

Organic-functionalization of Uranyl Peroxide Clusters to Impact Solubility

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Elemental Analysis Results

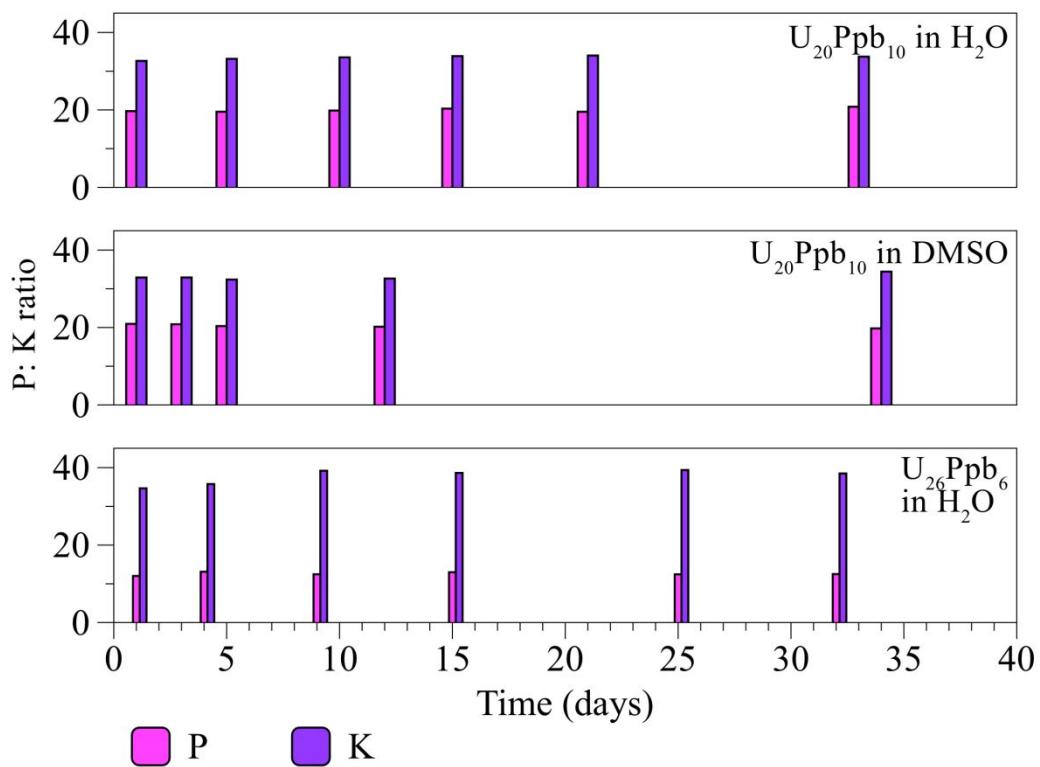


Figure S1. P: K ratios for saturated water or DMSO solutions of K- $\text{U}_{20}\text{Ppb}_{10}$ and K- $\text{U}_{26}\text{Ppb}_6$, measured by ICP-OES. Atomic ratios of P: K versus time in solutions are normalized to the number of U (i.e., 20 U for $\text{U}_{20}\text{Ppb}_{10}$ and 26 U for $\text{U}_{26}\text{Ppb}_6$).

ESI-MS Spectra Analyses

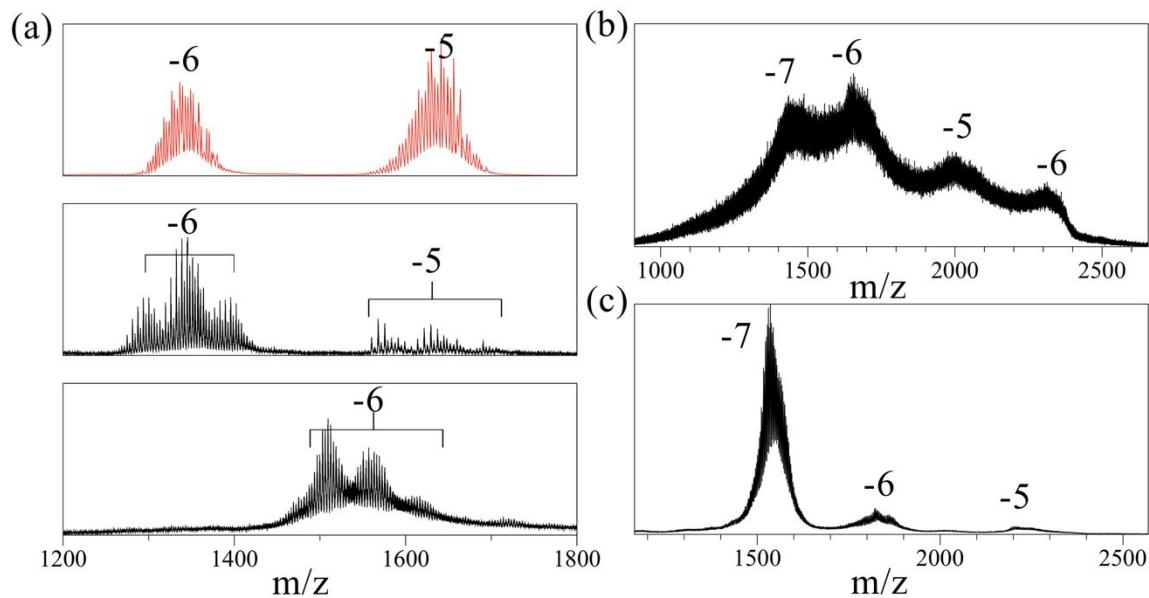


Figure S2. ESI-MS spectra of (a) K-U₂₀Pb₁₀ in water, (b) K-U₂₀Pb₁₀ in DMSO, and (c) K-U₂₆Pb₆ in water. Charge state is labeled on the top of each peak. In (a), the spectrum of fresh solution of K-U₂₀Pb₁₀ is shown on the bottom and that of the aged solution is shown in the middle, and the spectrum of K-U₂₄ that is retrieved from a reported work is shown in red on the top as a comparison.¹

Table S1. Detailed assignment of mass spectral data for K-U₂₀Ppb₁₀ and K-U₂₆Ppb₆K-U₂₀Ppb₁₀ in water

Ion	Charge	Calculated m/z	Observed m/z
K ₁₆ H ₁₈ [(UO ₂) ₂₀ (O ₂) ₂₀ (PO ₃) ₂₀ (C ₆ H ₄) ₁₀](H ₂ O) ₂	-6	1510.1	1509.4
K ₂₄ H ₁₀ [(UO ₂) ₂₀ (O ₂) ₂₀ (PO ₃) ₂₀ (C ₆ H ₄) ₁₀]H ₂ O	-6	1557.9	1557.0
K ₃₁ H ₃ [(UO ₂) ₂₀ (O ₂) ₂₀ (PO ₃) ₂₀ (C ₆ H ₄) ₁₀](H ₂ O) ₆	-6	1617.3	1616.6

K-U₂₀Ppb₁₀ in DMSO

Ion	Charge	Calculated m/z	Observed m/z
K ₃₀ H ₃ [(UO ₂) ₂₀ (O ₂) ₂₀ (PO ₃) ₂₀ (C ₆ H ₄) ₁₀](DMSO) ₆ H ₂ O	-7	1434.8	1435.0
K ₂₉ H ₅ [(UO ₂) ₂₀ (O ₂) ₂₀ (PO ₃) ₂₀ (C ₆ H ₄) ₁₀](DMSO) ₅ (H ₂ O)	-6	1654.8	1655.0
K ₂₈ H ₇ [(UO ₂) ₂₀ (O ₂) ₂₀ (PO ₃) ₂₀ (C ₆ H ₄) ₁₀](DMSO) ₆	-5	1990.3	1991.0
K ₂₂ H ₁₄ [(UO ₂) ₂₀ (O ₂) ₂₀ (PO ₃) ₂₀ (C ₆ H ₄) ₁₀]	-4	2313.8	2313.1

K-U₂₆Ppb₆ in water

Ion	Charge	Calculated m/z	Observed m/z
K ₂₄ H ₇ (UO ₂) ₂₆ (O ₂) ₃₃ (C ₆ H ₄ P ₂ O ₆) ₄ (H ₂ O) ₄₄	-7	1535.8	1535.9
K ₃₀ H ₂ (UO ₂) ₂₆ (O ₂) ₃₃ (C ₆ H ₄ P ₂ O ₆) ₄ (H ₂ O) ₄₄	-6	1830.1	1830.0
K ₂₆ H ₅ (UO ₂) ₂₆ (O ₂) ₃₃ (C ₆ H ₄ P ₂ O ₆) ₄ (H ₂ O) ₅₇	-5	2212.3	2212.5

Small-Angle X-ray Scattering (SAXS)

X-ray scattering data were collected using a Bruker Nanostar instrument equipped with a Cu microfocus source, Montel multilayer optics, and a HiSTAR multiwire detector. Aliquots of the solutions at steady states from the dissolution experiment were taken and each was placed into a 1.5 mm diameter capillary and sealed. Data for each sample, as well as the water and DMSO solution for the purpose of background subtraction, were collected for 2 h, with the solution located 26.3 cm from the detector. Data integration, normalization, and background subtraction were conducted using the Bruker Nanofit software. The radius of gyration (R_g) of each sample was derived via Guinier analysis from the slope of the experimental SAXS curve.

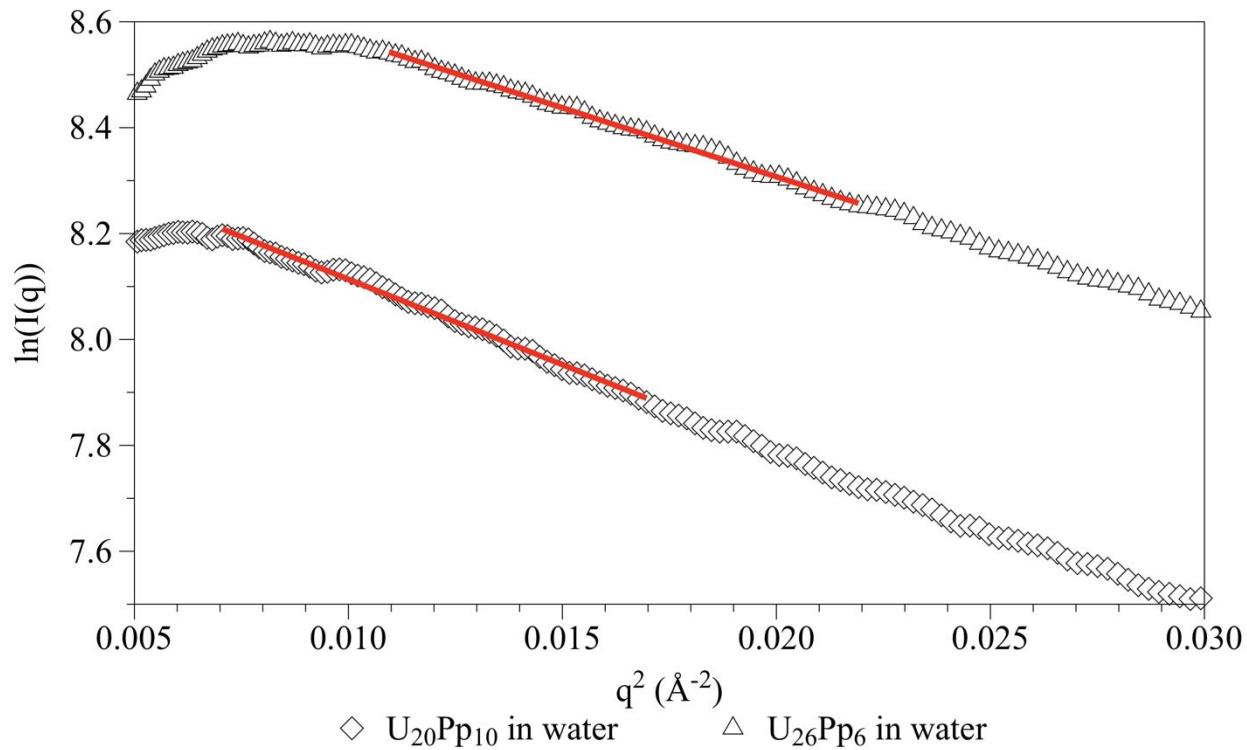


Figure S3. SAXS data of K-U₂₀Ppb₁₀ and K-U₂₆Ppb₆ in water in Guinier plot. The solutions were obtained from the end solutions from the dissolution experiment. The SAXS profile gives a $R_g = 9.84 \text{ \AA}$ for K-U₂₀Ppb₁₀, and 8.69 \AA for K-U₂₆Ppb₁₆.

Table S2. Crystal data and structure refinement for K-U₂₀Ppb₁₀

Identification code	c2m
Empirical formula	C ₆₀ H ₃₆ K _{22.30} O _{187.50} P ₂₀ U ₂₀
Formula weight	10008.82
Temperature	180(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/m
<i>a</i>	36.081(4) Å
<i>b</i>	32.094(4) Å
<i>c</i>	23.080(3) Å
α	90°
β	94.8286(18)°
γ	90°
Volume	26631(5) Å ³
<i>Z</i>	4
Density (calculated)	2.496 g.cm ⁻³
Absorption coefficient (μ)	12.683 mm ⁻¹
F(000)	17839
Crystal size	0.100 × 0.060 × 0.020 mm ³
θ range for data collection	0.850 to 22.947°
Index ranges	-39 ≤ <i>h</i> ≤ 39, -34 ≤ <i>k</i> ≤ 34, -25 ≤ <i>l</i> ≤ 25
Reflections collected	110798
Independent reflections	18545 [$R_{\text{int}} = 0.1520$]
Completeness to $\theta = 22.947^\circ$	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7448 and 0.5923
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	18545 / 0 / 834
Goodness-of-fit on F ²	1.046
Final R indices [I>2σ(I)]	$R_1 = 0.0656$, $wR_2 = 0.1669$
R indices (all data)	$R_1 = 0.1233$, $wR_2 = 0.2025$
Extinction coefficient	n/a
Largest diff. peak and hole	2.604 and -2.253 e ⁻ .Å ⁻³

**Table S3. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2)
for K-U₂₀Ppb₁₀. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.**

	x	y	z	U(eq)
U(1)	-0.31224(4)	0.5000	-0.33405(6)	0.025(1)
U(2)	-0.54807(4)	0.5000	-0.74307(6)	0.025(1)
U(3)	-0.18403(4)	0.5000	0.12299(6)	0.029(1)
U(4)	-0.31760(3)	0.60850(3)	-0.44422(4)	0.026(1)
U(5)	-0.17490(3)	0.56688(3)	-0.16210(4)	0.029(1)
U(6)	-0.17956(3)	0.60928(3)	0.01493(4)	0.030(1)
U(7)	-0.04338(4)	0.5000	0.23676(6)	0.027(1)
U(8)	-0.32627(3)	0.56622(3)	-0.62191(4)	0.026(1)
U(9)	-0.53850(3)	0.66874(3)	-0.57660(4)	0.030(1)
U(10)	-0.47547(3)	0.60356(3)	-0.69504(4)	0.030(1)
U(11)	-0.03649(3)	0.66857(3)	0.06957(4)	0.031(1)
U(12)	0.02863(3)	0.60302(3)	0.20400(4)	0.031(1)
K(1)	-0.4301(3)	0.5000	-0.6451(4)	0.045(2)
K(2)	-0.1495(3)	0.5000	-0.0279(4)	0.040(2)
K(3)	-0.3474(2)	0.5000	-0.4936(4)	0.037(2)
K(4)	0.0723(3)	0.5000	0.1626(4)	0.046(2)
K(5)	-0.0827(2)	0.4346(2)	0.1083(3)	0.052(2)
K(6)	0.0770(2)	0.3944(2)	0.0623(3)	0.060(2)
K(7)	-0.58526(18)	0.4349(2)	-0.6241(3)	0.045(2)
K(8)	-0.1921(2)	0.5000	-0.3162(4)	0.034(2)
K(9)	-0.2713(2)	0.5000	-0.1776(4)	0.042(2)
K(10)	-0.2798(2)	0.6183(2)	-0.2683(3)	0.058(2)
K(11)	-0.4215(2)	0.6041(2)	-0.5435(3)	0.056(2)
K(12)	-0.2348(3)	0.5000	-0.6422(6)	0.084(4)
K(13A)	-0.2015(4)	0.6244(4)	0.1904(6)	0.048(4)
K(13B)	-0.2187(11)	0.6275(11)	0.1622(17)	0.028(9)
K(14)	-0.0414(4)	0.6952(4)	0.3628(6)	0.062(4)
K(15)	-0.0415(4)	0.8059(4)	0.1295(7)	0.069(5)
K(16)	-0.0510(6)	0.7621(6)	-0.0626(9)	0.027(5)

K(17A)	0.1906(5)	0.3022(5)	0.1305(7)	0.070(5)
K(17B)	0.2171(9)	0.3226(10)	0.1255(14)	0.067(9)
P(1)	-0.39016(19)	0.5678(2)	-0.7549(3)	0.027(2)
P(2)	-0.6247(2)	0.7002(2)	-0.5166(3)	0.034(2)
P(3)	-0.36326(19)	0.5544(2)	-0.2267(3)	0.028(2)
P(4)	-0.1270(2)	0.6692(2)	0.1291(3)	0.034(2)
P(5)	-0.6304(2)	0.6672(2)	-0.6574(3)	0.034(2)
P(6)	-0.1234(2)	0.7005(2)	-0.0117(3)	0.032(2)
P(7)	-0.3850(2)	0.6545(2)	-0.6709(3)	0.038(2)
P(8)	0.1186(2)	0.6552(2)	0.2001(3)	0.043(2)
P(9)	-0.11485(19)	0.5677(2)	-0.2833(3)	0.029(2)
P(10)	-0.1325(2)	0.4463(2)	0.2444(3)	0.039(2)
O(1)	-0.3585(6)	0.5000	-0.3696(9)	0.026(6)
O(2)	-0.1977(6)	0.5000	-0.1392(9)	0.026(6)
O(3)	-0.0964(5)	0.4562(5)	0.2182(7)	0.032(4)
O(4)	-0.0491(7)	0.5000	0.3127(10)	0.035(6)
O(5)	-0.6018(4)	0.4570(5)	-0.7370(7)	0.028(4)
O(6)	-0.5429(6)	0.5000	-0.6645(9)	0.022(5)
O(7)	-0.3004(6)	0.5000	-0.5952(10)	0.031(6)
O(8)	-0.2925(5)	0.5438(5)	-0.4089(7)	0.033(4)
O(9)	-0.0247(5)	0.5704(5)	0.2374(7)	0.030(4)
O(10)	-0.1832(6)	0.5000	-0.1984(9)	0.024(5)
O(11)	-0.3630(5)	0.5997(5)	-0.2082(7)	0.036(4)
O(12)	-0.1376(6)	0.5000	0.0978(10)	0.030(6)
O(13)	-0.4729(5)	0.6346(5)	-0.7589(7)	0.031(4)
O(14)	-0.2051(4)	0.5440(5)	0.0448(7)	0.030(4)
O(15)	0.0273(5)	0.5705(5)	0.1400(8)	0.040(5)
O(16)	0.0130(5)	0.6612(5)	0.1424(7)	0.038(5)
O(17)	-0.5290(5)	0.4285(5)	-0.7390(7)	0.037(5)
O(18)	-0.5543(7)	0.5000	-0.8185(10)	0.033(6)
O(19)	-0.3042(5)	0.5688(5)	-0.3594(7)	0.032(4)
O(20)	-0.1512(4)	0.5614(5)	-0.2532(6)	0.024(4)
O(21)	-0.3150(6)	0.5000	-0.6571(9)	0.027(6)
O(22)	-0.3547(4)	0.5598(5)	-0.7177(7)	0.026(4)
O(23)	-0.2837(4)	0.5815(5)	-0.6492(7)	0.027(4)
O(24)	-0.3691(4)	0.5515(5)	-0.5940(6)	0.024(4)

O(25)	-0.3628(5)	0.5843(5)	-0.4556(7)	0.033(4)
O(26)	0.0322(5)	0.6352(5)	0.2687(7)	0.034(4)
O(27)	-0.1987(5)	0.5707(5)	-0.0697(7)	0.033(4)
O(28)	-0.2298(7)	0.5000	0.1469(10)	0.036(6)
O(29)	-0.1594(5)	0.6471(5)	0.0999(7)	0.035(4)
O(30)	-0.0398(6)	0.5000	0.1596(10)	0.030(6)
O(31)	-0.5154(5)	0.6892(5)	-0.4809(7)	0.039(5)
O(32)	0.0801(5)	0.5625(5)	0.2412(8)	0.040(5)
O(33)	-0.4757(5)	0.5723(5)	-0.6305(7)	0.038(5)
O(34)	-0.5245(5)	0.6465(5)	-0.6702(7)	0.032(4)
O(35)	-0.4234(5)	0.5641(5)	-0.7200(7)	0.038(5)
O(36)	-0.3500(5)	0.6336(5)	-0.6467(7)	0.035(4)
O(37)	-0.3126(5)	0.6120(5)	-0.5439(7)	0.032(4)
O(38)	-0.0412(4)	0.7218(5)	0.0925(7)	0.030(4)
O(39)	-0.4978(5)	0.5447(5)	-0.7499(7)	0.037(5)
O(40)	-0.0886(5)	0.6750(5)	-0.0005(7)	0.039(5)
O(41)	-0.1923(5)	0.5693(5)	0.0963(7)	0.032(4)
O(42)	-0.2729(5)	0.6321(5)	-0.4327(7)	0.032(4)
O(43)	-0.1866(5)	0.6127(5)	-0.0861(8)	0.041(5)
O(44)	-0.3288(5)	0.5444(5)	-0.2577(7)	0.032(4)
O(45)	0.0846(5)	0.6334(6)	0.1741(8)	0.043(5)
O(46)	-0.0334(5)	0.6153(5)	0.0463(7)	0.035(4)
O(47)	-0.5355(5)	0.6153(5)	-0.5528(7)	0.032(4)
O(48)	-0.4899(5)	0.6619(5)	-0.6387(7)	0.040(5)
O(49)	0.0161(5)	0.6880(5)	0.0219(7)	0.038(5)
O(50)	-0.2979(5)	0.5715(5)	-0.5236(7)	0.032(4)
O(51)	-0.5440(5)	0.7222(5)	-0.6024(7)	0.031(4)
O(52)	0.0079(5)	0.5453(5)	0.2556(7)	0.038(5)
O(53)	-0.2253(4)	0.6319(5)	0.0164(7)	0.030(4)
O(54)	-0.5893(5)	0.6752(6)	-0.5186(8)	0.043(5)
O(55)	-0.1662(5)	0.5435(5)	0.2021(7)	0.038(5)
O(56)	-0.1584(5)	0.6741(5)	-0.0171(7)	0.034(4)
O(57)	-0.6236(5)	0.7274(6)	-0.4628(8)	0.044(5)
O(58)	-0.1306(4)	0.5529(5)	-0.1261(7)	0.026(4)
O(59)	-0.2191(5)	0.5796(5)	-0.1976(7)	0.031(4)
O(60)	-0.2657(7)	0.5000	-0.2973(10)	0.034(6)

O(61)	-0.1337(5)	0.5850(5)	0.0139(7)	0.036(4)
O(62)	-0.3414(5)	0.6725(5)	-0.4780(7)	0.033(4)
O(63)	-0.3355(5)	0.6450(5)	-0.3598(7)	0.033(4)
O(64)	0.1195(6)	0.7008(6)	0.1821(9)	0.060(6)
O(65)	-0.3929(5)	0.5382(5)	-0.8084(8)	0.041(5)
O(66)	-0.0914(5)	0.6511(5)	0.1151(8)	0.041(5)
O(67)	-0.6318(5)	0.6683(6)	-0.7250(8)	0.046(5)
O(68)	-0.5949(5)	0.6484(6)	-0.6321(8)	0.043(5)
O(69)	-0.1294(6)	0.6693(7)	0.1967(9)	0.066(6)
O(70)	-0.3828(6)	0.7012(6)	-0.6497(9)	0.057(6)
O(71)	-0.4194(6)	0.6341(6)	-0.6526(9)	0.055(6)
O(72)	-0.0207(5)	0.6456(5)	0.1660(7)	0.039(5)
O(73)	-0.1149(5)	0.5378(5)	-0.3363(7)	0.036(4)
O(74)	-0.1543(5)	0.6343(6)	-0.1864(8)	0.044(5)
O(75)	-0.1216(6)	0.7268(6)	-0.0678(8)	0.053(6)
O(76)	-0.1330(7)	0.4008(7)	0.2626(10)	0.074(7)
OW1	0.0249(5)	0.8034(6)	0.1565(8)	0.049(5)
OW2	-0.2725(6)	0.5569(7)	-0.0885(9)	0.064(6)
OW3	-0.2289(6)	0.5530(7)	-0.7376(9)	0.068(6)
OW4	-0.2968(6)	0.5461(7)	0.2115(10)	0.073(7)
OW5	-0.2805(7)	0.5536(8)	0.0337(11)	0.094(8)
OW6	-0.2120(8)	0.6223(9)	-0.3193(12)	0.020(7)
OW7	-0.0659(7)	0.8830(8)	0.1727(11)	0.090(8)
OW8	-0.2963(7)	0.6260(8)	-0.1519(11)	0.085(8)
OW9	-0.2171(9)	0.5558(9)	-0.3984(13)	0.027(8)
OW10	0.0237(8)	0.6928(9)	0.3551(12)	0.020(7)
OW11	-0.0610(9)	0.6158(9)	0.3210(13)	0.027(8)
OW12	-0.2240(9)	0.5479(10)	-0.5316(14)	0.033(9)
OW13	0.4776(15)	0.0000	0.431(2)	0.045(14)
OW14	-0.0538(10)	0.7945(11)	0.2460(15)	0.041(10)
OW15	-0.0409(10)	0.7294(11)	-0.2009(15)	0.043(10)
OW16	-0.0554(10)	0.7034(11)	0.2427(15)	0.037(9)
OW17	0.4515(11)	0.0512(12)	0.4150(17)	0.054(11)
OW18	0.4486(11)	0.4452(12)	0.0774(16)	0.049(11)
OW19	0.0365(11)	0.2326(12)	0.3082(17)	0.052(11)
OW20	-0.0648(18)	0.5000	-0.008(3)	0.069(19)

OW21	0.1028(11)	0.1056(12)	0.0040(16)	0.049(11)
OW22	-0.0460(11)	0.8316(12)	0.0050(17)	0.054(11)
OW23	-0.1788(13)	0.8739(14)	-0.0225(19)	0.071(13)
OW24	-0.0451(12)	0.6707(13)	0.4884(19)	0.068(13)
OW25	-0.2079(16)	0.6269(17)	0.324(2)	0.100(18)
OW26	0.2139(13)	0.3008(14)	0.357(2)	0.075(14)
OW27	0.2709(13)	0.1995(14)	0.343(2)	0.075(14)
OW28	-0.2173(14)	0.7139(16)	0.185(2)	0.089(16)
OW29	-0.0778(14)	0.6369(15)	0.263(2)	0.081(15)
OW30	-0.3177(10)	0.5000	0.1012(15)	0.087(11)
OW31	-0.4350(14)	0.5000	-0.499(2)	0.041(14)
OW32	0.4763(10)	0.5000	0.0675(15)	0.078(10)
OW33	0.1965(6)	0.1918(7)	0.4171(9)	0.066(6)
OW34	0.0523(6)	0.2597(7)	0.4499(9)	0.066(6)
OW35	0.0242(7)	0.0525(8)	0.1409(11)	0.012(7)
OW36	-0.2210(8)	0.8050(9)	0.0074(12)	0.020(7)
OW37	0.2816(8)	0.2248(9)	0.0491(13)	0.022(8)
OW38	0.2809(10)	0.2754(11)	0.4043(15)	0.042(10)
OW39	0.0259(11)	0.4450(12)	0.3746(17)	0.057(11)
OW40	0.1074(12)	0.0276(13)	0.0796(18)	0.065(13)
C(1)	-0.3861(8)	0.6543(8)	-0.7486(12)	0.039(7)
C(2)	-0.3832(8)	0.6942(9)	-0.7766(13)	0.048(8)
C(3)	-0.3828(9)	0.6982(11)	-0.8328(15)	0.070(10)
C(4)	-0.3830(10)	0.6631(12)	-0.8713(18)	0.082(12)
C(5)	-0.3865(9)	0.6235(10)	-0.8445(14)	0.056(9)
C(6)	-0.3888(7)	0.6200(8)	-0.7831(11)	0.029(6)
C(7)	-0.3610(7)	0.5213(8)	-0.1622(11)	0.034(7)
C(8)	-0.3603(8)	0.5433(10)	-0.1097(13)	0.053(8)
C(9)	-0.3590(8)	0.5204(8)	-0.0545(13)	0.050(8)
C(10)	-0.6322(7)	0.7214(8)	-0.6366(11)	0.029(6)
C(11)	-0.6363(8)	0.7513(9)	-0.6816(13)	0.050(8)
C(12)	-0.6358(10)	0.7935(12)	-0.6689(17)	0.079(11)
C(13)	-0.6327(9)	0.8056(11)	-0.6128(15)	0.068(10)
C(14)	-0.6289(8)	0.7766(9)	-0.5649(14)	0.052(8)
C(15)	-0.6284(8)	0.7346(8)	-0.5763(12)	0.039(7)
C(16)	-0.1256(6)	0.7363(7)	0.0506(10)	0.023(6)

C(17)	-0.1287(9)	0.7785(11)	0.0361(16)	0.068(10)
C(18)	-0.1319(10)	0.8071(12)	0.0809(16)	0.072(10)
C(19)	-0.1339(10)	0.7944(12)	0.1350(17)	0.081(12)
C(20)	-0.1325(9)	0.7532(10)	0.1512(14)	0.059(9)
C(21)	-0.1292(7)	0.7239(8)	0.1060(11)	0.034(7)
C(22)	-0.1354(8)	0.4781(8)	0.3090(12)	0.044(7)
C(23)	-0.1394(9)	0.4533(12)	0.3623(15)	0.070(10)
C(24)	-0.1426(10)	0.4802(11)	0.4115(17)	0.089(13)
C(25)	-0.1177(8)	0.6193(8)	-0.3122(12)	0.037(7)
C(26)	0.1182(8)	0.6554(9)	0.2787(12)	0.039(7)
C(27)	0.1207(10)	0.6937(12)	0.3049(16)	0.078(11)
C(28)	0.1213(10)	0.6969(11)	0.3651(16)	0.071(10)
C(29)	-0.1180(10)	0.6638(12)	-0.3994(16)	0.073(11)
C(30)	-0.1161(9)	0.6229(10)	-0.3730(14)	0.059(9)
H(2)	-0.3814	0.7186	-0.7532	0.058
H(3)	-0.3825	0.7254	-0.8488	0.084
H(4)	-0.3809	0.6661	-0.9118	0.099
H(5)	-0.3873	0.5990	-0.8677	0.067
H(8)	-0.3607	0.5729	-0.1097	0.063
H(9)	-0.3582	0.5352	-0.0188	0.060
H(11)	-0.6394	0.7424	-0.7209	0.060
H(12)	-0.6376	0.8136	-0.6993	0.094
H(13)	-0.6330	0.8346	-0.6044	0.082
H(14)	-0.6268	0.7865	-0.5260	0.062
H(17)	-0.1286	0.7875	-0.0031	0.082
H(18)	-0.1327	0.8361	0.0724	0.086
H(19)	-0.1363	0.8149	0.1643	0.097
H(20)	-0.1336	0.7448	0.1905	0.071
H(21)	-0.1295	0.6950	0.1147	0.041
H(23)	-0.1398	0.4237	0.3637	0.085
H(24)	-0.1450	0.4670	0.4478	0.107
H(27)	0.1220	0.7182	0.2819	0.094

Table S4. Anisotropic displacement parameters (\AA^2) for K-U₂₀Ppb₁₀.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[\mathbf{h}^2\mathbf{a}^{*2}\mathbf{U}_{11} + \dots + 2\mathbf{hka}^{*}\mathbf{b}^{*}\mathbf{U}_{12}]$$

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
U(1)	0.0185(7)	0.0283(8)	0.0262(8)	0.000	-0.0048(6)	0.000
U(2)	0.0182(8)	0.0258(8)	0.0318(8)	0.000	-0.0010(6)	0.000
U(3)	0.0173(8)	0.0351(8)	0.0347(9)	0.000	-0.0004(6)	0.000
U(4)	0.0219(5)	0.0294(6)	0.0269(6)	-0.0003(4)	-0.0034(4)	-0.0023(4)
U(5)	0.0208(6)	0.0337(6)	0.0317(6)	-0.0034(5)	-0.0061(4)	0.0012(4)
U(6)	0.0221(6)	0.0334(6)	0.0322(6)	-0.0032(5)	-0.0028(4)	0.0033(4)
U(7)	0.0184(8)	0.0304(8)	0.0310(8)	0.000	-0.0019(6)	0.000
U(8)	0.0210(5)	0.0295(6)	0.0268(6)	0.0002(4)	0.0004(4)	0.0004(4)
U(9)	0.0278(6)	0.0272(6)	0.0347(6)	-0.0008(5)	-0.0010(5)	-0.0019(4)
U(10)	0.0207(6)	0.0307(6)	0.0389(6)	0.0040(5)	-0.0017(5)	-0.0025(4)
U(11)	0.0279(6)	0.0274(6)	0.0362(6)	-0.0010(5)	-0.0054(5)	-0.0002(4)
U(12)	0.0208(6)	0.0302(6)	0.0399(6)	0.0005(5)	-0.0044(5)	-0.0019(4)
K(1)	0.060(6)	0.031(5)	0.044(6)	0.000	0.000(5)	0.000
K(2)	0.049(6)	0.037(5)	0.033(5)	0.000	-0.003(4)	0.000
K(3)	0.044(6)	0.035(5)	0.033(5)	0.000	0.003(4)	0.000
K(4)	0.065(7)	0.029(5)	0.044(6)	0.000	0.006(5)	0.000
K(5)	0.065(5)	0.041(4)	0.049(4)	-0.015(3)	-0.016(4)	0.008(3)
K(6)	0.052(5)	0.080(5)	0.049(4)	-0.036(4)	0.015(4)	-0.013(4)
K(7)	0.043(4)	0.044(4)	0.050(4)	0.021(3)	0.009(3)	0.007(3)
K(8)	0.021(5)	0.039(5)	0.041(5)	0.000	-0.010(4)	0.000
K(9)	0.025(5)	0.063(6)	0.036(5)	0.000	-0.007(4)	0.000
K(10)	0.067(5)	0.046(4)	0.055(5)	-0.003(3)	-0.031(4)	-0.003(4)
K(11)	0.057(5)	0.064(5)	0.046(4)	-0.016(4)	-0.006(4)	0.011(4)
K(12)	0.048(7)	0.104(10)	0.105(10)	0.000	0.024(7)	0.000
K(14)	0.082(11)	0.034(8)	0.066(10)	-0.027(7)	-0.009(8)	0.003(7)
K(15)	0.072(11)	0.039(9)	0.098(13)	-0.021(8)	0.027(9)	-0.004(8)
K(16)	0.025(13)	0.017(11)	0.037(14)	0.015(10)	0.000(10)	0.010(9)

Table S5. Selected bond lengths [Å] for K-U₂₀Ppb₁₀.

atom-atom	distance	atom-atom	distance
U(1)-O(1)	1.80(2)	U(1)-O(60)	1.82(2)
U(1)-O(19)	2.309(16)	U(1)-O(19)#1	2.309(16)
U(1)-O(44)	2.382(16)	U(1)-O(44)#1	2.382(16)
U(1)-O(8)	2.382(17)	U(1)-O(8)#1	2.382(17)
U(2)-O(18)	1.74(2)	U(2)-O(6)	1.81(2)
U(2)-O(39)#1	2.329(17)	U(2)-O(39)	2.329(17)
U(2)-O(17)#1	2.396(17)	U(2)-O(17)	2.396(17)
U(2)-O(5)	2.395(16)	U(2)-O(5)#1	2.395(16)
U(3)-O(28)	1.78(2)	U(3)-O(12)	1.82(2)
U(3)-O(41)	2.318(16)	U(3)-O(41)#1	2.318(16)
U(3)-O(55)	2.346(17)	U(3)-O(55)#1	2.346(17)
U(3)-O(14)	2.367(16)	U(3)-O(14)#1	2.367(16)
U(4)-O(42)	1.781(16)	U(4)-O(25)	1.807(17)
U(4)-O(37)	2.326(16)	U(4)-O(62)	2.334(16)
U(4)-O(50)	2.342(16)	U(4)-O(19)	2.351(16)
U(4)-O(8)	2.382(16)	U(4)-O(63)	2.407(16)
U(5)-O(59)	1.779(16)	U(5)-O(58)	1.796(15)
U(5)-O(10)	2.315(8)	U(5)-O(20)	2.342(15)
U(5)-O(43)	2.353(18)	U(5)-O(27)	2.368(17)
U(5)-O(74)	2.370(18)	U(5)-O(2)	2.375(10)
U(6)-O(53)	1.804(16)	U(6)-O(61)	1.831(17)

U(6)-O(43)	2.326(18)	U(6)-O(41)	2.353(16)
U(6)-O(56)	2.356(17)	U(6)-O(29)	2.368(16)
U(6)-O(27)	2.367(16)	U(6)-O(14)	2.412(16)
U(7)-O(4)	1.78(2)	U(7)-O(30)	1.80(2)
U(7)-O(9)#1	2.356(16)	U(7)-O(9)	2.357(16)
U(7)-O(52)#1	2.364(17)	U(7)-O(52)	2.364(17)
U(7)-O(3)#1	2.385(16)	U(7)-O(3)	2.385(16)
U(8)-O(23)	1.780(16)	U(8)-O(24)	1.787(15)
U(8)-O(21)	2.323(9)	U(8)-O(37)	2.343(16)
U(8)-O(22)	2.366(15)	U(8)-O(36)	2.379(17)
U(8)-O(7)	2.382(10)	U(8)-O(50)	2.416(16)
U(9)-O(47)	1.802(16)	U(9)-O(51)	1.822(16)
U(9)-O(31)#4	2.354(17)	U(9)-O(54)	2.368(19)
U(9)-O(48)	2.368(18)	U(9)-O(34)	2.370(16)
U(9)-O(31)	2.385(17)	U(9)-O(68)	2.401(18)
U(10)-O(13)	1.788(16)	U(10)-O(33)	1.796(17)
U(10)-O(17)#1	2.343(17)	U(10)-O(34)	2.352(17)
U(10)-O(48)	2.362(17)	U(10)-O(35)	2.375(17)
U(10)-O(39)	2.377(17)	U(10)-O(71)	2.38(2)
U(11)-O(46)	1.798(17)	U(11)-O(38)	1.801(16)
U(11)-O(49)	2.356(18)	U(11)-O(16)	2.358(17)
U(11)-O(72)	2.368(17)	U(11)-O(49)#5	2.376(17)
U(11)-O(40)	2.384(17)	U(11)-O(66)	2.386(18)

U(12)-O(15)	1.806(17)	U(12)-O(26)	1.812(16)
U(12)-O(72)	2.354(17)	U(12)-O(52)	2.358(17)
U(12)-O(32)	2.369(18)	U(12)-O(9)	2.375(16)
U(12)-O(16)	2.385(17)	U(12)-O(45)	2.395(18)
K(1)-O(35)	2.712(18)	K(1)-O(35)#1	2.712(18)
K(1)-O(33)	2.880(18)	K(1)-O(33)#1	2.880(18)
K(1)-O(24)#1	2.921(17)	K(1)-O(24)	2.922(17)
K(1)-OW31	3.39(5)	K(2)-O(12)	2.90(2)
K(2)-O(61)	2.932(17)	K(2)-O(61)#1	2.932(17)
K(2)-O(58)#1	2.958(17)	K(2)-O(58)	2.958(17)
K(2)-O(2)	2.98(2)	K(2)-O(27)#1	2.990(17)
K(2)-O(27)	2.990(17)	K(2)-OW20	3.05(6)
K(2)-O(14)	3.067(18)	K(2)-O(14)#1	3.067(18)
K(3)-O(24)	2.900(16)	K(3)-O(24)#1	2.900(16)
K(3)-O(25)#1	2.912(17)	K(3)-O(25)	2.912(17)
K(3)-O(1)	2.92(2)	K(3)-O(7)	3.01(2)
K(3)-O(8)	3.013(18)	K(3)-O(8)#1	3.013(18)
K(3)-O(50)#1	3.023(17)	K(3)-O(50)	3.023(17)
K(3)-OW31	3.15(5)	K(4)-O(32)#1	2.704(18)
K(4)-O(32)	2.704(18)	K(4)-O(15)#1	2.810(18)
K(4)-O(15)	2.810(18)	K(4)-O(58)#5	2.881(18)
K(4)-O(58)#3	2.881(18)	K(5)-O(3)	2.716(18)
K(5)-O(66)#1	2.773(19)	K(5)-O(61)#1	2.803(18)

K(5)-O(30)	2.810(16)	K(5)-O(46)#1	2.861(18)
K(5)-O(12)	2.884(17)	K(6)-O(40)#3	2.697(18)
K(6)-O(45)#1	2.722(19)	K(6)-O(46)#3	2.862(18)
K(6)-O(15)#1	2.871(19)	K(6)-O(58)#3	2.879(17)
K(6)-O(61)#3	2.884(19)	K(7)-O(68)#1	2.698(19)
K(7)-O(5)	2.717(17)	K(7)-O(6)	2.795(16)
K(7)-O(25)#2	2.802(18)	K(7)-O(47)#1	2.834(17)
K(7)-O(1)#2	2.908(16)	K(8)-O(10)	2.71(2)
K(8)-OW9#1	2.71(3)	K(8)-OW9	2.71(3)
K(8)-O(60)	2.73(3)	K(8)-O(20)	2.796(16)
K(8)-O(20)#1	2.796(16)	K(8)-O(73)#1	3.107(18)
K(8)-O(73)	3.108(18)	K(9)-O(2)	2.73(2)
K(9)-OW2#1	2.75(2)	K(9)-OW2	2.75(2)
K(9)-O(60)	2.78(2)	K(9)-O(44)#1	3.018(17)
K(9)-O(44)	3.018(17)	K(9)-O(59)#1	3.230(17)
K(9)-O(59)	3.230(17)	K(9)-O(10)	3.25(2)
K(10)-O(19)	2.722(17)	K(10)-OW8	2.81(3)
K(10)-OW6	2.81(3)	K(10)-O(59)	2.898(17)
K(10)-O(63)	2.920(17)	K(10)-O(44)	2.980(18)
K(11)-O(71)	2.70(2)	K(11)-O(54)#4	2.704(19)
K(11)-O(47)#4	2.839(18)	K(11)-O(24)	2.857(17)
K(11)-O(33)	2.871(18)	K(11)-O(25)	2.878(17)
K(12)-O(7)	2.69(3)	K(12)-OW3	2.80(2)

K(12)-OW3#1	2.80(2)	K(12)-O(21)	2.89(2)
K(12)-OW12	2.98(3)	K(12)-OW12#1	2.98(3)
K(12)-O(23)	3.152(17)	K(12)-O(23)#1	3.152(17)
K(13A)-O(29)	2.78(2)	K(13A)-O(41)	2.84(2)
K(13A)-O(55)	2.89(2)	K(13A)-OW28	2.93(5)
K(13A)-O(69)	2.97(3)	K(13A)-O(76)#1	2.97(3)
K(13A)-OW3#8	3.05(3)	K(13A)-OW25	3.10(6)
K(13B)-O(41)	2.64(4)	K(13B)-O(29)	2.75(4)
K(13B)-OW28	2.82(6)	K(13B)-O(53)	3.36(4)
K(13B)-OW3#8	3.37(4)	K(13B)-O(55)	3.38(4)
K(14)-OW10	2.38(3)	K(14)-O(51)#9	2.77(2)
K(14)-OW16	2.79(4)	K(14)-OW11	2.79(3)
K(14)-OW24	3.02(5)	K(14)-OW29	3.16(5)
K(15)-OW1	2.42(3)	K(15)-OW14	2.79(4)
K(15)-O(38)	2.83(2)	K(15)-OW7	2.84(3)
K(15)-OW22	2.98(4)	K(16)-OW22	2.72(4)
K(16)-OW1#5	2.77(3)	K(16)-O(75)	2.78(3)
K(16)-O(49)#5	2.82(2)	K(16)-OW15	3.41(4)
K(17A)-O(74)#3	2.79(2)	K(17A)-O(56)#3	2.88(2)
K(17A)-O(64)#1	2.92(3)	K(17A)-O(43)#3	2.92(2)
K(17A)-O(75)#3	2.92(3)	K(17B)-O(43)#3	2.49(4)
K(17B)-O(74)#3	3.09(4)	K(17B)-O(56)#3	3.14(4)
K(17B)-OW8#3	3.31(4)	K(17B)-U(5)#3	3.98(3)

P(1)-O(22)	1.502(16)	P(1)-O(35)	1.505(18)
P(1)-O(65)	1.555(18)	P(1)-C(6)	1.80(3)
P(2)-O(62)#4	1.510(18)	P(2)-O(54)	1.513(19)
P(2)-O(57)	1.515(19)	P(3)-O(5)#2	1.498(17)
P(3)-O(11)	1.516(18)	P(3)-O(44)	1.519(18)
P(4)-O(66)	1.471(19)	P(4)-O(29)	1.480(18)
P(4)-O(69)	1.57(2)	P(5)-O(68)	1.490(19)
P(5)-O(63)#4	1.504(18)	P(5)-O(67)	1.557(19)
P(6)-O(40)	1.503(18)	P(6)-O(56)	1.518(18)
P(6)-O(75)	1.55(2)	P(7)-O(71)	1.49(2)
P(7)-O(36)	1.497(18)	P(7)-O(70)	1.58(2)
P(8)-O(45)	1.493(19)	P(8)-O(74)#5	1.51(2)
P(8)-O(64)	1.52(2)	P(9)-O(32)#5	1.529(18)
P(9)-O(20)	1.548(17)	P(9)-O(73)	1.552(18)
P(10)-O(3)	1.513(18)	P(10)-O(76)	1.52(2)
P(10)-O(55)#1	1.529(18)	O(1)-K(7)#4	2.907(17)
O(1)-K(7)#2	2.907(17)	O(2)-O(10)	1.50(3)
O(2)-U(5)#1	2.375(10)	O(5)-P(3)#2	1.498(17)
O(6)-K(7)#1	2.795(16)	O(7)-O(21)	1.48(3)
O(7)-U(8)#1	2.382(10)	O(8)-O(19)	1.49(2)
O(9)-O(52)	1.46(2)	O(10)-U(5)#1	2.315(8)
O(12)-K(5)#1	2.884(17)	O(14)-O(41)	1.48(2)
O(15)-K(6)#1	2.871(19)	O(16)-O(72)	1.46(2)

O(17)-O(39)#1	1.46(2)	O(17)-U(10)#1	2.342(17)
O(21)-U(8)#1	2.323(9)	O(25)-K(7)#2	2.802(18)
O(27)-O(43)	1.48(2)	O(30)-K(5)#1	2.810(16)
O(31)-O(31)#4	1.47(3)	O(31)-U(9)#4	2.354(17)
O(32)-P(9)#5	1.529(18)	O(34)-O(48)	1.48(2)
O(37)-O(50)	1.46(2)	O(39)-O(17)#1	1.46(2)
O(40)-K(6)#3	2.697(18)	O(43)-K(17B)#3	2.49(4)
O(43)-K(17A)#3	2.92(2)	O(45)-K(6)#1	2.722(19)
O(46)-K(5)#1	2.861(18)	O(46)-K(6)#3	2.862(18)
O(47)-K(7)#1	2.834(17)	O(47)-K(11)#4	2.839(18)
O(49)-O(49)#5	1.47(3)	O(49)-U(11)#5	2.376(17)
O(49)-K(16)#5	2.82(2)	O(51)-K(14)#11	2.77(2)
O(54)-K(11)#4	2.705(19)	O(55)-P(10)#1	1.529(18)
O(56)-K(17A)#3	2.88(2)	O(56)-K(17B)#3	3.14(4)
O(58)-K(6)#3	2.879(16)	O(58)-K(4)#3	2.881(18)
O(61)-K(5)#1	2.803(18)	O(61)-K(6)#3	2.884(19)
O(62)-P(2)#4	1.510(18)	O(63)-P(5)#4	1.504(18)
O(64)-K(17A)#1	2.92(3)	O(66)-K(5)#1	2.773(19)
O(68)-K(7)#1	2.698(19)	O(74)-P(8)#5	1.51(2)
O(74)-K(17A)#3	2.79(2)	O(74)-K(17B)#3	3.09(4)
O(75)-K(17A)#3	2.92(3)	O(76)-K(13A)#1	2.97(3)
OW1-K(16)#5	2.77(3)	OW3-K(13A)#7	3.05(3)
OW3-K(13B)#7	3.37(4)	OW8-K(17B)#3	3.31(4)

OW11-OW29	1.57(5)	OW40-OW40#12	1.77(8)
C(1)-C(6)	1.36(3)	C(1)-C(2)	1.44(4)
C(2)-C(3)	1.30(4)	C(3)-C(4)	1.43(5)
C(4)-C(5)	1.43(4)	C(5)-C(6)	1.43(4)
C(7)-C(7)#1	1.37(5)	C(7)-C(8)	1.40(4)
C(8)-C(9)	1.47(4)	C(9)-C(9)#1	1.31(5)
C(10)-C(11)	1.41(4)	C(10)-C(15)	1.45(3)
C(11)-C(12)	1.38(4)	C(12)-C(13)	1.35(4)
C(13)-C(14)	1.44(4)	C(14)-C(15)	1.37(4)
C(16)-C(21)	1.36(3)	C(16)-C(17)	1.40(4)
C(17)-C(18)	1.39(4)	C(18)-C(19)	1.32(4)
C(19)-C(20)	1.38(4)	C(20)-C(21)	1.41(4)
C(22)-C(22)#1	1.41(5)	C(22)-C(23)	1.48(4)
C(23)-C(24)	1.44(5)	C(24)-C(24)#1	1.27(7)
C(25)-C(26)#5	1.39(4)	C(25)-C(30)	1.41(4)
C(26)-C(27)	1.37(4)	C(26)-C(25)#5	1.39(4)
C(27)-C(28)	1.39(5)	C(28)-C(29)#5	1.34(4)
C(29)-C(28)#5	1.34(4)	C(29)-C(30)	1.45(4)

Symmetry transformations used to generate equivalent atoms:

```
#1 x,-y+1,z  #2 -x-1,-y+1,-z-1  #3 -x,-y+1,-z
#4 -x-1,y,-z-1  #5 -x,y,-z  #6 x,-y+1,z-1  #7 x,y,z-1
#8 x,y,z+1  #9 x+1/2,-y+3/2,z+1  #10 -x-1/2,-y+3/2,-z-1
#11 x-1/2,-y+3/2,z-1  #12 x,-y,z
```

Table S6. Crystal data and structure refinement for K-U₂₆Ppb₆.

Identification code	U ₂₆ Ppb ₆
Empirical formula	C18 H12 K14.01 O97.38 P6 U13.17
Formula weight	5655.34
Temperature	180(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	<i>C</i> 2/ <i>c</i>
<i>a</i>	30.435(4) Å
<i>b</i>	25.364(3) Å
<i>c</i>	32.902(4) Å
α	90°
β	105.1058(16)°
γ	90°
Volume	24521(5) Å ³
Z	8
Density (calculated)	3.064 g.cm ⁻³
Absorption coefficient (μ)	17.990 mm ⁻¹
F(000)	19737
Crystal size	0.150 × 0.080 × 0.020 mm ³
θ range for data collection	1.061 to 25.759°
Index ranges	-37 ≤ <i>h</i> ≤ 37, -30 ≤ <i>k</i> ≤ 31, -40 ≤ <i>l</i> ≤ 40
Reflections collected	128029
Independent reflections	23380 [R _{int} = 0.0995]
Completeness to $\theta = 25.242^\circ$	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7453 and 0.4205
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	23380 / 0 / 854
Goodness-of-fit on F ²	1.049
Final R indices [<i>I</i> >2σ(<i>I</i>)]	R ₁ = 0.0566, wR ₂ = 0.1438
R indices (all data)	R ₁ = 0.1038, wR ₂ = 0.1694
Extinction coefficient	n/a
Largest diff. peak and hole	2.943 and -3.439 e ⁻ .Å ⁻³

**Table S7. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2)
for K-U₂₆Ppb₆. U(eq) is defined as one third of the trace of the orthogonalized \mathbf{U}_{ij} tensor.**

	x	y	z	U(eq)
U(1)	0.51849(3)	0.28473(3)	0.49124(2)	0.030(1)
U(2)	0.46249(3)	0.10244(3)	0.39631(3)	0.042(1)
U(3)	0.53741(3)	0.03928(3)	0.31422(3)	0.046(1)
U(4)	0.33823(3)	0.11260(3)	0.18366(2)	0.036(1)
U(5)	0.33514(3)	0.13738(3)	0.31143(2)	0.036(1)
U(6)	0.29383(3)	0.29222(3)	0.33064(2)	0.031(1)
U(7)	0.26801(3)	0.36163(3)	0.21035(2)	0.034(1)
U(8)	0.34947(2)	0.49947(3)	0.22128(2)	0.027(1)
U(9)	0.40149(2)	0.48877(3)	0.11136(2)	0.026(1)
U(10)	0.45858(2)	0.52332(3)	0.38538(2)	0.027(1)
U(11)	0.41646(2)	0.39999(3)	0.45384(2)	0.027(1)
U(12)	0.29286(3)	0.25474(3)	0.12016(2)	0.037(1)
U(13)	0.36566(2)	0.34308(3)	0.04802(2)	0.030(1)
U(14)	0.49214(13)	0.30539(16)	0.26607(12)	0.026(2)
K(1)	0.37390(14)	0.40280(16)	0.31627(13)	0.030(2)
K(2)	0.41706(15)	0.24886(18)	0.38096(14)	0.039(2)
K(3)	0.50333(15)	0.37134(18)	0.38152(17)	0.047(2)
K(4A)	0.3472(10)	0.2462(6)	0.2385(4)	0.049(7)
K(4B)	0.3784(6)	0.2589(4)	0.2481(3)	0.036(4)
K(5)	0.44396(15)	0.45415(18)	-0.00224(13)	0.034(2)
K(6)	0.23019(16)	0.52193(19)	0.25217(16)	0.041(2)
K(7)	0.4485(2)	0.6294(2)	0.07426(17)	0.048(2)
K(8)	0.3200(2)	0.5860(3)	0.00788(19)	0.041(3)
K(9)	0.2205(3)	0.1218(3)	0.0865(2)	0.067(3)
K(10)	0.5593(3)	0.2145(3)	0.4014(2)	0.062(3)
K(11)	0.4813(3)	0.4589(5)	0.2837(3)	0.046(4)
K(12)	0.3528(3)	0.0212(4)	0.3940(3)	0.056(4)
K(13)	0.4631(3)	0.5959(4)	0.2001(3)	0.044(4)
K(14)	0.6468(4)	0.2110(5)	0.5400(4)	0.106(7)

K(15A)	0.4593(4)	0.1789(5)	0.2716(4)	0.057(5)
K(15B)	0.4424(3)	0.1303(4)	0.2788(3)	0.048(4)
K(16A)	0.3796(4)	0.3669(4)	0.1705(4)	0.032(4)
K(16B)	0.4056(9)	0.3525(6)	0.1894(7)	0.035(7)
K(17)	0.2968(6)	0.6631(7)	0.1811(6)	0.099(5)
K(18A)	0.7389(5)	0.2171(5)	0.5044(4)	0.052(3)
K(18B)	0.7500	0.2500	0.5000	0.041(8)
P(1)	0.42331(16)	0.59967(19)	0.28457(15)	0.027(1)
P(2)	0.34165(16)	0.54418(19)	0.32468(15)	0.026(1)
P(3)	0.29838(16)	0.41397(19)	0.39103(15)	0.027(1)
P(4)	0.33051(18)	0.2976(2)	0.44420(16)	0.033(1)
P(5)	0.43609(19)	0.1802(2)	0.48185(17)	0.039(1)
P(6)	0.5460(2)	0.1397(2)	0.49307(19)	0.044(1)
O(1)	0.4201(4)	0.3696(5)	0.4051(4)	0.030(3)
O(2)	0.4335(4)	0.4376(5)	0.1440(4)	0.030(3)
O(3)	0.3467(4)	0.2959(5)	0.3167(4)	0.028(3)
O(4)	0.4911(4)	0.3730(5)	0.4876(4)	0.026(3)
O(5)	0.4587(4)	0.3363(5)	0.4973(4)	0.034(3)
O(6)	0.4119(4)	0.4324(5)	0.5013(4)	0.032(3)
O(7)	0.2889(4)	0.4434(5)	0.1868(4)	0.034(3)
O(8)	0.4193(4)	0.4858(5)	0.4285(4)	0.029(3)
O(9)	0.3097(5)	0.1641(5)	0.1219(4)	0.039(3)
O(10)	0.4675(4)	0.4679(5)	0.4463(4)	0.028(3)
O(11)	0.2872(4)	0.4474(5)	0.2316(4)	0.035(3)
O(12)	0.3409(4)	0.4303(5)	0.4245(4)	0.030(3)
O(13)	0.3876(4)	0.4330(5)	0.0518(4)	0.031(3)
O(14)	0.2531(4)	0.3029(5)	0.2593(4)	0.035(3)
O(15)	0.3114(4)	0.5549(5)	0.2096(4)	0.032(3)
O(16)	0.3093(4)	0.3783(5)	0.3580(4)	0.029(3)
O(17)	0.3495(4)	0.4254(5)	0.0733(4)	0.036(3)
O(18)	0.4528(4)	0.4648(5)	0.3524(4)	0.031(3)
O(19)	0.3472(5)	0.4921(5)	0.1500(4)	0.037(3)
O(20)	0.3656(4)	0.3356(5)	0.4681(4)	0.036(3)
O(21)	0.3280(4)	0.3452(5)	0.2262(4)	0.033(3)
O(22)	0.3808(4)	0.1617(5)	0.2042(4)	0.033(3)
O(23)	0.4993(4)	0.2823(5)	0.4351(4)	0.034(3)

O(24)	0.4673(4)	0.5405(5)	0.1238(4)	0.034(3)
O(25)	0.4645(4)	0.5806(5)	0.4187(4)	0.029(3)
O(26)	0.2710(4)	0.4622(5)	0.3717(4)	0.035(3)
O(27)	0.5792(5)	0.3423(5)	0.4893(4)	0.039(3)
O(28)	0.3462(5)	0.2685(5)	0.1575(4)	0.039(3)
O(29)	0.3490(5)	0.5050(6)	0.2930(5)	0.053(4)
O(30)	0.4075(4)	0.3313(5)	0.0968(4)	0.029(3)
O(31)	0.3055(5)	0.3200(5)	0.0757(4)	0.040(3)
O(32)	0.3774(4)	0.1832(5)	0.3029(4)	0.033(3)
O(33)	0.2624(4)	0.3556(5)	0.2789(4)	0.032(3)
O(34)	0.3414(4)	0.0872(5)	0.2529(4)	0.035(3)
O(35)	0.2399(5)	0.2404(5)	0.0822(4)	0.042(3)
O(36)	0.3299(5)	0.2480(6)	0.4707(4)	0.045(4)
O(37)	0.2817(5)	0.2058(5)	0.3021(4)	0.038(3)
O(38)	0.5960(4)	0.2877(5)	0.4878(4)	0.037(3)
O(39)	0.4481(5)	0.5806(5)	0.3283(4)	0.042(3)
O(40)	0.3708(4)	0.5402(5)	0.0786(4)	0.035(3)
O(41)	0.3233(5)	0.3543(5)	-0.0013(4)	0.041(3)
O(42)	0.2087(5)	0.3783(6)	0.1936(5)	0.047(4)
O(43)	0.4643(4)	0.5058(5)	0.0865(4)	0.035(3)
O(44)	0.3870(5)	0.0631(6)	0.1525(4)	0.046(4)
O(45)	0.4782(5)	0.0129(6)	0.2560(5)	0.052(4)
O(46)	0.5373(5)	0.2857(6)	0.5480(4)	0.044(4)
O(47)	0.3063(5)	0.2016(5)	0.3473(4)	0.041(3)
O(48)	0.4735(5)	0.1566(6)	0.3647(4)	0.045(4)
O(49)	0.3239(4)	0.2716(5)	0.0618(4)	0.037(3)
O(50)	0.4786(5)	0.0422(6)	0.3478(4)	0.047(4)
O(51)	0.5481(5)	-0.0281(6)	0.3290(5)	0.050(4)
O(52)	0.2939(5)	0.0915(5)	0.3203(4)	0.041(3)
O(53)	0.5281(5)	0.1078(6)	0.2975(4)	0.044(4)
O(54)	0.2839(5)	0.1773(5)	0.1541(4)	0.043(3)
O(55)	0.3943(5)	0.0815(6)	0.3461(4)	0.044(4)
O(56)	0.5941(6)	0.1206(7)	0.5144(6)	0.071(5)
O(57)	0.2415(4)	0.2888(5)	0.3443(4)	0.037(3)
O(58)	0.2525(5)	0.2861(6)	0.1666(4)	0.045(4)
O(59)	0.3835(5)	0.1180(5)	0.3771(4)	0.041(3)

O(60)	0.2949(5)	0.0647(6)	0.1635(4)	0.046(4)
O(61)	0.3867(4)	0.4452(5)	0.2340(4)	0.034(3)
O(62)	0.4445(5)	0.1673(6)	0.4400(4)	0.046(4)
O(63)	0.4545(5)	0.2342(6)	0.4978(5)	0.048(4)
O(64)	0.3849(4)	0.5301(5)	0.1685(4)	0.036(3)
O(65)	0.4511(5)	0.0498(6)	0.4276(5)	0.054(4)
O(66)	0.3053(5)	0.1278(5)	0.2390(4)	0.042(3)
O(67)	0.3892(5)	0.0423(6)	0.1957(5)	0.050(4)
O(68)	0.5222(5)	0.0543(6)	0.3797(4)	0.044(4)
O(69)	0.2942(5)	0.5360(6)	0.3342(5)	0.055(4)
O(70)	0.3361(4)	0.2839(5)	0.4014(4)	0.038(3)
O(71)	0.4103(5)	0.5550(5)	0.2548(4)	0.042(3)
O(72)	0.2619(5)	0.3311(5)	0.1412(4)	0.040(3)
O(73)	0.3785(5)	0.5418(6)	0.3646(4)	0.045(4)
O(74)	0.5302(6)	0.1185(7)	0.4499(5)	0.068(5)
O(75)	0.4539(5)	0.6384(6)	0.2713(5)	0.057(4)
O(76)	0.3858(5)	0.1766(6)	0.4804(5)	0.054(4)
O(77)	0.5432(6)	0.1990(6)	0.4933(5)	0.059(4)
OW1	0.2857(5)	0.5789(6)	0.1192(5)	0.048(4)
OW2	0.3210(8)	0.4784(10)	-0.0150(7)	0.021(5)
OW3	0.3443(7)	0.4633(8)	-0.0482(6)	0.045(5)
OW4	0.4823(7)	0.0020(8)	0.0075(6)	0.034(5)
OW5	0.4086(8)	0.7269(9)	0.0547(7)	0.026(6)
OW6A	0.3485(12)	0.8128(14)	0.1654(11)	0.069(10)
OW6B	0.3475(13)	0.7553(15)	0.1657(12)	0.077(11)
OW7	0.8343(7)	0.3588(8)	0.2328(6)	0.085(6)
OW8	0.2969(8)	0.9450(9)	0.2001(7)	0.089(7)
OW9	0.2387(8)	0.6749(10)	0.0845(8)	0.083(7)
OW10	0.6284(9)	0.6421(11)	0.0840(9)	0.043(7)
OW11	0.1598(10)	0.4735(12)	0.1887(9)	0.048(8)
OW12	0.2721(12)	-0.0079(14)	0.3765(11)	0.067(10)
OW13	0.3266(10)	-0.1795(11)	0.3831(9)	0.044(7)
OW14	0.2581(10)	0.0303(12)	0.0714(9)	0.056(8)
OW15	0.5891(11)	0.6739(12)	0.1204(10)	0.066(8)
OW16	0.2524(11)	0.4384(13)	0.0415(10)	0.084(9)
OW17	0.3759(14)	0.9313(16)	0.2026(12)	0.081(11)

OW18	0.8475(13)	0.5050(15)	0.0778(11)	0.073(10)
OW19	0.3397(13)	0.0801(15)	0.4591(12)	0.077(11)
OW20	0.6152(18)	0.139(2)	0.4215(16)	0.039(13)
OW21	0.5237(11)	0.6841(12)	0.1268(9)	0.053(8)
OW22	0.4071(13)	0.0444(15)	0.0521(12)	0.078(11)
OW23	0.5256(15)	0.2289(18)	0.2216(14)	0.021(10)
OW24	0.5636(14)	0.2895(16)	0.2339(13)	0.088(12)
OW25	0.4742(11)	0.2749(13)	0.3326(10)	0.060(9)
OW26	0.3260(10)	0.5061(13)	-0.0058(10)	0.048(8)
OW27	0.4433(8)	0.3531(10)	0.2974(7)	0.028(6)
OW28	0.5329(14)	0.3610(16)	0.2316(13)	0.016(9)
OW29	0.4982(15)	0.3759(17)	0.2138(13)	0.020(10)
OW30	0.5495(15)	0.3161(18)	0.1991(13)	0.061(11)
OW31	0.706(2)	0.132(2)	0.4701(18)	0.046(15)
OW32	0.5576(9)	0.2110(11)	0.3442(9)	0.039(7)
OW33	0.5492(12)	0.2291(14)	0.3182(11)	0.061(9)
OW34	0.5067(9)	0.4980(12)	0.2210(8)	0.038(7)
OW35	0.2775(6)	0.6504(7)	0.1643(6)	0.058(5)
OW36	0.1134(17)	0.3492(19)	0.1614(15)	0.030(12)
OW37	0.6559(16)	0.2370(18)	0.6245(14)	0.027(11)
OW38	0.5004(17)	0.249(2)	0.1913(16)	0.050(13)
OW39	0.0000	0.406(3)	0.2500	0.026(15)
C(1)	0.3712(3)	0.6335(4)	0.2878(4)	0.028(4)
C(2)	0.3375(4)	0.6105(4)	0.3034(4)	0.025(4)
C(3)	0.2982(3)	0.6386(5)	0.3033(4)	0.032(4)
C(4)	0.2927(4)	0.6897(5)	0.2876(4)	0.044(5)
C(5)	0.3264(5)	0.7128(4)	0.2720(4)	0.060(7)
C(6)	0.3656(4)	0.6847(5)	0.2721(4)	0.038(5)
C(7)	0.2621(4)	0.3760(5)	0.4168(4)	0.034(5)
C(8)	0.2746(4)	0.3285(5)	0.4376(4)	0.035(5)
C(9)	0.2442(5)	0.3021(4)	0.4555(4)	0.048(6)
C(10)	0.2013(4)	0.3231(6)	0.4524(5)	0.060(7)
C(11)	0.1888(4)	0.3706(6)	0.4315(5)	0.060(7)
C(12)	0.2192(5)	0.3971(4)	0.4137(4)	0.050(6)
C(13)	0.4644(6)	0.1317(7)	0.5192(5)	0.059(7)
C(14)	0.5099(6)	0.1183(8)	0.5249(6)	0.069(8)

C(15)	0.5313(6)	0.0853(10)	0.5578(8)	0.135(15)
C(16)	0.5073(10)	0.0656(10)	0.5850(7)	0.20(2)
C(17)	0.4618(10)	0.0790(10)	0.5794(7)	0.136(15)
C(18)	0.4404(6)	0.1120(9)	0.5465(7)	0.094(10)
H(3A)	0.2752	0.6228	0.3140	0.038
H(4A)	0.2659	0.7089	0.2876	0.052
H(5A)	0.3226	0.7477	0.2613	0.072
H(6A)	0.3886	0.7005	0.2614	0.046
H(9A)	0.2527	0.2696	0.4697	0.057
H(10A)	0.1805	0.3051	0.4646	0.072
H(11A)	0.1594	0.3850	0.4294	0.072
H(12A)	0.2106	0.4295	0.3994	0.060
H(15A)	0.5624	0.0762	0.5616	0.162
H(16A)	0.5220	0.0430	0.6075	0.241
H(17A)	0.4454	0.0655	0.5981	0.163
H(18A)	0.4093	0.1211	0.5427	0.113

Table S8. Anisotropic displacement parameters (\AA^2) for K-U₂₆Ppb₆. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\mathbf{h}^2\mathbf{a}^{*2}\mathbf{U}_{11} + \dots + 2\mathbf{hka}^*\mathbf{b}^*\mathbf{U}_{12}]$

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
U(1)	0.0384(4)	0.0294(4)	0.0227(4)	0.0026(3)	0.0096(3)	0.0052(3)
U(2)	0.0524(5)	0.0400(5)	0.0412(5)	-0.0049(4)	0.0278(4)	-0.0113(4)
U(3)	0.0625(6)	0.0332(4)	0.0565(5)	0.0035(4)	0.0419(5)	-0.0012(4)
U(4)	0.0347(4)	0.0372(4)	0.0411(4)	-0.0155(3)	0.0200(4)	-0.0162(3)
U(5)	0.0408(5)	0.0356(4)	0.0379(4)	-0.0105(3)	0.0198(4)	-0.0171(3)
U(6)	0.0360(4)	0.0340(4)	0.0290(4)	-0.0076(3)	0.0196(3)	-0.0141(3)
U(7)	0.0324(4)	0.0453(5)	0.0289(4)	-0.0034(3)	0.0138(3)	-0.0044(3)
U(8)	0.0310(4)	0.0301(4)	0.0236(3)	0.0024(3)	0.0123(3)	0.0080(3)
U(9)	0.0262(4)	0.0309(4)	0.0235(3)	0.0007(3)	0.0126(3)	-0.0026(3)
U(10)	0.0248(4)	0.0286(4)	0.0265(4)	-0.0058(3)	0.0063(3)	0.0060(3)
U(11)	0.0299(4)	0.0297(4)	0.0250(4)	-0.0063(3)	0.0108(3)	0.0001(3)
U(12)	0.0362(4)	0.0493(5)	0.0269(4)	-0.0103(3)	0.0127(3)	-0.0189(4)
U(13)	0.0267(4)	0.0427(4)	0.0213(3)	-0.0038(3)	0.0085(3)	-0.0125(3)
U(14)	0.022(2)	0.030(3)	0.028(2)	-0.0044(17)	0.0108(17)	-0.0010(17)
K(1)	0.030(3)	0.032(3)	0.031(2)	0.0012(18)	0.0157(19)	-0.0024(18)
K(2)	0.039(3)	0.043(3)	0.035(3)	-0.004(2)	0.011(2)	-0.009(2)
K(3)	0.023(3)	0.037(3)	0.081(4)	0.015(2)	0.012(2)	0.0044(19)
K(4A)	0.076(18)	0.044(8)	0.034(7)	-0.009(6)	0.027(8)	-0.006(9)
K(4B)	0.056(10)	0.027(5)	0.033(5)	-0.002(4)	0.027(5)	-0.001(5)
K(5)	0.034(3)	0.039(3)	0.033(3)	0.013(2)	0.014(2)	0.003(2)
K(6)	0.032(3)	0.038(3)	0.053(3)	0.013(2)	0.014(2)	0.018(2)
K(7)	0.073(5)	0.041(4)	0.031(3)	0.008(2)	0.016(3)	0.016(3)
K(8)	0.042(4)	0.054(5)	0.029(4)	0.013(3)	0.012(3)	0.005(3)
K(9)	0.063(5)	0.079(6)	0.041(4)	-0.011(4)	-0.017(3)	-0.021(4)
K(10)	0.071(6)	0.060(5)	0.063(5)	-0.017(4)	0.032(4)	-0.008(4)
K(11)	0.035(6)	0.075(9)	0.030(6)	0.012(5)	0.013(4)	-0.006(5)
K(12)	0.056(7)	0.052(6)	0.055(6)	0.010(4)	0.009(5)	-0.027(5)
K(13)	0.036(6)	0.068(7)	0.038(6)	-0.011(4)	0.026(4)	-0.015(5)
K(14)	0.067(8)	0.098(11)	0.119(12)	0.040(8)	-0.034(7)	0.001(7)

K(15A)	0.053(8)	0.058(9)	0.067(8)	-0.004(6)	0.028(6)	0.013(6)
K(15B)	0.038(6)	0.070(8)	0.037(5)	-0.009(4)	0.014(4)	0.001(5)
K(16A)	0.036(7)	0.034(5)	0.026(5)	-0.002(4)	0.012(5)	-0.005(4)
K(16B)	0.046(14)	0.029(8)	0.035(10)	-0.002(7)	0.021(10)	-0.017(8)

Table S9. Selected bond lengths [Å] for K-U₂₆Ppb₆.

atom-atom	distance	atom-atom	distance
U(1)-O(23)	1.788(12)	U(1)-O(46)	1.805(14)
U(1)-O(5)	2.291(13)	U(1)-O(77)	2.297(16)
U(1)-O(27)	2.367(13)	U(1)-O(4)	2.381(12)
U(1)-O(63)	2.388(15)	U(1)-O(38)	2.392(13)
U(2)-O(65)	1.777(15)	U(2)-O(48)	1.807(14)
U(2)-O(62)	2.342(14)	U(2)-O(55)	2.351(14)
U(2)-O(50)	2.352(14)	U(2)-O(59)	2.354(14)
U(2)-O(68)	2.368(14)	U(2)-O(74)	2.372(18)
U(3)-O(51)	1.784(15)	U(3)-O(53)	1.822(14)
U(3)-O(45)#1	2.333(15)	U(3)-O(50)	2.335(15)
U(3)-O(67)#1	2.342(15)	U(3)-O(68)	2.350(14)
U(3)-O(44)#1	2.354(15)	U(3)-O(45)	2.359(15)
U(4)-O(60)	1.788(14)	U(4)-O(22)	1.797(13)
U(4)-O(66)	2.328(14)	U(4)-O(67)	2.329(15)
U(4)-O(34)	2.346(13)	U(4)-O(54)	2.352(14)
U(4)-O(44)	2.371(14)	U(4)-O(9)	2.381(13)
U(5)-O(52)	1.790(14)	U(5)-O(32)	1.808(13)
U(5)-O(47)	2.313(14)	U(5)-O(59)	2.329(14)
U(5)-O(66)	2.331(14)	U(5)-O(55)	2.342(14)
U(5)-O(37)	2.345(13)	U(5)-O(34)	2.356(13)

U(6)-O(57)	1.765(13)	U(6)-O(3)	1.789(12)
U(6)-O(33)	2.355(12)	U(6)-O(70)	2.358(13)
U(6)-O(16)	2.362(12)	U(6)-O(14)	2.366(13)
U(6)-O(47)	2.371(14)	U(6)-O(37)	2.375(13)
U(7)-O(42)	1.794(15)	U(7)-O(21)	1.811(13)
U(7)-O(33)	2.312(12)	U(7)-O(11)	2.314(13)
U(7)-O(14)	2.324(13)	U(7)-O(7)	2.360(13)
U(7)-O(72)	2.364(13)	U(7)-O(58)	2.370(14)
U(8)-O(61)	1.764(13)	U(8)-O(15)	1.799(12)
U(8)-O(19)	2.334(13)	U(8)-O(71)	2.359(14)
U(8)-O(29)	2.369(15)	U(8)-O(7)	2.369(13)
U(8)-O(64)	2.401(13)	U(8)-O(11)	2.405(13)
U(9)-O(40)	1.790(13)	U(9)-O(2)	1.801(12)
U(9)-O(43)	2.306(13)	U(9)-O(64)	2.319(13)
U(9)-O(19)	2.336(13)	U(9)-O(24)	2.339(13)
U(9)-O(13)	2.363(12)	U(9)-O(17)	2.370(13)
U(10)-O(25)	1.800(12)	U(10)-O(18)	1.821(12)
U(10)-O(8)	2.289(12)	U(10)-O(39)	2.330(14)
U(10)-O(43)#1	2.331(13)	U(10)-O(24)#1	2.393(13)
U(10)-O(73)	2.400(14)	U(10)-O(10)	2.405(12)
U(11)-O(6)	1.801(12)	U(11)-O(1)	1.808(12)
U(11)-O(5)	2.313(13)	U(11)-O(8)	2.339(12)
U(11)-O(4)	2.356(12)	U(11)-O(10)	2.375(12)

U(11)-O(12)	2.377(12)	U(11)-O(20)	2.378(13)
U(12)-O(28)	1.796(13)	U(12)-O(35)	1.799(14)
U(12)-O(31)	2.306(13)	U(12)-O(54)	2.312(14)
U(12)-O(58)	2.335(14)	U(12)-O(72)	2.336(14)
U(12)-O(9)	2.354(14)	U(12)-O(49)	2.388(13)
U(13)-O(30)	1.795(12)	U(13)-O(41)	1.813(14)
U(13)-O(31)	2.323(14)	U(13)-O(27)#1	2.325(13)
U(13)-O(49)	2.326(13)	U(13)-O(38)#1	2.331(13)
U(13)-O(17)	2.347(13)	U(13)-O(13)	2.371(12)
K(1)-OW27	2.67(2)	K(1)-O(16)	2.748(12)
K(1)-O(29)	2.752(16)	K(1)-O(3)	2.837(12)
K(1)-O(18)	2.856(13)	K(1)-O(1)	3.015(13)
K(1)-O(61)	3.031(13)	K(1)-O(21)	3.272(13)
K(1)-OW30#1	3.34(4)	K(2)-OW25	2.73(3)
K(2)-O(23)	2.798(13)	K(2)-O(62)	2.810(15)
K(2)-O(3)	2.849(13)	K(2)-O(70)	2.859(14)
K(2)-O(48)	3.031(15)	K(2)-O(32)	3.035(13)
K(2)-O(1)	3.159(13)	K(3)-O(30)#1	2.811(13)
K(3)-O(1)	2.837(13)	K(3)-O(2)#1	2.841(13)
K(3)-O(18)	2.853(13)	K(3)-O(23)	2.887(13)
K(3)-OW27	2.93(2)	K(3)-OW25	2.93(3)
K(3)-OW30#1	3.06(4)	K(3)-OW29#1	3.13(4)
K(4A)-O(21)	2.586(18)	K(4A)-O(32)	2.623(18)

K(4A)-O(28)	2.716(18)	K(4A)-O(22)	2.740(18)
K(4A)-OW24#1	2.85(5)	K(4A)-O(3)	2.867(17)
K(4A)-O(66)	3.26(3)	K(4A)-O(58)	3.37(3)
K(4A)-O(37)	3.40(2)	K(4A)-O(54)	3.42(3)
K(4B)-OW24#1	1.88(5)	K(4B)-O(32)	2.641(15)
K(4B)-O(21)	2.663(15)	K(4B)-OW30#1	2.82(5)
K(4B)-O(3)	2.834(14)	K(4B)-O(22)	2.867(16)
K(4B)-O(28)	2.896(17)	K(4B)-OW23#1	2.93(5)
K(4B)-OW27	3.25(3)	K(5)-O(8)#5	2.680(13)
K(5)-O(4)#1	2.806(12)	K(5)-O(10)#5	2.814(13)
K(5)-O(13)	2.827(13)	K(5)-O(10)#1	2.860(13)
K(5)-O(25)#5	2.964(13)	K(5)-O(27)#1	2.980(14)
K(5)-OW3	3.03(2)	K(5)-O(6)#5	3.051(13)
K(5)-O(43)	3.112(13)	K(6)-O(34)#6	2.708(14)
K(6)-OW8#2	2.76(2)	K(6)-O(11)	2.767(14)
K(6)-OW11	2.85(3)	K(6)-O(52)#6	2.903(14)
K(6)-O(69)	2.911(16)	K(6)-O(66)#6	2.938(15)
K(6)-O(60)#6	3.249(15)	K(6)-O(15)	3.250(13)
K(7)-O(24)	2.752(14)	K(7)-OW5	2.76(2)
K(7)-O(5)#5	2.772(13)	K(7)-O(6)#5	2.840(13)
K(7)-OW21	2.84(3)	K(7)-O(25)#1	2.877(14)
K(7)-O(43)	3.181(14)	K(7)-O(40)	3.302(14)
K(7)-O(4)#5	3.429(13)	K(8)-OW26	2.09(3)

K(8)-O(40)	2.699(14)	K(8)-OW2	2.83(3)
K(8)-O(6)#5	2.900(14)	K(8)-O(20)#5	2.925(14)
K(8)-O(12)#5	3.002(13)	K(9)-OW14	2.69(3)
K(9)-OW10#7	2.83(3)	K(9)-O(41)#8	2.837(15)
K(9)-O(9)	2.867(15)	K(9)-O(54)	2.902(15)
K(9)-OW3#8	2.97(2)	K(9)-O(35)	3.075(16)
K(9)-O(60)	3.265(16)	K(9)-OW31#1	3.27(6)
K(10)-OW32	1.87(3)	K(10)-OW20	2.54(5)
K(10)-OW33	2.70(4)	K(10)-O(23)	2.929(15)
K(10)-O(48)	2.965(16)	K(10)-O(30)#1	3.125(14)
K(10)-O(74)	3.163(19)	K(10)-O(77)	3.211(18)
K(10)-OW38#1	3.23(5)	K(10)-O(38)	3.334(15)
K(10)-OW25	3.33(3)	K(11)-OW34#1	1.08(3)
K(11)-OW29#1	2.19(4)	K(11)-OW28#1	2.55(4)
K(11)-OW34	2.58(3)	K(11)-O(18)	2.629(15)
K(11)-O(61)	2.937(16)	K(11)-OW27	3.00(3)
K(11)-O(2)#1	3.077(15)	K(11)-O(71)	3.232(18)
K(11)-OW29	3.25(4)	K(12)-OW12	2.48(4)
K(12)-OW19	2.72(4)	K(12)-O(55)	2.731(16)
K(12)-O(59)	2.737(16)	K(12)-OW11#2	2.91(3)
K(12)-O(65)	2.996(18)	K(12)-O(52)	3.164(16)
K(13)-O(75)	2.659(18)	K(13)-O(75)#1	2.679(18)
K(13)-OW34	2.81(3)	K(13)-O(64)	2.871(16)

K(13)-O(71)	2.902(16)	K(13)-O(24)	2.908(15)
K(13)-O(39)#1	3.102(16)	K(14)-OW13#9	2.57(3)
K(14)-O(38)	2.784(17)	K(14)-O(56)	2.80(2)
K(14)-OW37	2.80(5)	K(14)-O(35)#10	3.072(18)
K(14)-O(77)	3.14(2)	K(15A)-OW38#1	2.31(5)
K(15A)-O(53)	2.726(18)	K(15A)-O(22)	2.839(17)
K(15A)-OW24#1	2.88(4)	K(15A)-O(32)	2.938(17)
K(15A)-O(53)#1	3.004(18)	K(15A)-O(48)	3.034(18)
K(15A)-OW33	3.04(4)	K(15A)-OW25	3.11(4)
K(15B)-O(53)	2.583(17)	K(15B)-O(32)	2.675(15)
K(15B)-OW23#1	2.69(5)	K(15B)-O(22)	2.789(15)
K(15B)-O(48)	2.817(16)	K(15B)-O(53)#1	2.936(16)
K(15B)-O(34)	3.161(16)	K(15B)-O(50)	3.170(18)
K(15B)-O(55)	3.204(17)	K(15B)-O(45)	3.323(18)
K(16A)-O(28)	2.688(15)	K(16A)-O(2)	2.721(14)
K(16A)-O(21)	2.764(14)	K(16A)-O(61)	2.849(14)
K(16A)-O(30)	2.911(14)	K(16A)-O(19)	3.341(18)
K(16A)-O(17)	3.425(18)	K(16B)-OW29	2.79(5)
K(16B)-OW28#1	2.79(5)	K(16B)-O(28)	2.81(2)
K(16B)-O(2)	2.876(19)	K(16B)-O(61)	2.906(19)
K(16B)-OW24#1	2.93(5)	K(16B)-O(21)	2.93(2)
K(16B)-O(30)	3.108(19)	K(17)-OW35	0.76(2)
K(17)-O(37)#6	2.81(2)	K(17)-O(15)	2.90(2)

K(17)-OW1	2.91(2)	K(17)-OW6B	2.92(4)
K(17)-O(47)#6	3.19(2)	K(17)-OW9	3.22(3)
K(17)-O(52)#6	3.30(2)	K(17)-O(57)#6	3.42(2)
K(18A)-OW31	2.51(6)	K(18A)-O(35)#10	2.772(19)
K(18A)-O(49)#10	2.792(19)	K(18A)-O(31)#10	2.832(19)
K(18A)-O(49)#1	2.852(19)	K(18A)-O(35)#1	3.138(19)
K(18A)-O(41)#10	3.189(19)	K(18B)-O(49)#10	2.667(13)
K(18B)-O(49)#1	2.667(13)	K(18B)-O(35)#10	2.812(14)
K(18B)-O(35)#1	2.812(14)	K(18B)-O(31)#10	3.164(13)
K(18B)-O(31)#1	3.164(13)	K(18B)-OW31#11	3.31(6)
K(18B)-OW31	3.31(6)	P(1)-O(71)	1.483(14)
P(1)-O(75)	1.495(17)	P(1)-O(39)	1.519(14)
P(1)-C(1)	1.832(10)	P(2)-O(73)	1.490(15)
P(2)-O(29)	1.498(16)	P(2)-O(69)	1.569(16)
P(2)-C(2)	1.814(10)	P(3)-O(16)	1.515(13)
P(3)-O(12)	1.522(13)	P(3)-O(26)	1.524(14)
P(3)-C(7)	1.831(11)	P(4)-O(20)	1.500(14)
P(4)-O(70)	1.503(14)	P(4)-O(36)	1.533(15)
P(4)-C(8)	1.835(11)	P(5)-O(62)	1.501(15)
P(5)-O(63)	1.521(16)	P(5)-O(76)	1.523(16)
P(5)-C(13)	1.794(17)	P(6)-O(74)	1.477(18)
P(6)-O(77)	1.506(17)	P(6)-O(56)	1.528(19)
P(6)-C(14)	1.788(17)	O(2)-K(3)#1	2.841(13)

O(2)-K(11)#1	3.077(15)	O(4)-O(5)	1.454(17)
O(4)-K(5)#1	2.806(12)	O(4)-K(7)#3	3.429(13)
O(5)-K(7)#3	2.772(13)	O(6)-K(7)#3	2.840(13)
O(6)-K(8)#3	2.900(14)	O(6)-K(5)#3	3.051(13)
O(7)-O(11)	1.493(17)	O(8)-O(10)	1.502(17)
O(8)-K(5)#3	2.680(13)	O(9)-O(54)	1.512(18)
O(10)-K(5)#3	2.814(13)	O(10)-K(5)#1	2.860(13)
O(12)-K(8)#3	3.002(13)	O(13)-O(17)	1.517(17)
O(14)-O(33)	1.478(17)	O(19)-O(64)	1.501(18)
O(20)-K(8)#3	2.924(14)	O(24)-O(43)	1.492(17)
O(24)-U(10)#1	2.393(13)	O(25)-K(7)#1	2.877(14)
O(25)-K(5)#3	2.964(13)	O(27)-O(38)	1.481(18)
O(27)-U(13)#1	2.326(13)	O(27)-K(5)#1	2.980(14)
O(30)-K(3)#1	2.811(13)	O(30)-K(10)#1	3.125(14)
O(31)-O(49)	1.469(18)	O(31)-K(18A)#4	2.832(19)
O(31)-K(18B)#1	3.164(13)	O(34)-O(66)	1.489(18)
O(34)-K(6)#2	2.708(14)	O(35)-K(18A)#4	2.772(19)
O(35)-K(18B)#1	2.812(13)	O(35)-K(14)#4	3.072(18)
O(35)-K(18A)#1	3.138(19)	O(37)-O(47)	1.485(18)
O(37)-K(17)#2	2.81(2)	O(38)-U(13)#1	2.332(13)
O(39)-K(13)#1	3.102(16)	O(41)-K(9)#8	2.837(15)
O(41)-K(18A)#4	3.189(19)	O(43)-U(10)#1	2.331(13)
O(44)-O(67)	1.50(2)	O(44)-U(3)#1	2.354(14)

O(45)-O(45)#1	1.48(3)	O(45)-U(3)#1	2.333(15)
O(47)-K(17)#2	3.19(2)	O(49)-K(18B)#1	2.667(13)
O(49)-K(18A)#4	2.792(19)	O(49)-K(18A)#1	2.852(19)
O(50)-O(68)	1.49(2)	O(52)-K(6)#2	2.903(14)
O(52)-K(17)#2	3.30(2)	O(53)-K(15B)#1	2.936(16)
O(53)-K(15A)#1	3.004(18)	O(55)-O(59)	1.477(19)
O(57)-K(17)#2	3.42(2)	O(58)-O(72)	1.485(19)
O(60)-K(6)#2	3.249(15)	O(66)-K(6)#2	2.938(15)
O(67)-U(3)#1	2.342(15)	O(75)-K(13)#1	2.679(18)
OW2-OW26	0.76(3)	OW2-OW3	1.50(3)
OW3-K(9)#8	2.97(2)	OW4-OW4#12	1.30(4)
OW6A-OW6B	1.46(5)	OW8-K(6)#6	2.76(2)
OW10-K(9)#13	2.83(3)	OW11-K(12)#6	2.91(3)
OW13-OW37#9	1.59(5)	OW13-K(14)#9	2.57(3)
OW23-OW38	1.20(6)	OW23-K(15A)#1	1.35(5)
OW23-U(14)#1	2.08(5)	OW23-K(15B)#1	2.69(5)
OW23-K(4B)#1	2.93(5)	OW24-OW30	1.30(5)
OW24-U(14)#1	1.74(4)	OW24-K(4B)#1	1.88(5)
OW24-K(4A)#1	2.85(5)	OW24-K(15A)#1	2.88(4)
OW24-K(16B)#1	2.93(5)	OW25-OW38#1	1.40(6)
OW25-OW30#1	1.52(5)	OW27-OW30#1	0.97(4)
OW27-OW28#1	1.36(5)	OW28-OW29	1.13(6)
OW28-OW27#1	1.36(5)	OW28-U(14)#1	1.61(4)

OW28-OW30	1.72(6)	OW28-K(11)#1	2.55(4)
OW28-K(16B)#1	2.79(5)	OW29-U(14)#1	1.90(4)
OW29-K(11)#1	2.19(4)	OW29-K(3)#1	3.13(4)
OW30-OW27#1	0.97(4)	OW30-OW25#1	1.52(5)
OW30-U(14)#1	1.94(4)	OW30-K(4B)#1	2.82(5)
OW30-K(3)#1	3.06(4)	OW30-K(1)#1	3.34(4)
OW31-K(9)#1	3.27(6)	OW32-OW33	0.95(4)
OW33-OW38#1	1.54(6)	OW33-K(15A)#1	3.16(4)
OW34-K(11)#1	1.08(3)	OW37-OW13#9	1.59(5)
OW38-OW25#1	1.40(6)	OW38-OW33#1	1.54(6)
OW38-U(14)#1	1.98(5)	OW38-K(15A)#1	2.31(5)
OW38-K(10)#1	3.23(5)	C(1)-C(2)	1.3900
C(1)-C(6)	1.3900	C(2)-C(3)	1.3900
C(3)-C(4)	1.3900	C(4)-C(5)	1.3900
C(5)-C(6)	1.3900	C(7)-C(8)	1.3900
C(7)-C(12)	1.3900	C(7)-K(8)#3	3.205(15)
C(8)-C(9)	1.3900	C(8)-K(8)#3	3.208(15)
C(9)-C(10)	1.3900	C(10)-C(11)	1.3900
C(11)-C(12)	1.3900	C(13)-C(14)	1.3900
C(13)-C(18)	1.3900	C(14)-C(15)	1.3900
C(15)-C(16)	1.3900	C(16)-C(17)	1.3900
C(17)-C(18)	1.3900		

Symmetry transformations used to generate equivalent atoms:

```
#1 -x+1,y,-z+1/2  #2 -x+1/2,y-1/2,-z+1/2  #3 x,-y+1,z+1/2  
#4 x-1/2,-y+1/2,z-1/2  #5 x,-y+1,z-1/2  #6 -x+1/2,y+1/2,-z+1/2  
#7 x-1/2,y-1/2,z  #8 -x+1/2,-y+1/2,-z  #9 -x+1,-y,-z+1  
#10 x+1/2,-y+1/2,z+1/2  #11 -x+3/2,-y+1/2,-z+1  
#12 -x+1,-y,-z  #13 x+1/2,y+1/2,z
```

Table S10. Crystal data and structure refinement for K-U₂₀Ppb₆-U@U₂₈.

Identification code	c2m
Empirical formula	C0.22 K0.22 O2.56 P0.11 U0.44
Formula weight	161.17
Temperature	180(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/m
<i>a</i>	57.23(8) Å
<i>b</i>	28.72(3) Å
<i>c</i>	26.78(3) Å
α	90°
β	114.76(3)°
γ	90°
Volume	39980(86) Å ³
<i>Z</i>	442
Density (calculated)	2.959 g.cm ⁻³
Absorption coefficient (μ)	20.158 mm ⁻¹
F(000)	30246
Crystal size	0.100 × 0.060 × 0.040 mm ³
θ range for data collection	1.040 to 19.036°
Index ranges	-52 ≤ <i>h</i> ≤ 52, -26 ≤ <i>k</i> ≤ 26, -24 ≤ <i>l</i> ≤ 24
Reflections collected	81761
Independent reflections	15857 [$R_{\text{int}} = 0.1602$]
Completeness to $\theta = 19.036^\circ$	95.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7443 and 0.4199
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	15857 / 0 / 1010
Goodness-of-fit on F ²	0.961
Final R indices [I>2σ(I)]	$R_1 = 0.0810$, $wR_2 = 0.2168$
R indices (all data)	$R_1 = 0.1530$, $wR_2 = 0.2557$
Extinction coefficient	n/a
Largest diff. peak and hole	2.908 and -1.342 e ⁻ .Å ⁻³

**Table S11. Atomic coordinates and equivalent isotropic displacement parameters (\AA^2)
for K-U₂₀Ppb₆-U@U₂₈. U(eq) is defined as one third of the trace of the orthogonalized \mathbf{U}_{ij}
tensor.**

	x	y	z	U(eq)
U(1)	-0.73384(5)	0.5000	-1.21741(11)	0.043(1)
U(2)	-0.73382(4)	0.25406(7)	-1.21987(9)	0.059(1)
U(3)	-0.80980(4)	0.37426(8)	-1.45616(9)	0.068(1)
U(4)	-0.67846(4)	0.37431(8)	-1.36681(10)	0.066(1)
U(5)	-0.86705(6)	0.5000	-1.30617(17)	0.083(1)
U(6)	-0.66127(4)	0.30165(7)	-1.10934(9)	0.064(1)
U(7)	-0.39393(6)	0.0000	-0.99620(13)	0.056(1)
U(8)	-0.84746(4)	0.37199(8)	-1.35191(10)	0.069(1)
U(9)	-0.47363(4)	0.37972(8)	-0.66073(10)	0.067(1)
U(10)	-0.59886(6)	0.5000	-1.11974(17)	0.084(1)
U(11)	-0.44834(6)	0.0000	-1.15997(14)	0.066(1)
U(12)	-0.79978(5)	0.29849(8)	-1.20331(10)	0.071(1)
U(13)	-0.49373(4)	0.12071(8)	-1.18876(9)	0.064(1)
U(14)	-0.70753(8)	0.5000	-1.44693(15)	0.084(1)
U(15)	-0.74253(4)	0.29556(8)	-1.37779(10)	0.067(1)
U(16)	-0.59272(4)	0.37655(8)	-0.65098(11)	0.072(1)
U(17)	-0.62673(4)	0.37465(7)	-1.20091(10)	0.066(1)
U(18)	-0.57150(4)	0.07519(7)	-1.25107(9)	0.062(1)
U(19)	-0.79103(6)	0.38048(9)	-1.06896(12)	0.092(1)
U(20)	-0.65461(6)	0.37860(9)	-0.97804(10)	0.094(1)
U(21)	-0.40150(4)	0.42402(8)	-0.53761(9)	0.068(1)
U(22)	-0.51385(6)	0.5000	-0.73813(13)	0.067(1)
U(23)	-0.78901(8)	0.5000	-1.50027(14)	0.089(1)
U(24)	-0.46435(5)	0.20157(8)	-1.04133(11)	0.079(1)
U(25)	-0.61398(8)	0.5000	-0.97859(15)	0.099(2)
U(26)	-0.71927(7)	0.42463(10)	-0.95838(11)	0.107(1)
U(27)	-0.52351(5)	0.29886(8)	-0.61174(13)	0.091(1)
U(28)	-0.83526(8)	0.5000	-1.13441(19)	0.098(1)

U(29)	-0.59581(4)	0.12209(7)	-1.08171(10)	0.063(1)
U(30)	-0.58574(6)	0.5000	-0.73050(12)	0.060(1)
K(1)	-0.4628(3)	0.5000	-0.5758(8)	0.076(6)
K(2)	-0.5882(4)	0.5000	-0.5840(7)	0.074(6)
K(3)	-0.6761(4)	0.5000	-1.2622(9)	0.092(7)
K(4)	-0.8028(4)	0.5000	-1.3509(9)	0.096(7)
K(5)	-0.4204(4)	0.0000	-0.8777(10)	0.090(7)
K(6)	-0.4690(3)	-0.1359(5)	-0.9085(6)	0.094(5)
K(7)	-0.5419(3)	0.3606(6)	-0.4977(7)	0.017(5)
K(8)	-0.7289(4)	0.3834(6)	-1.1258(7)	0.025(5)
K(9)	-0.6758(3)	0.1662(6)	-1.1405(9)	0.146(8)
K(10)	-0.8006(4)	0.4358(7)	-1.2152(8)	0.037(6)
K(11)	-0.5929(3)	0.2646(5)	-1.1097(7)	0.127(7)
K(12)	-0.7427(4)	0.4356(7)	-1.3719(8)	0.041(6)
K(13)	-0.6569(4)	0.4355(7)	-1.1125(8)	0.041(6)
K(14)	-0.7757(4)	0.3583(9)	-1.2988(9)	0.040(6)
K(15A)	-0.6987(4)	0.3591(8)	-1.2472(9)	0.041(6)
K(15B)	-0.7056(6)	0.3846(11)	-1.2415(11)	0.076(9)
K(16A)	-0.5257(4)	0.4387(8)	-0.6137(10)	0.048(7)
K(16B)	-0.5322(6)	0.4205(10)	-0.6475(13)	0.078(9)
K(17)	-0.5164(4)	0.0000	-1.1487(12)	0.119(9)
K(18)	-0.7596(6)	0.5000	-1.0872(11)	0.036(8)
K(19A)	-0.5370(4)	0.0598(7)	-0.9625(8)	0.037(6)
K(19B)	-0.5481(6)	0.0772(9)	-0.9490(11)	0.072(8)
P(1)	-0.6276(3)	0.0780(5)	-1.2219(6)	0.064(5)
P(2)	-0.5934(3)	0.1799(6)	-1.2006(7)	0.070(5)
P(3)	-0.5231(4)	0.2654(8)	-1.0639(9)	0.107(7)
P(4)	-0.5299(5)	0.2332(8)	-0.4985(10)	0.114(7)
P(5)	-0.3898(4)	0.3171(6)	-0.4501(7)	0.083(5)
P(6)	-0.3581(3)	0.4181(6)	-0.3941(7)	0.074(5)
O(1)	-0.5866(7)	0.2301(12)	-1.2017(14)	0.068(11)
O(2)	-0.6514(8)	0.0431(15)	-1.2361(17)	0.100(14)
O(3)	-0.4247(9)	0.0000	-0.9955(18)	0.056(14)
O(4)	-0.7544(7)	0.2530(12)	-1.3171(14)	0.069(11)
O(5)	-0.8190(6)	0.4051(11)	-1.3202(12)	0.054(9)
O(6)	-0.3820(7)	0.0564(12)	-0.9297(15)	0.077(12)

O(7)	-0.5095(10)	0.5000	-0.671(2)	0.079(17)
O(8)	-0.5122(8)	0.3385(14)	-0.6779(16)	0.093(13)
O(9)	-0.8329(7)	0.3392(12)	-1.4133(14)	0.068(11)
O(10)	-0.6888(7)	0.2569(11)	-1.1764(14)	0.065(10)
O(11)	-0.6799(6)	0.3506(11)	-1.1354(12)	0.052(9)
O(12)	-0.5856(8)	0.0891(14)	-1.3244(16)	0.095(13)
O(13)	-0.6280(7)	0.3353(12)	-1.1256(14)	0.066(10)
O(14)	-0.6399(8)	0.3864(13)	-1.2951(16)	0.085(13)
O(15)	-0.7762(7)	0.2544(12)	-1.2375(15)	0.073(11)
O(16)	-0.5584(6)	0.0609(11)	-1.1786(13)	0.057(10)
O(17)	-0.6328(9)	0.5000	-1.1432(19)	0.063(15)
O(18)	-0.8463(7)	0.3837(11)	-1.4363(13)	0.061(10)
O(19)	-0.4229(7)	0.1613(12)	-1.0016(15)	0.075(11)
O(20)	-0.4818(7)	0.4462(13)	-0.7169(15)	0.079(12)
O(21)	-0.5395(7)	0.1257(12)	-1.2387(14)	0.071(11)
O(22)	-0.6759(7)	0.4085(13)	-1.0355(15)	0.079(12)
O(23)	-0.3800(7)	0.4124(13)	-0.5674(15)	0.080(12)
O(24)	-0.4107(6)	0.0246(10)	-1.0854(13)	0.061(10)
O(25)	-0.7054(17)	0.5000	-1.509(3)	0.17(3)
O(26)	-0.7127(10)	0.5000	-1.386(2)	0.073(16)
O(27)	-0.7007(8)	0.3049(14)	-1.3591(16)	0.090(13)
O(28)	-0.4616(8)	0.1633(14)	-1.1169(16)	0.089(13)
O(29)	-0.7406(6)	0.3483(10)	-1.3385(11)	0.043(8)
O(30)	-0.5560(7)	0.5260(11)	-0.7632(13)	0.066(11)
O(31)	-0.7327(7)	0.1899(12)	-1.2192(14)	0.072(11)
O(32)	-0.7767(9)	0.5000	-1.4274(18)	0.057(14)
O(33)	-0.7767(7)	0.4088(13)	-1.1063(15)	0.078(12)
O(34)	-0.5987(8)	0.4195(13)	-1.1271(15)	0.082(12)
O(35)	-0.5666(7)	0.4110(12)	-0.5985(14)	0.073(11)
O(36)	-0.8758(8)	0.3389(14)	-1.3853(16)	0.092(13)
O(37)	-0.8180(8)	0.2493(13)	-1.2022(15)	0.086(12)
O(38)	-0.4877(7)	0.1874(12)	-1.1371(14)	0.071(11)
O(39)	-0.4983(7)	0.0902(11)	-1.1376(13)	0.062(10)
O(40)	-0.4886(8)	0.3130(13)	-0.6338(15)	0.083(12)
O(41)	-0.5160(7)	0.3468(12)	-0.5688(14)	0.074(11)
O(42)	-0.7879(8)	0.3119(13)	-1.1127(16)	0.089(13)

O(43)	-0.7172(7)	0.3310(13)	-1.4141(15)	0.078(12)
O(44)	-0.6449(7)	0.3106(12)	-1.1762(14)	0.069(11)
O(45)	-0.3656(7)	0.4307(13)	-0.4529(15)	0.082(12)
O(46)	-0.7822(7)	0.3507(11)	-1.2082(13)	0.062(10)
O(47)	-0.6541(6)	0.4077(10)	-1.2066(12)	0.047(9)
O(48)	-0.4634(9)	0.0000	-1.1190(18)	0.057(14)
O(49)	-0.6924(6)	0.4054(11)	-1.3310(13)	0.054(9)
O(50)	-0.5732(6)	0.1890(11)	-1.0381(13)	0.057(10)
O(51)	-0.6139(6)	0.0677(11)	-1.2570(13)	0.058(10)
O(52)	-0.8348(10)	0.5000	-1.286(2)	0.073(16)
O(53)	-0.6100(7)	0.0783(11)	-1.1640(14)	0.067(11)
O(54)	-0.6774(9)	0.4420(15)	-1.4112(18)	0.108(15)
O(55)	-0.6746(9)	0.4145(16)	-0.9301(18)	0.110(15)
O(56)	-0.8131(8)	0.3364(13)	-1.1431(15)	0.082(12)
O(57)	-0.8261(7)	0.3081(12)	-1.2979(14)	0.064(10)
O(58)	-0.4780(7)	0.0560(13)	-1.2161(15)	0.077(12)
O(59)	-0.4789(8)	0.4089(13)	-0.6142(15)	0.083(12)
O(60)	-0.7451(8)	0.2458(13)	-1.4192(15)	0.083(12)
O(61)	-0.7877(7)	0.3055(12)	-1.4218(15)	0.076(12)
O(62)	-0.7346(6)	0.3166(10)	-1.2209(12)	0.042(9)
O(63)	-0.7637(6)	0.2541(11)	-1.1798(13)	0.053(9)
O(64)	-0.8309(8)	0.3443(14)	-1.5167(16)	0.094(13)
O(65)	-0.7746(7)	0.3284(13)	-1.4491(15)	0.078(12)
O(66)	-0.7905(7)	0.4031(12)	-1.3964(14)	0.072(11)
O(67)	-0.4320(12)	0.0000	-1.202(2)	0.096(19)
O(68)	-0.5868(11)	0.0000	-1.277(2)	0.075(16)
O(69)	-0.4238(6)	0.4377(10)	-0.5085(12)	0.045(9)
O(70)	-0.6094(11)	0.5000	-0.801(2)	0.079(17)
O(71)	-0.6421(8)	0.2525(13)	-1.0797(16)	0.088(13)
O(72)	-0.4887(7)	0.1553(13)	-1.2405(15)	0.081(12)
O(73)	-0.6073(7)	0.5553(12)	-0.7038(13)	0.065(10)
O(74)	-0.5672(6)	0.0902(11)	-1.0604(13)	0.060(10)
O(75)	-0.5635(12)	0.5000	-1.100(2)	0.096(19)
O(76)	-0.8052(9)	0.3477(16)	-1.0315(18)	0.114(15)
O(77)	-0.5883(7)	0.5812(11)	-0.7240(14)	0.067(11)
O(78)	-0.6243(7)	0.1559(12)	-1.1017(14)	0.071(11)

O(79)	-0.7207(7)	0.4378(12)	-1.0215(14)	0.068(11)
O(80)	-0.8713(7)	0.4409(13)	-1.3673(16)	0.081(12)
O(81)	-0.3635(10)	0.0000	-0.995(2)	0.068(15)
O(82)	-0.4322(7)	0.4161(12)	-0.6258(13)	0.065(10)
O(83)	-0.5614(8)	0.3375(13)	-0.6734(15)	0.084(12)
O(84)	-0.4788(7)	0.1508(12)	-1.0267(14)	0.073(11)
O(85)	-0.8365(8)	0.3352(14)	-1.2681(16)	0.093(13)
O(86)	-0.3875(9)	0.5000	-0.5212(18)	0.054(13)
O(87)	-0.5671(7)	0.3115(12)	-0.6337(14)	0.067(11)
O(88)	-0.8622(8)	0.4724(13)	-1.2223(16)	0.097(14)
O(89)	-0.8086(10)	0.5000	-1.155(2)	0.077(17)
O(90)	-0.5630(10)	0.5000	-0.663(2)	0.074(16)
O(91)	-0.8693(8)	0.4201(13)	-1.3191(16)	0.089(13)
O(92)	-0.4300(8)	0.3717(13)	-0.5993(15)	0.080(12)
O(93)	-0.5322(7)	0.0823(13)	-1.2547(15)	0.076(12)
O(94)	-0.5610(12)	0.0000	-1.268(2)	0.092(19)
O(95)	-0.5066(6)	0.4201(11)	-0.7337(13)	0.058(10)
O(96)	-0.4548(7)	0.0799(12)	-1.1700(14)	0.073(11)
O(97)	-0.6984(7)	0.2556(12)	-1.1356(14)	0.072(11)
O(98)	-0.6439(9)	0.5000	-1.0392(17)	0.049(13)
O(99)	-0.5842(11)	0.5000	-0.914(2)	0.086(18)
O(100)	-0.5046(10)	0.2435(17)	-1.079(2)	0.130(17)
O(101)	-0.7680(6)	0.3836(11)	-1.2850(12)	0.032(8)
O(102)	-0.4097(11)	0.5000	-0.573(2)	0.077(17)
O(103)	-0.5993(7)	0.3393(13)	-1.1930(14)	0.078(12)
O(104)	-0.6302(9)	0.4448(15)	-0.9369(18)	0.107(15)
O(105)	-0.3930(7)	0.0812(11)	-0.9836(13)	0.061(10)
O(106)	-0.6373(10)	0.3336(18)	-1.026(2)	0.132(18)
O(107)	-0.6001(9)	0.4419(15)	-1.1812(18)	0.111(15)
O(108)	-0.6492(7)	0.3425(12)	-1.2892(13)	0.063(10)
O(109)	-0.7034(8)	0.4164(13)	-1.4435(15)	0.082(12)
O(110)	-0.8186(8)	0.4447(14)	-1.4972(16)	0.095(13)
O(111)	-0.7933(9)	0.4190(14)	-1.4986(17)	0.101(14)
O(112)	-0.6636(7)	0.3449(13)	-1.4004(14)	0.077(12)
O(113)	-0.9014(14)	0.5000	-1.329(3)	0.13(2)
O(114)	-0.6672(9)	0.3108(15)	-1.0280(18)	0.106(15)

O(115)	-0.4674(8)	0.3481(15)	-0.7111(17)	0.103(14)
O(116)	-0.5941(8)	0.4754(12)	-1.0326(16)	0.100(14)
O(117)	-0.7507(8)	0.4740(12)	-1.4959(15)	0.082(12)
O(118)	-0.6202(8)	0.3451(14)	-0.7030(16)	0.095(13)
O(119)	-0.7503(10)	0.3661(16)	-1.001(2)	0.127(17)
O(120)	-0.7645(11)	0.4190(19)	-0.994(2)	0.15(2)
O(121)	-0.8303(8)	0.4187(13)	-1.1179(16)	0.084(12)
O(122)	-0.8143(8)	0.4436(14)	-1.0674(17)	0.096(14)
O(123)	-0.6899(9)	0.3676(16)	-0.9550(19)	0.116(16)
O(124)	-0.6194(9)	0.4180(16)	-0.9739(19)	0.116(16)
O(125)	-0.6347(9)	0.3463(15)	-0.9169(17)	0.103(14)
O(126)	-0.3925(9)	0.3507(16)	-0.4967(18)	0.114(15)
O(127)	-0.4473(10)	0.2485(18)	-1.056(2)	0.134(18)
O(128)	-0.7167(10)	0.4038(18)	-0.894(2)	0.134(18)
O(129)	-0.731(2)	0.5000	-0.946(4)	0.20(4)
O(130)	-0.7018(17)	0.5000	-0.921(3)	0.15(3)
O(131)	-0.5311(10)	0.2486(18)	-0.656(2)	0.139(19)
O(132)	-0.8602(14)	0.5000	-1.111(3)	0.13(2)
O(133)	-0.5857(7)	0.1660(13)	-1.1447(15)	0.080(12)
O(134)	-0.3368(8)	0.4518(14)	-0.3542(16)	0.092(13)
O(135)	-0.3959(6)	0.2688(11)	-0.4727(13)	0.060(10)
O(136)	-0.5833(7)	0.1492(12)	-1.2309(14)	0.069(11)
O(137)	-0.5183(12)	0.5000	-0.806(2)	0.096(19)
O(138)	-0.7267(10)	0.2545(16)	-1.2961(19)	0.124(17)
O(139)	-0.8006(16)	0.5000	-1.577(3)	0.15(3)
O(140)	-0.5314(14)	0.242(2)	-1.026(3)	0.20(3)
O(141)	-0.5408(13)	0.285(2)	-1.114(3)	0.18(2)
O(142)	-0.5372(11)	0.2573(19)	-0.548(2)	0.15(2)
O(143)	-0.5557(11)	0.2200(18)	-0.493(2)	0.139(19)
O(144)	-0.4049(8)	0.3342(13)	-0.4230(16)	0.087(12)
O(145)	-0.3782(8)	0.4167(14)	-0.3733(17)	0.096(14)
O(146)	-0.5184(14)	0.271(2)	-0.469(3)	0.19(3)
OW1	-0.6691(15)	0.067(3)	-1.144(3)	0.08(2)
OW2	-0.4431(6)	0.3203(10)	-0.7829(11)	0.040(8)
OW3	-0.5871(5)	0.2292(8)	-0.6013(10)	0.020(7)
OW4	-0.4151(6)	0.4174(11)	-0.1495(13)	0.059(10)

OW5	-0.6439(6)	0.0000	-1.3361(13)	0.011(9)
OW6	-0.3313(8)	0.5000	-0.4436(16)	0.038(12)
OW7	-0.6919(7)	0.5000	-1.0466(14)	0.020(10)
OW8	-0.7438(14)	0.0000	-1.393(3)	0.03(2)
OW9	-0.6372(10)	0.5000	-1.294(2)	0.078(17)
OW10	-0.7818(9)	0.1634(15)	-1.1834(17)	0.008(12)
OW11	-0.1287(8)	0.2540(13)	-0.6933(15)	0.083(12)
OW12	-0.3643(10)	0.4019(17)	-0.182(2)	0.027(15)
OW13	-0.3895(11)	0.2138(19)	-1.021(2)	0.040(17)
OW14	-0.8491(14)	0.5000	-1.437(3)	0.03(2)
C(1)	-0.6282(6)	0.1764(15)	-1.2310(15)	0.082(19)
C(2)	-0.6410(8)	0.2188(11)	-1.2421(16)	0.063(16)
C(3)	-0.6678(8)	0.2200(12)	-1.2642(17)	0.10(2)
C(4)	-0.6817(6)	0.1787(17)	-1.2753(16)	0.11(2)
C(5)	-0.6689(8)	0.1362(12)	-1.2642(16)	0.069(17)
C(6)	-0.6421(8)	0.1351(11)	-1.2421(17)	0.09(2)
C(7)	-0.3573(6)	0.3184(15)	-0.4044(14)	0.048(14)
C(8)	-0.3445(9)	0.2759(11)	-0.3951(17)	0.081(19)
C(9)	-0.3181(9)	0.2739(13)	-0.363(2)	0.17(4)
C(10)	-0.3045(6)	0.3144(18)	-0.3407(17)	0.12(3)
C(11)	-0.3173(8)	0.3569(14)	-0.3500(16)	0.074(18)
C(12)	-0.3436(8)	0.3589(11)	-0.3818(17)	0.09(2)

Table S12. Anisotropic displacement parameters (\AA^2) for K-U₂₀Ppb₆-U@U₂₈.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[\mathbf{h}^2\mathbf{a}^{*2}\mathbf{U}_{11} + \dots + 2\mathbf{hka}^{*}\mathbf{b}^{*}\mathbf{U}_{12}]$$

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
U(1)	0.0332(19)	0.0481(18)	0.0429(18)	0.000	0.0100(15)	0.000
U(2)	0.0373(14)	0.0491(14)	0.0759(16)	0.0033(12)	0.0090(12)	-0.0005(11)
U(3)	0.0466(16)	0.0739(17)	0.0562(15)	-0.0127(13)	-0.0054(12)	-0.0055(13)
U(4)	0.0506(16)	0.0725(16)	0.0824(18)	-0.0052(14)	0.0357(14)	0.0043(13)
U(5)	0.038(2)	0.061(2)	0.145(4)	0.000	0.036(2)	0.000
U(6)	0.0461(15)	0.0492(14)	0.0752(17)	0.0083(12)	0.0033(13)	0.0046(12)
U(7)	0.035(2)	0.056(2)	0.074(2)	0.000	0.0194(17)	0.000
U(8)	0.0321(14)	0.0580(15)	0.104(2)	-0.0038(14)	0.0148(13)	-0.0068(12)
U(9)	0.0429(15)	0.0794(17)	0.0725(17)	-0.0247(14)	0.0170(13)	-0.0005(13)
U(10)	0.035(2)	0.055(2)	0.132(3)	0.000	0.006(2)	0.000
U(11)	0.047(2)	0.083(2)	0.069(2)	0.000	0.0253(18)	0.000
U(12)	0.0616(17)	0.0575(15)	0.098(2)	0.0124(14)	0.0379(15)	-0.0034(13)
U(13)	0.0527(16)	0.0637(16)	0.0665(16)	0.0120(13)	0.0147(13)	-0.0093(13)
U(14)	0.093(3)	0.098(3)	0.079(3)	0.000	0.055(2)	0.000
U(15)	0.0461(16)	0.0714(17)	0.0727(17)	-0.0120(13)	0.0144(13)	0.0000(13)
U(16)	0.0371(15)	0.0657(16)	0.0954(19)	0.0045(14)	0.0096(13)	-0.0109(13)
U(17)	0.0326(14)	0.0550(15)	0.1019(19)	-0.0008(14)	0.0186(13)	0.0060(12)
U(18)	0.0453(15)	0.0593(15)	0.0633(16)	0.0110(12)	0.0059(12)	0.0053(12)
U(19)	0.127(3)	0.0829(19)	0.096(2)	0.0127(16)	0.076(2)	-0.0027(18)
U(20)	0.111(2)	0.0715(18)	0.0582(17)	0.0165(14)	-0.0036(16)	0.0046(16)
U(21)	0.0386(15)	0.0777(17)	0.0737(17)	-0.0127(14)	0.0111(12)	0.0129(13)
U(22)	0.048(2)	0.095(3)	0.051(2)	0.000	0.0143(17)	0.000
U(23)	0.081(3)	0.106(3)	0.046(2)	0.000	-0.006(2)	0.000
U(24)	0.0517(17)	0.0533(15)	0.101(2)	-0.0135(14)	0.0028(14)	0.0013(13)
U(25)	0.089(3)	0.069(2)	0.073(3)	0.000	-0.031(2)	0.000
U(26)	0.160(3)	0.092(2)	0.0709(19)	0.0137(16)	0.051(2)	-0.003(2)
U(27)	0.0584(18)	0.0548(16)	0.147(3)	0.0046(16)	0.0318(18)	0.0016(14)
U(28)	0.107(4)	0.087(3)	0.141(4)	0.000	0.091(3)	0.000

U(29)	0.0347(14)	0.0568(15)	0.0809(17)	0.0088(13)	0.0079(12)	0.0073(12)
U(30)	0.043(2)	0.063(2)	0.057(2)	0.000	0.0027(17)	0.000
K(1)	0.050(13)	0.051(12)	0.085(14)	0.000	-0.013(11)	0.000
K(2)	0.079(15)	0.071(13)	0.069(13)	0.000	0.028(11)	0.000
K(3)	0.072(16)	0.078(14)	0.129(19)	0.000	0.047(14)	0.000
K(5)	0.074(16)	0.037(11)	0.16(2)	0.000	0.051(15)	0.000
K(6)	0.042(9)	0.107(12)	0.120(13)	-0.018(10)	0.022(9)	-0.009(8)
K(8)	0.029(13)	0.022(12)	0.029(12)	-0.005(9)	0.016(10)	0.007(10)
K(9)	0.062(12)	0.085(12)	0.25(2)	0.014(13)	0.024(13)	0.021(10)
K(11)	0.096(14)	0.080(11)	0.145(15)	0.009(11)	-0.008(11)	0.024(10)
K(17)	0.045(14)	0.060(14)	0.22(3)	0.000	0.021(16)	0.000

Table S13. Bond lengths [Å] for K-U₂₀Ppb₆-U@U₂₈.

atom-atom	distance	atom-atom	distance
U(1)-O(101)#1	3.91(3)	U(1)-O(101)	3.91(3)
U(2)-O(62)	1.80(3)	U(2)-O(31)	1.85(3)
U(2)-O(138)	2.24(5)	U(2)-O(15)	2.27(4)
U(2)-O(97)	2.32(4)	U(2)-O(10)	2.34(4)
U(2)-O(4)	2.37(3)	U(2)-O(63)	2.37(3)
U(3)-O(66)	1.73(4)	U(3)-O(64)	1.79(4)
U(3)-O(111)	2.18(4)	U(3)-O(110)	2.26(4)
U(3)-O(9)	2.31(3)	U(3)-O(61)	2.32(4)
U(3)-O(65)	2.35(4)	U(3)-O(18)	2.38(3)
U(4)-O(112)	1.70(4)	U(4)-O(49)	1.73(3)
U(4)-O(108)	2.25(3)	U(4)-O(14)	2.26(4)
U(4)-O(109)	2.29(4)	U(4)-O(54)	2.29(4)
U(4)-O(43)	2.39(4)	U(4)-O(27)	2.42(4)
U(5)-O(52)	1.69(5)	U(5)-O(113)	1.80(7)
U(5)-O(88)	2.29(4)	U(5)-O(88)#1	2.29(4)
U(5)-O(91)	2.32(4)	U(5)-O(91)#1	2.32(4)
U(5)-O(80)#1	2.30(4)	U(5)-O(80)	2.30(4)
U(6)-O(11)	1.73(3)	U(6)-O(71)	1.76(4)
U(6)-O(10)	2.23(3)	U(6)-O(106)	2.26(5)
U(6)-O(13)	2.33(3)	U(6)-O(114)	2.36(4)

U(6)-O(44)	2.36(3)	U(6)-O(97)	2.35(4)
U(7)-O(81)	1.73(5)	U(7)-O(3)	1.77(5)
U(7)-O(24)#2	2.28(3)	U(7)-O(24)	2.28(3)
U(7)-O(6)	2.29(4)	U(7)-O(6)#2	2.29(4)
U(7)-O(105)#2	2.35(3)	U(7)-O(105)	2.35(3)
U(8)-O(36)	1.76(4)	U(8)-O(5)	1.77(3)
U(8)-O(91)	2.27(4)	U(8)-O(18)	2.31(3)
U(8)-O(9)	2.33(3)	U(8)-O(85)	2.32(4)
U(8)-O(57)	2.34(3)	U(8)-O(80)	2.34(4)
U(9)-O(59)	1.63(4)	U(9)-O(115)	1.78(4)
U(9)-O(92)	2.36(4)	U(9)-O(40)	2.33(4)
U(9)-O(20)	2.35(4)	U(9)-O(8)	2.37(4)
U(9)-O(82)	2.40(3)	U(9)-O(95)	2.38(3)
U(10)-O(17)	1.77(5)	U(10)-O(75)	1.87(6)
U(10)-O(34)	2.32(4)	U(10)-O(34)#1	2.32(4)
U(10)-O(107)#1	2.32(4)	U(10)-O(107)	2.32(4)
U(10)-O(116)#1	2.34(4)	U(10)-O(116)	2.34(4)
U(11)-O(48)	1.65(5)	U(11)-O(67)	1.73(6)
U(11)-O(96)#2	2.32(3)	U(11)-O(96)	2.32(3)
U(11)-O(24)	2.35(3)	U(11)-O(24)#2	2.35(3)
U(11)-O(58)	2.36(4)	U(11)-O(58)#2	2.37(4)
U(12)-O(37)	1.76(4)	U(12)-O(46)	1.84(3)
U(12)-O(42)	2.26(4)	U(12)-O(63)	2.28(3)

U(12)-O(15)	2.30(4)	U(12)-O(56)	2.32(4)
U(12)-O(85)	2.34(4)	U(12)-O(57)	2.36(3)
U(13)-O(39)	1.74(3)	U(13)-O(72)	1.82(4)
U(13)-O(38)	2.30(4)	U(13)-O(58)	2.31(4)
U(13)-O(28)	2.37(4)	U(13)-O(96)	2.38(4)
U(13)-O(21)	2.40(4)	U(13)-O(93)	2.43(4)
U(14)-O(25)	1.71(8)	U(14)-O(26)	1.79(5)
U(14)-O(54)	2.30(4)	U(14)-O(54)#1	2.30(5)
U(14)-O(117)	2.38(4)	U(14)-O(117)#1	2.38(4)
U(14)-O(109)	2.41(4)	U(14)-O(109)#1	2.41(4)
U(15)-O(60)	1.78(4)	U(15)-O(29)	1.82(3)
U(15)-O(65)	2.23(4)	U(15)-O(27)	2.25(4)
U(15)-O(43)	2.30(4)	U(15)-O(138)	2.31(5)
U(15)-O(61)	2.36(4)	U(15)-O(4)	2.35(3)
U(16)-O(118)	1.84(4)	U(16)-O(35)	1.85(4)
U(16)-O(87)	2.30(3)	U(16)-O(145)#5	2.33(4)
U(16)-O(73)#1	2.35(3)	U(16)-O(144)#5	2.38(4)
U(16)-O(83)	2.40(4)	U(16)-O(77)#1	2.40(3)
U(17)-O(47)	1.78(3)	U(17)-O(103)	1.81(4)
U(17)-O(13)	2.34(3)	U(17)-O(44)	2.34(3)
U(17)-O(34)	2.34(4)	U(17)-O(14)	2.34(4)
U(17)-O(108)	2.36(3)	U(17)-O(107)	2.38(5)
U(18)-O(16)	1.81(3)	U(18)-O(12)	1.83(4)

U(18)-O(21)	2.25(4)	U(18)-O(68)	2.33(2)
U(18)-O(93)	2.30(4)	U(18)-O(94)	2.34(2)
U(18)-O(136)	2.36(4)	U(18)-O(51)	2.38(3)
U(19)-O(33)	1.74(4)	U(19)-O(76)	1.80(5)
U(19)-O(56)	2.25(4)	U(19)-O(122)	2.26(4)
U(19)-O(120)	2.24(5)	U(19)-O(42)	2.34(4)
U(19)-O(119)	2.32(5)	U(19)-O(121)	2.35(4)
U(20)-O(22)	1.74(4)	U(20)-O(125)	1.81(4)
U(20)-O(124)	2.27(5)	U(20)-O(114)	2.30(4)
U(20)-O(106)	2.32(5)	U(20)-O(55)	2.29(4)
U(20)-O(104)	2.34(4)	U(20)-O(123)	2.37(5)
U(21)-O(23)	1.76(4)	U(21)-O(69)	1.80(3)
U(21)-O(86)	2.303(16)	U(21)-O(82)	2.29(3)
U(21)-O(126)	2.33(5)	U(21)-O(45)	2.35(4)
U(21)-O(92)	2.32(4)	U(21)-O(102)	2.35(2)
U(22)-O(7)	1.72(5)	U(22)-O(137)	1.74(6)
U(22)-O(20)	2.28(4)	U(22)-O(20)#1	2.28(4)
U(22)-O(30)	2.34(3)	U(22)-O(30)#1	2.34(3)
U(22)-O(95)#1	2.33(3)	U(22)-O(95)	2.33(3)
U(23)-O(32)	1.78(4)	U(23)-O(139)	1.87(8)
U(23)-O(117)#1	2.27(4)	U(23)-O(117)	2.27(4)
U(23)-O(111)	2.34(4)	U(23)-O(111)#1	2.34(4)
U(23)-O(110)#1	2.35(4)	U(23)-O(110)	2.35(4)

U(24)-O(84)	1.80(4)	U(24)-O(127)	1.80(5)
U(24)-O(140)#4	2.25(7)	U(24)-O(50)#4	2.34(3)
U(24)-O(28)	2.37(4)	U(24)-O(38)	2.38(4)
U(24)-O(100)	2.42(5)	U(24)-O(19)	2.45(4)
U(25)-O(98)	1.80(4)	U(25)-O(99)	1.86(6)
U(25)-O(116)	2.30(4)	U(25)-O(116)#1	2.30(4)
U(25)-O(104)	2.34(4)	U(25)-O(104)#1	2.34(4)
U(25)-O(124)#1	2.39(4)	U(25)-O(124)	2.39(4)
U(26)-O(79)	1.70(3)	U(26)-O(128)	1.76(5)
U(26)-O(55)	2.36(5)	U(26)-O(123)	2.32(5)
U(26)-O(120)	2.36(6)	U(26)-O(129)	2.34(4)
U(26)-O(119)	2.36(5)	U(26)-O(130)	2.42(4)
U(27)-O(41)	1.73(4)	U(27)-O(131)	1.80(5)
U(27)-O(87)	2.34(4)	U(27)-O(40)	2.35(4)
U(27)-O(83)	2.38(4)	U(27)-O(8)	2.41(4)
U(27)-O(142)	2.47(6)	U(27)-O(146)#5	2.60(7)
U(28)-O(132)	1.79(7)	U(28)-O(89)	1.83(5)
U(28)-O(122)	2.34(4)	U(28)-O(122)#1	2.34(4)
U(28)-O(121)#1	2.37(4)	U(28)-O(121)	2.37(4)
U(28)-O(88)	2.35(4)	U(28)-O(88)#1	2.35(4)
U(29)-O(74)	1.75(3)	U(29)-O(78)	1.78(4)
U(29)-O(19)#4	2.32(4)	U(29)-O(50)	2.34(3)
U(29)-O(53)	2.37(3)	U(29)-O(6)#4	2.36(4)

U(29)-O(133)	2.37(4)	U(29)-O(105)#4	2.41(3)
U(30)-O(90)	1.74(5)	U(30)-O(70)	1.81(5)
U(30)-O(73)#1	2.30(3)	U(30)-O(73)	2.30(3)
U(30)-O(77)	2.35(3)	U(30)-O(77)#1	2.35(3)
U(30)-O(30)#1	2.34(3)	U(30)-O(30)	2.34(3)
K(1)-O(7)	2.81(6)	K(1)-O(69)	2.84(3)
K(1)-O(69)#1	2.84(3)	K(1)-O(59)	2.82(4)
K(1)-O(59)#1	2.82(4)	K(1)-O(102)	3.01(6)
K(2)-O(69)#6	2.90(3)	K(2)-O(69)#5	2.90(3)
K(2)-O(35)#1	2.94(4)	K(2)-O(35)	2.94(4)
K(2)-O(145)#5	2.98(4)	K(2)-O(145)#6	2.98(4)
K(2)-O(90)	3.01(5)	K(2)-O(73)	3.33(4)
K(2)-O(73)#1	3.33(4)	K(3)-OW9	2.70(6)
K(3)-O(47)	3.04(3)	K(3)-O(47)#1	3.04(3)
K(3)-O(26)	3.09(6)	K(3)-O(17)	3.11(5)
K(3)-O(49)#1	3.19(3)	K(3)-O(49)	3.19(3)
K(4)-OW14	2.69(8)	K(4)-O(52)	3.01(6)
K(4)-O(32)	3.00(5)	K(4)-O(5)#1	3.10(3)
K(4)-O(5)	3.10(3)	K(4)-O(66)#1	3.23(4)
K(4)-O(66)	3.23(4)	K(4)-O(101)	3.91(3)
K(4)-O(101)#1	3.91(3)	K(5)-O(53)#4	2.78(4)
K(5)-O(53)#3	2.78(4)	K(5)-O(16)#4	2.89(4)
K(5)-O(16)#3	2.89(4)	K(5)-O(74)#3	3.00(3)

K(5)-O(74)#4	3.00(3)	K(5)-O(3)	3.06(5)
K(6)-O(84)#3	2.79(4)	K(6)-O(74)#3	2.85(4)
K(6)-O(39)#3	2.95(4)	K(6)-O(133)#3	2.97(4)
K(6)-O(84)#2	3.00(4)	K(6)-O(16)#3	3.08(3)
K(6)-O(100)#3	3.40(5)	K(7)-O(35)	2.86(4)
K(7)-O(146)	2.86(7)	K(7)-O(41)	2.89(4)
K(7)-O(144)#5	2.99(4)	K(7)-O(69)#5	3.01(3)
K(7)-O(41)#5	3.06(4)	K(7)-O(59)#5	3.05(4)
K(7)-O(142)	3.31(6)	K(8)-O(22)	3.07(4)
K(8)-O(46)	3.07(4)	K(8)-O(11)	3.07(4)
K(8)-O(33)	3.08(4)	K(8)-O(79)	3.06(4)
K(8)-O(62)	3.09(3)	K(9)-O(78)	2.70(4)
K(9)-O(10)	2.77(4)	K(9)-OW1	2.87(8)
K(9)-O(97)	2.90(4)	K(9)-O(71)	3.14(4)
K(9)-O(31)	3.13(4)	K(9)-C(4)	3.50(5)
K(10)-O(89)	2.61(4)	K(10)-O(46)	2.64(4)
K(10)-O(5)	2.70(4)	K(10)-O(33)	2.76(4)
K(10)-O(52)	2.78(4)	K(10)-O(101)	3.48(3)
K(11)-O(13)	2.76(4)	K(11)-O(50)	2.80(4)
K(11)-O(1)	2.81(4)	K(11)-O(103)	3.00(4)
K(11)-O(133)	3.06(4)	K(11)-O(44)	3.06(4)
K(11)-O(141)	3.09(7)	K(11)-O(71)	3.26(4)
K(11)-O(140)	3.35(7)	K(12)-O(32)	2.65(4)

K(12)-O(29)	2.65(3)	K(12)-O(26)	2.65(4)
K(12)-O(66)	2.70(4)	K(12)-O(49)	2.76(4)
K(12)-O(101)	3.55(4)	K(12)-O(117)	3.34(4)
K(12)-O(111)	3.45(5)	K(13)-O(98)	2.57(4)
K(13)-O(17)	2.64(4)	K(13)-O(47)	2.71(3)
K(13)-O(11)	2.72(4)	K(13)-O(22)	2.81(4)
K(14)-O(101)	0.85(3)	K(14)-O(46)	2.61(4)
K(14)-O(29)	2.65(4)	K(14)-O(5)	2.67(4)
K(14)-O(62)	2.68(4)	K(14)-O(66)	2.71(4)
K(14)-O(57)	3.23(4)	K(15A)-O(29)	2.63(4)
K(15A)-O(47)	2.70(4)	K(15A)-O(62)	2.72(4)
K(15A)-O(11)	2.74(4)	K(15A)-O(49)	2.76(4)
K(15A)-O(44)	3.18(4)	K(15A)-O(101)	3.73(4)
K(15B)-O(29)	2.73(4)	K(15B)-O(47)	2.77(4)
K(15B)-O(101)	3.26(4)	K(15B)-O(49)	2.86(4)
K(15B)-O(62)	2.76(4)	K(15B)-O(11)	2.77(4)
K(16A)-O(90)	2.65(5)	K(16A)-O(35)	2.66(4)
K(16A)-O(7)	2.73(5)	K(16A)-O(59)	2.82(5)
K(16A)-O(41)	2.86(4)	K(16B)-O(35)	2.80(4)
K(16B)-O(59)	2.81(5)	K(16B)-O(90)	2.81(4)
K(16B)-O(83)	2.83(5)	K(16B)-O(7)	2.82(4)
K(16B)-O(41)	2.85(4)	K(16B)-O(8)	2.88(5)
K(16B)-O(77)#1	3.00(5)	K(16B)-O(30)#1	3.21(4)

K(16B)-O(95)	3.21(4)	K(17)-O(39)#2	2.76(3)
K(17)-O(39)	2.76(3)	K(17)-O(16)	2.80(4)
K(17)-O(16)#2	2.80(4)	K(17)-O(48)	2.80(5)
K(17)-O(94)	3.14(6)	K(18)-O(89)	2.63(6)
K(18)-O(33)#1	2.77(4)	K(18)-O(33)	2.77(4)
K(18)-O(79)	2.82(4)	K(18)-O(79)#1	2.82(4)
K(18)-O(129)	3.44(10)	K(19A)-O(74)	2.61(4)
K(19A)-O(3)#3	2.64(4)	K(19A)-O(39)#4	2.74(4)
K(19A)-O(48)#3	2.77(4)	K(19A)-O(84)#4	2.82(4)
K(19B)-O(39)#4	2.72(4)	K(19B)-O(74)	2.74(4)
K(19B)-O(3)#3	2.76(4)	K(19B)-O(48)#3	2.77(4)
K(19B)-O(84)#4	2.85(4)	K(19B)-O(19)#4	2.92(5)
K(19B)-O(28)#4	2.95(5)	K(19B)-O(105)#4	3.09(5)
K(19B)-O(96)#4	3.12(4)	K(19B)-O(24)#4	3.24(4)
P(1)-O(53)	1.45(4)	P(1)-O(51)	1.48(3)
P(1)-O(2)	1.60(4)	P(1)-C(6)	1.81(3)
P(2)-O(133)	1.43(4)	P(2)-O(136)	1.47(4)
P(2)-O(1)	1.50(4)	P(2)-C(1)	1.81(3)
P(3)-O(140)	1.45(7)	P(3)-O(141)	1.43(6)
P(3)-O(100)	1.43(5)	P(4)-O(146)	1.34(7)
P(4)-O(142)	1.39(5)	P(4)-O(143)	1.59(5)
P(5)-O(144)	1.43(4)	P(5)-O(135)	1.50(3)
P(5)-O(126)	1.53(5)	P(5)-C(7)	1.75(3)

P(6)-O(45)	1.49(4)	P(6)-O(145)	1.48(4)
P(6)-O(134)	1.57(4)	P(6)-C(12)	1.86(3)
O(3)-K(19A)#3	2.64(4)	O(3)-K(19A)#4	2.64(4)
O(3)-K(19B)#3	2.76(4)	O(3)-K(19B)#4	2.76(4)
O(4)-O(138)	1.45(6)	O(6)-O(105)	1.49(4)
O(6)-U(29)#4	2.36(4)	O(7)-K(16A)#1	2.73(5)
O(7)-K(16B)#1	2.82(4)	O(8)-O(40)	1.56(5)
O(9)-O(18)	1.48(4)	O(10)-O(97)	1.41(4)
O(13)-O(44)	1.48(4)	O(14)-O(108)	1.40(4)
O(15)-O(63)	1.40(4)	O(16)-K(5)#3	2.89(4)
O(16)-K(6)#3	3.08(3)	O(17)-K(13)#1	2.64(4)
O(19)-O(50)#4	1.42(4)	O(19)-U(29)#4	2.32(4)
O(19)-K(19B)#4	2.92(5)	O(20)-O(95)	1.50(4)
O(21)-O(93)	1.44(4)	O(24)-O(24)#2	1.41(6)
O(24)-K(19B)#4	3.24(4)	O(26)-K(12)#1	2.65(4)
O(27)-O(43)	1.57(5)	O(28)-O(38)	1.53(5)
O(28)-K(19B)#4	2.95(5)	O(30)-O(30)#1	1.50(6)
O(30)-K(16B)#1	3.21(4)	O(32)-K(12)#1	2.65(4)
O(34)-O(107)	1.56(5)	O(39)-K(19B)#4	2.72(4)
O(39)-K(19A)#4	2.74(4)	O(39)-K(6)#3	2.95(4)
O(41)-K(7)#5	3.06(4)	O(42)-O(56)	1.50(5)
O(48)-K(19B)#4	2.77(4)	O(48)-K(19B)#3	2.77(4)
O(48)-K(19A)#4	2.77(4)	O(48)-K(19A)#3	2.77(4)

O(50)-O(19)#4	1.42(4)	O(50)-U(24)#4	2.34(3)
O(52)-K(10)#1	2.78(4)	O(53)-K(5)#3	2.78(4)
O(54)-O(109)	1.56(5)	O(55)-O(123)	1.59(6)
O(57)-O(85)	1.42(5)	O(58)-O(96)	1.54(5)
O(59)-K(7)#5	3.05(4)	O(61)-O(65)	1.41(5)
O(68)-O(94)	1.39(7)	O(68)-U(18)#2	2.33(2)
O(69)-K(2)#6	2.90(3)	O(69)-K(7)#5	3.01(3)
O(73)-O(77)	1.59(4)	O(73)-U(16)#1	2.35(3)
O(74)-K(6)#3	2.85(4)	O(74)-K(5)#3	3.00(3)
O(77)-U(16)#1	2.40(3)	O(77)-K(16B)#1	3.00(5)
O(80)-O(91)	1.38(5)	O(82)-O(92)	1.44(4)
O(83)-O(87)	1.44(4)	O(84)-K(6)#3	2.79(4)
O(84)-K(19A)#4	2.82(4)	O(84)-K(19B)#4	2.85(4)
O(84)-K(6)#2	3.00(4)	O(86)-O(102)	1.43(6)
O(86)-U(21)#1	2.303(16)	O(88)-O(88)#1	1.59(8)
O(89)-K(10)#1	2.61(4)	O(90)-K(16A)#1	2.65(5)
O(90)-K(16B)#1	2.81(4)	O(94)-U(18)#2	2.34(2)
O(96)-K(19B)#4	3.12(4)	O(98)-K(13)#1	2.57(4)
O(100)-K(6)#3	3.40(5)	O(102)-U(21)#1	2.35(2)
O(104)-O(124)	1.57(6)	O(105)-U(29)#4	2.41(3)
O(105)-K(19B)#4	3.09(5)	O(110)-O(111)	1.64(6)
O(116)-O(116)#1	1.42(7)	O(117)-O(117)#1	1.50(7)
O(119)-O(120)	1.77(7)	O(121)-O(122)	1.47(5)

O(129)-O(130)	1.54(12)	O(129)-U(26)#1	2.34(4)
O(130)-U(26)#1	2.42(4)	O(133)-K(6)#3	2.97(4)
O(140)-U(24)#4	2.25(7)	O(144)-U(16)#5	2.38(4)
O(144)-K(7)#5	2.99(4)	O(145)-U(16)#5	2.33(4)
O(145)-K(2)#6	2.98(4)	O(146)-U(27)#5	2.60(7)
C(1)-C(2)	1.3900	C(1)-C(6)	1.3900
C(2)-C(3)	1.3900	C(3)-C(4)	1.3900
C(4)-C(5)	1.3900	C(5)-C(6)	1.3900
C(7)-C(8)	1.3900	C(7)-C(12)	1.3900
C(8)-C(9)	1.3900	C(9)-C(10)	1.3900
C(10)-C(11)	1.3900	C(11)-C(12)	1.3900

Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1,z #2 x,-y,z #3 -x-1,-y,-z-2 #4 -x-1,y,-z-2

#5 -x-1,y,-z-1 #6 -x-1,-y+1,-z-1

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