammonium cations, which are reported herein.

Table 1. Crystallographic characteristics and structural complexity parameters of organically templated synthetic uranyl sulfates and selenates.

No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/β, °	*c*, Å/γ, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	Ammonium, NH_4^+						2.322/11.610			
5	$[NH_4][(UO_2)(SO_4)F]$	*cc*2–1:1–7	$Pb2_1a$	8.681(3)/90	11.319(8)/90	6.729(6)/90		3.170/114.117	3.585/172.078	[1]
6	$[NH_4]_2[UO_2(SO_4)_2(H_2O)](H_2O)$	*cc*2–1:2–2	$P2_1/c$	7.783(5)/90	7.403(2)/102.25(4)	20.918(9)/90		4.250/322.840	4.858/563.526	[2]
7	$[NH_4]_4[(UO_2)_2(SO_4)O_2)_2](H_2O)$	$5^24^33^2$	$C2/m$	8.6987(15)/90	14.166(2)/104.117(4)	17.847(3)/90		4.150/281.950	4.956/564.949	[3]
8	$[NH_4]_2[(UO_2)_2(SO_4)O_2)]$	$5^24^33^2$	$Cmca$	14.2520(9)/90	8.7748(5)/90	17.1863(10)/90		2.780/144.420	3.654/336.168	[3]
9	$[NH_4]_2[(UO_2)(SeO_4)_2(H_2O)](H_2O)_2$	*cc*2–1:2–3	$P2_12_12_1$	8.2036(9)/90	11.631(2)/90	14.028(2)/90		4.000/256.000	5.000/640.000	[4]
	Methylamine, $CH_3NH_3^+$						3.000/24.000			
10	$[CH_6N]_2[(UO_2)_2(SO_4)_3]$	*cc*2–2:3–14	$P1$	8.4784(6)/90.170(2)	9.7873(8)/95.744(2)	9.8121(7)/90.136(2)		5.390/226.480	6.209/459.500	[5]
11	$[CH_6N][(UO_2)(SO_4)(OH)]$	$6^15^24^23^2$	$Pbca$	11.5951(8)/90	9.2848(6)/90	14.5565(9)/90		3.320/265.750	4.170/600.469	[6]
12	$[CH_6N]_2[(UO_2)(SeO_4)_2\ (H_2O)](H_2O)$	*cc*1–1:2–1	$Pnma$	7.5496(7)/90	12.0135(9)/90	15.8362(13)/90		3.250/208.000	4.272/598.100	[7]
13	$[CH_6N]_2[(UO_2)(SeO_4)_2\ (H_2O)]$	*cc*2–1:2–3	$P2_1/c$	8.2366(10) /90	7.5888(6)/104.566(9)	22.260(2)/90		4.000/256.000	5.000/640.000	[7]
14	$[CH_6N][H_3O][(UO_2)_2\ (SeO_4)_3(H_2O)](H_2O)$	*cc*2–2:3–12	$P2_1/c$	8.4842(10)/90	10.2368(8)/102.803(9)	24.228(2)/90		4.590/440.160	5.285/824.523	[7]
15	$[CH_6N]_2[(UO_2)_2(SeO_4)_3]$	*cc*2–2:3–14	$P2_1$	8.5827(13)/90	10.0730(15)/95.980(12)	10.0915(14)/90		4.390/184.480	5.209/385.500	[7]
16	$[CH_6N]_4[(UO_2)_3(SeO_4)_5](H_2O)_4$	*cc*2–3:5–2	$Pnma$	16.4221(14)/90	18.4773(9)/90	10.3602(5)/90		4.230/608.470	5.311/1657.045	[7]
17	$[CH_6N][H_5O_2][H_3O]_2(UO_2)_3(SeO_4)_5]\ (H_2O)_4$	*cc*2–3:5–2	$Ibca$	20.956(2)/90	34.767(8)/90	18.663(2)/90		5.170/1488.940	6.150/3493.056	[7]
18	$[CH_6N]_2[H_3O]_2[(UO_2)_5\ (SeO_4)_8(H_2O)](H_2O)_4$	*cc*2–5:8–2	$Pca2_1$	31.505(2)/90	10.3688(6)/90	16.2424(11)/90		5.860/1359.050	6.807/3049.695	[7]
19	$[CH_6N]_{1.5}[H_5O_2]_{1.5}[H_3O]_3$ $[(UO_2)_5(SeO_4)_8(H_2O)]\ (H_2SeO_4)_{2.6}(H_2O)_3$	*cc*2–5:8–3	$Pnma$	30.9728(19)/90	37.022(2)/90	10.4171(5)/90		5.880/2776.610	6.749/5614.766	[7]
	Ethylamine, $C_2H_5NH_3^+$						3.459/38.054			
20	$[C_2H_8N][(UO_2)Cl(SO_4)(H_2O)]$	*cc*2–1:1–1	$P2_1/c$	8.3545(17)/90	10.550(2)/102.64(3)	12.370(3)/90		3.585/172.078	4.524/416.168	[8]
21	$[C_2H_8N]_2[(UO_2)(SeO_4)_2(H_2O)](H_2O)_2$	*cc*1–1:2–1	$Pnma$	7.6176(9)/90	12.1811(16)/90	19.258(2)/90		3.250/208.000	4.724/944.771	[9]
22	$[C_2H_8N][H_3O][(UO_2)(SeO_4)_2(H_2O)]$	*cc*1–1:2–1	$P1$	7.5635(15)/79.559(15)	7.6188(15)/89.272(16)	12.101(2)/82.356(16)		4.000/128.000	4.954/307.160	[9]
23	$[C_2H_8N]_3[(UO_2)(SeO_4)_2(HSeO_4)]$	*cc*1–1:3–2	$P2_1/c$	12.7463(11)/90	12.4261(7)/113.433(6)	14.9928(11)/90		4.248/322.842	5.700/1185.691	[9]
24	$[C_2H_8N][(UO_2)(SeO_4)(SeO_2OH)]$	*cc*2–1:2–4	$P2_1/n$	8.475(3)/90	12.264(2)/95.23(3)	10.404(3)/90		3.700/192.423	4.954/614.320	[9]
25	$[C_2H_8N]_2[(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–10	$P2_1$	8.2897(14)/90	12.349(2)/104.439(4)	11.0379(18)/90		4.585/220.078	5.524/508.168	[10]

Table 1. *Cont.*

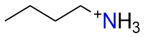
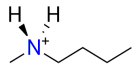
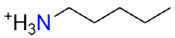
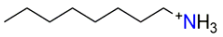
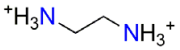
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	1-butylamine, $C_4H_7NH_3^+$						3.907/58.603			
26	$[C_4H_{10}N]_3[(UO_2)_2(SO_4)_3(OH)]$ $(H_2O)_2$	*cc*2–2:3–10	$P2_1$	8.439(5)/90	11.912(7)/102.79(10)	10.636(6)/90		4.459/196.215	5.426/466.659	[11]
27	$[C_4H_{10}N]_8[(UO_2)_5(SO_4)_9](H_2O)$	framework	$P2_12_12_1$	9.4586(8)/90	26.769(2)/90	32.377(3)/90		5.907/1417.654	7.500/5429.888	[11]
28	$[C_4H_{10}N]_2[(UO_2)_6(SO_4)_7(H_2O)_2]$	framework	$C222_1$	10.2776(12)/90	18.339(2)/90	22.788(3)/90		4.800/527.950	5.421/921.596	[11]
29	$[C_4H_{12}N][H_3O][(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–10	$P2_1/c$	10.7691(9)/90	12.5019(12)/98.172(7)	15.4620(14)/90		4.585/440.156	5.492/988.534	[12,13]
30	$[C_4H_{12}N][H_5O_2][(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–10	$P2_1$	8.3908(11)/90	12.3602(11)/101.567(10)	10.9150(13)/90		4.459/196.215	5.358/439.319	[14]
31	$[C_4H_{12}N]_{14}[(UO_2)_{10}(SeO_4)_{17}(H_2O)]$	*cc*2–3:5–2 nanotubules	$I2mm$	10.8864(5)/90	29.532(2)/90	47.439(2)/90		5.999/1403.665	7.547/5268.064	[15]
	N-methylbutylamine, $C_5H_{12}NH_2^+$						4.322/86.439			
32	$[C_5H_{14}N]_4[(UO_2)_3(SeO_4)_4$ $(HSeO_3)(H_2O)](H_2SeO_3)(HSeO_4)$	*cc*2–3:5–3	$P1$	11.7068(9)/73.899(6)	14.8165(12)/76.221(7)	16.9766(15)/89.861(6)		5.209/385.500	7.011/1808.897	[16]
33	$[C_5H_{14}N]_2[H_3O][(UO_2)_3(SeO_4)_4(HSeO_4)$ $(H_2O)]$	*cc*2–3:5–3	C2/c	16.7572(13)/90	11.7239(12)/98.875(6)	19.0490(13)/90		4.215/295.050	5.306/817.085	[17]
34	$[C_5H_{14}N]_2[H_3O][(UO_2)_3$ $(SeO_4)_4(HSeO_4)(H_2O)](H_2O)$	*cc*2–3:5–3	$P2_1/n$	10.8252(10)/90	19.0007(10)/100.324(7)	18.6463(15)/90		5.129/718.100	6.267/1930.170	[17]
	Pentylamine, $C_5H_{11}NH_3^+$						4.322/86.439			
35	$[C_5H_{14}N][(UO_2)(SeO_4)(SeO_2OH)]$	*cc*2–1:2–4	$P2_1/n$	11.553(2)/90	10.6445(16)/108.045(15)	12.138(2)/90		3.700/192.423	5.044/665.860	[18]
	Octylamine, $C_8H_{17}NH_3^+$						4.858/140.881			
36	$[C_8H_{20}N]_2[(UO_2)(SeO_4)_2$ $(H_2O)](H_2O)$	*cc*2–1:2–2	$P1$	7.498(3)/89.69(3)	11.897(4)/90.05(4)	32.056(14)/88.80(3)		5.000/320.000	7.267/2238.170	[19]
	Ethylenediamine, $C_2H_4(NH_3)_2^{2+}$						3.807/53.303			
37	$[C_2H_{10}N_2][(UO_2)(SeO_4)_2$ $(H_2O)](H_2O)$	*cc*2–1:2–2	$C2/c$	11.787(2)/90	7.7007(10)/102.016(14)	16.600(3)/90		3.125/100.000	4.225/304.235	[20]
38	$[C_2H_{10}N_2][(UO_2)(SeO_4)_2$ $(H_2O)](H_2O)_2$	*cc*2–1:2–2	$P2_1/c$	11.677(2)/90	7.908(1)/98.813(3)	15.698(2)/90		4.000/256.000	5.170/744.469	[10]
39	$[C_2H_{10}N_2][(UO_2)(SeO_3)$ $(HSeO_3)](NO_3)(H_2O)_{0.5}$	*cc*2–1:2–4	$Pbca$	13.170(3) /90	11.055(2)/90	18.009(4)/90		3.585/344.156	4.954/1228.641	[21]
40	$[C_2H_4(NH_3)_2][UO_2(SO_4)_2H_2O]$	*cc*1–1:2–1	$C2/c$	15.6163(4)/90	7.3018(2)/118.731(2)	11.7114(3)/90		3.125/100.000	3.974/238.413	[22]

Table 1. *Cont.*

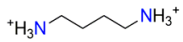
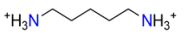
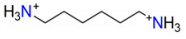
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/β, °	*c*, Å/γ, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	1.3-diaminopropane, $C_3H_6(NH_3)_2^{2+}$						4.087/69.487			
41	$[C_3H_{12}N_2][UO_2(H_2O)(SO_4)_2]$	*cc*1–1:2–1	*P*2/*c*	7.2582(2)/90	7.3697(2)/99.4053(19)	11.8514(3)/90		3.125/100.000	4.135/272.930	[23]
42	$[C_3H_{12}N_2][(UO_2)_2(H_2O)(SO_4)_3]$	*cc*2–2:3–4	$P2_1/n$	10.7391(3)/90	10.3791(3)/106.942(1)	18.0265(7)/90		4.585/440.156	5.358/878.639	[23]
43	$[N_2C_3H_{12}][UO_2F(SO_4)]_2(H_2O)$	*cc*2–1:1–10	$P2_1$	6.7745(2)/90	8.1589(2)/94.556(1)	14.3661(4)/90		4.170/150.117	5.248/398.842	[24]
	1.4-diaminobutane, $C_4H_8(NH_3)_2^{2+}$						4.322/86.439			
44	$[C_4H_{14}N_2]_2[UO_2(SO_4)_3](H_2O)_2$	*cc*0–1:3–4	*P*1	8.4584(1)/100.8158(5)	10.2830(1)/96.3926(5)	15.2943(2)/112.5170(5)		4.170/150.117	6.000/768.000	[22]
45	$[C_4H_{14}N_2][UO_2(H_2O)(SO_4)_2]$	*cc*2–1:2–1	*P*1	7.4199(2)/79.1237(9)	7.8380(2)/79.9015(9)	12.0319(3)/83.1098(9)		4.000/128.000	5.170/372.235	[25]
46	$[C_4H_{14}N_2][UO_2F(SO_4)]_2$	*cc*2–1:1–10	$P2_1/c$	6.7754(5)/90	8.4094(8)/93.245(3)	14.1492(14)/90		3.170/114.117	4.248/322.842	[25]
47	$[C_4H_{14}N_2][(UO_2)_2(SeO_4)_3(H_2O)](H_2O)_2$	*cc*2–2:3–4	$P2_1/c$	11.068(3)/90	10.455(3)/114.555(19)	20.266(3)/90		4.585/440.156	5.644/1128.771	[12,13]
48	$(C_4H_{14}N_2)[(UO_2)_2(SO_4)_3(H_2O)]\cdot 2H_2O$	*cc*2–2:3–4	$P2_1/n$	10.9075(4)/90	10.4513(4)/97.908(2)	17.7881(7)/90		4.585/440.156	5.644/1128.771	[26]
49	$[C_4H_{14}N_2][(UO_2)(SO_4)_2(H_2O)]\cdot 2H_2O$	*cc*2–1:2–3	$P2_1/n$	8.8570(4)/90	7.3299(3)/95.140(2)	20.4260(9)/90		4.000/256.000	5.000/640.000	[26]
	1.5-diaminopentane, $C_5H_{10}(NH_3)_2^{2+}$						4.524/104.042			
50	$[C_5H_{16}N_2][UO_2(SO_4)_2]$	*cc*2–1:2–21	$P2_1/c$	7.9825(1)/90	19.8458(4)/111.6563(9)	9.7868(2)/90		3.700/192.423	5.170/744.469	[22]
51	$[C_5H_{16}N_2][(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–10	$P2_1$	8.0491(11)/90	12.2633(16)/99.918(11)	10.7239(16)/90		4.585/220.078	5.555/522.131	[12,13]
	1.6-diaminohexane, $C_6H_{12}(NH_3)_2^{2+}$						4.700/122.211			
52	$[C_6H_{18}N_2][UO_2(SO_4)_2]H_2O$	*cc*1–1:2–12	$P2_1/m$	10.1385(3)/90	6.9537(3)/99.287(2)	11.7233(4)/90		3.393/88.211	4.880/478.242	[22]
53	$[C_6H_{18}N_2][(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–10	$P2_1$	8.4020(18)/90	12.411(3)/102.951(17)	10.923(2)/90		4.585/220.078	5.644/564.386	[12,13]
	1.7-diaminoheptane, $C_7H_{14}(NH_3)_2^{2+}$						4.858/140.881			
54	$[C_7H_{20}N_2][(UO_2)_2(SeO_4)_3(H_2O)](H_2O)$	*cc*2–2:3–10	$P2_1$	8.7100(16)/90	12.4174(14)/101.348(14)	10.8838(18)/90		4.585/220.078	5.807/650.424	[12,13]

Table 1. *Cont.*

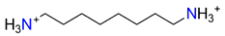
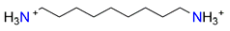
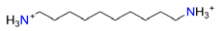
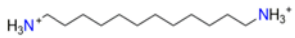
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	1.8-diaminooctane, $C_8H_{16}(NH_3)_2^{2+}$						5.000/160.000			
55	$[C_8H_{22}N_2][(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–10	$P2_1$	8.7793(16)/90	12.4874(15)/100.609(14)	10.9331(18)/90		4.585/220.078	5.807/650.424	[12,13]
	1.9-diaminononane, $C_9H_{18}(NH_3)_2^{2+}$						5.129/179.525			
56	$[C_9H_{24}N_2][(UO_2)(SeO_4)(SeO_2OH)]$ (NO_3)	*cc*2–1:2–4	$P1$	10.7480(7) /109.960(1)	13.8847(9)/103.212(2)	14.6363(10)/90.409(1)		4.700/244.423	6.700/1393.691	[27]
57	$[C_9H_{24}N_2]_2[(UO_2)_3(SeO_4)_5(H_2O)_2](H_2O)x$	*cc*2–3:5–4	$P6_3/mmc$	19.5572(5)/90	19.5572(5)/90	47.878(2)/120		4.670/2017.408	5.755/5190.982	[28]
	1.10-diaminodecane, $C_{10}H_{20}(NH_3)_2^{2+}$						5.248/199.421			
58	$[C_{10}H_{26}N_2][(UO_2)(SeO_4)_2(H_2O)]$ $(H_2SeO_4)_{0.85}(H_2O)_2$	*cc*1–1:2–1	$P1$	7.5461(6)/77.678(6)	14.9910(12)/85.463(6)	22.3789(17)/82.717(6)		5.000/320.000	6.895/1640.967	[19]
59	$[C_{10}H_{26}N_2][(UO_2)(SeO_4)_2]$ $(H_2SeO_4)_{0.5}(H_2O)$	*cc*2–1:2–4	$C2/c$	29.280(2)/90	13.3013(10)/93.295(5)	11.4513(7)/90		3.700/192.423	5.879/1375.665	[19]
	1.12-diaminododecane, $C_{12}H_{24}(NH_3)_2^{2+}$						5.459/240.215			
60	$[C_{12}H_{30}N_2]_3[H_3O]_2[(UO_2)_4(SeO_4)_8]$ $(H_2O)_5$	*cc*2–1:2–13	$P2_1/n$	11.3437(7)/90	24.8042(12)/96.701(5)	29.2496(19)/90		5.700/1185.691	7.622/6006.177	[29]
	Dimethylamine, $C_2H_6NH_2^+$						3.459/38.054			
61	$[C_2H_8N]_2[(UO_2)(SeO_4)_2(H_2O)]$	*cc*1–1:2–1	$P2_12_12_1$	7.5363(7)/90	12.2021(11)/90	16.7601(16)/90		4.000/256.000	5.248/797.685	[30]
62	$[C_2H_8N]_2[(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–4	$P2_12_12_1$	11.2154(5)/90	11.2263(5)/90	16.9138(8)/90		4.585/440.156	5.524/1016.335	[30]
63	$[C_2H_8N]_3[H_5O_2][(UO_2)_2(SeO_4)_3(H_2O)_2]_2$ $(H_2O)_5$	*cc*2–2:3–5	$P2_1/c$	12.451(5)/90	31.126(5)/120.39(2)	14.197(4)/90		5.524/1016.335	6.658/2689.917	[30]
64	$[C_2H_8N]_2[H_3O][(UO_2)_3$ $(SeO_4)_4(HSeO_3)(H_2O)](H_2SeO_3)_{0.2}$	*cc*2–3:5–3	$P2_1/m$	8.3116(4)/90	18.6363(8)/97.582(1)	11.5623(5)/90		4.264/289.947	5.078/619.550	[30]
65	$[C_2H_8N][(H_5O_2)(H_2O)]$ $[(UO_2)_2(SeO_4)_3(H_2SeO_3)](H_2O)$	*cc*2–1:2–14	$P2_1/n$	14.7979(8)/90	10.0238(6)/111.628(1)	16.4176(9)/90		4.755/513.528	5.672/1157.175	[31]
66	$[C_2H_8N]_3[C_2H_7N][(UO_2)_3(SeO_4)_4$ $(HSeO_3)(H_2O)]$	*cc*2–3:5–3	*Pnma*	11.6591(11)/90	14.9556(17)/90	22.194(2)/90		4.472/715.508	5.607/1883.819	[30]
67	$[C_2H_8N]_3[H_3O][(UO_2)_3(SeO_4)_4(SeO_3)$ $(H_2O)](H_2O)$	*cc*2–3:5–3	$P2_1/m$	8.941(2)/90	19.300(4)/97.510(4)	11.377(3)/90		4.329/303.050	5.599/996.681	[30]

Table 1. *Cont.*

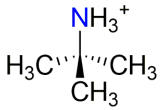
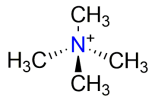
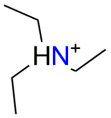
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	Isopropylamine, $C_3H_7NH_3^+$						3.807/53.303			
1	$[C_3H_{10}N]_2[(UO_2)_6(SO_4)_7(H_2O)_2]$	framework	$C222_1$	10.2560(2)/90	18.4062(4)/90	22.8900(4)/90		4.900/578.152	5.454/949.072	This work
2	$[C_3H_{10}N]_2[(UO_2)_2(SeO_4)_3(H_2O)](H_2O)$	*cc*2–2:3–4	$P2_1/c$	11.4644(2)/90	11.2426(2)/99.421(2)	18.7555(4)/90		4.585/440.156	5.781/1271.899	This work, [12,13]
3	$[C_3H_{10}N]_2[(UO_2)_2(SO_4)_3(H_2O)](H_2O)$	*cc*2–2:3–4	$P2_1/c$	11.0470(1)/90	10.8926(1)/100.180(1)	18.5397(2)/90		4.585/440.156	5.781/1271.899	This work
4	$[C_3H_{10}N](H_3O)[(UO_2)_2(SeO_4)_3(H_2O)](H_2SeO_3)$	*cc*2–2:3–4	$P2_1/c$	11.2894(4)/90	11.1012(3)/94.717(3)	18.1368(6)/90		4.585/440.156	5.585/1072.313	This work
	Tert-butylamine, $C_4H_9NH_3^+$						4.087/69.487			
68	$[C_4H_{12}N]_2[(UO_2)(SeO_4)_2(H_2O)]$	*cc*2–1:2–3	$C2/c$	27.212(10)/90	7.372(3)/117.75(2)	23.113(7)/90		4.000/256.000	5.644/1128.771	[20]
69	$[C_4H_{12}N]_2[(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–4	$P2_1/c$	11.3478(14)/90	11.3850(9)/91.865(11)	18.959(3)/90		4.585/440.156	5.858/1359.052	[12,13]
	Tetramethylammonium, $C_4H_{12}N^+$						4.087/69.487			
70	$[C_4H_{12}N][(UO_2)(SO_4)(H_2O)_2]Cl$	*cc*1–1:1–2	$P2_1$	8.989(6)/90	6.877(4)/109.77(4)	10.981(8)/90		3.807/106.606	5.000/320.000	[32]
71	$[C_4H_{12}N][(UO_2)(SO_4)(NO_3)]$	*cc*1–1:2–12	$C2/m$	21.106(1)/90	6.9350(3)/97.5468(18)	8.4284(5)/90		3.252/78.039	4.306/249.763	[33]
72	$[C_4H_{12}N][(UO_2)(SeO_4)(NO_3)]$	*cc*1–1:2–12	$C2/m$	21.244(5)/90	7.1092(11)/97.693(17)	8.6581(18)/90		3.252/78.039	4.375/280.000	[34]
73	$[C_4H_{12}N]_2[(UO_2)_6(SO_4)_7(H_2O)_2]$	framework	$C222_1$	10.3466(2)/90	18.5415(3)/90	22.7001(4)/90		4.800/527.950	5.487/976.681	[35]
	Triethylamine, $C_6H_{15}NH^+$						4.524/104.042			
74	$[C_6H_{16}N][H_3O][(UO_2)_2(SeO_4)_3(H_2O)]\ (H_2O)$	*cc*2–2:3–4	$P2_1$	8.8162(16)/90	12.4459(15)/103.695(14)	10.8212(19)/90		4.585/220.078	5.755/621.528	[12,13]
75	$[C_6H_{16}N][H_5O_2][(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–10	$P2_1$	8.8477(3)/90	12.4835(5)/103.382(1)	10.8373(4)/90		4.585/220.078	5.755/621.528	[36]
76	$(H_5O_2)[C_6H_{16}N][(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–10	$P2_1/c$	10.753(1)/90	12.3221(8)/91.050(9)	18.142(2)/90		4.585/440.156	5.755/1243.056	[13]

Table 1. *Cont.*

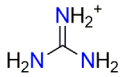
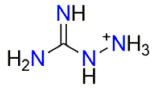
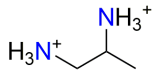
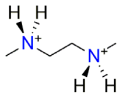
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	Guanidine, $CH_6N_3^+$						3.322/33.219			
77	$[CH_6N_3]_2[(UO_2)(SO_4)(H_2O)_2](NO_3)_2\ (H_2O)$	*cc*1–1:1–2	$P2_1/n$	12.3824(7)/90	7.0329(4)/99.598(2)	21.5362(12)/90		3.807/213.212	5.492/988.534	[37]
78	$[CH_6N_3]_2[(UO_2)(SO_4)_2(H_2O)](H_2O)_2$	*cc*2–1:2–2	$C2/c$	11.220(8)/90	8.027(4)/101.00(7)	18.681(8)/90		3.125/100.000	4.440/372.955	[38]
79	$[CH_6N_3]_2[(UO_2)_2(SO_4)_3]$	*cc*2–2:3–14	$P2_12_12$	9.907(3)/90	9.597(3)/90	9.762(3)/90		3.440/144.477	4.480/367.319	[39]
80	$[CH_6N_3]_2[(UO_2)(SeO_4)_2(H_2O)](H_2O)_{1.5}$	*cc*2–1:2–2	$C2/c$	37.314(4)/90	7.1771(6)/109.267(8)	13.2054(14)/90		4.000/256.000	5.352/867.056	[20]
81	$[CH_6N_3]_3[(UO_2)_2(SeO_4)_3(HSeO_4)](H_2O)_2$	*cc*2–1:2–4	$P2_12_12_1$	10.7261(9)/90	13.9178(16)/90	18.3213(17)/90		4.755/513.528	5.977/1506.275	[20]
82	$[CH_6N_3]_2[(UO_2)_2(SeO_4)_3]$	*cc*2–2:3–14	$P2$	9.9448(15)/90	9.727(2)/90.213(12)	10.1508(15)/90		4.440/186.477	5.480/449.319	[5]
	Aminoguanidine, $CH_7N_4^+$						3.585/43.020			
83	$[CH_7N_4]_2[(UO_2)(SO_4)_2(H_2O)]$	*cc*2–1:2–2	$C2/c$	11.297(2)/90	7.8336(16)/100.18(3)	17.984(4)/90		3.125/100.000	4.627/444.156	[40]
	1,2-diaminopropane, $C_3H_{12}N_2^{2+}$						4.087/69.487			
84	$[C_3H_{12}N_2]_2[(UO_2)_2(SO_4)_4(H_2O)_4](H_2O)_2$	*cc*1–1:2–1	$P1$	7.3983(2)/95.1761(12)	7.6333(2)/94.6412(13)	12.5946(5)/96.578(2)		4.248/161.421	5.285/412.261	[41]
85	$[C_3H_{12}N_2][UO_2(H_2O)(SO_4)_2]$	*cc*1–1:1–1	$P1$	7.3296(2)/92.0309(13)	7.3702(2)/106.041(1)	11.6822(2)/93.6783(9)		4.000/128.000	5.044/332.930	[42]
86	$[C_3H_{12}N_2][UO_2F(SO_4)]_2{\cdot}H_2O$	*cc*2–1:1–9	*Pnma*	13.5775(3)/90	14.6180(4)/90	8.1168(2)/90		3.170/228.235	4.752/912.313	[24]
87	$[C_3H_{12}N_2][(UO_2)(SeO_4)_2(H_2O)_2](H_2O)$	*cc*0–1:2–3	$P1$	7.5611(16)/94.604(18)	7.7650(17)/94.405(17)	12.925(3)/96.470(17)		4.248/161.421	5.285/412.261	[34]
	N.N-dimethylethylene diamine, $C_4H_{14}N_2^{2+}$						4.322/86.439			
88	$[C_4H_{14}N_2][UO_2(SO_4)_2]$	*cc*2–1:2–20	$P2_12_12_1$	9.3322(1)/90	9.7743(2)/90	13.8897(3)/90		3.700/192.423	5.044/665.860	[43]
89	$[C_4H_{14}N_2][(UO_2)_2(H_2O)(SO_4)_3](H_2O)$	*cc*2–2:3–4	$P2_1/c$	11.2460(2)/90	10.5387(2)/92.9884(6)	17.0432(3)/90		4.585/440.156	5.555/1044.263	[43]
90	$[C_4H_{14}N_2][(UO_2)(SeO_4)_2(H_2O)]$	*cc*2–1:2–8	$P1$	6.853(2)/99.62(3)	10.537(3)/94.45(3)	10.574(3)/100.52(3)		4.000/128.000	5.170/372.235	[34]
91	$[C_4H_{14}N_2][(UO_2)_2(SeO_4)_3(H_2O)](H_2O)$	*cc*2–2:3–4	$P2_1/c$	11.568(4)/90	10.857(4)/95.545(11)	17.229(7)/90		4.585/440.156	5.555/1044.263	[36]

Table 1. *Cont.*

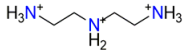
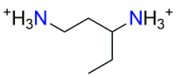
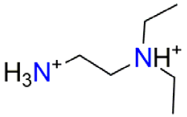
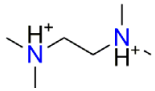
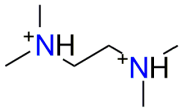
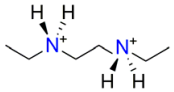
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	Diethylenetriamine, $C_4H_{15}N_3^{3+}$						4.459/98.107			
92	$[C_4H_{15}N_3][H_3O]_{0.5}[(UO_2)_2(SeO_4)_3\ (H_2O)](NO_3)_{0.5}$	*cc*2–2:3–4	$P2_1/c$	11.1679(4)/98.019(1)	10.9040(4)/90	17.9913(6)/90		4.459/392.430	5.615/1100.483	[30]
	1.3-diaminopentane, $C_5H_{16}N_2^{2+}$						4.524/104.042			
93	$[C_5H_{16}N_2]_2[(UO_2)(SeO_4)_2(H_2O)](NO_3)_2$	*cc*1–1:2–1	$C2/c$	28.916(5)/90	8.0836(10)/110.909(11)	11.9856(16)/90		3.125/100.000	5.158/722.100	[34]
	N,N-Diethylethylenediamine, $C_6H_{18}N_2^{2+}$						4.700/122.211			
94	$[C_3H_8N]_2[(UO_2)_2(SeO_4)_3(H_2O)](H_2O)$	*cc*2–2:3–4	$P2_1/c$	12.0301(15)/90	10.7845(9)/91.865(10)	17.490(2)/90		4.585/440.156	5.728/1214.319	[13]
	Tetramethylethylenediamine, $C_6H_{18}N_2^{2+}$						4.700/122.211			
95	$[C_6H_{18}N_2][(UO_2)_2(SO_4)_3(H_2O)]$	*cc*2–2:3–4	$P2_1$	8.4460(7)/90	11.966(1)/104.043(2)	10.6635(9)/90		4.585/220.078	5.644/564.386	[36]
	1.2-ethylamino ethane, $C_6H_{18}N_2^{2+}$						4.700/122.211			
96	$[C_6H_{18}N_2][(UO_2)_2(H_2O)_3(SO_4)_3]$	*cc*1–1:1–2 *cc*1–1:2–8	$P1$	6.8234(1)/101.3691(6)	8.7384(1)/98.1340(6)	19.2381(4)/90.0480(11)		4.907/294.413	5.807/650.424	[42]
	N,N-*diethylethane-1,2-diamine*, $C_6H_{18}N_2^{2+}$						4.700/122.211			
97	$[C_6H_{18}N_2]_2[UO_2F(SO_4)]_4\cdot H_2O$	*cc*2–1:1–6	$P1$	10.8832(2)/75.6604(8)	10.9386(2)/73.6101(7)	16.5325(3)/89.7726(7)		5.285/412.261	6.508/1184.419	[24]

Table 1. *Cont.*

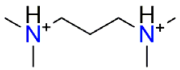
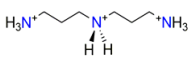
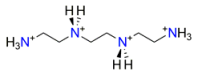
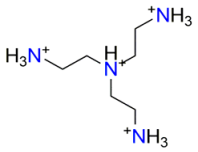
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	N,N,N′,N′-tetramethyl-1,3-propanediamine, $C_7H_{20}N_2^{2+}$						4.858/140.881			
98	$[C_7H_{20}N_2][(UO_2)_2(SO_4)_3(H_2O)]$	*cc*2–2:3–17	*P*1	6.7861(1)/88.6230(9)	8.5143(1)/81.6364(8)	19.0442(3)/84.8577(6)		4.585/220.078	5.728/607.160	[44]
	N-(3-aminopropyl)-1,3-propanediamine, $N_3C_6H_{20}^{3+}$						4.858/140.881			
99	$(N_3C_6H_{20})(H_5O_2)[(UO_2)_4(SO_4)_6(H_2O)_2]\cdot 4H_2O$	*cc*2–2:3–4	$P2_1/n$	10.8576(1)/90	10.4120(1)/97.518(1)	17.8726(3)/90		4.585/440.156	5.858/1359.052	[45]
100	$(N_3C_6H_{20})[(UO_2)(SO_4)_2(SO_3OH)]\cdot H_2O$	*cc*1–1:3–2	*P*1	7.9164(1)/92.892(1)	11.0632(1)/97.938(1)	11.3354(1)/107.497(1)		4.248/161.421	5.672/578.587	[45]
	Triethylenetetramine, $C_6H_{22}N_4^{4+}$						5.000/160.000			
101	$[C_6H_{22}N_4][UO_2(H_2O)(SO_4)_2]_2(H_2O)_6$	*cc*1–1:2–8	*P*1	6.7186(5)/72.337(2)	9.2625(7)/89.198(2)	13.1078(9)/70.037(1)		4.000/128.000	5.358/439.319	[46]
102	$[C_6H_{22}N_4][UO_2(SO_4)_2]_2$	*cc*2–1:2–20	*Pbca*	9.3771(2)/90	12.9523(3)/90	18.9065(6)/90		3.700/384.846	4.858/1127.052	[47]
103	$[C_6H_{22}N_4][(UO_2)(SeO_4)_2(H_2O)](H_2O)$	*cc*2–1:2–3	$P2_1/n$	13.002(2)/90	7.962(1)/114.077(2)	14.754(2)/90		4.000/256.000	5.129/718.100	[10]
104	$[N_4C_6H_{22}][UO_2(H_2O)(SO_4)_2]_2(H_2O)_6$	*cc*1–1:2–8	*P*1	6.7318(1)/72.3395(6)	9.2975(1)/89.1401(7)	13.1457(3)/70.0267(12)		4.000/128.000	5.358/439.319	[47]
	Tris(2-aminoethyl)-amine, $C_6H_{21}N_4^{4+}$						5.000/160.000			
105	$[C_6H_{21}N_4][(UO_2)(SeO_4)_2(HSeO_4)]$	*cc*1–1:3–2	$P2_1/m$	9.2218(6)/90	12.2768(9)/116.165(1)	9.4464(7)/90		3.616/137.421	4.931/512.846	[10]
106	$(N_4C_6H_{22})[(UO_2)_2(SO_4)_4(H_2O)_2]\cdot 3H_2O$	*cc*2–1:2–2	$P2_1/n$	7.4982(1)/90	16.9531(5)/90.729(2)	11.4496(2)/90		4.000/256.000	5.700/1185.691	[45]
107	$[C_6H_{22}N_4]_2[(UO_2)_2(SO_4)_6](H_2O)$	*cc*0–1:3–4	*P*1	11.2315(1)/88.4073(5)	13.2136(1)/74.5896(5)	14.3521(2)/66.5370(6)		5.170/372.235	6.687/1377.419	[22]

Table 1. *Cont.*

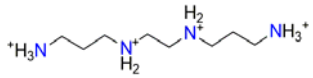
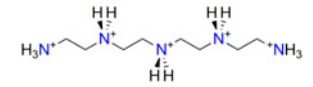
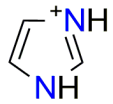
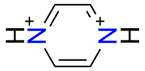
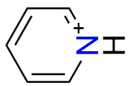
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	1,5,8,12-tetraazadodecane, $C_8H_{26}N_4^{4+}$						5.248/199.421			
108	$[C_8H_{26}N_4][(UO_2)(SeO_4)_2(H_2O)](H_2O)$	*cc*2–1:2–2	$P2_1/n$	7.8198(11)/90	16.516(3)/90.662(11)	11.6831(16)/90		4.000/256.000	5.285/824.523	[48]
109	$[C_8H_{26}N_4]_{0.5}[(UO_2)_2(SO_4)_3(H_2O)](H_2O)_2$	*cc*2–2:3–12	$P2_1/n$	11.8400(2)/90	10.3190(2)/107.7718(9)	16.5919(4)/90		4.585/440.156	5.615/1100.483	[49]
	Tetraethylenepentamine, $C_8H_{28}N_5^{5+}$						5.358/219.660			
110	$[C_8H_{28}N_5]_2[(UO_2)_5(H_2O)_5(SO_4)_{10}]H_2O$	*cc*2–1:2–2	*Pbnm*	7.7638(5)/90	14.16890(5)/90	56.46930(5)/90		5.372/1719.017	6.409/4229.773	[47]
	Imidazole, $C_3H_5N_2^+$						3.322/33.219			
111	$[C_3H_5N_2]_2[(UO_2)_2(SO_4)_3]$	*cc*2–2:3–14	$P2_12_12_1$	9.7683(3)/90	10.0252(3)/90	19.9136(7)/90		4.392/368.955	5.358/878.639	[42]
	Pyrazine, $C_4H_5N_2^{2+}$						3.459/38.054			
112	$(C_4H_5N_2)_2[(UO_2)(SeO_4)_2(H_2O)]$	*cc*2–1:2–1	*C*2/*c*	18.2026(8)/90	7.9997(3)/106.947(2)	11.6866(5)/90		3.125/100.000	4.301/326.842	[50]
113	$(C_4H_5N_2)_2[(UO_2)_2(SeO_4)_3(H_2O)]\cdot 3H_2O$	*cc*2–2:3–11	*P*1	8.8130(5)/108.286(2)	11.5642(6)/94.279(2)	13.1308(7)/105.157(2)		4.755/256.764	5.781/635.950	[50]
114	$(H_3O)(C_4H_5N_2)_2[(UO_2)_3(SeO_4)_5(H_2O)]\cdot H_2O$	*cc*2–3:5–3	*Pbcm*	11.573(3)/90	19.220(6)/90	14.465(5)/90		4.472/715.508	5.469/1465.712	[50]
	Pyridine, $C_5H_6N^+$						3.585/43.020			
115 [1]	$[C_5H_6N][(UO_2)(SeO_4)(HSeO_3)]$	*cc*2–1:2–4	$P2_1/n$	8.993(3)/90	13.399(5)/108.230(4)	10.640(4)/90		-	-	[51]
116	$[C_5H_6N]_2[(UO_2)_2(SeO_4)_3]$	*cc*2–2:3–14	*Pccn*	9.987(7)/90	10.251(7)/90	20.957(14)/90		3.440/288.955	4.589/789.318	[52]
117	$(C_5H_6N)_2[(UO_2)_2(SeO_4)_3(H_2O)]\cdot 3H_2O$	*cc*2–2:3–10	$P2_1/n$	10.6354(4)/90	12.3334(5)/103.182(1)	18.8810(8)/90		4.585/440.156	5.755/1243.056	[50]

Table 1. *Cont.*

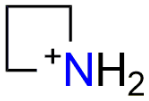
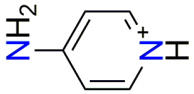
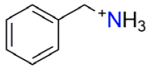
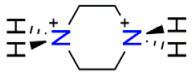
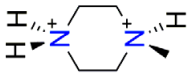
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	Azetidine, $C_3H_8N^+$						3.585/43.020			
118	$[C_3H_8N]_2[(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–4	$P2_12_12_1$	10.8620(5)/90	11.1105(5)/90	17.8815(8)/90		4.585/440.156	5.585/1072.313	[53]
	4-aminopyridine, $C_5H_7N_2^+$						3.907/58.603			
119	$[C_5H_7N_2]_2[(UO_2)(SO_4)_2]$	*cc*1–1:2–12	*P*1	7.0126(9)/68.187(5)	10.3352(13)/78.940(5)	13.8027(19)/71.339(3)		3.700/96.211	5.426/466.659	[37]
	Benzylamine, $NC_7H_{10}^+$						4.170/75.059			
120	$[NC_7H_{10}]_2[(UO_2)_2(SO_4)_3]\cdot H_2O$	*cc*2–2:3–14	$P2_1/n$	10.3238(2)/90	9.1710(2)/91.414(2)	27.1113(7)/90		4.392/368.955	5.907/1417.654	[45]
121	$[C_7H_{10}N]_2[(UO_2)(SeO_4)_2(H_2O)](H_2O)$	*cc*2–1:2–2	$Pna2_1$	24.221(2)/90	11.9169(11)/90	7.4528(7)/90		4.000/256.000	5.781/1271.899	[10]
	Piperazine, $C_4H_{12}N_2^{2+}$						4.170/75.059			
122	$[C_4H_{12}N_2][UO_2(H_2O)(SO_4)_2]$	*cc*1–1:2–1	*C*2/*c*	14.7676(3)/90	7.6585(2)/104.837(2)	11.6807(2)/90		3.125/100.000	4.146/281.947	[54]
123	$[C_4H_{12}N_2][(UO_2)(SeO_4)_2\ (H_2O)]$	*cc*1–1:2–1	*C*2/*c*	15.7651(10)/90	7.4093(5)/101.121(2)	11.9639(8)/90		3.125/100.000	4.146/281.947	[50]
124	$[C_4H_{12}N_2]_{0.5}[(UO_2)(HSeO_3)(SeO_3)]$	*cc*2–1:2–20	$P2_1/c$	10.9378(5)/90	8.6903(4)/90.3040(8)	9.9913(5)/90		3.585/172.078	4.392/368.955	[55]
	1-methylpiperazine, $C_5H_{14}N_2^{2+}$						4.392/92.239			
125	$[C_5H_{14}N_2][UO_2(H_2O)(SO_4)_2]$	*cc*1–1:2–1	*P*1	8.0031(2)/72.704(1)	8.1873(2)/81.7766(11)	10.8911(3)/78.7917(9)		4.000/128.000	5.209/385.500	[56]

Table 1. *Cont.*

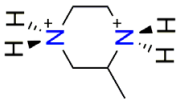
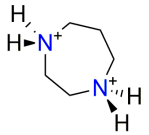
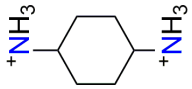
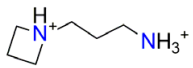
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	2-methylpiperazine, $C_5H_{14}N_2^{2+}$						4.392/92.239			
126	$[C_5H_{14}N_2][UO_2(H_2O)(SO_4)_2]$	*cc*1–1:2–4	*P*1	10.7537(2)/87.998(1)	11.4297(2)/79.660(1)	11.5797(2)/80.6313(6)		5.000/320.000	6.209/918.999	[54]
127	$[C_5H_{14}N_2][UO_2F(H_2O)(SO_4)]_2$	*cc*2–1:1–7	$P2_1/n$	8.4354(2)/90	15.5581(4)/96.666(1)	14.8442(6)/90		4.585/440.156	5.585/1072.313	[24]
	Homopiperazine, $C_5H_{14}N_2^{2+}$						4.392/92.239			
128	$[C_5H_{14}N_2]_2[UO_2(SO_4)_3]$	*cc*0–1:3–2	*C*2/*c*	14.4975(3)/90	11.9109(3)/110.475(1)	13.0157(3)/90		3.281/118.117	4.940/592.827	[43]
129	$[C_5H_{14}N_2][UO_2(H_2O)(SO_4)_2]$	*cc*1–1:1–2	$P22_12_1$	7.6955(2)/90	11.7717(3)/90	14.7038(4)/90		4.125/264.000	4.125/264.000	[43]
	1.4-diaminocyclohexane, $C_6H_{16}N_2^{2+}$						4.585/110.039			
130	$[N_2C_6H_{16}][UO_2F_2(SO_4)]$	*cc*1–1:1–13	*P*1	6.9105(2)/72.659(1)	9.6605(2)/87.068(1)	10.1033(2)/77.957(1)		3.322/66.439	5.087/345.947	[24]
131	$[C_6H_{16}N_2][UO_2F_2(SO_4)]$	*cc*2–1:1–14	*Pmmn*	6.9503(1)/90	17.2147(4)/90	7.0867(1)/90		2.948/106.117	4.309/534.320	[24]
132	$[C_6H_{16}N_2][UO_2(SO_4)_2]\cdot 2H_2O$	*cc*1–1:2–12	*P*1	6.7813(1)/76.7537(7)	10.0636(2)/75.6074(7)	12.9753(3)/74.3971(13)		3.700/96.211	5.426/466.659	[57]
	Azetidinopropaneamine, $C_6H_{16}N_2^{+}$						4.585/110.039			
133	$[C_6H_{16}N_2][(UO_2)_2(SeO_4)_3(H_2O)](H_2O)$	*cc*2–2:3–4	$P2_1/c$	11.3575(5)/90	11.021(5)/90.608(1)	17.8038(8)/90		4.585/440.156	5.728/1214.319	[53]
134	$[C_3H_8N]_2(H_5O_2)[(UO_2)_2(SO_4)_3(HSO_4)]$	*cc*2–1:2–13	$P2_1/n$	8.677(3)/90	10.294(3)/97.521(7)	26.474(8)/90		4.755/513.528	5.858/1359.052	[53]

Table 1. *Cont.*

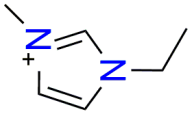
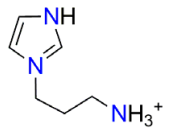
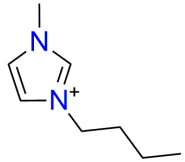
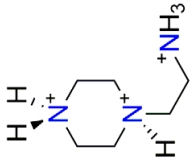
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	1-ethyl-3-methyl imidazolium, $C_6H_{11}N_2^+$						4.248/80.711			
135 [1]	$[C_6H_{11}N_2]_2[(UO_2)(SO_4)_2]$	*cc*1–1:2–12	*C*2/*c*	31.90(1)/90	9.383(5)/93.999(7)	13.770(7)/90		-	-	[58]
136	$[C_6N_2H_{11}](Na)[(UO_2)_4(SO_4)_2(OH)_2(O)_2]\cdot 3(H_2O)$	$5^2\,4^3\,3^2$	$P2_1/c$	17.182(5)/90	8.852(3)/100.693(4)	17.162(5)/90		4.755/513.528	5.803/1288.360	[59]
137	$[C_6N_2H_{11}](H_9O_4)[(UO_2)(SO_4)_2]$	*cc*1–1:2–12	*P*1	6.9504(11)/95.993(2)	9.9247(15)/95.024(2)	14.966(2)/103.323(2)		3.700/96.211	5.931/723.550	[59]
138	$[C_6N_2H_{11}]_2[(UO_2)_2(SO_4)_3(H_2O)]$	*cc*2–2:3–22	*P*1	9.5715(11)/81.803(1)	10.4399(12)/81.394(1)	13.7023(16)/86.480(1)		4.585/220.078	5.954/738.320	[59]
139	$[C_6N_2H_{11}]_2[(UO_2)_2(SO_4)_3(H_2O)_2]\cdot 2(H_2O)$	*cc*1–2:3–3	$P2_1/n$	12.952(2)/90	19.302(3)/116.891(2)	13.224(2)/90		4.755/513.528	6.150/1746.528	[59]
140	$[C_6N_2H_{11}][(UO_2)_2(SO_4)(OH)(O)]$	$5^2\,4^3\,3^2$	*P*1	8.859(2)/107.671(3)	8.926(2)/97.350(3)	9.893(3)/104.502(3)		3.807/106.606	5.044/332.930	[59]
	1-(3-aminopropyl) imidazole, $N_3C_6H_{13}^+$						4.459/98.107			
141	$[N_3C_6H_{13}][(UO_2)(SO_4)_2]$	*cc*1–1:2–12	*P*1	6.8164(1)/76.749(1)	7.6357(1)/88.091(1)	14.1979(2)/86.533(1)		3.700/96.211	5.129/359.050	[45]
	1-butyl-3-methylimidazole, $C_8H_{15}N_2^+$						4.644/116.096			
142	$[C_8H_{15}N_2]_2[(UO_2)_4(SeO_3)_5]$	$6^1\,5^2\,4^2\,3^2$	*Pnma*	18.860(2)/90	18.010(2)/90	11.140(1)/90		4.250/544.000	5.455/1789.277	[52]
	2-piperazinoethylamine, $C_6H_{18}N_3^{3+}$						4.755/128.382			
143	$[C_6H_{18}N_3][(UO_2)_2(H_2O)(SO_4)_3(HSO_4)]\,(H_2O)_{4.5}$	*cc*2–1:2–12	$P2_1/a$	15.7673(4)/90	10.5813(3)/99.9216(9)	16.7710(5)/90		4.907/588.827	6.129/1716.199	[60]
144	$[C_6H_{18}N_3]_2[(UO_2)_5(H_2O)(SO_4)_8](H_2O)_5$	*cc*2–5:8–2	$P2_1/n$	21.5597(3)/90	10.2901(2)/96.7436(7)	22.8403(3)/90		5.858/1359.052	6.989/3550.252	[60]

Table 1. *Cont.*

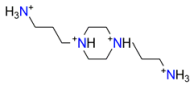
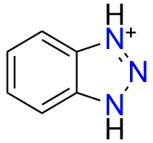
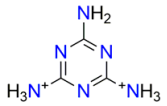
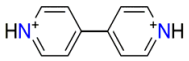
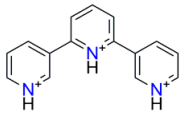
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	1,4-bis(3-aminopropyl)piperazine, $C_{10}H_{28}N_4^{4+}$						5.392/226.477			
145	$(N_4C_{10}H_{28})_{0.5}[(UO_2)(SO_4)_2(H_2O)]\cdot H_2O$	*cc*2–1:2–2	$P2_1/n$	7.5484(2)/90	16.9859(4)/90.580(2)	11.4581(3)/90		4.000/256.000	5.322/851.508	[45]
146	$[C_{10}H_{28}N_4][(UO_2)_2(SO_4)_4]$	*cc*2–1:2–20	*Pbca*	9.5831(2)/90	15.6060(3)/90	18.1212(3)/90		3.700/384.846	5.087/1383.790	[61]
	1,2,3-benzotriazole, $C_6H_6N_3^+$						3.907/58.603			
147	$[C_6H_6N_3][H_5O_2][(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–10	$P2_1/c$	12.167(3)/90	12.316(3)/108.270(4)	14.909(3)/90		4.585/440.156	5.392/905.909	[36]
148	$[C_6H_6N_3][H_7O_3][(UO_2)_2(SO_4)_3(H_2O)]$ (H_2O)	*cc*2–2:3–10	*C*2	19.678(7)/90	10.600(4)/95.979(7)	10.925(4)/90		4.585/220.078	5.720/594.846	[36]
	Melamine, $C_3H_8N_6^{2+}$						4.087/69.487			
149	$[C_3H_8N_6][(UO_2)_2(SO_4)_3(H_2O)](H_2O)$	*cc*2–2:3–4	$P2_1/n$	11.1194(4)/90	10.5921(3)/101.405(2)	17.0143(6)/90		4.585/440.156	5.459/960.860	[62]
150	$[(C_3H_8N_6)(SeO_4)]$ $[(UO_2)(SeO_4)$ $(H_2SeO_3)_2]$	*cc*2–1:3–6	$P2_1/c$	16.247(4)/90	8.680(2)/90.615(5)	13.347(3)/90		4.644/464.386	5.392/905.909	[63]
	4.4′-Bipyridine, $C_{10}H_{10}N_2^{2+}$						4.459/98.107			
151	$[C_{10}H_{10}N_2][UO_2(SO_4)_2]H_2O$	*cc*1–1:2–12	*P*1	6.9507(1)/79.1992(7)	7.7097(1)/80.1403(8)	15.9200(4)/80.9717(14)		3.700/96.211	5.248/398.842	[42]
	Terpyridine, $C_{15}H_{14}N_3^{3+}$						5.000/160.000			
152	$[C_{15}H_{14}N_3][(UO_2)(SO_4)_2](NO_3)(H_2O)_2$	*cc*1–1:2–12	*P*1	6.9732(7)/111.809(2)	13.569(1)/102.386(2)	13.641(1)/93.833(2)		3.700/96.211	5.781/635.950	[46]

Table 1. *Cont.*

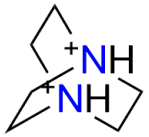
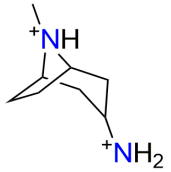
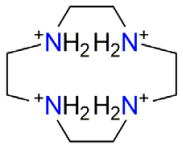
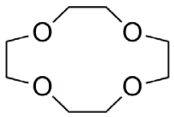
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	1.4-diazabicyclo(2.2.2)octane, $C_6H_{14}N_2^{2+}$						4.459/98.107			
153	$[C_6H_{14}N_2][UO_2(H_2O)(SO_4)_2]$	*cc*2–1:2–3	$P2_1/n$	8.6480(1)/90	7.7135(1)/90.7254(9)	21.2554(3)/90		4.000/256.000	5.248/797.685	[54]
	3-Aminotropane, $C_8H_{18}N_2^{2+}$						4.807/134.606			
154	$[C_8H_{18}N_2](H_5O_2)_2[(UO_2)_3(SeO_4)_5(H_2O)]$ (H_2O)	*cc*2–3:5–5	$P2_1/n$	10.210(2)/90	19.151(4)/98.959(3)	17.819(3)/90		5.209/770.999	6.340/2054.111	[64]
155	$[C_8H_{18}N_2](H_5O_2)_2[(UO_2)_3(SO_4)_5(H_2O)]$ (H_2O)	*cc*2–3:5–5	$P2_1/n$	10.147(3)/90	18.726(6)/99.043(7)	17.076(5)/90		5.209/770.999	6.322/2023.017	[64]
	Cyclen, $C_8H_{24}N_4^{4+}$						5.170/186.117			
156	$[C_8H_{24}N_4][(UO_2)_3(SO_4)_5]$ $(H_2O)_3$	*cc*2–3:5–2	$Pna2_1$	16.8623(10)/90	18.0113(11)/90	10.1928(6)/90		5.087/691.895	6.304/1991.995	[64]
157	$(C_8H_{24}N_4)(H_3O)_2[(UO_2)_4(SeO_4)_7(H_2O)]$ $(H_2O)_{6.75}$	*cc*2–4:7–3	$P1$	8.7587(14)/73.807(3)	13.067(2)/88.980(4)	23.009(4)/86.129(3)		5.644/564.386	6.977/1758.275	[64]
	12-crown-4 ether, $C_8H_{16}O_4$						4.807/134.606			
158	$[C_8H_{16}O_4]_{0.5}[UO_2(SO_4)(H_2O)](H_2O)$	*cc*1–1:1–2	$P1$	7.007(1)/91.31(1)	8.0408(6)/93.60(2)	10.776(2)/100.18(1)		3.585/86.039	4.858/281.763	[65]
159	$[C_8H_{16}O_4]_2[(H_5O_2)_3(H_9O_4)]$ $[(UO_2)_2(SeO_4)_3(H_2O)]_2$	*cc*2–2:3–10	$P2_1/c$	10.7328(6)/90	12.2828(5)/110.102(5)	22.7085(17)/90		4.585/440.156	6.087/1655.790	[66,67]

Table 1. *Cont.*

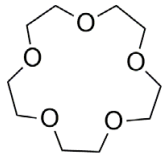
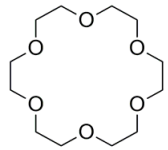
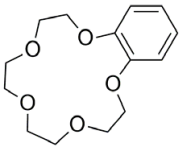
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	15-crown-5-ether, $C_{10}H_{20}O_5$						5.129/179.525			
160	$[K@(C_{10}H_{20}O_5)][(UO_2)(SeO_4)(HSeO_4)\ (H_2O)]$	*cc*1–1:2–1	*Pnma*	15.386(3)/90	10.771(2)/90	13.239(3)/90		3.382/229.947	4.860/1030.319	[68]
161	$[(H_5O_2)(H_3O)_3](C_{10}H_{20}O_5)[(UO_2)_3\ (SeO_4)_5(H_2O)]$	*cc*2–3:5–3	$P2_1/m$	11.6754(5)/90	18.9887(10)/112.282(3)	12.2047(5)/90		4.399/325.500	6.064/1491.859	[66,67]
162	$[(H_5O_2)x(H_3O)_{4-x}](C_{10}H_{20}O_5)$ $[(UO_2)_3(SeO_4)_5(H_2O)](H_2O)_y$	*cc*2–3:5–3	$C2/c$	24.2575(15)/90	11.7501(7)/101.996(1)	18.9243(12)/90		4.362/340.261	6.012/1527.126	[66,67]
	18-crown-6 ether, $C_{12}H_{24}O_6$						5.392/226.477			
163	$[C_{12}H_{24}O_6]_{0.5}[(UO_2)(SO_4)(H_2O)_3]$	*cc*1–1:1–1	$P2_1/n$	9.314(5)/90	9.339(3)/103.62(3)	16.734(3)/90		4.087/277.947	5.248/797.685	[65]
164	$[(H_3O)@(C_{12}H_{24}O_6)]_2(H_3O)_8$ $[(UO_2)_{14}(SO_4)_{19}(H_2O)_4](H_2O)_{20.5}$	framework	$I4/m$	28.023(1)/90	28.023(1)/90	19.6840(7)/90		5.313/1583.312	6.531/4375.972	[69]
165	$[K@(C_{12}H_{24}O_6)][(UO_2)(SeO_4)(NO_3)]\ (H_2O)$	*cc*1–1:2–12	$P2_1/c$	7.2402(2)/90	21.2024(7)/91.581(1)	15.7322(5)/90		3.585/172.078	5.858/1359.052	[70]
166	$[(H_3O)@(C_{12}H_{24}O_6)]K[H_3O]_2\ [(UO_2)_3(SeO_4)_5](H_2O)_4$	*cc*2–3:5–2 nanotubules	*Ccmm*	11.292(1)/90	37.158(1)/90	38.504(1)/90		5.264/1431.790	6.622/4754.269	[69]
	Benzo-15-crown-5 ether, $C_{14}H_{20}O_5$						5.285/206.131			
167	$[C_{14}H_{20}O_5]_{0.5}[(UO_2)(SO_4)(H_2O)_2](H_2O)$	*cc*1–1:1–2	*P*1	6.908(2)/79.46(2)	8.717(4)/75.28(2)	13.578(2)/89.98(3)		3.807/106.606	5.524/508.168	[65]

Table 1. *Cont.*

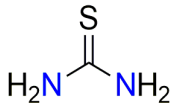
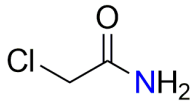
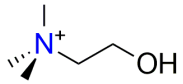
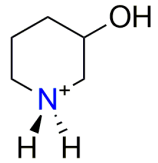
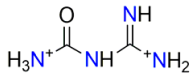
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	Thiourea, CN_2H_4S						3.000/24.000			
168	$[CN_2H_4S]_2[UO_2(SO_4)_2]\cdot 0.3H_2O$	*cc*1–1:2–12	$P2_12_12_1$	6.9283(1)/90	13.3983(3)/90	15.2250(3)/90		3.700/192.423	5.044/665.860	[71]
	Chloroacetamide, $ClCH_2CONH_2$						3.322/33.219			
169	$(C_2H_4NCOCl)[UO_2(SO_4)(H_2O)_2]$	*cc*1–1:1–2	$P1$	6.892(3)/104.40(3)	8.786(6)/109.71(3)	9.494(6)/90.33(3)		3.807/106.606	4.524/208.084	[72]
	Choline, $C_5H_{12}NO^+$						4.248/80.711			
170	$[C_5H_{12}NO][(UO_2)(SeO_4)Cl(H_2O)]$	*cc*2–1:1–1	$P2_1/n$	10.745(4)/90	11.236(4)/114.580(5)	12.477(4)/90		3.585/172.078	5.044/665.860	[73]
	3-hydroxypiperidine, $C_5H_7NO^+$						3.807/53.303			
171	$[(C_5H_7NO)_2(H_2O)][(UO_2)_2(SeO_4)_3\ (H_2O)_2](H_2O)$	*cc*2–2:3–11	$P1$	9.4248(7)/85.456(1)	11.2711(8)/79.571(1)	13.1059(10)/73.439(1)		4.585/220.078	5.781/635.950	[36]
	Carbamoylguanidine, $C_2N_4H_7O_2^{2+}$						3.907/58.603			
172	$[C_2N_4H_7O][(UO_2)(SO_4)(OH)](H_2O)_{0.5}$	$6^{\,1}\,5^{\,2}\,4^{\,2}\,3^{\,2}$	$P2_1/c$	10.5135(7)/90	11.3744(7)/110.880(2)	9.2731(5)/90		3.170/114.117	4.747/503.160	[74]

Table 1. *Cont.*

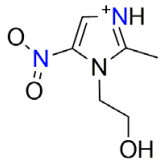
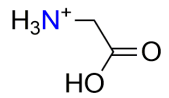
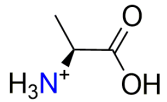
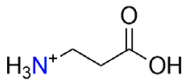
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	1-(hydroxyethyl)-5-nitroimidazole (Metronidazole), $C_6H_{10}N_3O_3^+$						4.459/98.107			
173	$[(C_6H_{10}N_3O_3)(H_5O_2)_2(H_2O)][(H_5O_2)_3(H_2O)][(UO_2)_5(SO_4)_8(H_2O)]$	*cc*2–5:8–2	*P*2/*c*	18.1693(17)/90	10.0732(10)/103.427(2)	30.098(3)/90		5.858/1359.052	6.858/3182.103	[75]
	Glycine, $C_2H_5NO_2^+$						3.322/33.219			
174	$[(glyH_2^+)(H_2O)]_2[(UO_2)(SO_4)_2(H_2O)]$	*cc*2–1:2–2	*C*2/*c*	11.5914(5)/90	7.3412(3)/103.993(2)	23.5958(9)/90		3.125/100.000	4.684/468.386	[76]
175 [2]	$[(glyH^+)(H_2O)]_2[(UO_2)(SeO_4)_2(H_2O)]$	*cc*2–1:2–2	*C*2/*c*	11.5854(5)/90	7.3322(3)/103.623(2)	23.5768(9)/90		3.125/100.000	4.684/468.386	[76]
176	$(glyH^+)_2[(UO_2)(SeO_4)_2(H_2O)$	*cc*2–1:2–2	*P*2/*c*	7.646(2)/90	9.496(3)/104.832(6)	11.477(3)/90		3.125/100.000	4.301/326.842	[76]
177 [3]	$(glyH^+)_2[(UO_2)(SO_4)_2(H_2O)]$	*cc*2–1:2–2	*P*2/*c*	7.690(2)/90	9.505(3)/104.805(6)	11.433(3)/90		3.125/100.000	4.301/326.842	[76]
	α-alanine, $C_3H_8NO_2^+$						3.807/53.303			
178	$(\alpha\text{-}AlaH^+)(H_5O_2)(H_2O)_3[(UO_2)_2(SO_4)_3\ (H_2O)_2]$	*cc*2–2:3–5	$P2_1/c$	11.000(2)/90	15.402(3)/91.320(6)	13.688(3)/90		4.755/513.528	5.644/1128.771	[76]
179 [4]	$(\alpha\text{-}AlaH^+)(H_5O_2)(H_2O)_3[(UO_2)_2(SeO_4)_3\ (H_2O)_2]$	*cc*2–2:3–5	$P2_1/c$	11.150(3)/90	15.510(2)/92.00(2)	13.500(5)/90		4.755/513.528	5.644/1128.771	[76]
	β-alanine, $C_3H_8NO_2^+$						3.807/53.303			
180	$(\beta\text{-}AlaH^+)_2[(UO_2)(SO_4)_2(H_2O)]$	*cc*1–1:2–1	*C*2/*c*	20.660(3)/90	7.3138(11)/91.934(5)	11.8449(17)/90		3.125/100.000	4.739/492.846	[76]
181	$(\beta\text{-}AlaH^+)_2[(UO_2)(SeO_4)_2(H_2O)]$	*cc*1–1:2–1	*C*2/*c*	20.909(2)/90	7.4754(8)/92.589(2)	12.1693(13)/90		3.125/100.000	4.505/396.430	[76]

Table 1. *Cont.*

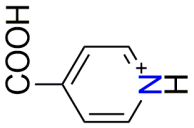
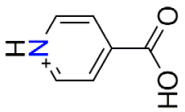
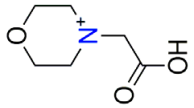
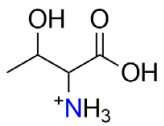
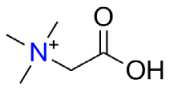
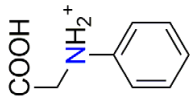
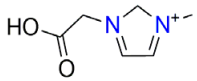
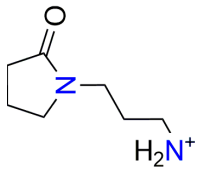
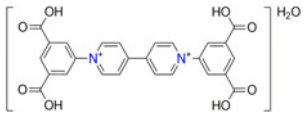
No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	Nicotinic acid, $C_6H_6NO_2^+$						3.907/58.603			
182	$[(nicH^+)(H_5O_2)(H_2O)][(UO_2)(SO_4)_2\ (H_2O)]$	*cc*2–2:3–10	$P2_1/n$	12.4322(9)/90	11.9693(9)/106.574(2)	14.5768(11)/90		4.585/440.156	5.487/976.681	[76]
183	$[(nicH^+)(H_5O_2)(H_2O)][(UO_2)(SeO_4)_2\ (H_2O)]$	*cc*2–2:3–10	$P2_1/n$	12.616(2)/90	12.329(3)/107.221(5)	14.819(3)/90		4.585/440.156	5.550/1032.284	[76]
	Isonicotinic acid, $C_6H_6NO_2^+$						3.907/58.603			
184	$(IsonicH^+)_2[(UO_2)(SO_4)_2(H_2O)]$	*cc*1–1:2–1	$P1$	8.5774(9)/97.034(2)	11.2800(12)/105.214(2)	11.4608(12)/106.737(2)		4.000/128.000	5.524/508.168	[76]
185	$(IsonicH^+)_2[(UO_2)(SeO_4)_2(H_2O)]$	*cc*1–1:2–1	$P1$	8.629(2)/98.22(5)	11.588(3)/105.180(4)	11.588(3)/105.180(4)		5.044/166.465	6.524/600.168	[76]
	Protonated morpholino-N-acetic acid, $C_6H_6O_3^+$						3.907/58.603			
186	$Na(C_6H_6O_3)[(UO_2)_2(SeO_4)_3(H_2O)](H_2O)_2$	*cc*2–2:3–10	$P2_1/c$	10.7767(5)/90	12.2679(5)/92.126(1)	17.9043(8)/90		4.585/440.156	5.728/1214.319	[77]
187	$Na_2(SO_3OH)(C_6H_6O_3)[(UO_2)(SO_4)_2]$	*cc*1–1:2–12	$P1$	6.860(3)/85.186(6)	10.546(4)/88.017(5)	13.047(5)/79.752(5)		3.700/96.211	5.426/466.659	[77]
	Threonine, $C_4H_9NO_3^+$						4.087/69.487			
188	$[(TrhH^+)(H_2O)]_2[(UO_2)_2(SO_4)_3(H_2O)]$	*cc*2–2:3–4	$P2_12_12_1$	10.5155(6)/90	10.516(1)/90	17.3804(12)/90		4.585/440.156	5.492/988.534	[76]
189 [5]	$[(TrhH^+)(H_2O)]_2[(UO_2)_2(SeO_4)_3(H_2O)]$	*cc*2–2:3–4	$P2_12_12_1$	10.5602(6)/90	10.485(5)/90	17.5804(2)/90		4.585/440.156	5.492/988.534	[76]

Table 1. *Cont.*

No.	Chemical Formulae	Topology	Sp. Gr.	*a*, Å/*α*, °	*b*, Å/*β*, °	*c*, Å/*γ*, °	Structural Complexity Parameters, Bits per Atom/Bits per Unit Cell			Ref.
							Organic Molecule	U-Bearing Unit	Entire Structure	
	Trimethylglycine, $C_5H_{12}NO_2^+$						4.322/86.439			
190	$[C_5H_{12}NO_2][UO_2(Cl)(SO_4)(H_2O)]$	*cc*2–1:1–1	$P2_1/n$	9.0486(7)/90	12.5735(9)/111.4560(7)	12.3064(9)/90		3.585/172.078	5.000/640.000	[78]
	Protonated N-phenylglycine, $C_8H_9NO_2^+$						4.322/86.439			
191	$Na(C_6H_5CH(NH_2)CO_2)_7[(UO_2)_6(SO_4)_{10}]\ (H_2O)_{3.5}$	*cc*2–3:5–2 nanotubules	$R3m$	44.001(10)/90	44.001(10)/90	10.367(2)/90		5.329/1119.149	6.062/2218.650	[79]
	1-methyl-3-carboxy methylimidazolium, $C_6H_{10}N_2O_2^+$						4.322/86.439			
192	$(C_7H_{15}N_2O_2)(H_3O)[(UO_2)_2(SO_4)_3(H_2O)]\cdot 1.5H_2O$	*cc*2–2:3–4	$P2_1/n$	10.7858(6)/90	10.7092(6)/98.493(1)	19.776(1)/90		4.585/440.156	5.755/1243.056	[80]
	N-(3-aminopropyl)-2-pyrrolidinone, $C_7H_{14}N_2O^+$						4.585/110.039			
193	$(N_2C_6H_{17}COOH)[(UO_2)_2(SO_4)_3(H_2O)]$	*cc*2–2:3–4	$P2_1/c$	11.4656(3)/90	10.6562(2)/99.604(3)	17.7267(5)/90		4.585/440.156	5.728/1214.319	[45]
	N,N′-bis(3,5-dicarboxylatophenyl)-4,4′-bipyridinium dihydrate, $C_{26}H_{16}N_2O_8^{2+}$						5.700/296.423			
194	$(C_{26}H_{16}N_2O_8)_{0.5}[(UO_2)(SO_4)(H_2O)_2]\cdot H_2O$	*cc*1–1:1–2	$C2/c$	6.8993(14)/90	18.396(4)/93.191(7)	27.847(5)/90		3.807/213.212	5.426/933.318	[81]

[1]—Structural data not available; [2]—assumed to be the structural analog of **174**; [3]—assumed to be the structural analog of **176**; [4]—assumed to be the structural analog of **178**; [5]—assumed to be the structural analog of **188**.

2. Results and Discussion

2.1. Crystal Structure Description

The crystal structure of **1** contains three crystallographically non-equivalent U^{6+} atoms, which are strongly bonded to two O^{2-} atoms, forming linear (within 2.5°) $O^{2-}{\equiv}U^{6+}{\equiv}O^{2-}$ uranyl cations (*Ur*) with $U^{6+}{\equiv}O^{2-}$ bond lengths ranging from 1.738(10) to 1.784(10) Å. The *Ur*1 and *Ur*2 ions are coordinated in the equatorial plane by five O atoms of sulfate tetrahedra, which results in the formation of UrO_5 pentagonal bipyramids (U1,2–O_{eq} = 2.337(9)–2.449(8) Å). The *Ur*3 ion is coordinated by four O atoms of sulfate tetrahedra and an H_2O molecule to form a $Ur3O_4(H_2O)$ pentagonal bipyramid (U3–O_{eq} = 2.337(10)–2.539(9) Å). Four non-equivalent S^{6+} cations are tetrahedrally coordinated by 4 O, each with S^{6+}–O^{2-} bond lengths ranging from 1.437(10) to 1.482(9) Å. All sulfate tetrahedra are four-dentate bridging. Uranyl pentagonal bipyramids and sulfate tetrahedra share common edges to form a microporous framework of a $[(UO_2)_6(SO_4)_7(H_2O)_2]^{2-}$ composition (Figure 1a) with elliptical spiral channels passing along the *c*-axis of c.a. 7.6 × 6.8 Å in diameter, if calculated as the shortest distance between terminal O atoms, which is equal to c.a. 4.9 × 4.1 Å of a free diameter (assuming a O^{2-} radii of 1.35 Å). One crystallographically non-equivalent isopropylammonium cation is arranged within the channel, compensating for the negative charge of the framework and forming strong (N–H···O) and weak (C–H···O) H-bonding systems with uranyl and bridging O atoms. The topology of the uranyl sulfate framework in **1** was similar to that found in isotypic uranyl sulfate compounds templated by protonated 1-butylamine $[C_4H_{10}N]_2[(UO_2)_6(SO_4)_7(H_2O)_2]$ (**28**) [11] and tetramethylammonium $[C_4H_{12}N]_2[(UO_2)_6(SO_4)_7(H_2O)_2]$ (**74**) [35] cations, as well as in a number of inorganic and organically templated uranyl molybdates [82–84].

The crystal structures of **2** and **3** are fully isotypic. There are two non-equivalent U^{6+} atoms, forming *Ur* with $U^{6+}{\equiv}O^{2-}$ bond lengths falling in the range of 1.757(4)–1.766(3) and 1.763(2)–1.781(2) Å (for **2** and **3**, respectively). The *Ur*1 ions are coordinated in the equatorial plane by five O atoms of selenate/sulfate tetrahedra, which results in the formation of UrO_5 pentagonal bipyramids (U1–O_{eq} = 2.352(3)–2.438(3) and 2.340(2)–2.440(2) Å, for **2** and **3**). The *Ur*2 ion is coordinated by four O atoms of selenate/sulfate tetrahedra and an H_2O molecule to form a $Ur2O_4(H_2O)$ pentagonal bipyramid (U2–O_{eq} = 2.343(3)–2.512(4) and 2.341(2)–2.483(2) Å, for **2** and **3**, respectively). There are three non-equivalent tetrahedral sites occupied by Se^{6+} (**2**) and S^{6+} (**3**) ions that are surrounded by 4 O atoms each with T^{6+}–O^{2-} bond lengths falling in the range of 1.603(4)–1.653(3) and 1.441(2)–1.496(2) Å (for **2** and **3**, respectively). All tetrahedral groups are three-dentate bridging. Uranyl pentagonal bipyramids and selenate/sulfate tetrahedra share common edges to form a layered complex of $[(UO_2)_2(TO_4)_3(H_2O)]^{2-}$ (*T* = S, Se) composition (Figure 1b) and are arranged parallel to (001). The negative charge of the layer is compensated by two non-equivalent isopropylammonium cations that are arranged within the interlayer space along with one additional H_2O molecule.

The crystal structure of **4** is very similar to **2** and **3**. It is also based on the layered complexes of a $[(UO_2)_2(SeO_4)_3(H_2O)]^{2-}$ composition with the following bond-length ranges: U≡O_{Ur} = 1.759(4)–1.767(3) Å; U1–O_{eq} = 2.374(3)–2.443(3) Å; U2–O_{eq} = 2.359(3)–2.480(4) Å; and Se^{6+}–O = 1.612(4)–1.658(3) Å. The difference between structures **2** and **4** lies in the interlayer space. If there are two isopropylammonium cations and one H_2O molecule in the structure of **2**, the structure of **4** contains one isopropylammonium cation, one hydronium ion, and an additional selenous acid molecule $[H_2SeO_3]^0$ with Se^{4+}–O = 1.681(4)–1.732(5) Å. It is also of interest that quite unusual interatomic interactions are observed in the structure of **4** between the Se4(IV) atom of the $[H_2SeO_3]^0$ molecule and O2 of the *Ur*2 ion (Se4···O6 = 3.000(4) Å and O20–Se4···O2 = 172.2(2)°), terminal non-shared O17 atom of the $[Se1O_4]^{2-}$ selenate tetrahedra (Se4···O17 = 3.112(4) Å and O19–Se4···O17 = 140.4(2)°), O13 of the *Ur*1 ion (Se4···O13 = 3.359(4) Å and O19–Se4···O13 = 148.1(2) °); however, the closest contact is observed between Se4 and O6 of the *Ur*1 ion (Se4···O6 = 2.730(4) Å and O21–Se4···O6 = 176.8(2)°). All these interatomic distances, especially the latter, are lower

than the sum of the Se and O van der Waals radii (1.9 + 1.55 = 3.45 Å [85]); therefore, they can be attributed to chalcogen bonding [86–89].

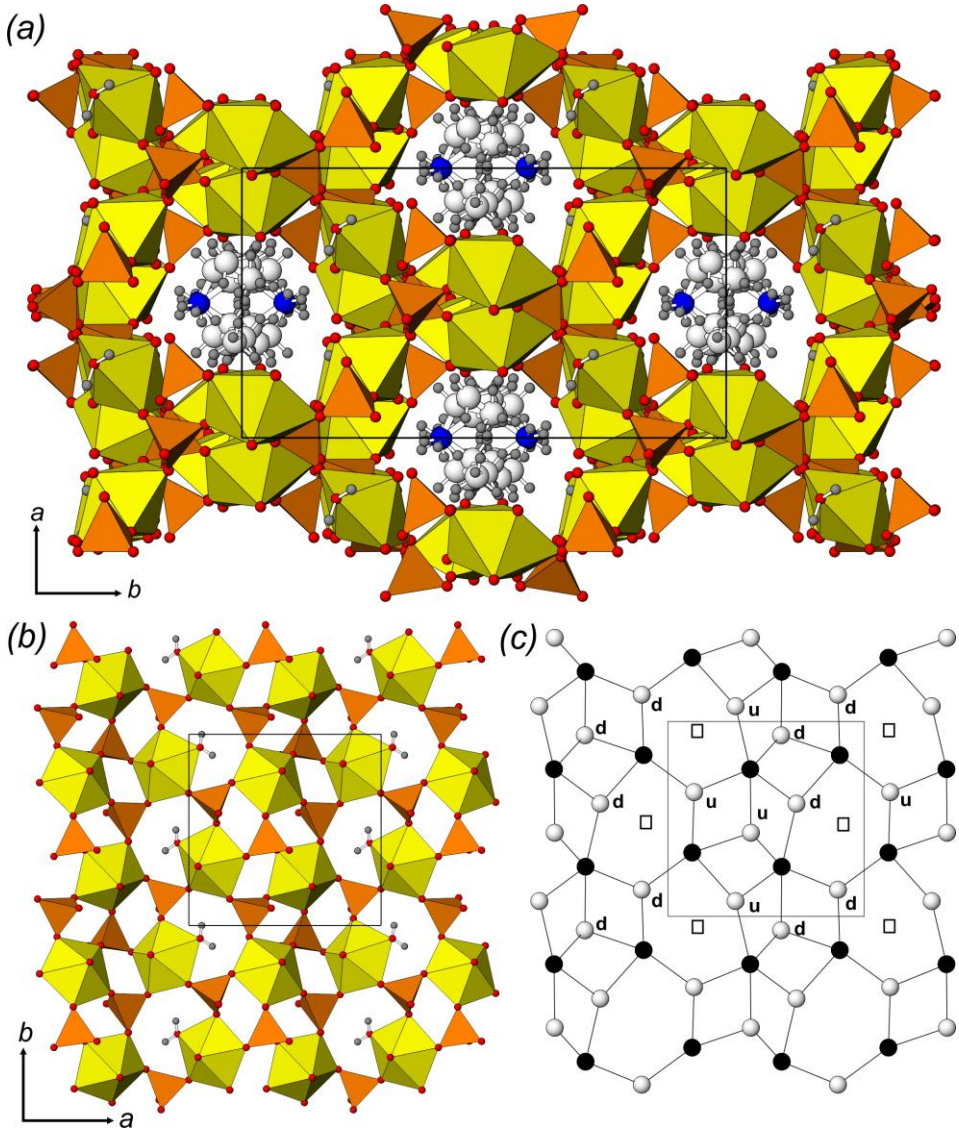


Figure 1. The crystal structure of **1**: (**a**) polyhedral representation of layers in the structures of **2**–**4** (**b**), and topology of its interpolyhedral linkage (**c**). Legend: U polyhedra = yellow, TO_4 (T = S, Se) tetrahedra = orange; O atoms = red, N atoms = blue, C atoms = white, H atoms = gray; black nodes = U atoms, white nodes = T atoms.

2.2. Structural Topology

The layered complexes in the structures of **2**–**4** belong to one of the most common topological types (*cc*2–2:3–4) among uranyl compounds of both pure inorganic or organically templated origin. The topology of the layer can be represented by a black-and-white graph where *Ur* polyhedra are denoted by black vertices, SO_4 or SeO_4 coordination polyhedra are denoted by white vertices, and two vertices are connected by a line if the corresponding polyhedra have a common O atom (Figure 1c). Within the current review, the structures of 24 organically templated uranyl sulfates and selenates are based on the layers of this topology, including compounds **2**–**4**. Being tridentate bridging, sulfate and selenate tetrahedra have their fourth non-shared O atom arranged up or down relative to the plane of the layer. This variability can generate the formation of geometrical isomers with various orientations of tetrahedral groups that can be described by the orientation matrices [90].

Symbols **u** (up), **d** (down), or □ (tetrahedra missing in the graph) are assigned to each tetrahedral site (white vertex) at the graph of the layer (Figure 1c). The aforementioned change in the interlayer space filling results, however, does not entail differences in the geometric isomerism of the layers. Thus, the orientation matrix for the U-bearing layers in the structures of **2**–**4** can be written as (**uud**□)/(□**udd**). Moreover, the degree of layer distortion is also the same. Layer undulation (Figure 2a,b) can be calculated as the shortest interatomic distance between the neighbor wave crests, and the thickness can be calculated as the normal distance between the mean planes that pass through the most protruding parts of the layer (i.e., terminal O atoms of the tetrahedra). The layer undulation and thickness parameters are 7.5 and 5.9 Å, 7.2 and 5.6 Å, 7.4 and 5.9 Å for **2**–**4**, respectively. The substitution of the isopropylammonium cation and H_2O molecule by a selenous acid molecule and H_3O ion results in the orthogonalization of the unit cell of **4**, and in the alignment of neighboring layers.

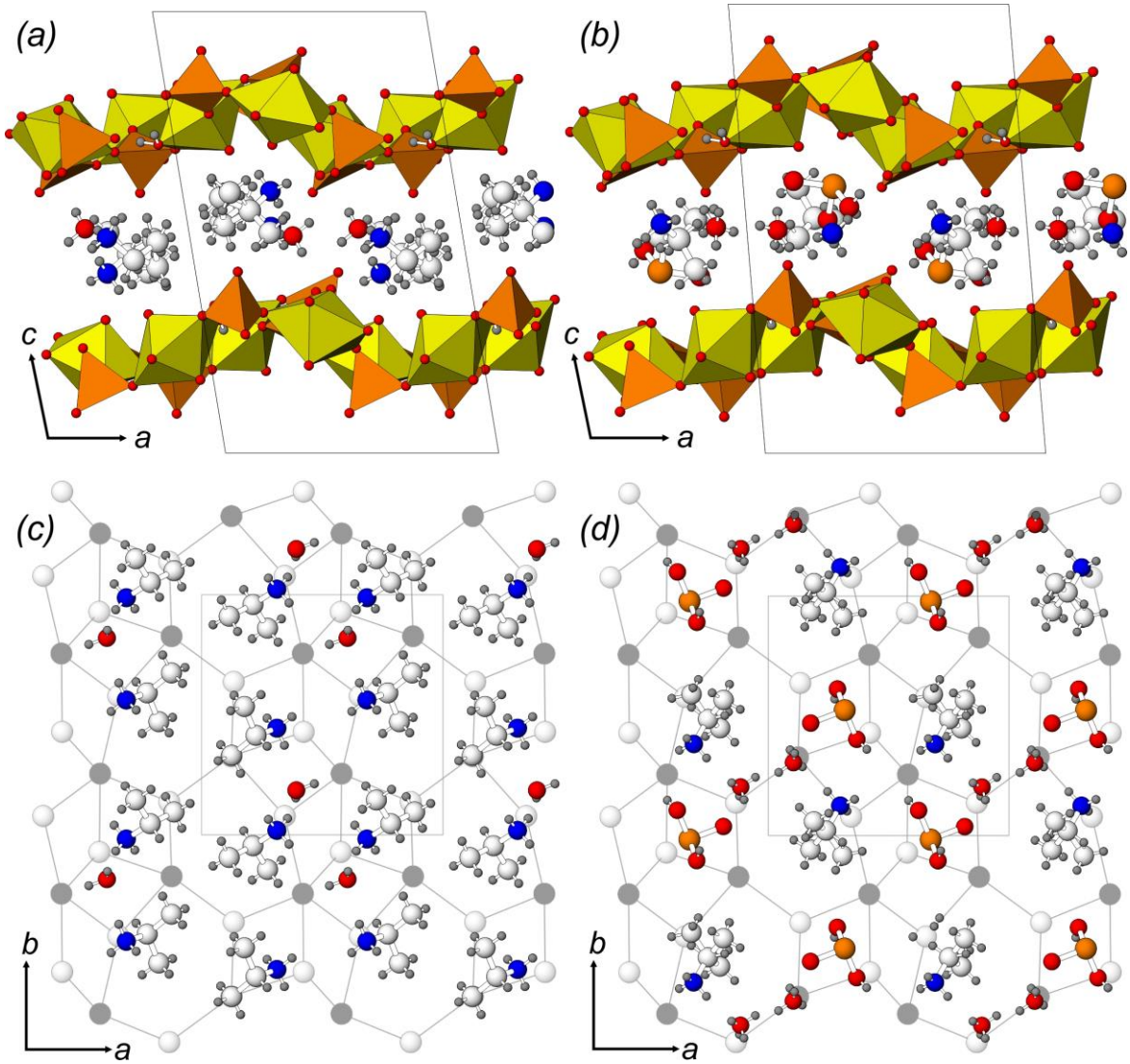


Figure 2. The crystal structures of **2** (**a**) and **4** (**b**): location of the interlayer species in the structures of **2** (**c**) and **4** (**d**) relative to the black-and-white graph of the inorganic layer. Legend: see Figure 1.

It is known that hydrophilic amine groups of organic cations in the structures of organically templated uranyl compounds prefer to associate with dense fragments of U-bearing substructural complexes (four-membered rings of the graph), while hydrocarbon

components of the molecules, which do not play a charge-compensating role, are usually arranged in front of rarefied zones (six-membered rings of the graph). It is of interest that the arrangement of the isopropylammonium cation in the structure of **4** fully corresponds to that in the structures of **2** and **3** (Figure 2c,d). The arrangement of the selenous acid molecule in **4** plays a role of the hydrocarbon part of the second isopropylammonium cation in **2** and **3**, so that the H_3O^+ molecule occupies a position different from H_2O in the structures of **2** and **3**, and functions as an amino group.

3. Discussion

3.1. Isotypic Uranyl Sulfates and Selenates

An aforementioned example demonstrates the rather high resistance of the U-bearing structural type to substitutions in the oxyanion substructural complex. However, this case in the total amount of known structural data is not so frequent. Only 11 pairs of isotypic sulfate–selenate compounds, excluding those reported here, are known. Most of them account for the uranyl compounds templated by various amino acid molecules (**174**–**185**, **188**, **189** [76]). Two pairs correspond to quite rare piperazine (**122** [47], **123** [48]) and 3-Aminotropane (**154**, **155** [64]) molecules. Additionally, only two pairs of compounds represent more common organic molecules that were used in the synthetic experiments: 1-butylamine (**26** [11], **30** [14]) and tetramethylammonium (**71** [33], **72** [34]). There are also several examples of a very close structural architecture, for example, compounds templated by 1,4-diaminobutane (**47** [12,13], **48** [26]) and N.N-dimethylethylenediamine (**89** [43], **91** [36]). Those pairs of compounds have the same topology of the U-bearing layers, and even close unit cell parameters; however, an arrangement of the respective organic and additional H_2O molecules in the interlayer space differs, which leads to the impossibility of classifying them as isotypic compounds.

3.2. Topology of U-Bearing Complexes

An analysis of Table 1 demonstrates the following distribution of U-bearing substructural complexes. There are four compounds, of which the structures contain isolated uranyl sulfate or selenate moieties, which possess three different topologies. The crystal structures of 49 compounds are based on the 1D U-bearing chains of 9 various topological types, among which two topologies *cc*1–1:2–12 (13 compounds with $[UO_2(TO_4)_2]^{2-}$ or $[UO_2(TO_4)(NO_3)]^-$ (T = S, Se) composition) and *cc*1–1:2–1 (17 compounds with $[UO_2(TO_4)_2H_2O]$ (T = S, Se) composition) account for more than half of all the considered chain-based crystal structures (Figure 3a-e). Compound **96** [42] should be especially mentioned, since it is the only compound within those under consideration, of which the crystal structure is based on units of different topological types (*cc*1–1:1–2 and *cc*1–1:2–8). The vast majority of organically templated uranyl sulfates and selenates (135 compounds) have their structures based on layered U-bearing complexes, which is fully consistent with the general trend for U(VI) compounds [48,91–93]. Among them, three topologies that prevail over others can be quite clearly distinguished as well. Those are *cc*2–1:2–2 (16 compounds with $[(UO_2)(TO_4)_2(H_2O)]^{2-}$ (T = S, Se) composition), *cc*2–2:3–10 (17 compounds with $[(UO_2)_2(TO_4)_3(H_2O)]^{2-}$ (T = S, Se) composition), and *cc*2–2:3–4 (22 compounds with $[(UO_2)_2(TO_4)_3(H_2O)]^{2-}$ (T = S, Se) composition) (Figure 3f-k). Moreover, the *cc*2–2:3–10 topology of the layered U-bearing complexes was observed in the structures of the compounds templated by 11 various organic molecules; the *cc*2–1:2–2 topology was described for 11 molecules of various shapes and sizes, and the most common topological type, *cc*2–2:3–4, was observed in the structures with 17 various amine molecules. There were five compounds, including compound **1**, of which the structures were based on microporous frameworks. Additionally, the crystal structures of **31**, **166**, and **191** contained nanotubules, formed by vertex-sharing of *Ur* bipyramids and sulfate or selenate tetrahedra. It is of interest that nanotubules in all three compounds can be unfolded into the planar fragments of the *cc*2–3:5–2 topological type.

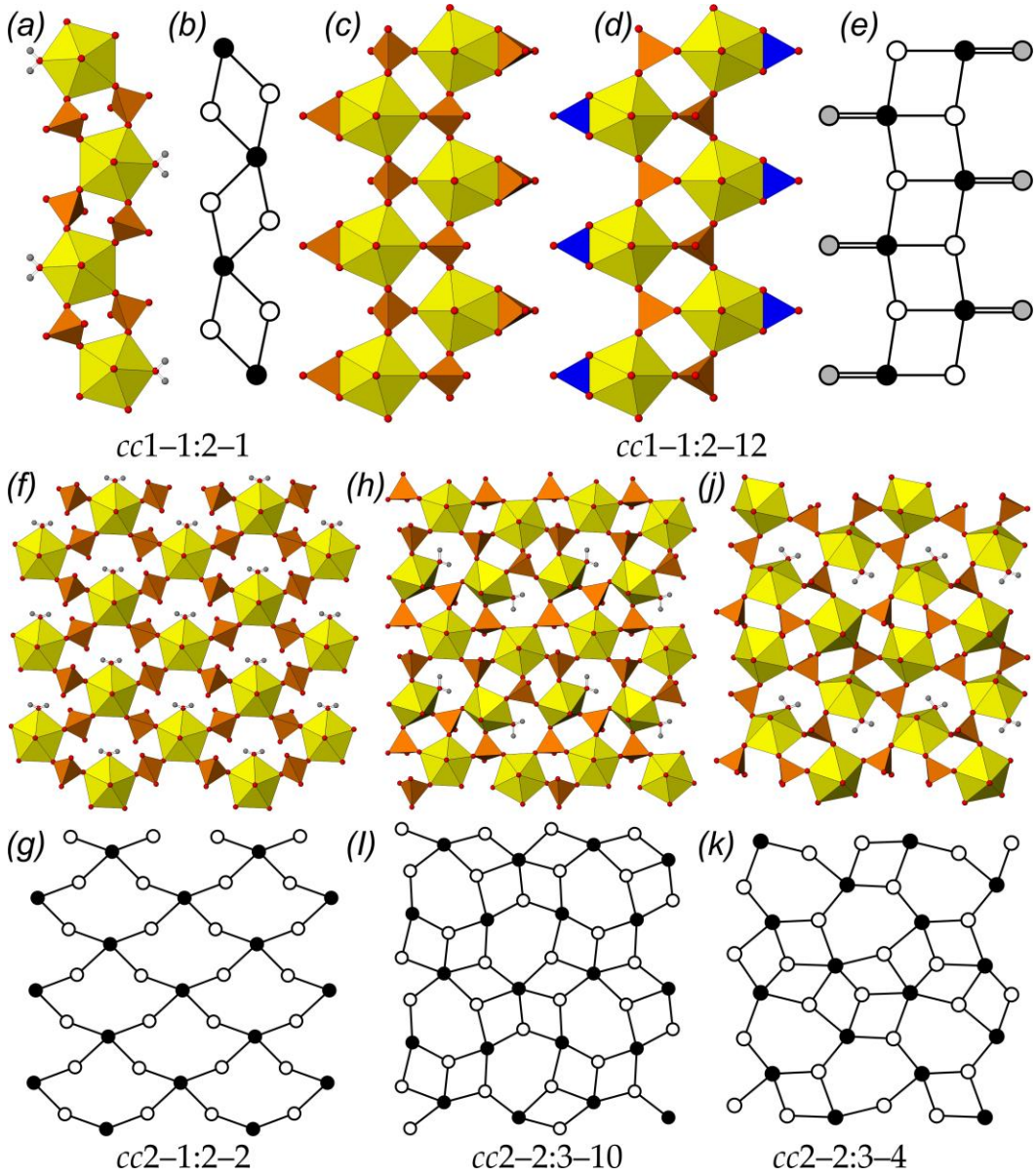


Figure 3. The most common topologies of the U-bearing substructural units among organically templated uranyl sulfate and selenate compounds: chains of *cc*1–1:2–1 (**a**) and *cc*1–1:2–12 (**c**,**d**) types and their black-and-white graphs ((**b**,**e**), respectively); layers of *cc*2–1:2–2 (**f**), *cc*2–2:3–10 (**h**), and *cc*2–2:3–4 (**j**) topologies and their respective graphs (**g**,**i**,**k**). Legend: see Figure 1; blue triangles = NO_3 groups; gray nodes and double line = edge-shared TO_4 tetrahedra or NO_3 group.

3.3. Structural Complexity

The method of calculating and analyzing structural complexity parameters has been quite successfully used in the study of mineral associations [94–97], as well as in the analysis of various groups of inorganic compounds, including uranyl compounds [98–101].

Considering the full set of available structural data, the only obvious correlation was observed between complexities of the U-bearing structural unit and entire structure (Figure 4a).

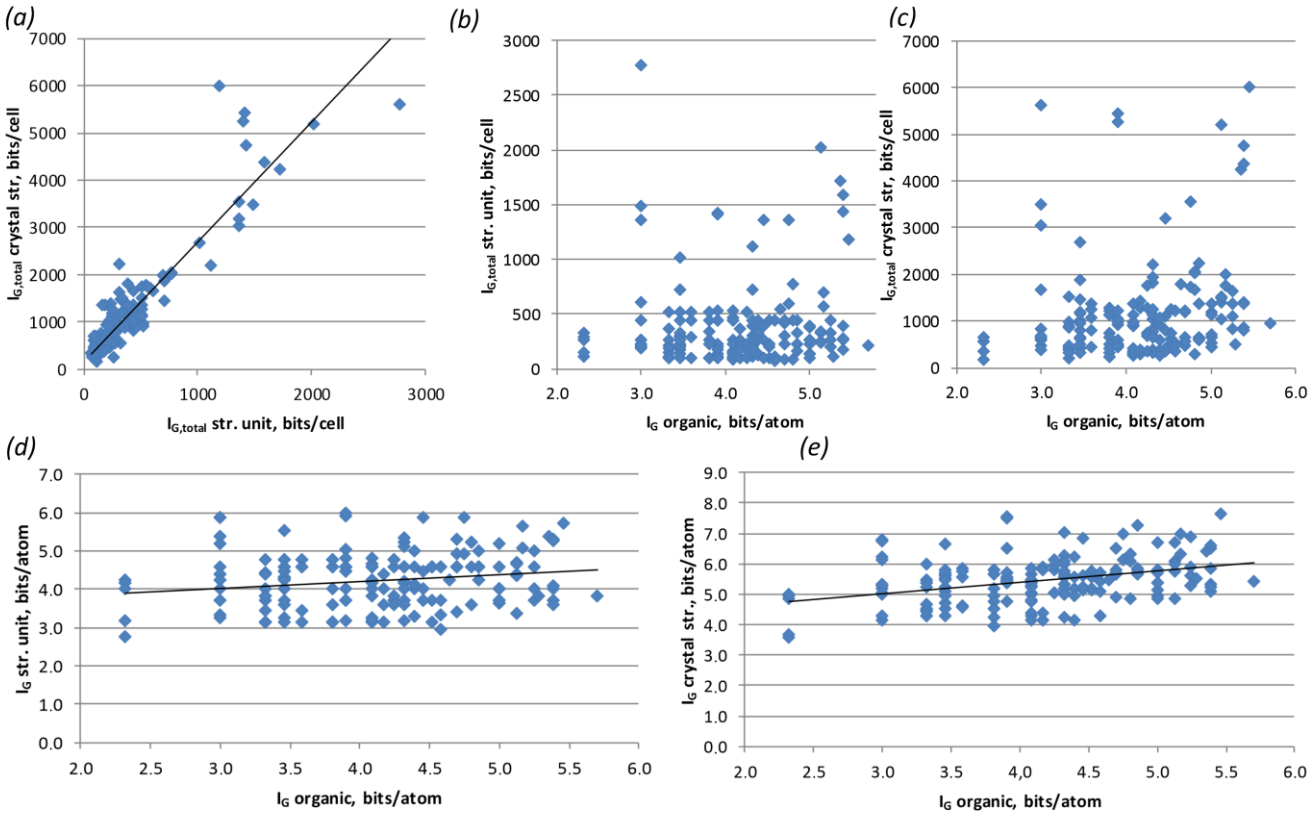


Figure 4. Correlation graphs of structural complexity parameters: complexity of U-bearing structural unit vs. complexity of the entire structure (**a**); complexity of organic molecule vs. complexity of U-bearing structural unit and of the entire structure per unit cell (**b**,**c**) and per atom (**d**,**e**).

On the one hand, this trend is rather obvious: the more complex the structural unit, the more complex the structure is. However, one should keep in mind that the most accurate comparison and analysis of the calculated complexity values are possible for compounds with similar chemical compositions (polymorph modifications). Deviations in the chemical composition or, to be more precise, in a number of atoms in the crystal structure automatically create certain allowances, since the complexity parameters directly depend on the number and multiplicity of atomic sites. For example, a single H_2O molecule introduces three atomic sites into the calculation. Therefore, organic molecules should contribute to the overall complexity due to the large number of atomic sites compared to the inorganic substructural unit. However, there is no such tendency observed in the graphs, if complexity values per unit cell are taken into account (Figure 4b,c). The situation becomes somewhat better when using complexity parameters per atom (Figure 4d,e). However, even here, there were no real trends, minor tendencies. This was mainly due to the fact that organic molecules with similar numbers of atoms had completely different functionalities (size, shape, number of amino groups, etc.), which presented different effects on the U-bearing structural complexes. Therefore, it made sense to consider some groups of molecules separately.

Thus, the most representative groups were the rows of chained amine and diamine molecules. For these groups, firstly, there was a long-term trend towards an increase in the hydrocarbon part of the molecule, and secondly, there were relatively large numbers of representatives to obtain better statistics. Both of these statements are more relevant to the group of diamines; however, in comparison with the other types of molecules, the statistics are, unfortunately, less obvious. As it can be seen from the graph (Figure 5), an increase in the length of the hydrocarbon moiety of the chain amine correlates both with an increase in the complexity of the entire structure (which is expected) and with an increase in the complexity of the uranyl-bearing substructural complex. Of course, the trend line

cannot be called absolute, but rather a trend of the average complexity values for each of the molecules.

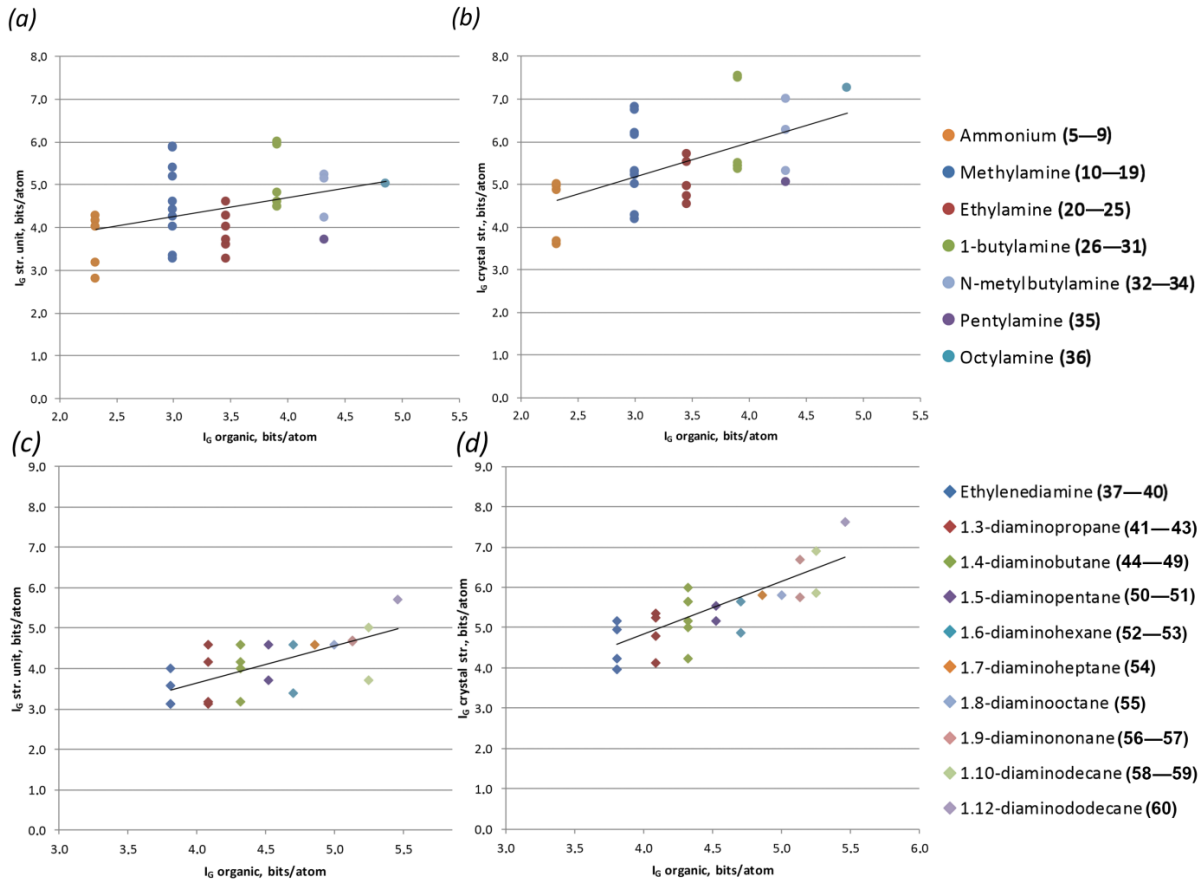


Figure 5. Correlation graphs of chained amine (**a**,**b**) and diamine molecule (**c**,**d**) complexity vs. complexity of U-bearing structural unit (**a**,**c**) and of the entire structure (**b**,**d**), per atom.

A rather good agreement with this tendency can also be observed for compounds with amino acid molecules (Figure 6).

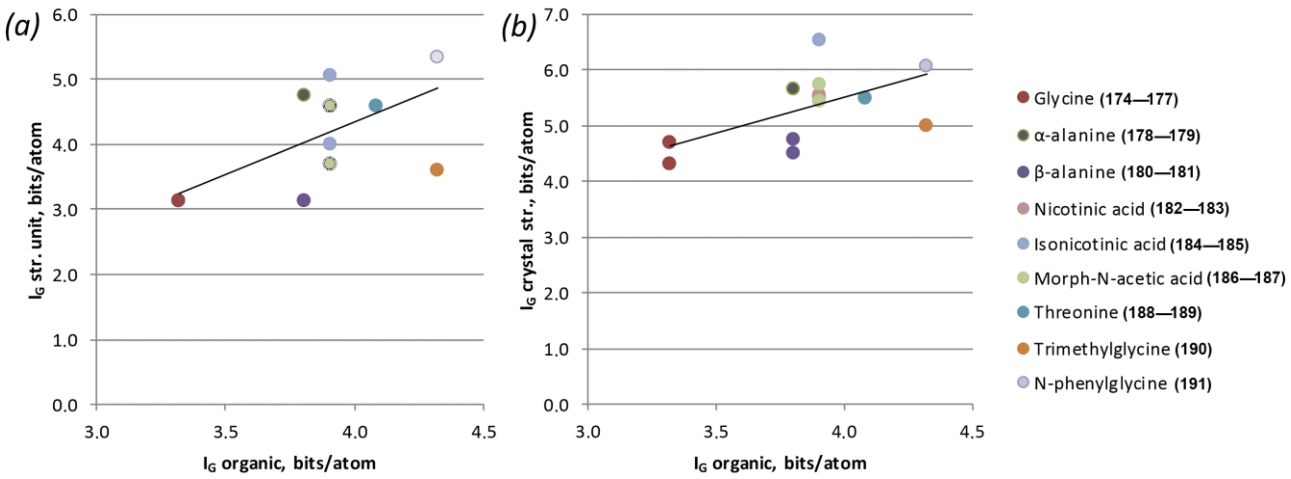


Figure 6. Correlation graphs of amino acid molecule complexity vs. complexity of U-bearing structural unit (**a**) and of the entire structure (**b**), per atom.

Most of the remaining groups of molecules did not have a large number of compounds available; therefore, it was rather difficult to analyze them. However, several interesting trends could be observed as well. Considering the features of cyclic molecules, one can notice that small strained molecules, such as azetidine, pyridine, imidazole, etc., are located at the beginning of the graph (Figure 7a,b). Those points correspond to rather complex U-bearing structural units, as well as structures in general. As the cycle increases and multiple bonds disappear, the complexity of the substructural building units decrease. Additionally, they begin to increase again as branches from the cyclic base appear.

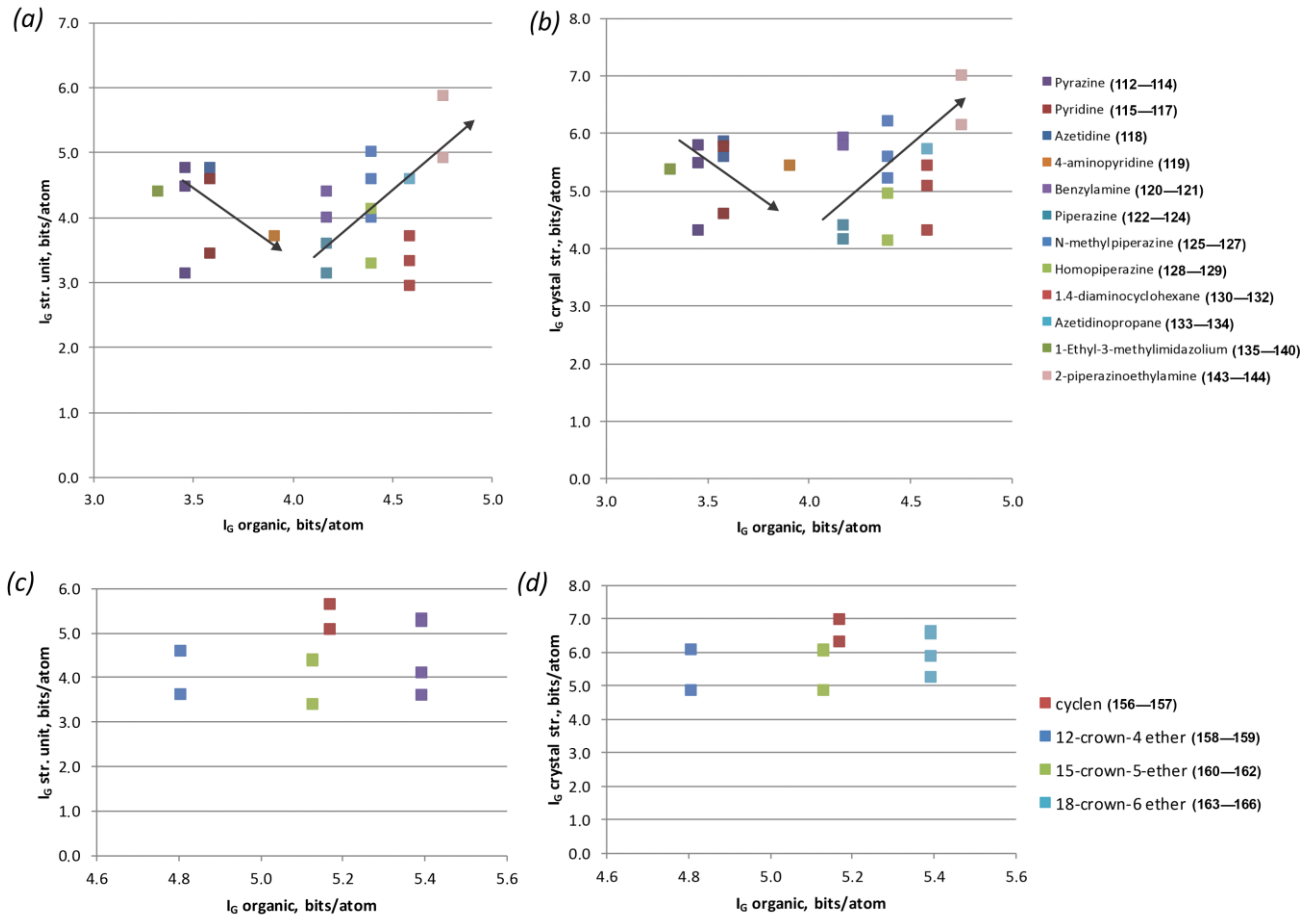


Figure 7. Correlation graphs of cyclic organic molecule complexity vs. complexity of U-bearing structural unit (**a**,**c**) and of the entire structure (**b**,**d**), per atom.

The importance of the number of atoms is well illustrated in the calculation of complexity parameters by the example of crown molecules (Figure 7c,d). Crown ether molecules do not contain amino groups and are electrically neutral within the structures of the corresponding compounds. Thus, the role of their size in the formation of more complex structures is not clearly traced. This is all the more obvious if one compares the molecules of 12-crown-4 ether and cyclene, which are nearly identical in size and shape. The presence of four amino groups in the structure of the latter, instead of four O atoms, firstly affects the complexity of the molecule itself (eight additional atoms), and secondly increases the complexity of substructural units due to the active participation of amino groups in a particular topology templating process.

4. Materials and Methods

4.1. Synthesis

Caution: *While isotopically depleted U was used in these experiments, precautions for handling radioactive materials should be followed*.

Uranyl nitrate hexahydrate ($(UO_2)(NO_3)_2{\cdot}6H_2O$, Vekton, 99%), uranyl acetate ($(UO_2)(CH_3COO)_2{\cdot}2H_2O$, Vekton, 99%), sulfuric acid (H_2SO_4, Aldrich, 98%), selenic acid (H_2SeO_4, 40 wt. % in H_2O, Aldrich, 99.95%), 1-butylamine ($C_4H_{11}N$, Aldrich, ≥99.5%), and isopropylamine (C_3H_9N, Aldrich, ≥99.5%) were used as received.

To reveal the features of the isotypic uranyl compounds' crystallization upon substitution in cationic and anionic substructural complexes, a series of synthetic experiments were conducted. Uranyl sulfate with a microporous structure $[C_4H_{12}N]_2[(UO_2)_6(SO_4)_7(H_2O)_2]$ (**28**) [11], in the channels of which small-chained molecules of 1-butylamine were arranged, was chosen as the starting point. A similar ratio of initial reagents was taken; however, another small amine with a branched aliphatic part, isopropylamine, was chosen as an organic template.

An aqueous solution of 0.1720 g (0.34 mmol) of uranyl nitrate was dissolved in 4 mL of deionized distilled water. Then, 0.500 mL (9.38 mmol) of H_2SO_4 and 0.012 mL (0.14 mmol) of isopropylamine were added to the solution, which was stirred until all solid material dissolved. The resulting yellowish transparent solution was left to evaporate in a watch glass at room temperature. Individual, single, flat, rhombic crystals of **1** (Figure 8a) began crystallizing after 3 days. It should be noted that compound **1** was also obtained using another protocol as follows. An aqueous solution of 0.6400 g (1.51 mmol) of uranyl acetate was dissolved in 1 mL of deionized distilled water. Then, 0.200 mL (3.75 mmol) of H_2SO_4 (98%) and 0.012 mL (0.14 mmol) of isopropylamine were added to the solution, which was stirred until all solid material dissolved. The resulting yellowish transparent solution was placed in a steel autoclave with a Teflon capsule, which was kept in an oven at a temperature of 180 °C for 24 h. After cooling, the solution was poured onto a watch glass, where individual crystals of **1** began crystallizing after 30 min.

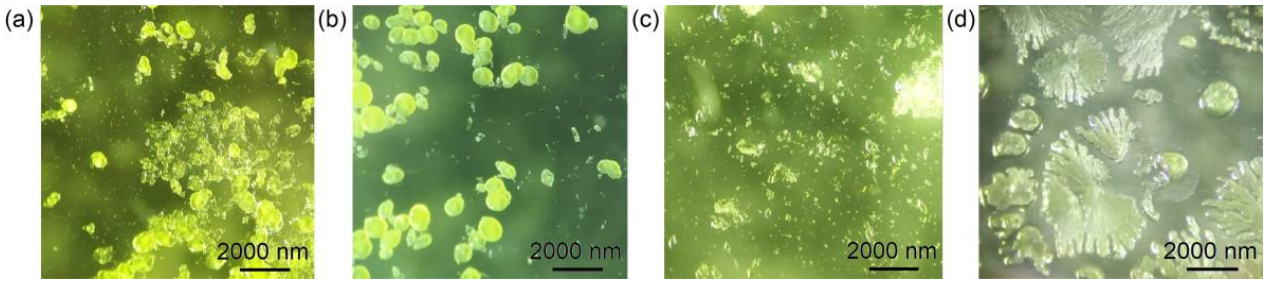


Figure 8. Crystals of **1**–**4** (**a**–**d**, respectively) formed in the described synthetic experiments.

An attempt to crystalize the selenate compound isotypic to **1** was unsuccessful. An analysis of the crystalline precipitate showed that a $[C_3H_{10}N]_2[(UO_2)_2(SeO_4)_3(H_2O)](H_2O)$ (**2**) phase was formed, which was previously reported in [12,13]. To avoid the accidental crystallization of the compound **2**, several experiments were performed in an extended range of initial reagent concentrations with approximately the same molar ratios. The best-quality single crystals of **2** were formed under the following conditions. An aqueous solution of 0.0880 g (0.18 mmol) of uranyl nitrate was dissolved in 2 mL of deionized distilled water. Then, 0.220 mL (1.79 mmol) of H_2SeO_4 (40%) and 0.006 mL (0.07 mmol) of isopropylamine were added to the solution, which was stirred until all solid material dissolved. The resulting yellowish transparent solution was left to evaporate in a watch glass at room temperature. The formation of crystals started in 2 days (Figure 8b). Although the crystal structure of **2** was previously described [12,13], we reported here on the refinement of its structural model with better precision.

To obtain a sulfate compound isotypic to **2**, the following experiment was conducted. An aqueous solution of 0.0880 g (0.18 mmol) of uranyl nitrate was dissolved in 2 mL of deionized distilled water. Then, 0.103 mL (1.92 mmol) of H_2SO_4 (98%) and 0.006 mL (0.07 mmol) of isopropylamine were added to the solution, which was stirred until all solid material dissolved. The resulting yellowish transparent solution was left to evaporate in a watch glass at room temperature. The formation of individual, flat, octagonal crystals of **3** started in 3 days (Figure 8c).

The final attempt to substitute isopropylamine in the synthetic protocol of **2** with 1-butylamine molecules was unsuccessful and resulted in the formation of a $[C_4H_{12}N][H_3O][(UO_2)_2(SeO_4)_3(H_2O)]$ (**29**) compound, where the structure was based on the layered complexes with another topology [12,13].

It is of interest that, for the synthesis of **2**, a newly obtained selenic acid was used, while compound **4** was synthesized using a selenic acid reagent stored for ~2 years (Figure 8d). This resulted in the incorporation of electroneutral H_2SeO_3 molecules in the interlayer space of **4** (see Chapter 2 for details). The Se(VI) reduction to the 4+ oxidation state during the long-term storage of the selenic acid reagent is a rather frequent process, which was repeatedly noted previously [27,30,100].

4.2. Chemical Analysis

The chemical analyses of small pieces of individual single crystals of **1**–**4**, preliminary checked using a single-crystal X-ray diffractometer, were performed using a Hitachi TM 3000 scanning electron microscope equipped with an Oxford EDX spectrometer, with an acquisition time of 30 s per point in an energy dispersive mode (acceleration voltage: 15 kV). The following standards and X-ray lines were used: S—pyrite (FeS_2), K_α; Se—PbSe, K_α; and U—U_3O_8, M_β.

Analytical calculations. Compound **1,** atomic ratio from structural data: U 6.0, S 7.0; found by EDX: U 5.94, S 7.06. Compound **2,** structural data: U 2.0, Se 3.0; found by EDX: U 1.92, Se 3.08. Compound **3,** structural data: U 2.0, S 3.0; found by EDX: U 2.02, S 2.98. Compound **4,** structural data: U 2.0, Se 4.0; found by EDX: U 2.11, S 3.89.

4.3. Single-Crystal X-ray Diffraction

Single crystals of **1**–**4** were selected under an optical microscope in polarized light, immersed in an oil-based cryoprotectant, and fixed on cryoloops. Diffraction data were collected at 100 K using a Rigaku XtaLAB Synergy S X-ray diffractometer operated with a monochromated microfocus MoKα PhotonJet-S (λ = 0.71073 Å) source at 50 kV and 1.0 mA, and equipped with a CCD HyPix 6000HE hybrid photon-counting detector [102]. The frame width was 0.5 or 1.0° in ω, and there was a 1 to 16 s count time for each frame. Diffraction data were integrated and corrected for polarization, background, and Lorentz effects using the *CrysAlisPro* program [103]. An empirical absorption correction was applied based on the spherical harmonics (SCALE3 ABSPACK algorithm). The unit-cell parameters (Table 2) were refined using least-squares techniques. The structures were solved by a dual-space algorithm and refined using *SHELX* programs [104,105] incorporated in the *OLEX2* program package [106]. The final models included coordinates and anisotropic displacement parameters for all non-H atoms. The carbon-, nitrogen- and oxygen-bound H atoms were placed in calculated positions and were included in the refinement in the 'riding' model approximation, with U_{iso}(H) set to 1.5U_{eq}(C) and C–H 0.98 Å for CH_3 groups, U_{iso}(H) set to 1.2U_{eq}(C) and C–H 1.00 Å for tertiary CH groups, U_{iso}(H) set to 1.2U_{eq}(N) and N–H 0.91 Å for NH_3 groups, U_{iso}(H) set to 1.5U_{eq}(O) and O–H 0.84 Å for OH^- groups, and U_{iso}(H) set to 1.5U_{eq}(O) and O–H 0.87 Å for H_2O molecules. Supplementary crystallographic data for **1**–**4** can be downloaded from the Supplementary Materials section and from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures/.

Table 2. Crystallographic data and refinement parameters for **1**–**4**.

Compound	1	2	3	4
Crystallographic Data				
Space Group	$C222_1$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a [Å]	10.2560(2)	11.4644(2)	11.0470(1)	11.2894(4)
b [Å]	18.4062(4)	11.24259(17)	10.8926(1)	11.1012(3)
c [Å]	22.8900(4)	18.7555(4)	18.5397(2)	18.1368(6)
β [°]	90	99.421(2)	100.180(1)	94.717(3)
V [Å^3]	4321.03(15)	2384.77(8)	2195.77(4)	2265.30(12)
Z	4	4	4	4
Data Collection Parameters				
Angle range 2θ [°]	6.94–55.00	7.12–52.00	6.49–55.00	6.65–55.00
Total reflections	21,967	28,650	71,790	18,562
Unique reflections	4968	4656	5027	5195
Reflections with $F^2 > 2\sigma(F^2)$	4715	4326	4773	4616
R_{int}, R_σ [%]	4.19, 3.63	4.14, 2.93	7.86, 2.72	2.77, 2.93
Refinement Parameters				
R_1 ($F^2 > 2\sigma(F^2)$), wR_2 ($F^2 > 2\sigma(F^2)$) [%]	2.88, 6.61	2.29, 4.99	1.86, 4.48	2.44, 4.69
R_1 and wR_2 (all data) [%]	3.12, 6.69	2.61, 5.09	2.02, 4.53	3.11, 4.86
S	1.052	1.068	1.048	1.024
ρ_{max}, ρ_{min} [e$^-$ Å^{-3}]	2.008/−1.932	1.940/−1.026	1.477/−1.733	1.453/−0.883
CCDC	2,285,071	2,285,072	2,285,073	2,285,074

4.4. Structural Complexity Calculations

A structural complexity approach was recently developed by S.V. Krivovichev [107–112]. This method allows estimating the information content of each particular crystal structure, as well as its substructural components. It appears to be quite useful for comparing isotypic or similar structures and quantitatively characterizing the contribution of each substructural component (uranyl sulfate or selenate complexes, interstitial organic template, etc.) to the formation of the whole structural architecture of the compound. The approach is based on the Shannon information content calculations of per atom (I_G) and per unit cell ($I_{G,total}$) using the following equations:

$$I_G = -\sum_{i=1}^{k} p_i \log_2 p_i \ \text{(bits/atom)} \quad (1)$$

$$I_{G,total} = -v\, I_G = -v \sum_{i=1}^{k} p_i \log_2 p_i \ \text{(bits/cell)} \quad (2)$$

where k is the number of different crystallographic orbits (independent sites) in the structure and p_i is the random choice probability for an atom from the i-th crystallographic orbit, that is:

$$p_i = m_i/v \quad (3)$$

where m_i is the multiplicity of the crystallographic orbit (i.e., the number of atoms of a specific Wyckoff site in the reduced unit cell) and v is the total number of atoms in the reduced unit cell.

It should be noted that all calculations for already-studied crystal structures were based on the original cif files, which were obtained from structural databases (CCDC and ICSD) and respective publications. In addition, if H-atom sites were not reported in the original entries, they were assigned manually considering the distribution of the H-bonding system. Complexity parameters for the organic molecules and U-bearing substructural

complexes were calculated manually, while the parameters for the whole structure were determined using *ToposPro* software [113].

5. Conclusions

In this paper, we reviewed the state of the art in the structural chemistry of organically templated uranyl sulfates and selenates, which were considered as the most representative groups of U-bearing synthetic compounds. In total, there were 194 compounds known for both groups, including three novel ones reported here, the crystal structures of which contained 84 various organic molecules. Such statistics illustrates both the great work already performed in the field of syntheses and structural studies, but also the obvious insufficiency of specific system studies, since it turned out that, on average, there were slightly more than two compounds per molecule. Nevertheless, quite clear regularities could be formulated for a number of groups of compounds. Thus, in accordance with the analysis, an increase in the size of the hydrocarbon part and number of charge functional groups of the organic cation led to the formation of rare and more complex topologies.

The presence, albeit in a small number, of isostructural compounds for complex molecules and the absence of such compounds for simpler ones indicated a very fine interaction between the inorganic oxyanion and organic positively charged parts of the structures. Large molecules, apparently, created a kind of a buffer due to their size and the distribution of charge-carrying amino groups, which made it possible to level the difference in the sizes of the sulfate and selenate tetrahedra. However, even in the given examples, the difficulties in obtaining isostructural sulfates and uranyl selenates were very well observed. Thus, compounds **175**, **177**, **179**, and **189** [76] were designated as isostructural, only by the similarity of unit cell parameters, since the quality of the obtained crystals (and all of them were selenates) did not allow one to solve their structures directly. The problem of the presence of a correlation between the uranyl-bearing structural complex topology and the size and shape of the amine molecule has already been raised [12–14,64], and it is obvious, at present, that the structural architecture of the entire compound depends on the combination of the organic and oxyanion parts. For example, the most common layer topologies *cc*2–2:3–10, *cc*2–1:2–2, and *cc*2–2:3–4 (see Ch. 3.2) were described in the structures templated by amine molecules of various sizes and shapes (chained, cyclic, etc.); however, the arrangement preserved a certain position of the amino- or other charge-carrying groups. At the same time, changes in the oxyanion substructure can be sometimes realized with symmetry breaking, whilst maintaining the topology of the complex (e.g., **147**, **148** [36]).

This review demonstrated the ability to form isotypic compounds, which, by analogy with recently performed studies in purely inorganic uranyl systems [98,114,115], indicated the probability of the isomorphic sulfate–selenate series' existence with substitutions in both cationic and oxyanionic moieties. At the same time, the results of the structural studies and topological analysis of all known compounds within the groups under consideration clearly indicate complex crystal chemical limitations in terms of the isomorphic substitution implementation, since the existence of isotypic phases has to date been confirmed only for 24 compounds out of 194, which is slightly above 12%.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/ijms241613020/s1.

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References

1. Serezhkin, V.N.; Soldatkina, M.A. Crystal Structure of the $NH_4[UO_2SO_4F]$. *Coord. Chem.* **1985**, *11*, 103–105.
2. Niinistö, L.; Toivonen, J.; Valkonen, J. Uranyl(VI) Compounds. I. The Crystal Structure of Ammonium Uranyl Sulfate Dihydrate, $(NH_4)_2UO_2(SO_4)_2{\cdot}_2H_2O$. *Acta Chem. Scand.* **1978**, *A32*, 647–651. [CrossRef]
3. Burns, P.C.; Deely, K.M.; Hayden, L.A. The crystal chemistry of the zippeite group. *Can. Mineral.* **2003**, *41*, 687–706. [CrossRef]
4. Mikhailov, Y.N.; Gorbunova, Y.E.; Serezhkina, L.B.; Demchenko, E.A.; Serezhkin, V.N. Crystal Structure of the $[(NH_4)_2][UO_2(SeO_4)_2]\cdot 3H_2O$. *Russ. J. Inorg. Chem.* **1997**, *42*, 1413–1417.
5. Gurzhiy, V.V.; Tyshchenko, D.V.; Krivovichev, S.V.; Tananaev, I.G. Symmetry Reduction in Uranyl Compounds with $[(UO_2)_2(TO_4)_3]^{2-}$ (T = Se, S, Mo) Layers: Crystal Structures of the New Guanidinium Uranyl Selenate and Methylammonium Uranyl Sulfate. *Z. Krist.-Cryst. Mater.* **2014**, *229*, 368–377. [CrossRef]
6. Nazarchuk, E.V.; Charkin, D.O.; Siidra, O.I.; Gurzhiy, V.V. Synthesis and Crystal Structures of New Layered Uranyl Compounds Containing Dimers $[(UO_2)_2O_8]$ of Edge-Linked Pentagonal Bipyramids. *Radiochemistry* **2018**, *60*, 498–506. [CrossRef]
7. Kovrugin, V.M.; Gurzhiy, V.V.; Krivovichev, S.V. Structural Topology and Dimensional Reduction in Uranyl Oxysalts: Eight Novel Phases in the Methylamine–$(UO_2)(NO_3)_2$–H_2SeO_4–H_2O System. *Struct. Chem.* **2012**, *23*, 2003–2017. [CrossRef]
8. Guo, H.X.; Weng, W.; Li, X.Z. Hydrothermal Synthesis, Crystal Structure and Luminescent Properties of an Organically Templated 2-D Uranyl Sulfate. *Chin. J. Struct. Chem.* **2008**, *27*, 1455–1458.
9. Gurzhiy, V.V.; Krivovichev, S.V.; Tananaev, I.G. Dehydration-Driven Evolution of Topological Complexity in Ethylamonium Uranyl Selenates. *J. Solid State Chem.* **2017**, *247*, 105–112. [CrossRef]
10. Ling, J.; Sigmon, G.E.; Burns, P.C. Syntheses, Structures, Characterizations and Charge-Density Matching of Novel Amino-Templated Uranyl Selenates. *J. Solid State Chem.* **2009**, *182*, 402–408. [CrossRef]
11. Bharara, M.S.; Gorden, A.E.V. Amine Templated Two- and Three-Dimensional Uranyl Sulfates. *Dalton Trans.* **2010**, *39*, 3557. [CrossRef] [PubMed]
12. Krivovichev, S.V.; Gurzhii, V.V.; Tananaev, I.G.; Myasoedov, B.F. Topology of Inorganic Complexes as a Function of Amine Molecular Structure in Layered Uranyl Selenates. *Dokl. Phys. Chem.* **2006**, *409*, 228–232. [CrossRef]
13. Krivovichev, S.V.; Gurzhiy, V.V.; Tananaev, I.G.; Myasoedov, B.F. Amine-Templated Uranyl Selenates with Chiral $[(UO_2)_2(SeO_4)_3(H_2O)]^{2-}$ Layers: Topology, Isomerism, Structural Relationships. *Z. Krist.-Cryst. Mater.* **2009**, *224*, 316–324. [CrossRef]
14. Gurzhiy, V.V.; Mikhailenko, P.A.; Krivovichev, S.V.; Tananaev, I.G.; Myasoedov, B.F. Synthesis and Structure of a New Uranyl Selenate Complex with 1-Butylamine $[CH_3(CH_2)_3NH_3](H_5O_2)[(UO_2)_2(SeO_4)_3(H_2O)]$. *Russ. J. Gen. Chem.* **2012**, *82*, 23–26. [CrossRef]
15. Krivovichev, S.V.; Kahlenberg, V.; Tananaev, I.G.; Kaindl, R.; Mersdorf, E.; Myasoedov, B.F. Highly Porous Uranyl Selenate Nanotubules. *J. Am. Chem. Soc.* **2005**, *127*, 1072–1073. [CrossRef] [PubMed]
16. Krivovichev, S.V.; Tananaev, I.G.; Kahlenberg, V.; Myasoedov, B.F. Synthesis and Crystal Structure of a New Uranyl Selenite(IV)-Selenate(VI), $[C_5H_{14}N]_4[(UO_2)_3(SeO_4)_4(HSeO_3)(H_2O)](H_2SeO_3)(HSeO_4)$. *Radiochemistry* **2006**, *48*, 217–222. [CrossRef]
17. Krivovichev, S.V.; Tananaev, I.G.; Myasoedov, B.F. Geometric Isomerism of Layered Complexes of Uranyl Selenates: Synthesis and Structure of $(H_3O)[C_5H_{14}N]_2[(UO_2)_3(SeO_4)_4(HSeO_4)(H_2O)]$ and $(H_3O)[C_5H_{14}N]_2[(UO_2)_3(SeO_4)_4(HSeO_4)(H_2O)](H_2O)$. *Radiochemistry* **2006**, *48*, 552–560. [CrossRef]
18. Krivovichev, S.V.; Tananaev, I.G.; Kalenberg, V.; Myasoedov, B.F. Synthesis and Crystal Structure of the First Uranyl Selenite (IV)-Selenate (VI), $[C_5H_{14}N][(UO_2)(SeO_4)(SeO_2OH)]$. *Dokl. Akad. Nauk.* **2005**, *403*, 124–127. [CrossRef]
19. Krivovichev, S.V.; Tananaev, I.G.; Myasoedov, B.F. Charge-Density Matching in Organic–Inorganic Uranyl Compounds. *C. R. Chim.* **2007**, *10*, 897–904. [CrossRef]
20. Krivovichev, S.V.; Kahlenberg, V.; Tananaev, I.G.; Myasoedov, B.F. Amine-Templated Uranyl Selenates with Layered Structures. I Structural Diversity of Sheets with a U:Se Ratio of 1:2. *Z. Anorg. Allg. Chem.* **2005**, *631*, 2358–2364. [CrossRef]
21. Liu Liu, D.-S.; Kuang, H.-M.; Chen, W.-T.; Luo, Q.-Y.; Sui, Y. Synthesis, Structure, and Photoluminescence Properties of an Organically-Templated Uranyl Selenite. *Z. Anorg. Allg. Chem.* **2015**, *641*, 2009–2013. [CrossRef]
22. Norquist, A.J.; Doran, M.B.; O'Hare, D. The Effects of Linear Diamine Chain Length in Uranium Sulfates. *Solid State Sci.* **2003**, *5*, 1149–1158. [CrossRef]
23. Thomas, P.M.; Norquist, A.J.; Doran, M.B.; O'Hare, D. Organically Templated Uranium(vi) Sulfates: Understanding Phase Stability Using Composition Space. *J. Mater. Chem.* **2003**, *13*, 88–92. [CrossRef]
24. Doran, M.B.; Cockbain, B.E.; O'Hare, D. Structural Variation in Organically Templated Uranium Sulfate Fluorides. *Dalton Trans.* **2005**, *10*, 1774–1780. [CrossRef]
25. Doran, M.B.; Cockbain, B.E.; Norquist, A.J.; O'Hare, D. The effects of hydrofluoric acid addition on the hydrothermal synthesis of templated uranium sulfates. *Dalton Trans.* **2004**, *2004*, 3810–3814. [CrossRef]

26. Jouffret, L.J.; Wylie, E.M.; Burns, P.C. Amine Templating Effect Absent in Uranyl Sulfates Synthesized with 1,4-n-Butyldiamine. *J. Solid State Chem.* **2013**, *197*, 160–165. [CrossRef]
27. Gurzhiy, V.V.; Krivovichev, S.V.; Burns, P.C.; Tananaev, I.G.; Myasoedov, B.F. Supramolecular Templates for the Synthesis of New Nanostructured Uranyl Compounds: Crystal Structure of $[NH_3(CH_2)_9NH_3][(UO_2)(SeO_4)(SeO_2OH)](NO_3)$. *Radiochemistry* **2010**, *52*, 1–6. [CrossRef]
28. Krivovichev, S.V.; Gurzhiy, V.V.; Burns, P.C.; Tananaev, I.G.; Myasoedov, B.F. Partially Ordered Organic-Inorganic Nanocomposites in the System UO_2SeO_4–H_2O–$NH_3(CH_2)_9NH_3$. *Radiochemistry* **2010**, *52*, 7–11. [CrossRef]
29. Krivovichev, S.V.; Kahlenberg, V.; Avdontseva, E.Y.; Mersdorf, E.; Kaindl, R. Self-Assembly of Protonated 1,12-Dodecanediamine Molecules and Strongly Undulated Uranyl Selenate Sheets in the Structure of Amine-Templated Uranyl Selenate: $(H_3O)_2[C_{12}H_{30}N_2]_3[(UO_2)_4(SeO_4)_8](H_2O)_5$. *Eur. J. Inorg. Chem.* **2005**, *2005*, 1653–1656. [CrossRef]
30. Gurzhiy, V.V.; Kovrugin, V.M.; Tyumentseva, O.S.; Mikhaylenko, P.A.; Krivovichev, S.V.; Tananaev, I.G. Topologically and Geometrically Flexible Structural Units in Seven New Organically Templated Uranyl Selenates and Selenite–Selenates. *J. Solid State Chem.* **2015**, *229*, 32–40. [CrossRef]
31. Kovrugin, V.M.; Gurzhiy, V.V.; Krivovichev, S.V.; Tananaev, I.G.; Myasoedov, B.F. Unprecedented layer topology in the crystal structure of a new organically templated uranyl selenite-selenate. *Mendeleev Commun.* **2012**, *22*, 11–12. [CrossRef]
32. Serezhkina, L.N.; Trunov, V.K. Crystal structure of $(N(CH_3)_4)[UO_2SO_4x2H_2O]Cl$. *Zh. Neorg. Khim.* **1989**, *34*, 968–970.
33. Doran, M.B.; Norquist, A.J.; O'Hare, D. *catena*-Poly-[tetra-methyl-ammonium-[[(nitrato-κ2O,O′)-dioxouranium]-μ3-sulfato]]. *Acta Crystallogr.* **2004**, *E59*, m373–m375.
34. Krivovichev, S.V.; Kahlenberg, V. Low-Dimensional Structural Units in Amine-Templated Uranyl Oxoselenates(VI): Synthesis and Crystal Structures of $[C_3H_{12}N_2][(UO_2)(SeO_4)_2(H_2O)_2](H_2O)$, $[C_5H_{16}N_2]_2[(UO_2)(SeO_4)_2(H_2O)](NO_3)_2$, $[C_4H_{12}N][(UO_2)(SeO_4)(NO_3)]$, and $[C_4H_{14}N_2][(UO_2)(SeO_4)_2(H_2O)]$. *Z. Anorg. Allg. Chem.* **2005**, *631*, 2352–2357. [CrossRef]
35. Doran, M.; Norquist, A.J.; O'Hare, D. $[NC_4H_{12}]_2[(UO_2)_6(H_2O)_2(SO_4)_7]$: The First Organically Templated Actinide Sulfate with a Three-Dimensional Framework Structure. *Chem. Commun.* **2002**, *2002*, 2946–2947. [CrossRef] [PubMed]
36. Nazarchuk, E.V.; Charkin, D.O.; Kozlov, D.V.; Siidra, O.I.; Kalmykov, S.N. Topological Analysis of the Layered Uranyl Compounds Bearing Slabs with UO_2:TO_4 Ratio of 2:3. *Radiochem. Acta* **2020**, *108*, 249–260. [CrossRef]
37. Nazarchuk, E.V.; Charkin, D.O.; Siidra, O.I.; Gurzhiy, V.V. Crystal-Chemical Features of U(VI) Compounds with Inorganic Complexes Derived from $[(UO_2)(TO_4)(H_2O)_n]$, T = S, Cr, Se: Synthesis and Crystal Structures of Two New Uranyl Sulfates. *Radiochemistry* **2018**, *60*, 345–351. [CrossRef]
38. Baggio, R.F.; De Benyacar, M.A.R.; Perazzo, B.O.; De Perazzo, P.K. Crystal Structure of Ferroelectric Guanidinium Uranyl Sulphate Trihydrate. *Acta Crystallogr. B* **1977**, *33*, 3495–3499. [CrossRef]
39. Gurzhiy, V.V.; Tyumentseva, O.S.; Belova, E.V.; Krivovichev, S.V. Chemically Induced Symmetry Breaking in the Crystal Structure of Guanidinium Uranyl Sulfate. *Mendeleev Commun.* **2019**, *29*, 408–410. [CrossRef]
40. Medrish, I.V.; Vologzhanina, A.V.; Starikova, Z.A.; Antipin, M.Y. Synthesis and Crystal Structure of the Aminoguanidinium Uranyl Sulfate. *Russ. J. Inorg. Chem.* **2005**, *50*, 412–416.
41. Doran, M.B.; Norquist, A.J.; O'Hare, D. $(C_3H_{12}N_2)_2[UO_2(H_2O)_2(SO_4)_2]_2{\cdot}2H_2O$: An Organically Templated Uranium Sulfate with a Novel Dimer Type. *Acta Crystallogr. E* **2005**, *61*, m881–m884. [CrossRef]
42. Norquist, A.J.; Doran, M.B.; Thomas, P.M.; O'Hare, D. Structural Diversity in Organically Templated Uranium Sulfates. *Dalton Trans.* **2003**, *2003*, 1168–1175. [CrossRef]
43. Doran, M.B.; Norquist, A.J.; O'Hare, D. Exploration of Composition Space in Templated Uranium Sulfates. *Inorg. Chem.* **2003**, *42*, 6989–6995. [CrossRef] [PubMed]
44. Norquist, A.J.; Doran, M.B.; O'Hare, D. $(C_7H_{20}N_2)[(UO_2)_2(SO_4)_3(H_2O)]$: An Organically Templated Uranium Sulfate with a Novel Layer Topology. *Acta Crystallogr. Sect. E Struct. Rep. Online* **2005**, *61*, m807–m810. [CrossRef]
45. Kohlgruber, T.A.; Perry, S.N.; Sigmon, G.E.; Oliver, A.G.; Burns, P.C. Hydrogen Bond Network and Bond Valence Analysis on Uranyl Sulfate Compounds with Organic-Based Interstitial Cations. *J. Solid State Chem.* **2022**, *307*, 122871. [CrossRef]
46. Ling, J.; Sigmon, G.E.; Ward, M.; Roback, N.; Carman Burns, P. Syntheses, Structures, and IR Spectroscopic Characterization of New Uranyl Sulfate/Selenate 1D-Chain, 2D-Sheet and 3D-Framework. *Z. Kristallogr. Cryst. Mater.* **2010**, *225*, 230–239. [CrossRef]
47. Norquist, A.J.; Doran, M.B.; O'Hare, D. The Role of Amine Sulfates in Hydrothermal Uranium Chemistry. *Inorg. Chem.* **2005**, *44*, 3837–3843. [CrossRef]
48. Krivovichev, S.V.; Burns, P.C. Actinide compounds containing hexavalent cations of the VI group elements (S, Se, Mo, Cr, W). In *Structural Chemistry of Inorganic Actinide Compounds*; Krivovichev, S.V., Burns, P.C., Tananaev, I.G., Eds.; Elsevier: Amsterdam, The Netherlands, 2007; pp. 95–182.
49. Doran, M.B.; Norquist, A.J.; Stuart, C.L.; O'Hare, D. $(C_8H_{26}N_4)_{0.5}[(UO_2)_2(SO_4)_3(H_2O)]{\cdot}2H_2O$, an Organically Templated Uranyl Sulfate with a Novel Layer Type. *Acta Crystallogr. Sect. E Struct. Rep. Online* **2004**, *60*, m996–m998. [CrossRef]
50. Williams, J.M.; Pyrch, M.M.; Unruh, D.K.; Lightfoot, H.; Forbes, T.Z. Influence of Heterocyclic N-Donors on the Structural Topologies and Vibrational Spectra of Uranyl Selenate Phases. *J. Solid State Chem.* **2021**, *304*, 122619. [CrossRef]
51. Jouffret, L.J.; Wylie, E.M.; Burns, P.C. Influence of the Organic Species and Oxoanion in the Synthesis of Two Uranyl Sulfate Hydrates, $(H_3O)_2[(UO_2)_2(SO_4)_3(H_2O)]{\cdot}7H_2O$ and $(H_3O)_2[(UO_2)_2(SO_4)_3(H_2O)]{\cdot}4H_2O$, and a Uranyl Selenate-Selenite $[C_5H_6N][(UO_2)(SeO_4)(HSeO_3)]$. *Z. Anorg. Allg. Chem.* **2012**, *638*, 1796–1803. [CrossRef]

52. Wylie, E.M.; Smith, P.A.; Peruski, K.M.; Smith, J.S.; Dustin, M.K.; Burns, P.C. Effects of Ionic Liquid Media on the Cation Selectivity of Uranyl Structural Units in Five New Compounds Produced Using the Ionothermal Technique. *Cryst. Eng. Commun.* **2014**, *16*, 7236–7243. [CrossRef]
53. Gurzhiy, V.V.; Tyumentseva, O.S.; Britvin, S.N.; Krivovichev, S.V.; Tananaev, I.G. Ring Opening of Azetidine Cycle: First Examples of 1-Azetidinepropanamine Molecules as a Template in Hybrid Organic-Inorganic Compounds. *J. Mol. Struct.* **2018**, *1151*, 88–96. [CrossRef]
54. Norquist, A.J.; Thomas, P.M.; Doran, M.B.; O'Hare, D. Synthesis of Cyclical Diamine Templated Uranium Sulfates. *Chem. Mater.* **2002**, *14*, 5179–5184. [CrossRef]
55. Almond, P.M.; Albrecht-Schmitt, T.E. Do Secondary and Tertiary Ammonium Cations Act as Structure-Directing Agents in the Formation of Layered Uranyl Selenites. *Inorg. Chem.* **2003**, *42*, 5693–5698. [CrossRef] [PubMed]
56. Stuart, C.L.; Doran, M.B.; Norquist, A.J.; O'Hare, D. *Catena*-Poly[1-Methylpiperazinium [[Aquadioxouranium(VI)]-Di-μ-Sulfato-κ^4 *O*:*O*′]]. *Acta Crystallogr. Sect. E Struct. Rep. Online* **2003**, *59*, m446–m448. [CrossRef]
57. Doran, M.B.; Norquist, A.J.; O'Hare, D. *Catena*-Poly[Cyclohexane-1,4-Diammonium [[Dioxo(Sulfato-κ^2 *O*,*O*′)Uranium(VI)]-μ-Sulfato] Dihydrate]. *Acta Crystallogr. E* **2003**, *59*, m765–m767. [CrossRef]
58. Wylie, E.M.; Dustin, M.K.; Smith, J.S.; Burns, P.C. Ionothermal Synthesis of Uranyl Compounds That Incorporate Imidazole Derivatives. *J. Solid State Chem.* **2013**, *197*, 266–272. [CrossRef]
59. Kohlgruber, T.A.; Felton, D.E.; Perry, S.N.; Oliver, A.G.; Burns, P.C. Effect of Ionothermal Conditions on the Crystallization of Organically Templated Uranyl Sulfate Compounds. *Cryst. Growth Des.* **2021**, *21*, 861–868. [CrossRef]
60. Norquist, A.J.; Doran, M.B.; Thomas, P.M.; O'Hare, D. Controlled Structural Variations in Templated Uranium Sulfates. *Inorg. Chem.* **2003**, *42*, 5949–5953. [CrossRef]
61. Doran, M.B.; Norquist, A.J.; O'Hare, D. Poly[[1,4-Bis-(3-Aminopropyl)Piperazinium] [[Dioxouranium(VI)]-Di-μ_2,μ_3 -Sulfato]]. *Acta Crystallogr. Sect. E Struct. Rep. Online* **2003**, *59*, m762–m764. [CrossRef]
62. Tyshchenko, D.V. Structural Study of Uranyl Sulfates with Inorganic and Organic Cations. Master's Thesis, St. Petersburg State University, St. Petersburg, Russia, 2014.
63. Kuporev, I.V.; Gurzhiy, V.V.; Krivovichev, S.V. Synthesis and Structural Study of the New Modular Uranyl selenite-Selenate with Melamine $[(UO_2)(SeO_4)(H_2SeO_3)][(SeO_4)(C_3H_8N_6)]$. In *IV Conference and School for Young Scientists: Non-Ambient Diffraction and Nanomaterials*; Book of Abstracts; St. Petersburg State University: St. Petersburg, Russia, 2020; p. 101.
64. Gurzhiy, V.V.; Tyumentseva, O.S.; Krivovichev, S.V.; Tananaev, I.G. Cyclic Polyamines as Templates for Novel Complex Topologies in Uranyl Sulfates and Selenates. *Z. Kristallogr.* **2018**, *233*, 233–245. [CrossRef]
65. Rogers, R.D.; Bond, A.H.; Hipple, W.G.; Rollins, A.N.; Henry, R.F. Synthesis and Structural Elucidation of Novel Uranyl-Crown Ether Compounds Isolated from Nitric, Hydrochloric, Sulfuric, and Acetic Acids. *Inorg. Chem.* **1991**, *30*, 2671–2679. [CrossRef]
66. Gurzhiy, V.V.; Tyumentseva, O.S.; Tyshchenko, D.V.; Krivovichev, S.V.; Tananaev, I.G. Crown-Ether-Templated Uranyl Selenates: Novel Family of Mixed Organic-Inorganic Actinide Compounds. *Mendeleev Commun.* **2016**, *26*, 309–311. [CrossRef]
67. Krivovichev, S.V.; Gurzhiy, V.V.; Tananaev, I.G.; Myasoedov, B.F. Uranyl Selenates with Organic Templates: Principles of Structure and Characteristics of Self-Organization. *Russ. J. Gen. Chem.* **2009**, *79*, 2723–2730. [CrossRef]
68. Gurzhiy, V.V.; Tyumentseva, O.S.; Krivovichev, S.V.; Tananaev, I.G. Hybrid One-Dimensional 15-Crown-5-Ether-Uranyl-Selenate Polymers in $[K@(C_{10}H_{20}O_5)][(UO_2)(SeO_4)(HSeO_4)(H_2O)]$: Synthesis and Characterization. *Z. Anorg. Allg. Chem.* **2015**, *641*, 1110–1113. [CrossRef]
69. Alekseev, E.V.; Krivovichev, S.V.; Depmeier, W. A Crown Ether as Template for Microporous and Nanostructured Uranium Compounds. *Angew. Chem. Int. Ed.* **2008**, *47*, 549–551. [CrossRef]
70. Gurzhiy, V.V.; Tyumentseva, O.S.; Krivovichev, S.V.; Tananaev, I.G. Novel Type of Molecular Connectivity in One-Dimensional Uranyl Compounds: $[K@(18\text{-Crown-6})(H_2O)][(UO_2)(SeO_4)(NO_3)]$, a New Potassium Uranyl Selenate with 18-Crown-6 Ether. *Inorg. Chem. Commun.* **2014**, *45*, 93–96. [CrossRef]
71. Charkin, D.O.; Bezzubov, S.I.; Siidra, O.I.; Borisov, A.S.; Kalmykov, S.N. Preparation and Crystal Structure of a New Uranyl Sulfate Templated by a Bis-Isothiouronium Cation. *Z. Anorg. Allg. Chem.* **2020**, *646*, 540–543. [CrossRef]
72. Mikhajlov, Y.N.; Mistryukov, V.E.; Gorbunova, Y.E.; Serezhkina, L.B.; Demchenko, E.A.; Serezhkin, V.N. Crystal Structure of $[UO_2SO_4x2H_2O]XCH_2ClCONH_2$. *Zhurnal Neorg. Khimii* **1995**, *40*, 1288–1290.
73. Tyumentseva, O.S.; Gurzhiy, V.V.; Krivovichev, S.V.; Tananaev, I.G.; Myasoedov, B.F. First Organic–Inorganic Uranyl Chloroselenate: Synthesis, Crystal Structure and Spectroscopic Characteristics. *J. Chem. Crystallogr.* **2013**, *43*, 517–522. [CrossRef]
74. Grechishnikova, E.V.; Serezhkina, L.B.; Virovets, A.V.; Peresypkina, E.V. Synthesis and Crystal Structure of $(C_2N_4H_7O)[UO_2(SO_4)(OH)] \cdot 0.5H_2O$. *Russ. J. Inorg. Chem.* **2005**, *50*, 1800–1805.
75. Nazarchuk, E.V.; Siidra, O.I.; Charkin, D.O. Specific Features of the Crystal Chemistry of Layered Uranyl Compounds with the Ratio UO_2:TO_4 = 5:8 (T = S^{6+}, Cr^{6+}, Se^{6+}, Mo^{6+}). *Radiochemistry* **2018**, *60*, 352–361. [CrossRef]
76. Nazarchuk, E.V.; Ikhalaynen, Y.A.; Charkin, D.O.; Siidra, O.I.; Petrov, V.G.; Kalmykov, S.N.; Borisov, A.S. Effect of Solution Acidity on the Structure of Amino Acid-Bearing Uranyl Compounds. *Radiochem. Acta* **2019**, *107*, 311–325. [CrossRef]
77. Siidra, O.I.; Nazarchuk, E.V.; Charkin, D.O.; Chukanov, N.V.; Zakharov, A.Y.; Kalmykov, S.N.; Ikhalaynen, Y.A.; Sharikov, M.I. Open-Framework Sodium Uranyl Selenate and Sodium Uranyl Sulfate with Protonated Morpholino-N-Acetic Acid. *Z. Kristallogr. Cryst. Mater.* **2019**, *234*, 109–118. [CrossRef]

78. Smith, P.A.; Burns, P.C. Ligand Mediated Morphology of the Two-Dimensional Uranyl Aqua Sulfates $[UO_2(X)(SO_4)(H_2O)]$ [X = Cl^- or $(CH_3)_3NCH_2COO$]. *Z. Anorg. Allg. Chem.* **2019**, *645*, 504–508. [CrossRef]
79. Siidra, O.; Nazarchuk, E.; Charkin, D.; Chukanov, N.; Depmeier, W.; Bocharov, S.; Sharikov, M. Uranyl Sulfate Nanotubules Templated by N-Phenylglycine. *Nanomaterials* **2018**, *8*, 216. [CrossRef]
80. Smith, P.A.; Aksenov, S.M.; Jablonski, S.; Burns, P.C. Structural Unit Charge Density and Molecular Cation Templating Effects on Orientational Geometric Isomerism and Interlayer Spacing in 2-D Uranyl Sulfates. *J. Solid State Chem.* **2018**, *266*, 286–296. [CrossRef]
81. Hu, K.; Zeng, L.; Kong, X.; Huang, Z.; Yu, J.; Mei, L.; Chai, Z.; Shi, W. Viologen-Based Uranyl Coordination Polymers: Anion-Induced Structural Diversity and the Potential as a Fluorescent Probe. *Eur. J. Inorg. Chem.* **2021**, *2021*, 5077–5084. [CrossRef]
82. Tabachenko, V.V.; Kovba, L.M.; Serezhkin, V.N. Crystal structures of magnesium and strontium molybdateouranilates of $Mg(UO_2)_6(MoO_4)_7{\cdot}18H_2O$ and $Sr(UO_2)_6(MoO_4)_7{\cdot}15H_2O$ composition. *Koord. Khim.* **1984**, *10*, 558–562.
83. Krivovichev, S.V.; Armbruster, T.; Chernyshov, D.Y.; Burns, P.C.; Nazarchuk, E.V.; Depmeier, W. Chiral open-framework uranyl molybdates. 2. Flexibility of the U:Mo = 6:7 frameworks: Syntheses and crystal structures of $(UO_2)_{0.82}[C_8H_{20}N]_{0.36}[(UO_2)_6(MoO_4)_7(H_2O)_2](H_2O)n$ and $[C_6H_{14}N_2][(UO_2)_6(MoO_4)_7(H_2O)_2](H_2O)m$. *Microporous Mesoporous Mater.* **2005**, *78*, 217–224. [CrossRef]
84. Krivovichev, S.V.; Armbruster, T.; Chernyshov, D.Y.; Burns, P.C.; Nazarchuk, E.V.; Depmeier, W. Chiral open-framework uranyl molybdates. 3. Synthesis, structure and the $C222_1$–$P2_12_12_1$ low-temperature phase transition of $[C_6H_{16}N]_2[(UO_2)_6(MoO_4)_7(H_2O)_2](H_2O)_2$. *Microporous Mesoporous Mater.* **2005**, *78*, 225–234. [CrossRef]
85. Batsanov, S.S. Van der Waals Radii of Elements. *Inorg. Mater.* **2001**, *37*, 871–885. [CrossRef]
86. Bleiholder, C.; Gleiter, R.; Werz, D.B.; Köppel, H. Theoretical Investigations on Heteronuclear Chalcogen−Chalcogen Interactions: On the Nature of Weak Bonds between Chalcogen Centers. *Inorg. Chem.* **2007**, *46*, 2249–2260. [CrossRef] [PubMed]
87. Pascoe, D.; Ling, K.; Cockroft, S. The Origin of Chalcogen-Bonding Interactions. *J. Amer. Chem. Soc.* **2017**, *139*, 15160–15167. [CrossRef]
88. Lenardão, E.J.; Santi, C.; Sancineto, L. Nonbonded Interaction: The Chalcogen Bond. In *New Frontiers in Organoselenium Compounds*; Springer: Cham, Switzerland, 2018; pp. 157–183.
89. Aakeroy, C.B.; Bryce, D.L.; Desiraju, G.R.; Frontera, A.; Legon, A.C.; Nicotra, F.; Rissanen, K.; Scheiner, S.; Terraneo, G.; Metrangolo, P.; et al. Definition of the chalcogen bond (IUPAC Recommendation). *Pure Appl. Chem.* **2019**, *91*, 1889–1892. [CrossRef]
90. Krivovichev, S.V.; Burns, P.C. Geometrical isomerism in uranyl chromates II. Crystal structures of $Mg_2[(UO_2)_3(CrO_4)_5](H_2O)_{17}$ and $Ca_2[(UO_2)_3(CrO_4)_5](H_2O)_{19}$. *Z. Kristallogr.* **2003**, *218*, 683–690. [CrossRef]
91. Burns, P.C. The Crystal Chemistry of Uranium. In *Uranium: Mineralogy, Geochemistry, and the Environment*; Reviews in Mineralogy; Burns, P.C., Finch, R., Eds.; Walter de Gruyter GmbH & Co KG.: Berlin, Germany, 1999; Volume 38, pp. 23–90.
92. Krivovichev, S.V. *Structural Crystallography of Inorganic Oxysalts*; Oxford University Press: Oxford, UK, 2008; 303p.
93. Lussier, A.J.; Lopez, R.A.K.; Burns, P.C. A revised and expanded structure hierarchy of natural and synthetic hexavalent uranium compounds. *Can. Mineral.* **2016**, *54*, 177–283. [CrossRef]
94. Krivovichev, S.V.; Hawthorne, F.C.; Williams, P.A. Structural complexity and crystallization: The Ostwald sequence of phases in the $Cu_2(OH)_3Cl$ system (botallackite–atacamite–clinoatacamite). *Struct. Chem.* **2017**, *28*, 153–159. [CrossRef]
95. Plášil, J. Structural complexity of uranophane and uranophane-β: Implications for their formation and occurrence. *Eur. J. Mineral.* **2018**, *30*, 253–257. [CrossRef]
96. Izatulina, A.R.; Gurzhiy, V.V.; Krzhizhanovskaya, M.G.; Kuz'mina, M.A.; Leoni, M.; Frank-Kamenetskaya, O.V. Hydrated Calcium Oxalates: Crystal Structures, Thermal Stability and Phase Evolution. *Cryst. Growth Des.* **2018**, *18*, 5465–5478. [CrossRef]
97. Krivovichev, V.G.; Krivovichev, S.V.; Charykova, M.V. Selenium Minerals: Structural and Chemical Diversity and Complexity. *Minerals* **2019**, *9*, 455. [CrossRef]
98. Kornyakov, I.V.; Tyumentseva, O.S.; Krivovichev, S.V.; Gurzhiy, V.V. Dimensional evolution in hydrated K+-bearing uranyl sulfates: From 2D-sheets to 3D frameworks. *CrystEngComm* **2020**, *22*, 4621–4629. [CrossRef]
99. Gurzhiy, V.V.; Plášil, J. Structural complexity of natural uranyl sulfates. *Acta Crystallogr.* **2019**, *B75*, 39–48. [CrossRef]
100. Gurzhiy, V.V.; Kuporev, I.V.; Kovrugin, V.M.; Murashko, M.N.; Kasatkin, A.V.; Plášil, J. Crystal chemistry and structural complexity of natural and synthetic uranyl selenites. *Crystals* **2019**, *9*, 639. [CrossRef]
101. Gurzhiy, V.V.; Kalashnikova, S.A.; Kuporev, I.V.; Plášil, J. Crystal chemistry and structural complexity of the uranyl carbonate minerals and synthetic compounds. *Crystals* **2021**, *11*, 704. [CrossRef]
102. Fraser, W. Diffractometers for modern X-ray crystallography: The XtaLAB Synergy X-ray diffractometer platform. *Rigaku J.* **2020**, *36*, 37–47.
103. *CrysAlisPro Software System*, Version 1.171.41.94a; Rigaku Oxford Diffraction: Oxford, UK, 2021.
104. Sheldrick, G.M. SHELXT—Integrated space-group and crystal structure determination. *Acta Crystallogr.* **2015**, *A71*, 3–8. [CrossRef]
105. Sheldrick, G.M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* **2015**, *C71*, 3–8.
106. Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschmann, H. OLEX2: A complete structure solution, refinement and analysis program. *J. Appl. Cryst.* **2009**, *42*, 339–341. [CrossRef]
107. Krivovichev, S.V. Topological complexity of crystal structures: Quantitative approach. *Acta Crystallogr.* **2012**, *A68*, 393–398. [CrossRef]
108. Krivovichev, S.V. Structural complexity of minerals: Information storage and processing in the mineral world. *Mineral. Mag.* **2013**, *77*, 275–326. [CrossRef]

109. Krivovichev, S.V. Which inorganic structures are the most complex? *Angew. Chem. Int. Ed.* **2014**, *53*, 654–661. [CrossRef] [PubMed]
110. Krivovichev, S.V. Structural complexity of minerals and mineral parageneses: Information and its evolution in the mineral world. In *Highlights in Mineralogical Crystallography*; Danisi, R., Armbruster, T., Eds.; Walter de Gruyter GmbH: Berlin, Germany; Boston, MA, USA, 2015; pp. 31–73.
111. Krivovichev, S.V. Structural complexity and configurational entropy of crystalline solids. *Acta Crystallogr.* **2016**, *B72*, 274–276.
112. Krivovichev, S.V. Ladders of information: What contributes to the structural complexity in inorganic crystals. *Z. Kristallogr.* **2018**, *233*, 155–161. [CrossRef]
113. Blatov, V.A.; Shevchenko, A.P.; Proserpio, D.M. Applied topological analysis of crystal structures with the program package ToposPro. *Cryst. Growth. Des.* **2014**, *14*, 3576–3586. [CrossRef]
114. Gurzhiy, V.V.; Tyumentseva, O.S.; Krivovichev, S.V.; Krivovichev, V.G.; Tananaev, I.G. Mixed uranyl sulfate-selenates: Variable composition and crystal structures. *Cryst. Growth Des.* **2016**, *16*, 4482–4492. [CrossRef]
115. Kornyakov, I.V.; Tyumentseva, O.S.; Krivovichev, S.V.; Tananaev, I.G.; Gurzhiy, V.V. Crystal chemistry of the $M^{2+}[(UO_2)(T^{6+}O_4)_2(H_2O)](H_2O)_4$ (M^{2+} = Mg, Mn, Fe, Co, Ni and Zn; T^{6+} = S, Se) compounds: The interplay between chemical composition, pH and structural architecture. *CrystEngComm* **2021**, *23*, 1140–1148. [CrossRef]