Supporting Information

Porous Anionic Uranyl–Organic Networks for Highly Efficient Cs^+ Adsorption and Mechanism Investigation

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Adsorption Kinetic Experiments

The adsorption kinetic experiments were investigated with different contacting time at initial Cs^+ concentration of 1 ppm. Pseudo-second-order kinetic model is described as the following function:

$$\frac{t}{q_t} = \frac{1}{k_s + q_e^2} + \frac{1}{q_e} t$$

where q_e represents the amount of Cs^+ on the adsorbent under equilibrium, and K_s is pseudo-second-order adsorption rate constant.

Selectivity Experiments

The selectivity experiments of Cs^+ adsorption from aqueous solution containing various metal cations were carried out at room temperature. The residual concentration in the supernatant of metal ions was determined by inductively coupled plasma mass spectrometry (ICP-MS). As a measurement of selectivity, K_d can be described as follows:

$$K_d = \frac{V}{m} \frac{(C_0 - C_f)}{C_f}$$

where C_0 and C_f are the initial and equilibrium ion concentrations, respectively. V is the volume (mL) of the testing solution and m is the mass of the sorbent (g).

Supplementary tables and figures

Table S1: Crystallographic data for compounds

compound	1	2	2-Cs
Formula	$C_{66}H_{33}O_{16}U_2$	$C_{66}H_{33}O_{16}U_2$	$C_{66}H_{32}Cs_2O_{16}U_2$
F_w	1557.98	1557.98	1822.79
Crystal system	monoclinic	orthorhombic	orthorhombic
Space group	C2/m	$Cmc2_1$	$Cmc2_1$
a, Å	30.196(6)	41.078(6)	39.501(3)
b, Å	17.028(3)	17.573(2)	17.761(1)
c, Å	22.538(4)	29.157(4)	28.789(2)
α, °	90	90	90
β, °	96.278(4)	90	90
γ, °	90	90	90
V, $Å^3$	11519(4)	21047(5)	20198(3)
Z	4	8	8
D_c, mg/mm^3	0.898	0.983	1.199
μ, mm^{-1}	2.844	3.113	3.955
reflection collected	34115	64286	62616
GOF on F^2	1.046	0.944	0.961
R_1/wR_2 ($I > 2\sigma(I)$)	0.0708/0.1851	0.0491/0.1036	0.0560/0.1258
R_1/wR_2 (all data)	0.1065/ 0.2003	0.0863/ 0.1148	0.0895/0.1392

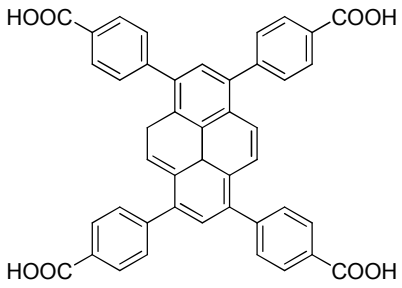


Figure S1. Chemical structure of ligand H_4TBAPy

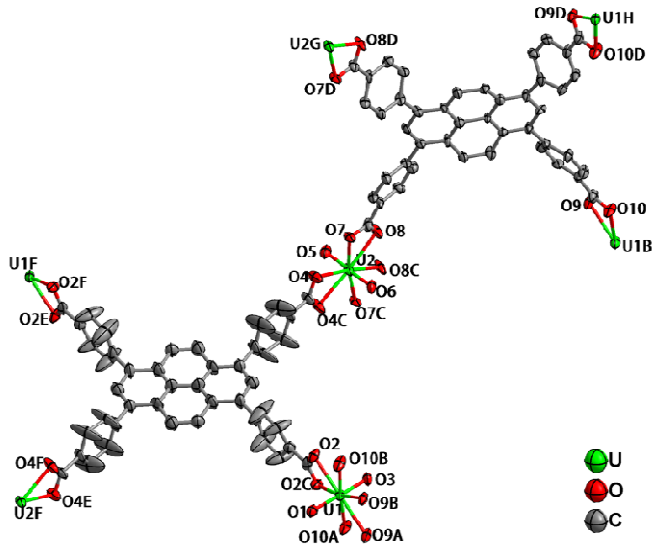


Figure S2. ORTEP representation of the coordination environment of compound **1** with thermal ellipsoids set at 50% probability. The asymmetric codes: A, 1-x,1-y, 1-z; B, 1-x, y,1-z; C, x, 1-y, z; D, x, -y, z; E, 2-x, 1-y, 1-z; F, 2-x, y, 1-z; G, x, -1+y, z; H, 1-x, -1+y, 1-z. Hydrogen atoms bonded to carbon atoms are omitted for clarity.

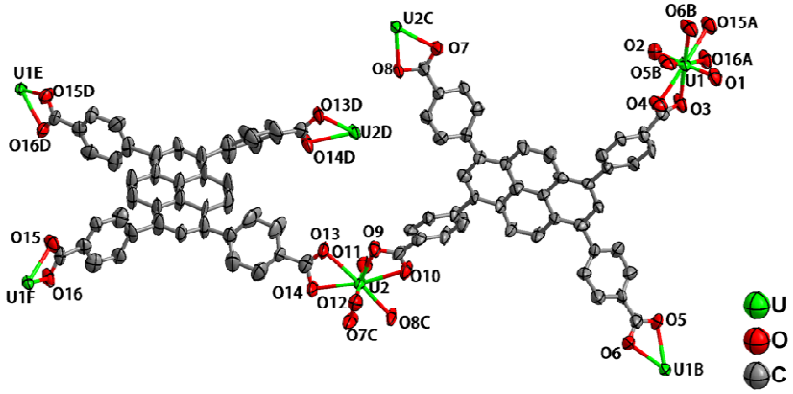


Figure S3. ORTEP representation of the coordination environment of compound **2** with thermal ellipsoids set at 50% probability. The asymmetric codes: A, x, 2+y, z; B, 0.5-x, 1.5-y,-0.5+z; C, x, -y, -0.5+z; D, -x, y, z; E, -x, -2+y, z; F, x, -2+y, z; G, 0.5-x, 1.5-y, -0.5+z. Hydrogen atoms bonded to carbon atoms are omitted for clarity.

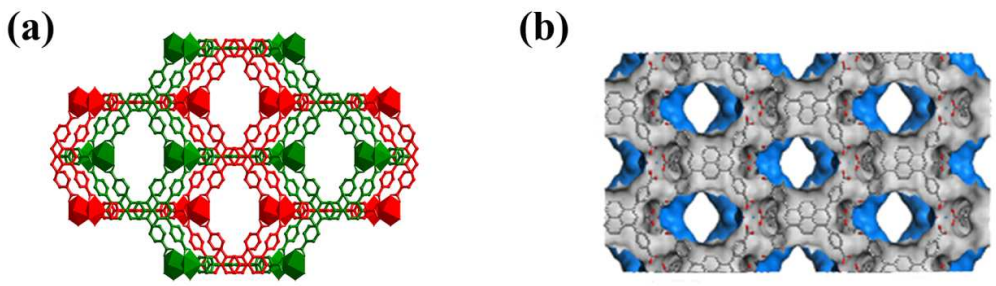


Figure S4. (a) The viewing of 2D layer network **1** along the c-axis . (b) Connolly surface representation showing the 2D structure **1**.

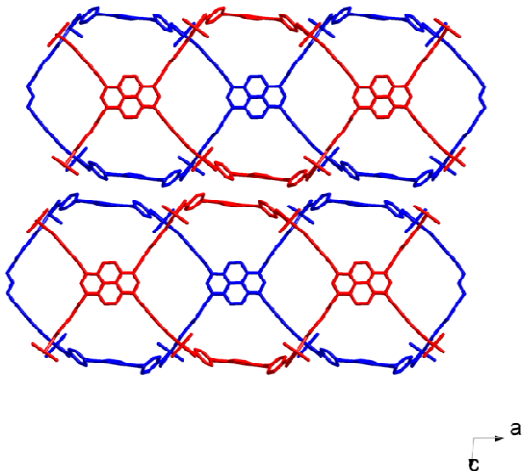


Figure S5. The 2D interpenetrated layer network of compound **1** along the *b*-axis

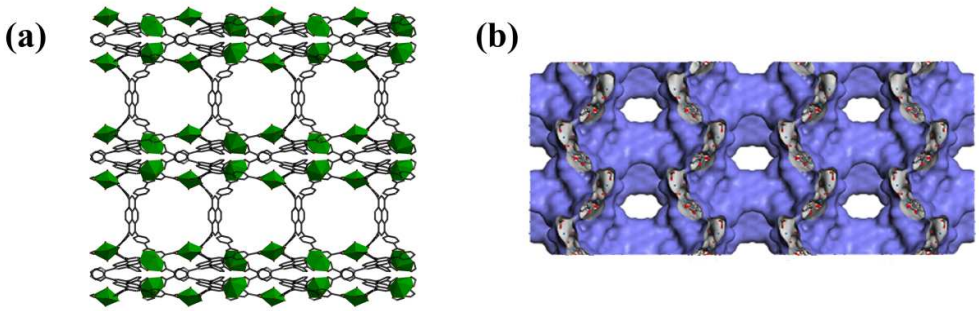


Figure S6. (a) The viewing of 3D structure **2**. (b) Connolly surface representation showing the 3D structure **2**.

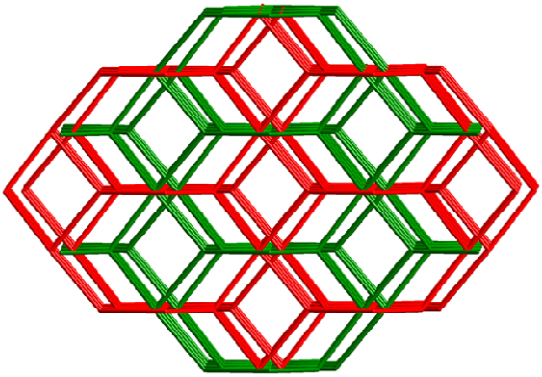


Figure S7. The simplified (3,4,4)-connected topological net of compound **1** analyzed using TOPOS software.

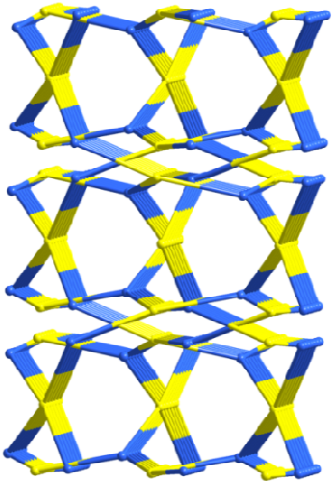


Figure S8. The simplified (3,3,4,4)-connected topological net of compound **2** analyzed using TOPOS software.

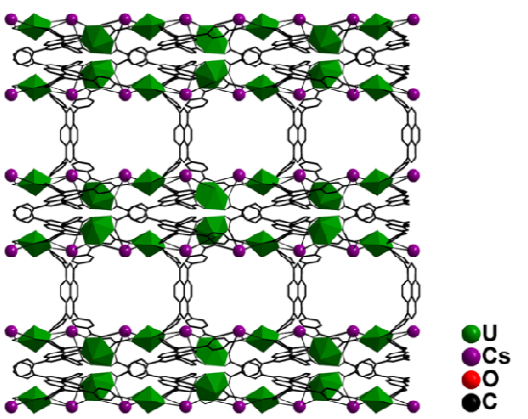


Figure S9. The 3D view of compound 2-Cs.

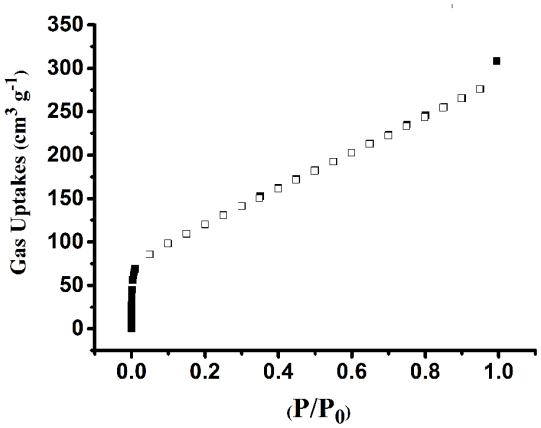


Figure S10. N_2 sorption isotherms for compound **1** at 77 K.

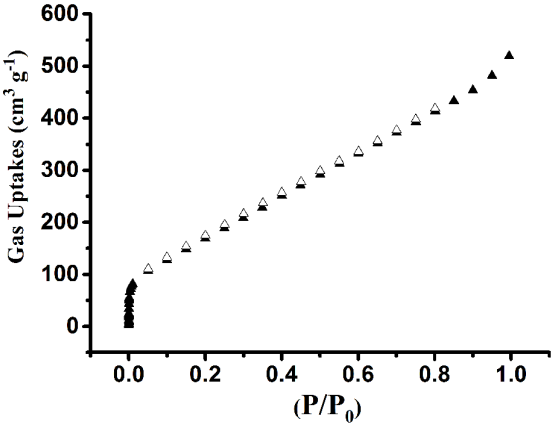


Figure S11. N_2 sorption isotherms for compound **2** at 77 K.

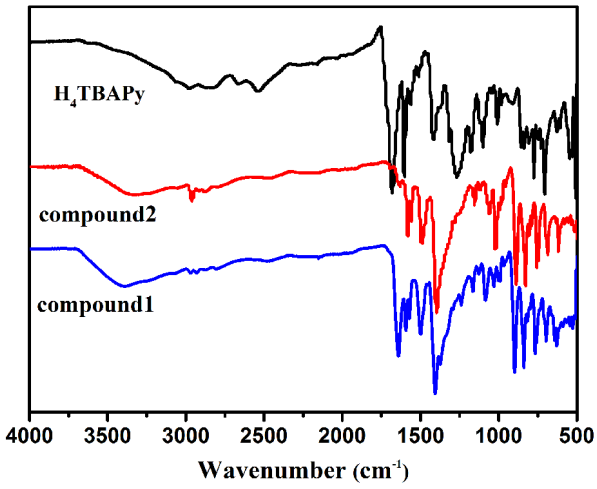


Figure S12. FT-IR spectra of H_4TBAPy ligand as well as compound **1** and **2**.

Thermo gravimetric Analysis (TGA)

The TGA curve of compound **1** shows a weight loss of 32.62 % between 25 and 280 °C, indicating the exclusion of solvent H_2O molecules and DMF molecules, with no further weight loss up to 320 °C. The subsequent weight loss of 45.13% occurs in 320–480 °C, which can be ascribed to decompose of skeleton structure. The TGA curve of compound **2** shows a weight loss of 40.56 % between 25 and 270 °C, indicating the exclusion of solvent H_2O molecules and DMF molecules, with no further weight loss up to 330 °C. The subsequent weight loss of 33.18% occurs in 330–490 °C, which can be ascribed to decompose of skeleton structure.

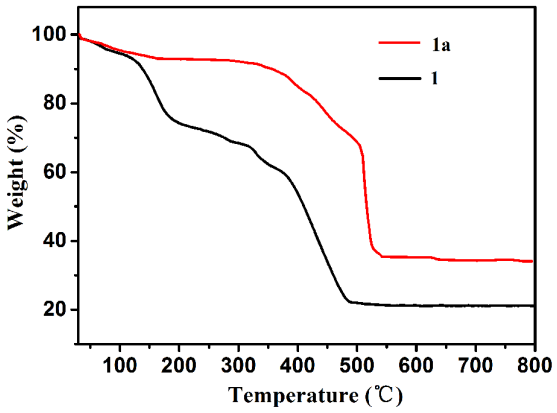


Figure S13. TGAs curves for the as-synthesized and activated samples of compound **1**.

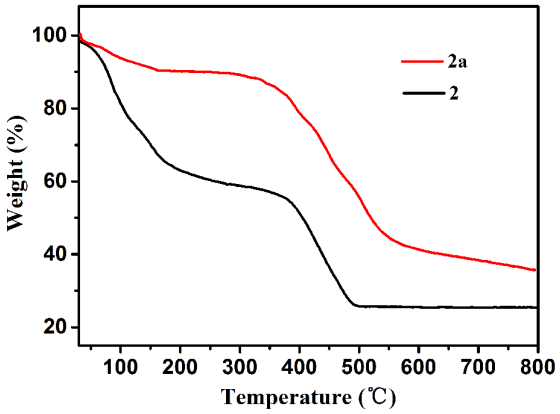


Figure S14. TGAs curves for the as-synthesized and activated samples of compound **2**.

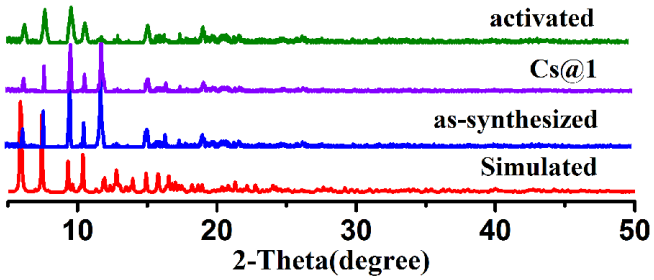


Figure S15. PXRD patterns for compound **1**: simulated compound **1**, as-synthesized compound **1**, Cs@**1** and activated.

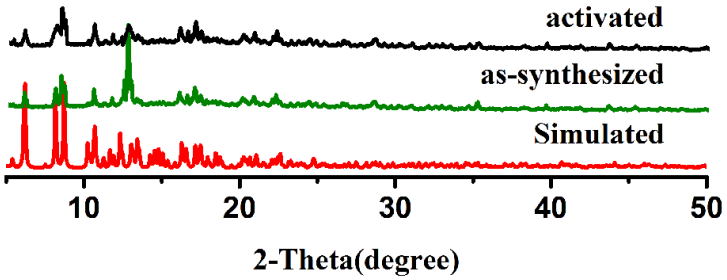


Figure S16. PXRD patterns for compound **2**: simulated compound **2**, as-synthesized compound **2** and activated.

Table S2: Selected bond lengths (Å) and angles (°) for compound **1**

U(1)-O(2)#1	2.436(6)	U(2)-O(3)#3	2.472(6)
U(1)-O(2)#2	2.436(6)	U(2)-O(3)	2.472(6)
U(1)-O(1)#2	2.481(6)	U(2)-O(4)#3	2.465(5)
U(1)-O(1)#1	2.481(6)	U(2)-O(4)	2.465(5)
U(1)-O(8)	1.738(8)	U(2)-O(5)	1.726(1)
U(1)-O(9)	1.773(8)	U(2)-O(7)	2.448(6)
U(1)-O(10)	2.470(6)	U(2)-O(7)#3	2.448(6)
U(1)-O(10)#3	2.470(6)	U(2)-O(6)	1.755(9)
O(2)#1-U(1)-O(2)#2	173.8(3)	O(4)-U(2)-O(3)#3	120.52(2)
O(2)#2-U(1)-O(1)#1	121.6(2)	O(4)#3-U(2)-O(3)#3	52.32(2)
O(2)#2-U(1)-O(1)#2	53.2(2)	O(4)-U(2)-O(3)	52.32(2)
O(2)#1-U(1)-O(1)#1	53.2(2)	O(4)#3-U(2)-O(3)	120.52(2)
O(2)#1-U(1)-O(1)#2	121.6(2)	O(4)-U(2)-O(4)#3	171.1(2)
O(2)#2-U(1)-O(10)#3	66.1(2)	O(5)-U(2)-O(3)#3	88.1(3)
O(2)#2-U(1)-O(10)	118.9(2)	O(5)-U(2)-O(3)	88.1(3)
O(2)#1-U(1)-O(10)#3	118.9(2)	O(5)-U(2)-O(4)	87.21(1)
O(2)#1-U(1)-O(10)	66.1(2)	O(5)-U(2)-O(4)#3	87.21(1)
O(8)-U(1)-O(2)#1	91.81(2)	O(5)-U(2)-O(7)#3	91.5(3)
O(8)-U(1)-O(2)#2	91.81(2)	O(5)-U(2)-O(7)	91.5(3)
O(8)-U(1)-O(1)#1	92.1(3)	O(5)-U(2)-O(6)	178.9(4)
O(8)-U(1)-O(1)#2	92.1(3)	O(7)-U(2)-O(3)	118.9(2)
O(8)-U(1)-O(9)	179.4(4)	O(7)-U(2)-O(3)#3	172.78(2)
O(8)-U(1)-O(10)	91.1(3)	O(7)#3-U(2)-O(3)#3	118.9(2)
O(8)-U(1)-O(10)#3	91.1(3)	O(7)#3-U(2)-O(3)	172.78(2)
O(9)-U(1)-O(2)#1	88.22(2)	O(7)-U(2)-O(4)#3	120.46(2)
O(9)-U(1)-O(2)#2	88.22(2)	O(7)#3-U(2)-O(4)	120.46(2)
O(9)-U(1)-O(1)#1	88.4(3)	O(7)-U(2)-O(4)	66.65(2)
O(9)-U(1)-O(1)#2	88.4(3)	O(7)#3-U(2)-O(4)#3	66.65(2)
O(9)-U(1)-O(10)#3	88.3(3)	O(7)-U(2)-O(7)#3	53.9(3)
O(9)-U(1)-O(10)	88.3(3)	O(6)-U(2)-O(3)	91.0(3)
O(10)-U(1)-O(1)#1	119.3(2)	O(6)-U(2)-O(3)#3	91.0(3)
O(10)#3-U(1)-O(1)#1	171.6(2)	O(6)-U(2)-O(4)	92.73(1)
O(10)-U(1)-O(1)#2	171.6(2)	O(6)-U(2)-O(4)#3	92.72(1)
O(10)#3-U(1)-O(1)#2	119.3(2)	O(6)-U(2)-O(7)	89.4(3)
O(10)#3-U(1)-O(10)	52.9(3)	O(6)-U(2)-O(7)#3	89.4(3)

Symmetry code: #1 1-X,+Y,1-Z; #2 1-X,1-Y,1-Z; #3 X,1-Y,+Z.

Table S3: Selected bond lengths (Å) and angles (°) for compound **2**

U(1)-O(6)#1	2.438(2)	U(2)-O(14)	2.442(1)
U(1)-O(3)	2.451(2)	U(2)-O(9)	2.476(2)
U(1)-O(16)#2	2.454(2)	U(2)-O(7)#3	2.500(1)
U(1)-O(2)	1.758(2)	U(2)-O(13)	2.516(2)
U(1)-O(5)#1	2.465(2)	U(2)-O(8)#3	2.446(2)
U(1)-O(15)#2	2.478(2)	U(2)-O(12)	1.749(2)
U(1)-O(4)	2.434(2)	U(2)-O(10)	2.445(2)
U(1)-O(1)	1.764(2)	U(2)-O(11)	1.690(2)
O(6)#1-U(1)-O(3)	175.9(6)	O(14)-U(2)-O(9)	67.3(6)
O(6)#1-U(1)-O(16)#2	118.7(6)	O(14)-U(2)-O(7)#3	170.2(6)
O(6)#1-U(1)-O(5)#1	52.8(5)	O(14)-U(2)-O(13)	52.7(5)
O(6)#1-U(1)-O(15)#2	66.3(6)	O(14)-U(2)-O(8)#3	119.1(5)
O(3)-U(1)-O(16)#2	65.0(6)	O(14)-U(2)-O(10)	120.6(5)
O(3)-U(1)-O(5)#1	123.6(5)	O(9)-U(2)-O(7)#3	122.3(6)
O(3)-U(1)-O(15)#2	117.3(6)	O(9)-U(2)-O(13)	118.5(5)
O(2)-U(1)-O(6)#1	92.3(7)	O(7)#3-U(2)-O(13)	117.5(6)
O(2)-U(1)-O(3)	89.7(7)	O(8)#3-U(2)-O(9)	172.8(6)
O(2)-U(1)-O(16)#2	89.7(7)	O(8)#3-U(2)-O(7)#3	51.4(6)
O(2)-U(1)-O(5)#1	91.4(7)	O(8)#3-U(2)-O(13)	68.6(5)
O(2)-U(1)-O(15)#2	89.6(7)	O(12)-U(2)-O(14)	87.3(7)
O(2)-U(1)-O(4)	84.3(7)	O(12)-U(2)-O(9)	93.3(8)
O(2)-U(1)-O(1)	179.6(8)	O(12)-U(2)-O(7)#3	93.3(6)
O(5)#1-U(1)-O(15)#2	119.1(6)	O(12)-U(2)-O(13)	96.3(8)
O(4)-U(1)-O(6)#1	122.6(6)	O(12)-U(2)-O(8)#3	83.9(7)
O(4)-U(1)-O(3)	54.0(5)	O(12)-U(2)-O(10)	87.8(8)
O(4)-U(1)-O(16)#2	118.6(6)	O(10)-U(2)-O(9)	53.9(5)
O(4)-U(1)-O(5)#1	70.0(5)	O(10)-U(2)-O(7)#3	69.2(6)
O(4)-U(1)-O(15)#2	169.3(6)	O(10)-U(2)-O(13)	171.8(6)
O(1)-U(1)-O(6)#1	87.6(7)	O(10)-U(2)-O(8)#3	119.2(5)
O(1)-U(1)-O(3)	90.4(6)	O(11)-U(2)-O(14)	93.1(7)
O(1)-U(1)-O(16)#2	90.0(7)	O(11)-U(2)-O(9)	86.2(8)
O(1)-U(1)-O(5)#1	88.8(7)	O(11)-U(2)-O(7)#3	86.4(6)
O(1)-U(1)-O(15)#2	90.0(7)	O(11)-U(2)-O(13)	84.5(8)
O(1)-U(1)-O(4)	96.1(7)	O(11)-U(2)-O(8)#3	96.4(7)

Symmetry code: #1 -1/2-X,1/2-Y,-1/2+Z; #2 1-X,+Y,1/2+Z; #3 1-X,+Y,-1/2+Z

Table S4: Cs–O bond lengths (Å) for compound **2-Cs**

Cs(1)-O(12)	3.063(1)	Cs(2)-O(3)#7	3.259(1)
Cs(1)-O(15)#10	3.066(1)	Cs(2)-O(6)#6	3.056(1)
Cs(1)-O(13)#11	3.229(1)	Cs(2)-O(14)	3.060(1)
Cs(1)-O(5)#8	3.141(1)	Cs(2)-O(10)#6	3.122(1)

Symmetry code: #6 X,-1+Y,+Z; #7 X,-2+Y,+Z; #10 3/2-X,3/2-Y,-1/2+Z;#11 3/2-X,1/2+Y,+Z

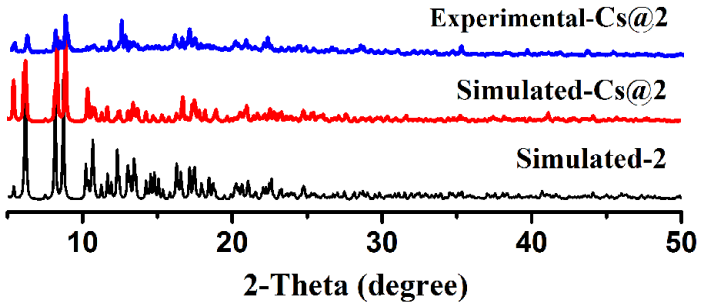


Figure S17. Simulated **2**, Simulated Cs@**2** and experimental XRD patterns of Cs@**2**

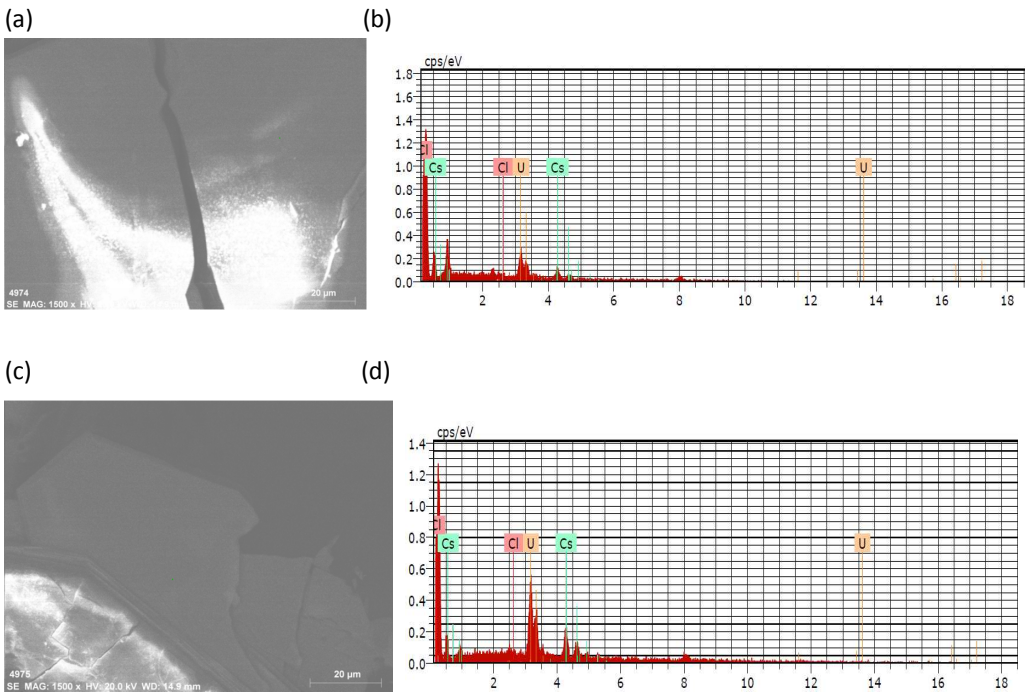


Figure S18. (a, b) The SEM images and the EDS patterns of the single crystal studied for Cs^+ adsorption of compound **1** (c, d) The SEM images and the EDS patterns of the single crystal studied for Cs^+ adsorption of compound **2**

Kinetic Studies for Compounds of Cs^+ Adsorption: The solutions of Cs^+ (1 ppm) were prepared at room temperature and V : m is 1000 mL/g (V = 10 mL, m =10 mg). All the samples were carried out under magnetic stirring. Then we took one sample one time at different time of ion-exchange.

Tables S5: Kinetics of Cs^+ adsorption using compound **1**

t (min)	0	5	10	20	30	40	50	60
Ce (ppm)	0.98	0.52	0.37	0.21	0.12	0.14	0.13	0.12
q	0	0.46	0.61	0.77	0.86	0.84	0.85	0.86
t/qt	0	10.87	16.39	25.97	34.88	47.62	58.82	69.77
K_d	0	885	1649	3667	7167	6000	6538	7167

Tables S6: Kinetics of Cs^+ adsorption using compound **2**

t (min)	0	5	10	20	30	40	50	60
Ce (ppm)	0.98	0.47	0.23	0.09	0.12	0.09	0.11	0.09
q	0	0.51	0.75	0.89	0.86	0.89	0.87	0.89
t/qt	0	9.80	13.23	22.47	34.88	44.94	57.47	67.42
K_d	0	1085	3261	9889	7167	9889	7909	9889

Tables S7: Adsorption behavior comparison for MOF-based materials

MOF	K_d (mL/g)	q_{max}(mg g^{-1})	Ref
MIL-101-SO_3H	-	453	29a
MOF/KNiFC	-	153	29b
MOF/Fe_3O_4/KNiFC	-	109	29b
uranyl-based MOF	7545	-	2a
compound 1	7167	108	this work
compound 2	9889	96	this work

Tables S8: The competitive ion-exchange experiments for compound **1**.
(mole ratio, Cs^+ : Rb^+ : K^+ : Na^+ = 1: 10 : 10 : 10)

Metal cations	C_o / ppm (initial concentration)	C_f / ppm (equilibrium concentration)	K_d / (mL/ g) (distribution coefficient)
Cs^+	45.78	31.44	4.56×10^2
Rb^+	289.4	244.8	1.82×10^2
K^+	152.7	139.8	0.92×10^2
Na^+	89.62	80.23	1.17×10^2

Tables S9: The competitive ion-exchange experiments for compound **2**.
(mole ratio, Cs^+ : Rb^+ : K^+ : Na^+ = 1: 10 : 10 : 10)

Metal cations	C_o / ppm (initial concentration)	C_f / ppm (equilibrium concentration)	K_d / (mL/ g) (distribution coefficient)
Cs^+	45.78	28.05	6.32×10^2
Rb^+	289.4	238.6	2.13×10^2
K^+	152.7	135.4	1.28×10^2
Na^+	89.62	81.10	1.05×10^2

Tables S10: The competitive ion-exchange experiments for compound **1**.

(mole ratio, Cs^+ : Mg^{2+} : Sr^{2+}: La^{3+} = 1: 10: 10: 10)

Metal cations	C_o / ppm (initial concentration)	C_f / ppm (equilibrium concentration)	K_d / (mL/ g) (distribution coefficient)
Cs^+	42.96	35.30	2.17×10^2
Mg^{2+}	98.35	87.97	1.18×10^2
Sr^{2+}	301.9	218.6	3.81×10^2
La^{3+}	517.4	507.8	0.19×10^2

Tables S11: The competitive ion-exchange experiments for compound **2**.

(mole ratio, Cs^+ : Mg^{2+} : Sr^{2+}: La^{3+} = 1: 10: 10: 10)

Metal cations	C_o / ppm (initial concentration)	C_f / ppm (equilibrium concentration)	K_d / (mL/ g) (distribution coefficient)
Cs^+	42.96	33.25	2.92×10^2
Mg^{2+}	98.35	89.25	1.02×10^2
Sr^{2+}	301.9	209.2	4.43×10^2
La^{3+}	517.4	505.8	0.23×10^2

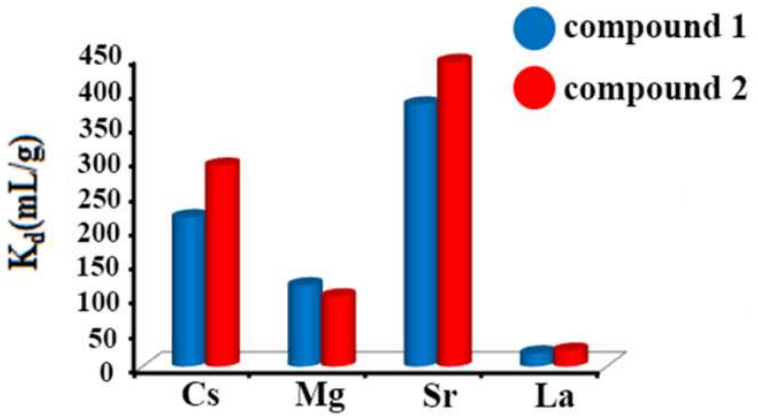


Figure S19. The selective adsorption of the test ions.

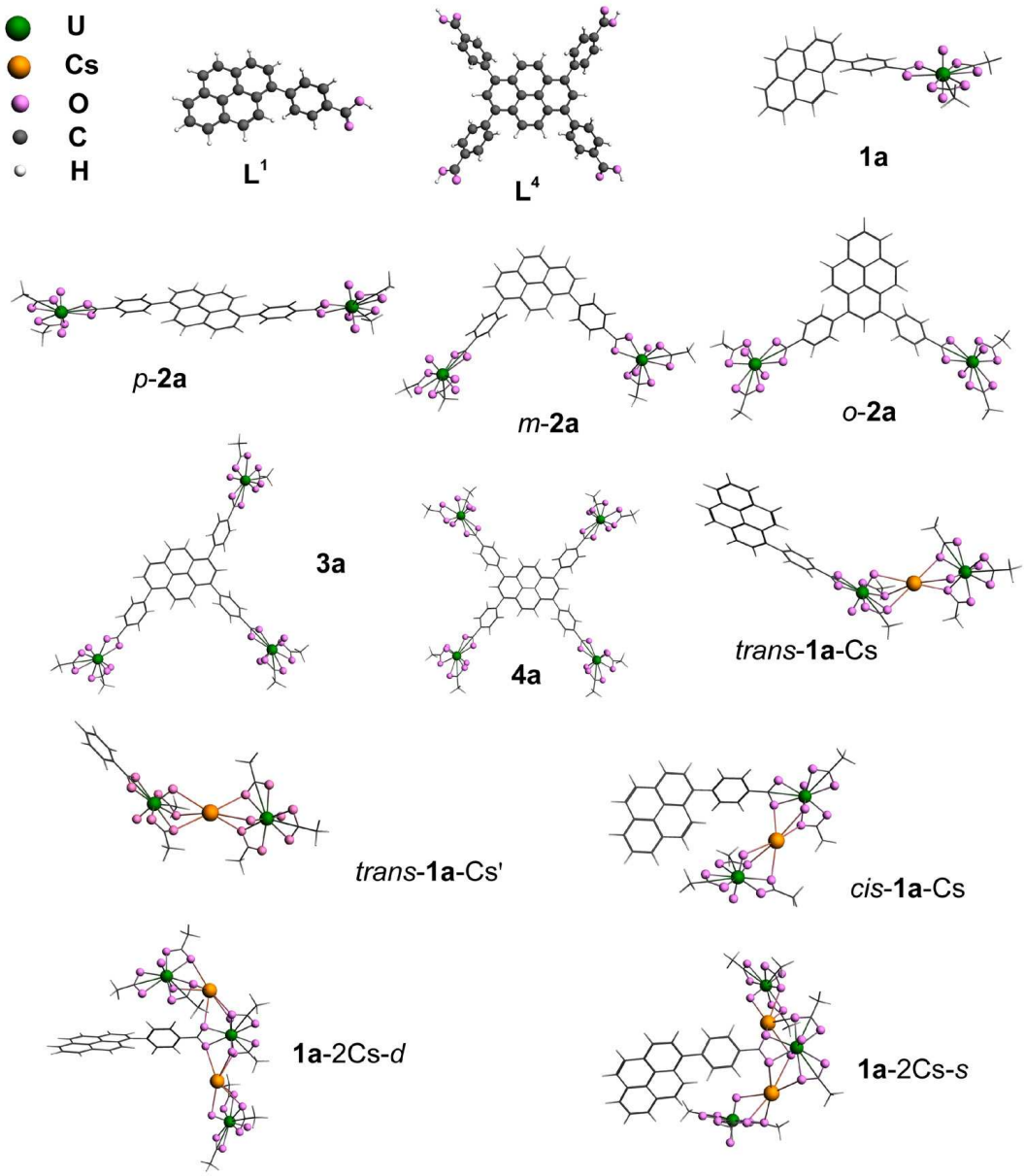
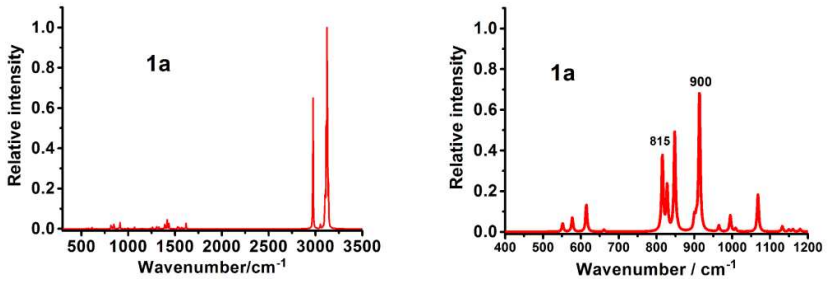


Figure S20. Optimized structures of ligands and model compounds.



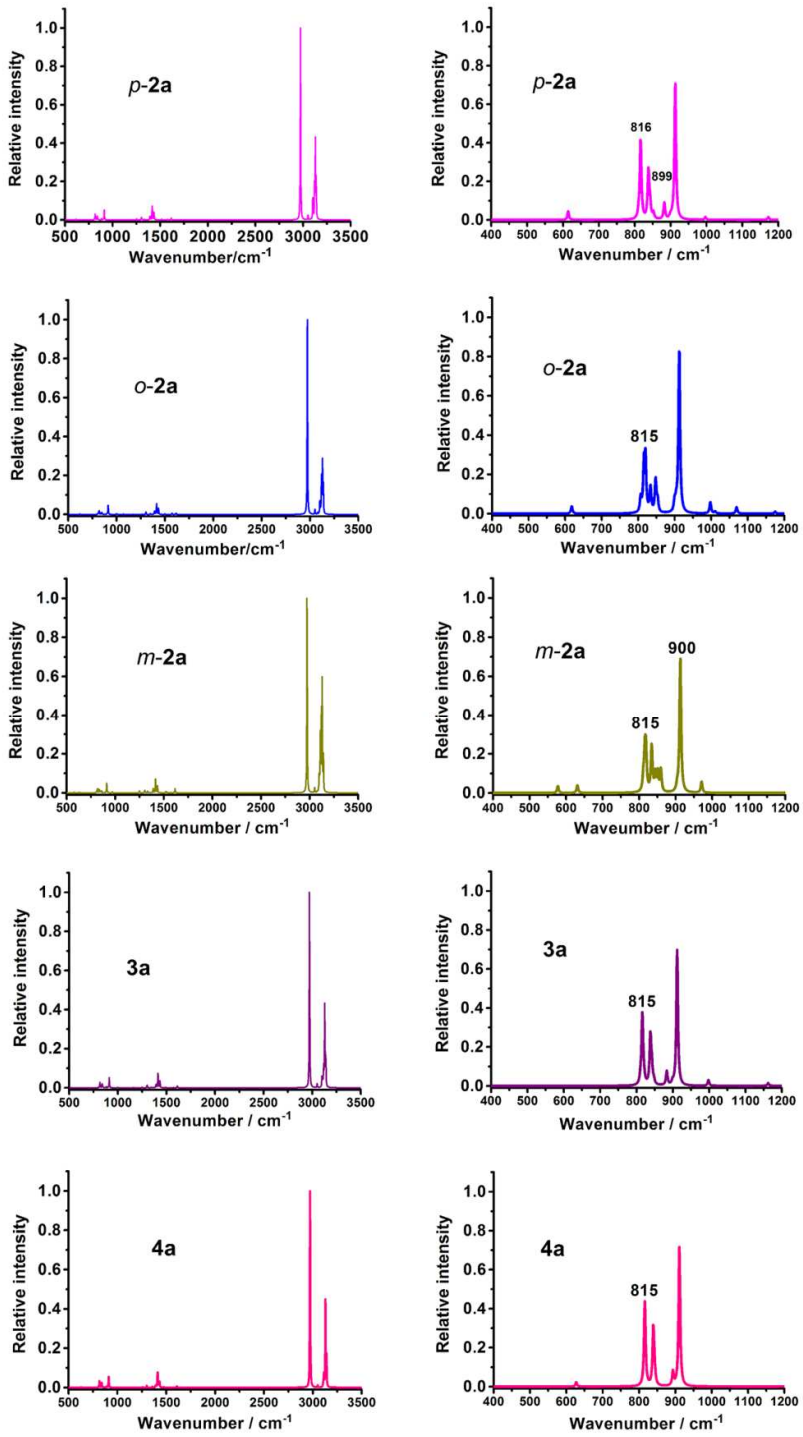


Figure S21. Theoretically simulated vibrational spectra of the model compounds **1a**~**4a**: the one spreading the region from 400 to 4000 cm^{-1} was presented on the left side, and the one between 400 and 1200 cm^{-1} on the right side where the U=O stretches were marked.

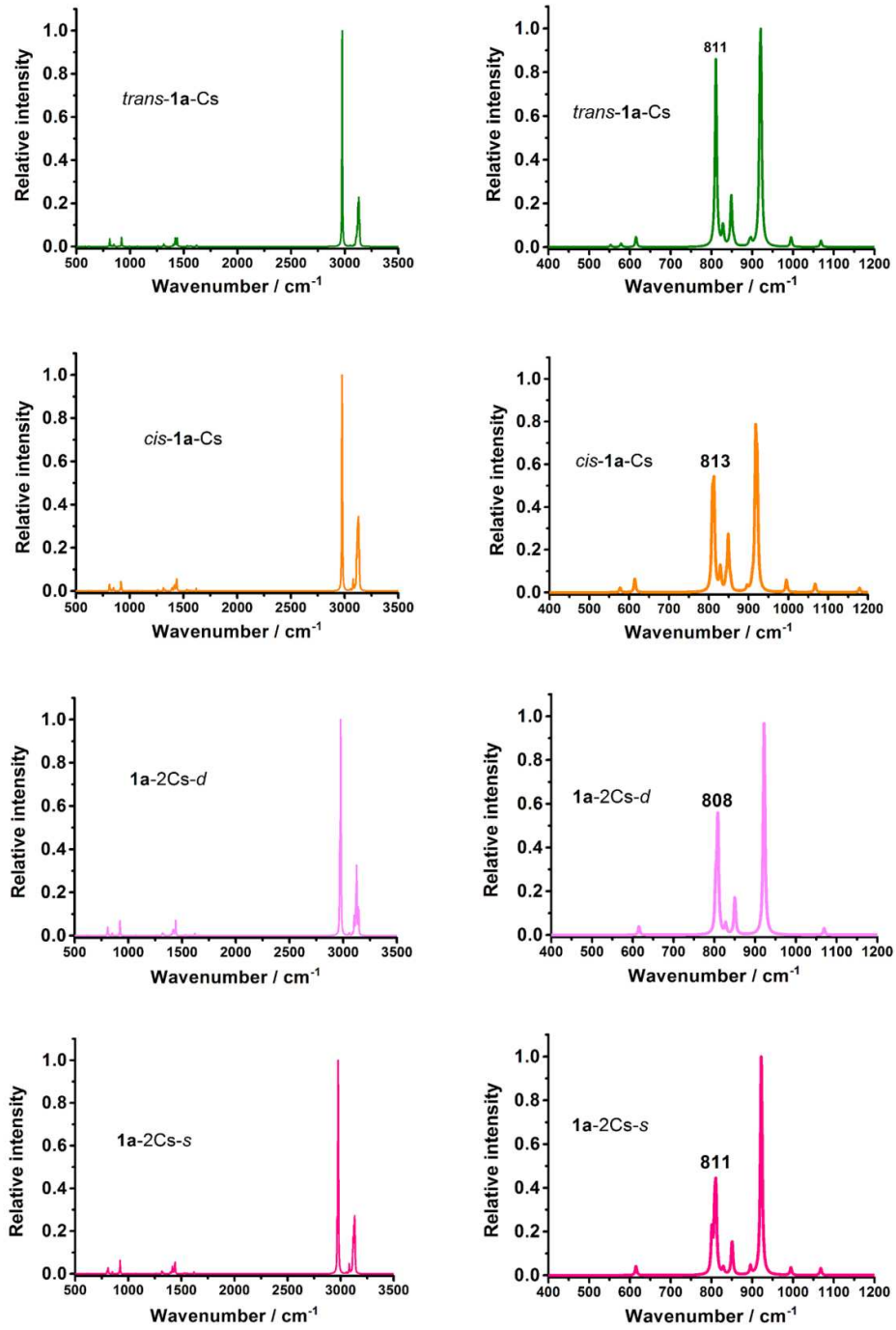


Figure S22. Theoretically simulated vibrational spectra of the model compounds of cesium analogues: the one spreading the region from 400 to 4000 cm^{-1} was presented on the left side, and the one between 400 and 1200 cm^{-1} on the right side where the U=O stretches were marked.

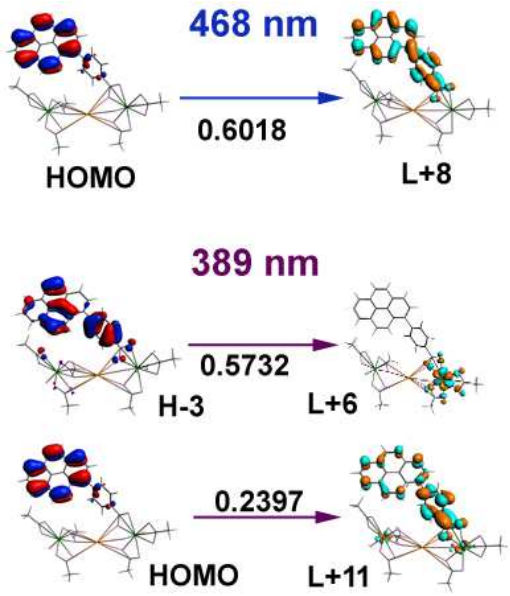


Figure S23. Electron transition diagrams in the TD-DFT calculation for absorptions of *cis*-**1a**-Cs.

Table S12. Investigated model compounds.

Formula	Number of atoms	Abbreviation
Pyrene-PhCOOH	39	L^1
Pyrene-$(PhCOOH)_4$	78	L^4 (H_4TBAPy)
{Pyrene-[(PhCOO)$(UO_2)$$(OOCMe)_2$]}$^-$	55	**1a**
para-{Pyrene-[(PhCOO)$(UO_2)$$(OOCMe)_2]_2$}$^{2-}$	84	*p*-**2a**
meta-{Pyrene-[(PhCOO)$(UO_2)$$(OOCMe)_2]_2$}$^{2-}$	84	*m*-**2a**
ortho-{Pyrene-[(PhCOO)$(UO_2)$$(OOCMe)_2]_2$}$^{2-}$	84	*o*-**2a**
{Pyrene-[(PhCOO)$(UO_2)$$(OOCMe)_2]_3$}$^{3-}$	113	**3a**
{Pyrene-[(PhCOO)$(UO_2)$$(OOCMe)_2]_4$}$^{4-}$	142	**4a**
trans-{Pyrene-[(PhCOO)$(UO_2)$$(OOCMe)_2$]Cs[$(UO_2)$$(OOCMe)_3$]}$^-$	80	*trans*-**1a**-Cs
trans-{[(PhCOO)$(UO_2)$$(OOCMe)_2$]Cs[$(UO_2)$$(OOCMe)_3$]}$^-$		*trans*-**1a**-Cs'
cis-{Pyrene-[(PhCOO)$(UO_2)$$(OOCMe)_2$]Cs[$(UO_2)$$(OOCMe)_3$]}$^-$	80	*cis*-**1a**-Cs
{Pyrene-[(PhCOO)$(UO_2)$$(OOCMe)_2$]$Cs_2$[$(UO_2)$$(OOCMe)_3]_2$}$^-$ (2Cs at different side of molecular plane)	105	**1a**-2Cs-*d*
{Pyrene-[(PhCOO)$(UO_2)$$(OOCMe)_2$]$Cs_2$[$(UO_2)$$(OOCMe)_3]_2$}$^-$ (same side of molecular plane)	105	**1a**-2Cs-*s*

Table S13. Optimized bond lengths (average values) of model compounds by the Priroda code. (Distances in Å)

		Unit1	Unit2	Unit3	Unit4
1a	$U=O_{yl}$	1.809			
	$U-O_{eq}$	2.501			
	U-C	2.864			
p-**2a**	$U=O_{yl}$	1.810	1.810		

	$U\text{-}O_{eq}$	2.501	2.501		
	U-C	2.865	2.865		
m-**2a**	$U{=}O_{yl}$	1.809	1.809		
	$U\text{-}O_{eq}$	2.501	2.501		
	U-C	2.865	2.865		
o-**2a**	$U{=}O_{yl}$	1.810	1.810		
	$U\text{-}O_{eq}$	2.501	2.501		
	U-C	2.866	2.866		
3a	$U{=}O_{yl}$	1.805	1.809	1.810	
	$U\text{-}O_{eq}$	2.502	2.502	2.502	
	U-C	2.867	2.867	2.867	
4a	$U{=}O_{yl}$	1.810	1.810	1.810	1.810
	$U\text{-}O_{eq}$	2.503	2.503	2.503	2.503
	U-C	2.868	2.868	2.868	2.868
trans-**1a**-Cs	$U{=}O_{yl}$	1.813	1.812		
	$U\text{-}O_{eq}$	2.496	2.496		
	U-C	2.869	2.868		
	$Cs\text{-}O_{eq}$		3.069		
	$Cs\text{-}O_{eq}$		3.079		
	$Cs\text{-}O_{yl}$		3.261		
	$Cs\text{-}O_{eq}$		3.084		
	$Cs\text{-}O_{eq}$		3.091		
	$Cs\text{-}O_{yl}$		3.290		
cis-**1a**-Cs	$U{=}O_{yl}$	1.813	1.812		
	$U\text{-}O_{eq}$	2.496	2.496		
	U-C	2.868	2.871		
	$Cs\text{-}O_{eq}$		3.117		
	$Cs\text{-}O_{eq}$		3.083		
	$Cs\text{-}O_{yl}$		3.271		
	$Cs\text{-}O_{eq}$		3.085		
	$Cs\text{-}O_{eq}$		3.096		
	$Cs\text{-}O_{yl}$		3.295		
1a-2Cs-*d*	$U{=}O_{yl}$	1.814	1.818	1.814	
	$U\text{-}O_{eq}$	2.494	2.486	2.495	
	U-C	2.869	2.870	2.872	
	$Cs\text{-}O_{eq}$		3.079	3.171	
	$Cs\text{-}O_{eq}$		3.055	3.143	
	$Cs\text{-}O_{yl}$		3.193	3.278	
	$Cs\text{-}O_{eq}$		3.088	3.010	
	$Cs\text{-}O_{eq}$		3.186	3.147	
	$Cs\text{-}O_{yl}$		3.296	3.116	
1a-2Cs-*s*	$U{=}O_{yl}$	1.814	1.816	1.813	
	$U\text{-}O_{eq}$	2.494	2.490	2.496	

	U-C	2.869	2.873	2.871	
	Cs-O_{eq}		3.049	3.054	
	Cs-O_{eq}		3.041	3.047	
	Cs-O_{yl}		3.229	3.185	
	Cs-O_{eq}		3.134	3.074	
	Cs-O_{eq}		3.095	3.216	
	Cs-O_{yl}		3.396	3.425	

Table S14. Optimized bond angles (average values in degree) of model compounds by the Priroda code.

		Unit1	Unit2	Unit3	Unit4
1a	O_{yl}=U=O_{yl}	179.6			
	O_{yl}=U-O_{eq}	90.3			
	O_{yl}=U-O_{eq}	90.1			
	O_{yl}=U-C	90.5			
	O_{eq}-U-O_{eq}	67.4			
p-**2a**	O_{yl}=U=O_{yl}	179.9	179.9		
	O_{yl}=U-O_{eq}	90.2	89.7		
	O_{yl}=U-O_{eq}	90.0	89.8		
	O_{yl}=U-C	90.3	89.5		
	O_{eq}-U-O_{eq}	67.4	67.4		
m-**2a**	O_{yl}=U=O_{yl}	179.8	179.8		
	O_{yl}=U-O_{eq}	90.3	89.7		
	O_{yl}=U-O_{eq}	90.1	89.9		
	O_{yl}=U-C	90.5	89.5		
	O_{eq}-U-O_{eq}	67.4	67.5		
o-**2a**	O_{yl}=U=O_{yl}	179.8	179.8		
	O_{yl}=U-O_{eq}	89.7	89.7		
	O_{yl}=U-O_{eq}	90.0	89.9		
	O_{yl}=U-C	89.6	89.5		
	O_{eq}-U-O_{eq}	67.5	67.5		
3a	O_{yl}=U=O_{yl}	179.4	179.4	179.4	
	O_{yl}=U-O_{eq}	89.9	89.5	89.6	
	O_{yl}=U-O_{eq}	90.0	89.9	89.9	
	O_{yl}=U-C	90.2	89.4	89.5	
	O_{eq}-U-O_{eq}	67.5	67.5	67.6	
4a	O_{yl}=U=O_{yl}	179.1	179.1	179.1	179.0
	O_{yl}=U-O_{eq}	89.3	89.6	89.9	89.7
	O_{yl}=U-O_{eq}	90.0	89.8	90.0	90.1
	O_{yl}=U-C	89.4	89.5	90.2	90.1
	O_{eq}-U-O_{eq}	67.7	67.6	67.6	67.7
trans-**1a**-Cs	O_{yl}=U=O_{yl}	176.9	177.1		
	O_{yl}=U-O_{eq}	87.8	85.9		
	O_{yl}=U-O_{eq}	91.8	91.8		
	O_{yl}=U-C	88.8	89.7		

	O_{eq}-U-O_{eq}	52.1	67.8	
	O_{eq}-Cs-O_{eq}		54.2	
	O_{eq}-Cs-O_{eq}		53.9	
cis-**1a**-Cs	O_{yl}=U=O_{yl}	177.0	177.2	
	O_{yl}=U-O_{eq}	90.6	92.4	
	O_{yl}=U-O_{eq}	92.0	85.6	
	O_{yl}=U-C	91.7	89.7	
	O_{eq}-U-O_{eq}	68.0	67.3	
	O_{eq}-Cs-O_{eq}		53.2	
	O_{eq}-Cs-O_{eq}		54.0	
1a-2Cs-*d*	O_{yl}=U=O_{yl}	176.7	177.7	177.3
	O_{yl}=U-O_{eq}	92.2	90.4	92.2
	O_{yl}=U-O_{eq}	91.5	92.6	82.6
	O_{yl}=U-C	91.9	91.9	88.0
	O_{eq}-U-O_{eq}	68.0	67.2	66.4
	O_{eq}-Cs-O_{eq}		54.0	51.8
	O_{eq}-Cs-O_{eq}		52.2	53.6
1a-2Cs-*s*	O_{yl}=U=O_{yl}	176.4	177.0	176.7
	O_{yl}=U-O_{eq}	91.5	93.7	90.5
	O_{yl}=U-O_{eq}	91.0	86.4	91.3
	O_{yl}=U-C	91.6	94.1	90.7
	O_{eq}-U-O_{eq}	68.1	67.5	67.7
	O_{eq}-Cs-O_{eq}		55.0	54.5
	O_{eq}-Cs-O_{eq}		53.2	52.0

Table S15. Calculated electron density [ρ(r)], Laplacian [$\nabla^2\rho(r)$], energy density [H(r)] and ellipticity (ε) at U-X bond critical points (BCPs) (all values in au.), together with bond orders calculated by different approaches.

		BCPs	ρ(*r*)	$\nabla^2\rho(r)$	H(*r*)	ε	Bond order[a]	Bond order[b]
1a	unit1	U-O_{eq1}	0.0524	0.1700	-0.0025	0.1517	0.41	0.47
		U-O_{eq2}	0.0522	0.1691	-0.0024	0.1509	0.41	0.46
		U-O_{eq3}	0.0568	0.1797	-0.0036	0.1651	0.47	0.52
		U-O_{eq4}	0.0567	0.1802	-0.0036	0.1682	0.46	0.52
		U-O_{eq5}	0.0568	0.1804	-0.0036	0.1684	0.46	0.52
		U-O_{eq6}	0.0567	0.1795	-0.0036	0.1651	0.47	0.51
		$(U\text{-}O_{eq})_{av}$	0.0553	0.1765	-0.0032	0.1616	0.45	0.50
		U-O_{yl1}	0.2799	0.1840	-0.2482	0.0013	2.21	2.37
		U-O_{yl2}	0.2799	0.1840	-0.2482	0.0013	2.21	2.37
		$(U\text{-}O_{yl})_{av}$	0.2799	0.1840	-0.2482	0.0013	2.21	2.37
4a	unit1	U-O_{eq1}	0.0551	0.1767	-0.0031	0.1672	0.44	0.51
		U-O_{eq2}	0.0557	0.1789	-0.0032	0.1688	0.44	0.51

	$U\text{-}O_{eq3}$	0.0557	0.1770	-0.0033	0.1636	0.46	0.50
	$U\text{-}O_{eq4}$	0.0536	0.1705	-0.0029	0.1545	0.45	0.49
	$U\text{-}O_{eq5}$	0.0539	0.1713	-0.0030	0.1554	0.45	0.50
	$U\text{-}O_{eq6}$	0.0561	0.1783	-0.0034	0.1644	0.46	0.50
	$(U\text{-}O_{eq})_{av}$	0.0550	0.1755	-0.0031	0.1623	0.45	0.50
	$U\text{-}O_{yl1}$	0.2795	0.1845	-0.2476	0.0004	2.21	2.37
	$U\text{-}O_{yl2}$	0.2795	0.1847	-0.2476	0.0006	2.21	2.37
	$(U\text{-}O_{yl})_{av}$	0.2795	0.1846	-0.2476	0.0005	2.21	2.37
unit2	$U\text{-}O_{eq1}$	0.0557	0.1788	-0.0032	0.1688	0.44	0.50
	$U\text{-}O_{eq2}$	0.0551	0.1770	-0.0031	0.1677	0.44	0.49
	$U\text{-}O_{eq3}$	0.0564	0.1795	-0.0035	0.1662	0.46	0.50
	$U\text{-}O_{eq4}$	0.0535	0.1701	-0.0029	0.1540	0.45	0.51
	$U\text{-}O_{eq5}$	0.0538	0.1710	-0.0029	0.1547	0.45	0.50
	$U\text{-}O_{eq6}$	0.0556	0.1766	-0.0033	0.1629	0.45	0.50
	$(U\text{-}O_{eq})_{av}$	0.0550	0.1755	-0.0031	0.1624	0.45	0.50
	$U\text{-}O_{yl1}$	0.2795	0.1849	-0.2474	0.0007	2.21	2.37
	$U\text{-}O_{yl2}$	0.2797	0.1842	-0.2478	0.0006	2.21	2.37
	$(U\text{-}O_{yl})_{av}$	0.2796	0.1845	-0.2476	0.0006	2.21	2.37
unit3	$U\text{-}O_{eq1}$	0.0558	0.1792	-0.0032	0.1690	0.44	0.50
	$U\text{-}O_{eq2}$	0.0551	0.1768	-0.0031	0.1671	0.44	0.50
	$U\text{-}O_{eq3}$	0.0562	0.1786	-0.0034	0.1648	0.46	0.50
	$U\text{-}O_{eq4}$	0.0539	0.1712	-0.0030	0.1554	0.45	0.50
	$U\text{-}O_{eq5}$	0.0537	0.1707	-0.0029	0.1547	0.45	0.51
	$U\text{-}O_{eq6}$	0.0556	0.1768	-0.0033	0.1634	0.46	0.50
	$(U\text{-}O_{eq})_{av}$	0.0550	0.1755	-0.0031	0.1624	0.45	0.50
	$U\text{-}O_{yl1}$	0.2795	0.1847	-0.2476	0.0006	2.21	2.37
	$U\text{-}O_{yl2}$	0.2796	0.1845	-0.2476	0.0004	2.21	2.37
	$(U\text{-}O_{yl})_{av}$	0.2795	0.1846	-0.2476	0.0005	2.21	2.37
unit4	$U\text{-}O_{eq1}$	0.0552	0.1771	-0.0031	0.1676	0.44	0.50
	$U\text{-}O_{eq2}$	0.0557	0.1787	-0.0032	0.1686	0.44	0.50
	$U\text{-}O_{eq3}$	0.0556	0.1767	-0.0033	0.1632	0.45	0.50
	$U\text{-}O_{eq4}$	0.0537	0.1707	-0.0029	0.1546	0.45	0.51
	$U\text{-}O_{eq5}$	0.0538	0.1711	-0.0030	0.1552	0.45	0.50
	$U\text{-}O_{eq6}$	0.0562	0.1785	-0.0034	0.1649	0.46	0.50
	$(U\text{-}O_{eq})_{av}$	0.0550	0.1755	-0.0031	0.1624	0.45	0.50
	$U\text{-}O_{yl1}$	0.2796	0.1845	-0.2476	0.0004	2.21	2.37
	$U\text{-}O_{yl2}$	0.2795	0.1848	-0.2475	0.0006	2.21	2.37

		$(U\text{-}O_{yl})_{av}$	0.2795	0.1846	-0.2476	0.0005	2.21	2.37
trans-**1a**-Cs	unit1	$U\text{-}O_{eq1}$	0.0582	0.1877	-0.0038	0.1835	0.45	0.44
		$U\text{-}O_{eq2}$	0.0584	0.1884	-0.0038	0.1841	0.45	0.44
		$U\text{-}O_{eq3}$	0.0575	0.1810	-0.0038	0.1641	0.46	0.52
		$U\text{-}O_{eq4}$	0.0524	0.1663	-0.0027	0.1535	0.47	0.51
		$U\text{-}O_{eq5}$	0.0523	0.1659	-0.0027	0.1526	0.46	0.51
		$U\text{-}O_{eq6}$	0.0573	0.1804	-0.0037	0.1634	0.45	0.52
		$(U\text{-}O_{eq})_{av}$	0.0560	0.1783	-0.0034	0.1669	0.46	0.49
		$U\text{-}O_{yl1}$	0.2727	0.2019	-0.2354	0.0038	2.22	2.32
		$U\text{-}O_{yl2}$	0.2835	0.1703	-0.2546	0.0048	2.23	2.38
		$(U\text{-}O_{yl})_{av}$	0.2781	0.1861	-0.2450	0.0043	2.22	2.35
	unit2	$U\text{-}O_{eq1}$	0.0512	0.1626	-0.0025	0.1499	0.46	0.43
		$U\text{-}O_{eq2}$	0.0513	0.1628	-0.0025	0.1497	0.46	0.43
		$U\text{-}O_{eq3}$	0.0565	0.1785	-0.0035	0.1629	0.45	0.51
		$U\text{-}O_{eq4}$	0.0608	0.1924	-0.0046	0.1918	0.49	0.55
		$U\text{-}O_{eq5}$	0.0607	0.1921	-0.0046	0.1914	0.49	0.51
		$U\text{-}O_{eq6}$	0.0567	0.1791	-0.0035	0.1635	0.45	0.55
		$(U\text{-}O_{eq})_{av}$	0.0562	0.1779	-0.0036	0.1682	0.47	0.50
		$U\text{-}O_{yl1}$	0.2714	0.2042	-0.2331	0.0026	2.21	2.38
		$U\text{-}O_{yl2}$	0.2826	0.1715	-0.2529	0.0040	2.22	2.31
		$(U\text{-}O_{yl})_{av}$	0.2770	0.1879	-0.2430	0.0033	2.22	2.35
		$Cs\text{-}O_{eq1}$	0.0130	0.0493	0.0013	0.1099	0.01	0.10
		$Cs\text{-}O_{eq2}$	0.0131	0.0500	0.0013	0.1095	0.01	0.10
		$Cs\text{-}O_{eq1'}$	0.0133	0.0506	0.0013	0.1105	0.01	0.10
		$Cs\text{-}O_{eq2'}$	0.0135	0.0518	0.0013	0.1089	0.01	0.10
		$Cs\text{-}O_{yl}$	0.0093	0.0329	0.0010	0.0800	0.01	
		$Cs\text{-}O_{yl'}$	0.0098	0.0350	0.0011	0.0742	-0.02	
cis-**1a**-Cs	unit1	$U\text{-}O_{eq1}$	0.0532	0.1716	-0.0027	0.1540	0.45	0.42
		$U\text{-}O_{eq2}$	0.0539	0.1732	-0.0028	0.1572	0.42	0.46
		$U\text{-}O_{eq3}$	0.0613	0.1938	-0.0048	0.1892	0.49	0.55
		$U\text{-}O_{eq4}$	0.0610	0.1927	-0.0047	0.1927	0.49	0.48
		$U\text{-}O_{eq5}$	0.0575	0.1817	-0.0037	0.1644	0.45	0.55
		$U\text{-}O_{eq6}$	0.0502	0.1584	-0.0024	0.1427	0.45	0.51
		$(U\text{-}O_{eq})_{av}$	0.0562	0.1786	-0.0035	0.1667	0.46	0.50
		$U\text{-}O_{yl1}$	0.2833	0.1700	-0.2542	0.0027	2.21	2.31
		$U\text{-}O_{yl2}$	0.2716	0.2043	-0.2334	0.0028	2.22	2.38
		$(U\text{-}O_{yl})_{av}$	0.2775	0.1872	-0.2438	0.0027	2.22	2.35

unit2	U-O_{eq1}	0.0597	0.1888	-0.0044	0.1866	0.48	0.42
	U-O_{eq2}	0.0590	0.1889	-0.0041	0.1892	0.43	0.44
	U-O_{eq3}	0.0570	0.1800	-0.0036	0.1633	0.45	0.51
	U-O_{eq4}	0.0523	0.1662	-0.0027	0.1522	0.46	0.51
	U-O_{eq5}	0.0513	0.1633	-0.0025	0.1505	0.45	0.52
	U-O_{eq6}	0.0573	0.1809	-0.0037	0.1641	0.45	0.53
	$(U\text{-}O_{eq})_{av}$	0.0561	0.5340	-0.0035	0.1676	0.45	0.49
	U-O_{yl1}	0.2729	0.2009	-0.2357	0.0032	2.21	2.38
	U-O_{yl2}	0.2832	0.1714	-0.2540	0.0041	2.22	2.32
	$(U\text{-}O_{yl})_{av}$	0.2780	0.1862	-0.2448	0.0037	2.22	2.35
	Cs-O_{eq1}	0.0135	0.0510	0.0013	0.0924	0.00	0.11
	Cs-O_{eq2}	0.0122	0.0465	0.0013	0.1123	0.02	0.07
	Cs-$O_{eq1'}$	0.0131	0.0500	0.0013	0.1076	0.01	0.09
	Cs-$O_{eq2'}$	0.0128	0.0488	0.0013	0.1110	0.02	0.11
	Cs-O_{yl}	0.0091	0.0326	0.0010	0.0809	-0.02	
	Cs-$O_{yl'}$	0.0096	0.0342	0.0011	0.0713	-0.02	

[a] Bond order of Mayer calculated with QTAIM

[b] Bond order of Mayer calculated with the Priroda code.

Table S16. Decomposition of the interaction energy between uranyl parts and Cs atom calculated by the ADF Code (Energies in eV).[a]

	$E_{Electro}$	E_{Pauli}	E_{Steric}	E_{Orbit}	$E_{Kinetic}$	E_{Coulm}	E_{XC}	ΔE_{TBE}
trans-**1a**-Cs [b]	-5.958	1.061	-4.897	-0.773	3.413	-1.635	-1.491	-5.670
cis-**1a**-Cs [b]	-5.994	1.162	-4.832	-0.937	4.091	-2.085	-1.780	-5.769
trans-**1a**-Cs' [b]	-5.992	1.060	-4.932	-0.767	3.355	-1.574	-1.487	-5.698
trans-**1a**-Cs' [c]	-6.094	1.083	-5.011	-0.743	2.141	-0.183	-1.618	-5.754

[a] $\Delta E_{TBE} = E_{Electro} + E_{Pauli} + E_{Orbit}$ $\Delta E_{TBE} = E_{Steric} + E_{Orbit}$

$$\Delta E_{TBE} = E_{Electro} + E_{Kinetic} + E_{Coulm} + E_{XC}$$

$E_{Electro}$, E_{Pauli}, E_{Orbit} and E_{Steric} denote the energy of electrostatic interaction, Pauli repulsion, orbital interactions and steric interaction, respectively. The terms $E_{Kinetic}$, E_{Coulm} and E_{XC} correspond to contributions from kinetic energy, Coulomb energy and exchange-correlation energy, respectively. Detailed description and discussion of the energy contributions are given in the paper of Bickelhaupt and Baerends.[1]

[b] Resutls from GGA-PBE calculations.

[c] Resutls from hybrid PBE0 calculations.

Table S17. Bond lengths (average values) of *trans*-**1a**-Cs' optimized by different functionals implemented in the Priroda code. (Distances in Å)

	PBE		**PBE0**	
	Unit1	Unit2	Unit1	Unit2
$U{=}O_{yl}$	1.813	1.812	1.773	1.771
$U{-}O_{eq}$	2.496	2.496	2.477	2.478
U-C	2.869	2.869	2.847	2.846
$Cs{-}O_{eq}$		3.079		3.049
$Cs{-}O_{eq}$		3.071		3.030
$Cs{-}O_{yl}$		3.273		3.320
$Cs{-}O_{eq}$		3.077		3.038
$Cs{-}O_{eq}$		3.092		3.056
$Cs{-}O_{yl}$		3.288		3.342

References:

[1] Bickelhaupt, F. M.; Baerends, E. J. Kohn-Sham Density Functional Theory: Predicting and Understanding Chemistry. *Rev. Comput. Chem.* **2000**, *15*, 1-86.

Cartesian coordinates of optimized model compounds and ligands

L^1

C	-2.08783360	8.66626715	14.42776573
C	-0.11046451	8.45065809	12.41431309
C	0.73508454	8.64439906	18.82958120
C	-2.46324747	8.58345977	13.04614088
C	-1.86681914	8.36921879	10.66025479
H	-1.08905595	8.27450793	9.89677187
C	-1.46191875	8.46540470	12.03144622
C	-0.24165816	8.63439124	16.18268045
C	-0.71057851	8.61345611	14.77491151
C	0.24968424	8.52666123	13.75374807
H	1.30589798	8.48239275	14.03257073
C	-3.13017422	8.84597685	15.39900266
H	-2.85181469	8.96396932	16.44773181
C	-0.70021807	7.69214211	17.12367231
C	0.72099754	9.57413723	16.59423120
H	-1.42536217	6.93595279	16.81313570
H	1.07766795	10.31801907	15.87706226
C	-0.21730236	7.69758940	18.42666358
C	1.20305268	9.58406774	17.90007818
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H	1.94140531	10.32537351	18.21003528
O	0.83281735	7.80560304	21.07699031
O	2.13660333	9.56740208	20.50869439
C	1.20836268	8.59856137	20.23987689
C	-3.83929211	8.62427544	12.67217056
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C	-4.85238450	8.76839331	13.67044661
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C	-6.20271047	8.80247223	13.27925328
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C	-6.55826669	8.69735301	11.93576864
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H	-5.21903270	9.03588376	15.79847108
H	-7.61281476	8.72447561	11.64982246
H	2.36912686	9.43811561	21.45349103
H	0.66134343	8.36278750	11.64430483
H	-6.97416753	8.91476099	14.04651916
H	-5.86301493	8.48182723	9.89999863

L^4 (H_4TBAPy)

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1a

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p-**2a**

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m-**2a**

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