Two New Layered Uranyl Fluoride Complexes with U^{VI}=O-Alkali (Na, Cs) Interactions: Experimental and Theoretical Studies

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Supplementary Information

Table S1 Selected bond length in compound 1

Bond	Length(Å)	Bond	Length (Å)	Bond	Length(Å)	Bond	Length (Å)
U1-O1	1.774(4)	U1-O2	1.778(5)	U1-O4	2.234(3)	U1-O3	2.237(3)
U1-F2	2.3114(3)	U1-F1	2.387(3)	U1-F1	2.415(3)	U1-Na1	3.6472(11)
U1-Na2	3.731(2)	U1-U1	4.0476(7)	U1-Na2	4.069(3)	Na1-O3	2.272(4)
Na1-O3	2.272(4)	Na1-O4	2.353(4)	Na1-O4	2.353(4)	Na1-O2	2.464(5)
Na1-O2	2.464(5)	Na1-U1	3.6472(11)	Na2-O4	2.205(4)	Na2-O3	2.282(4)
Na2-F1	2.352(4)	Na2-O5	2.375(5)	Na2-O1	2.398(5)	Na2-O5	2.543(6)
Na2-U1	3.731(2)	Na2-Na2	3.733(5)	Na2-U1	4.069(3)	O5-Na2	2.375(5)
F-Na2	2.352(4)	F-U1	2.415(3)	F2-U1	2.3114(3)	O1-Na2	2.398(5)
		O2-Na1	2.464(5)	O3-Na2	2.282(4)		

Table S2 Selected bond angles in compound 1.

Bond Angles	Value(deg)	Bond Angles	Value(deg)	Bond Angles	Value(deg)
O1-U1-O2	177.7(2)	O1-U1-O4	90.86(17)	O2-U1-O4	91.47(18)
O1-U1-O3	89.12(18)	O2-U1-O3	91.67(18)	O4-U1-O3	74.38(12)
O1-U1-F2	90.03(15)	O2-U1-F2	90.31(15)	O4-U1-F2	77.43(9)
O3-U1-F2	151.79(8)	O1-U1-F1	86.18(17)	O2-U1-F1	91.70(18)
O4-U1-F1	150.73(12)	O3-U1-F1	134.56(12)	O1-U1-F1	90.50(16)
O2-U1-F1	87.71(16)	O4-U1-F1	144.12(11)	O3-U1-F1	69.79(11)
F2-U1-F1	138.43(7)	F1-U1-F1	65.10(13)	O3-Na2-O1	113.81(17)
O3-Na1-O3	92.5(2)	O3-Na1-O4	71.48(12)	O3-Na1-O4	163.89(17)
O4-Na1-O4	124.6(2)	O3-Na1-O2	89.75(15)	O3-Na1-O2	85.19(15)
O4-Na1-O2	92.97(15)	O4-Na1-O2	90.43(15)	O3-Na1-O2	85.19(15)

O3-Na1-O2	89.75(15)	O4-Na1-O2	90.43(15)	O4-Na1-O2	92.97(15)
O2-Na1-O2	172.7(3)	O4-Na2-O3	146.66(19)	O4-Na2-F1	98.79(15)
O3-Na2-F1	70.20(13)	O4-Na2-O5	108.15(17)	O3-Na2-O5	89.58(16)
F1-Na2-O5	152.40(17)	O4-Na2-O1	96.38(17)	F1-Na2-O1	87.29(16)
O5-Na2-O1	83.93(18)	O4-Na2-O5	84.74(16)	O3-Na2-O5	70.17(15)
F1-Na2-O5	108.25(17)	O5-Na2-O5	80.69(18)	O1-Na2-O5	164.12(19)
Na2-F1-U1	135.82(16)	Na2-F1-U1	103.00(13)	U1-F1-U1	114.90(13)
U1-F2-U1	180.000(10)	U1-O1-Na2	154.2(3)	U1-O2-Na1	171.0(3)
U1-O3-Na1	107.95(15)	U1-O3-Na2	111.30(15)	Na1-O3-Na2	133.92(18)
Na2-O4-U1	139.63(19)	Na2-O4-Na1	108.25(17)	U1-O4-Na1	105.31(15)
		Na2-O5-Na2	98.72(18)		

Table S3 Selected bond length in compound 2.

Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)	Bond	Length(Å)
U1-O1	1.77 (1)	U1-O2	1.76(1)	U1-F1	2.266(3)	U1-F2	2.314(6)
U1-F3	2.326(5)	U2-O3	1.74(1)	U2-O8	1.78(1)	U2-F2	2.318(6)
U2-F3	2.309(5)	U2-F4	2.267(2)	Cs1-F2	3.367(7)	Cs1-F3	3.144(7)
Cs1-O3	3.632(4)	Cs1-O1	3.297(4)	Cs1-O8	3.211(5)	Cs1-O2	3.654(6)

Table S4 Selected bond angle in compound 2.

Bond Angle	Value(deg)	Bond Angle	Value(deg)	Bond Angle	Value(deg)
F2-U2-F3	70.7(2)	F2-U2-F4	70.7(3)	F2-U2-O3	88.3(4)
F2-U2-O8	92.1(4)	F2-U2-F2	140.9(2)	F2-U2-F3	148.3(2)
F3-U2-F4	141.0(3)	F3-U2-O3	90.7(4)	F3-U2-O8	88.5(3)
F3-U2-F2	148.3(2)	F3-U2-F3	77.7(2)	F4-U2-O3	92.8(4)
F4-U2-O8	88.3(4)	F4-U2-F2	70.7(3)	F4-U2-F3	141.0(3)
O3-U2-O8	179.0(4)	O3-U2-F2	88.3(4)	O3-U2-F3	90.7(4)
O8-U2-F2	92.1(4)	O8-U2-F3	88.5(3)	F2-U2-F3	70.7(2)
F1-U1-O1	91.4(4)	F1-U1-O2	89.5(4)	F1-U1-F3	70.6(3)
F1-U1-F2	141.5(3)	F1-U1-F2	141.5(3)	F3-U1-O1	88.8(4)
F3-U1-O2	91.5(4)	F3-U1-F3	141.0(2)	F3-U1-F2	147.9(2)
F3-U1-F2	71.0(2)	O1-U1-O2	179.0(5)	O1-U1-F3	88.8(4)
O1-U1-F2	89.7(4)	O1-U1-F2	89.7(4)	O2-U1-F3	91.5(4)
O2-U1-F2	89.5(4)	O2-U1-F2	89.5(4)	F3-U1-F2	71.0(2)

F3-U1-F2	147.9(2)	F2-U1-F2	77.0(2)	U1-F1-U1	146.2(5)
Cs1-F2-U2	97.5(2)	Cs1-F2-Cs1	115.7(2)	Cs1-F2-U1	104.6(2)
U2-F2-Cs1	91.3(2)	U2-F2-U1	156.3(3)	Cs1-F2-U1	87.1(2)
Cs1-F3-U2	104.0(2)	Cs1-F3-U1	100.4(2)	U2-F3-U1	154.8(3)
U2-F4-U2	155.0(5)	Cs1-O3-U2	101.4(4)	F2-U2-F3	70.7(2)
F2-U2-O3	88.3(4)	F2-U2-O8	92.1(4)	F2-U2-F2	140.9(2)
F2-U2-F4	70.7(3)	F3-U2-O3	90.7(4)	F3-U2-O8	88.5(3)
F3-U2-F2	148.3(2)	F3-U2-F3	77.7(2)	F3-U2-F4	141.0(3)
O3-U2-O8	179.0(4)	O3-U2-F2	88.3(4)	O3-U2-F3	90.7(4)
O3-U2-F4	92.8(4)	O8-U2-F2	92.1(4)	O8-U2-F3	88.5(3)
O8-U2-F4	88.3(4)	F2-U2-F3	70.7(2)	F2-U2-F4	70.7(3)
F3-U2-F4	141.0(3)	F1-U1-F3	70.6(3)	F1-U1-O1	91.4(4)
F1-U1-O2	89.5(4)	F1-U1-F3	70.6(3)	F1-U1-F2	141.5(3)
F1-U1-F2	141.5(3)	F3-U1-O1	88.8(4)	F3-U1-O2	91.5(4)
F3-U1-F3	141.0(2)	F3-U1-F2	147.9(2)	F3-U1-F2	71.0(2)
O1-U1-O2	179.0(5)	O1-U1-F3	88.8(4)	O1-U1-F2	89.7(4)
O1-U1-F2	89.7(4)	O2-U1-F3	91.5(4)	O2-U1-F2	89.5(4)
O2-U1-F2	89.5(4)	F3-U1-F2	71.0(2)	F3-U1-F2	147.9(2)
F2-U1-F2	77.0(2)	U1-F3-U2	154.8(3)	U2-F2-U1	156.3(3)
F2-U1-O2	89.5(4)	F2-U1-O2	89.5(4)		

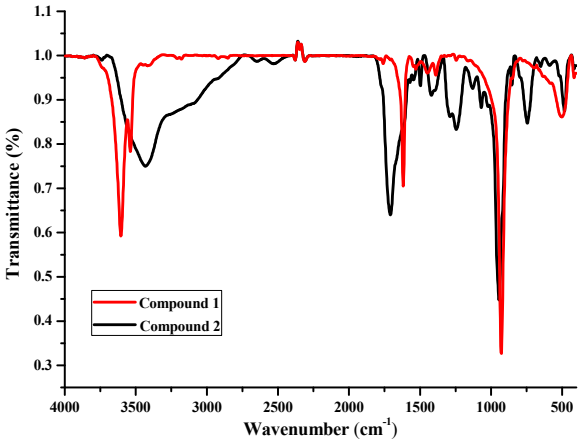
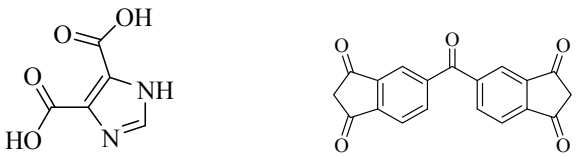


Figure S1. IR spectra of compounds 1and 2.

The IR spectra of inorganic compounds are always difficult to identify because there is very little reference in the literature. For simple ionic compounds, such as sodium chloride, potassium bromide, and calcium fluoride, etc, the only vibrations originate from lattice vibrations, in which the individual ions undergo translational oscillations. The resulting spectral bands are broad and are responsible for the long wave-length cutoff in transmission.[1] For somewhat complicated inorganic compounds 1 and 2, their IR spectra are shown in figure S1. The peaks positioned at 750, 944 and 928 cm−1 are assigned to the symmetric and asymmetric stretching modes of the uranyl cation in 1 and 2, respectively. The peaks resolved at 483 and 501 cm−1 can be assigned to M-F stretches according to the literature,[1, 2] Besides, the peaks of compound 2 at 3605 and 3538 nm are assigned to O-H stretches of the hydroxide. The peaks of compound 1 at 3432 nm are assigned to absorption band of water in crystal. The broad band from 1200-1600 nm imply the influence of water resulting in certain changes in structures, this judgement agrees with the literature as well.[2]



a b

Figure S2. (a)Structure of 1H-imidazole-4,5-dicarboxylic acid (H3IDC) and (b) 3,3′,4,4′-benzophenonetetracarboxylic dianhydride (3,3′,4,4′-BTDA)

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