Supporting information

Single-Crystal Time-of-Flight Neutron Diffraction and Magic Angle Spinning NMR Spectroscopy Resolve the Structure and ^{1}H and ^{7}Li Dynamics of the Uranyl Peroxide Nanocluster U_{60}

Travis A. Olds,[1] Mateusz Dembowski,[2] Xiaoping Wang,[3] Christina Hoffman,[3] Todd M. Alam,[4] Sarah Hickam,[1] Kristi L. Pellegrini,[1] He Junhong,[5] and Peter C. Burns[1,2*]

[1] Department of Civil and Environmental Engineering and Earth Sciences, University of Notre Dame, Notre Dame, Indiana 46556, United States

[2] Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, Indiana 46556, United States

[3] Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States

[4] Department of Organic Material Science, Sandia National Laboratories, Albuquerque, New Mexico 87185, United States

[5] Instrument and Source Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States

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1) **Raman spectroscopy**

Raman spectra were measured using a Bruker Sentinel system equipped with a Peltier cooled CCD detector and fiber optic diode laser which was calibrated internally with polystyrene and NIST SRM 2065 standards. Crystals of U_{60} were placed onto carbon tape, and the spectrum was collected from 80 to 3200 cm^{-1} at 400 mW, 785 nm, and 5 cm^{-1} resolution. The spectrum reveals two major bands, assigned to the v_1 symmetric vibrations of $(UO_2)^{2+}$ at 803.5 cm^{-1}, and a symmetric stretching mode of bridging peroxide at 842 cm^{-1}. The values correspond well to those determined previously.[1] A series of weak bands found in the 410-131 cm^{-1} region are attributed to various ν (U–OH_{ligand}) stretches.

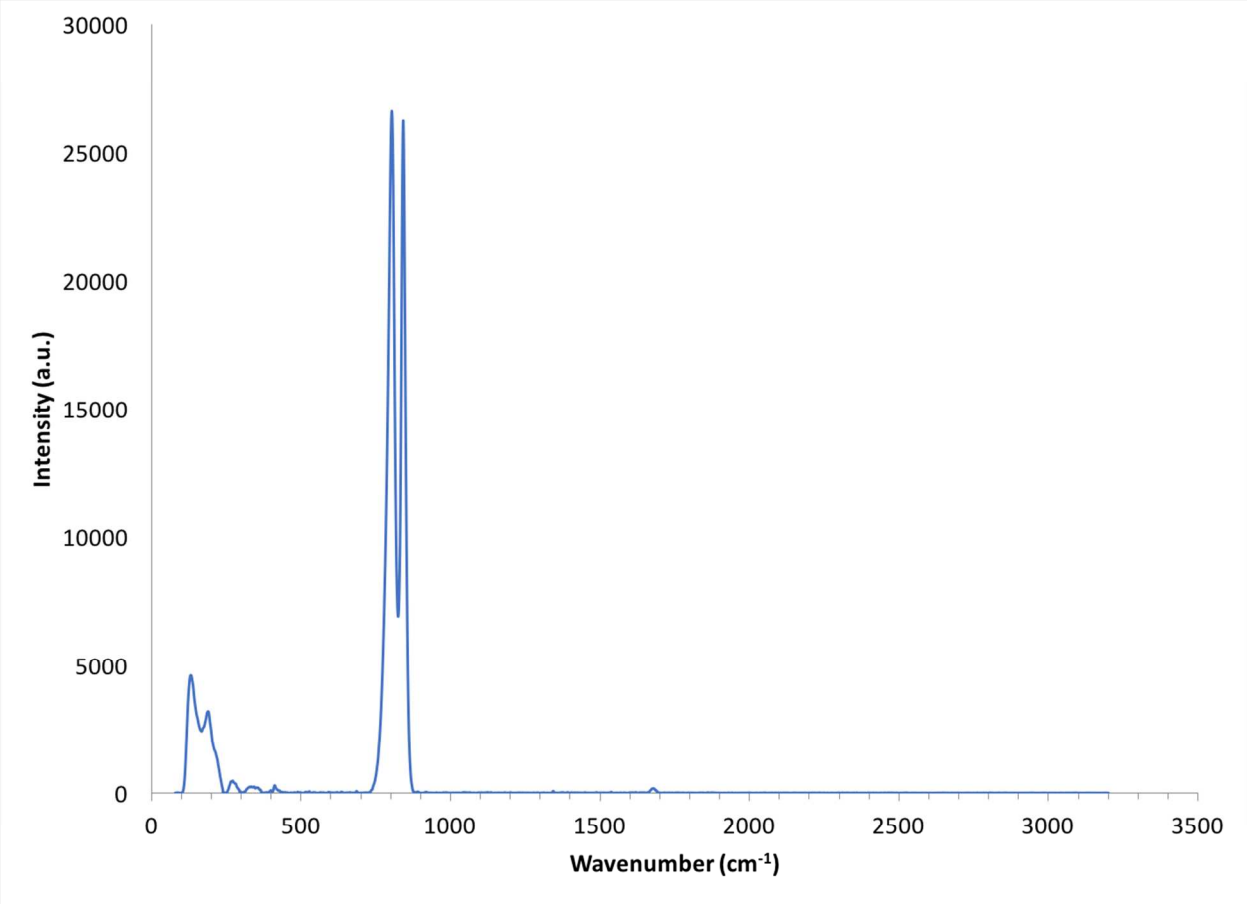

Figure S1. Raman spectra of U_{60} from 80 to 3200 cm^{-1}.

Bartlett and Cooney[2] provide an empirical relationship to derive the approximate U–O_{yl} bond lengths from the band position assigned to the ν_1 $(UO_2)^{2+}$ stretching vibration, which gives 1.807 Å (803.5 cm^{-1}). This corresponds well with the average value from the single crystal neutron data (1.813 Å).

2) **Inductively Coupled Plasma Optical Emission Spectroscopy**

The empirical cation formula for U_{60} was determined using a PerkinElmer Optima 8000 DV ICP-OES instrument for multi-elemental analysis (K, Li, and U). A standard solution of U_{60} (85 mg of crystals/mL) was diluted using 5% nitric acid. External calibration standards were prepared for concentrations ranging from 0.5 to 10 ppm for K and Li, and from 18 to 60 ppm for U. To monitor instrumental drift and matrix effects, each standard, blank, and sample was spiked with 0.5 ppm Y. An average of 5 analyses gives ~17 K^+ and 44 Li^+ per 60 U (Table S1), which corresponds well with that determined previously.[3]

Table S1. Elemental analyses of U_{60}, and the number of K and Li atoms per 60 U.

# K/U_{60}	# Li/U_{60}
16.90	43.69
17.32	45.42
17.37	43.81
16.81	43.66
17.51	44.76
Avg: 17.10	Avg: 44.14

3) **Thermogravimetric Analysis (TGA)**

Thermogravimetric analysis measurements were performed on a Mettler Toledo TGA/DSC-1 Thermal Gravimetric Analyzer. Washed, air-dried crystals of U_{60} (8.4 mg) were placed in a 70 µL alumina crucible and heated from 25 to 800°C at 5°C/min, under N_2 atmosphere with an N_2 flow rate of 50 mL/min.

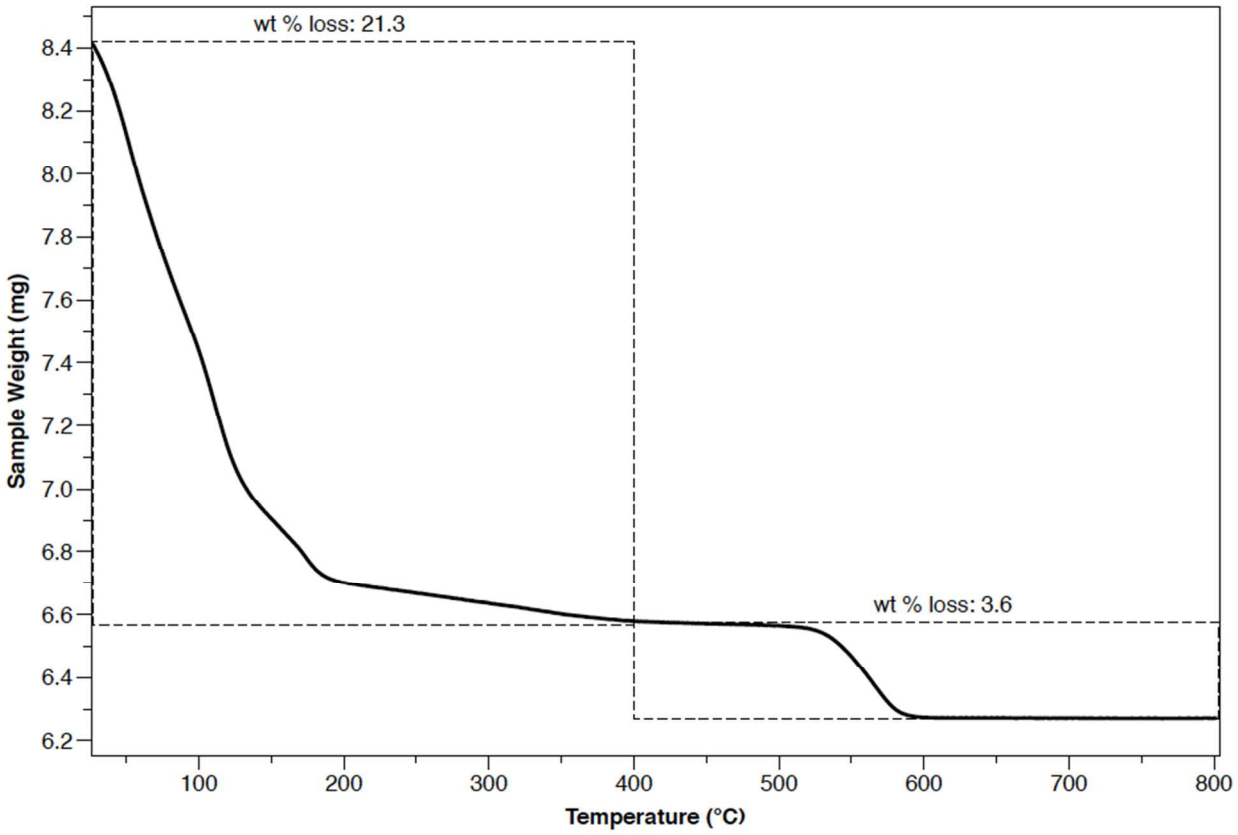

Fig S2. TGA curve of U_{60}. Weight loss up to 400 °C (21.3%) corresponds to 300 H_2O molecules.

4) **Supplementary Crystallographic Information**

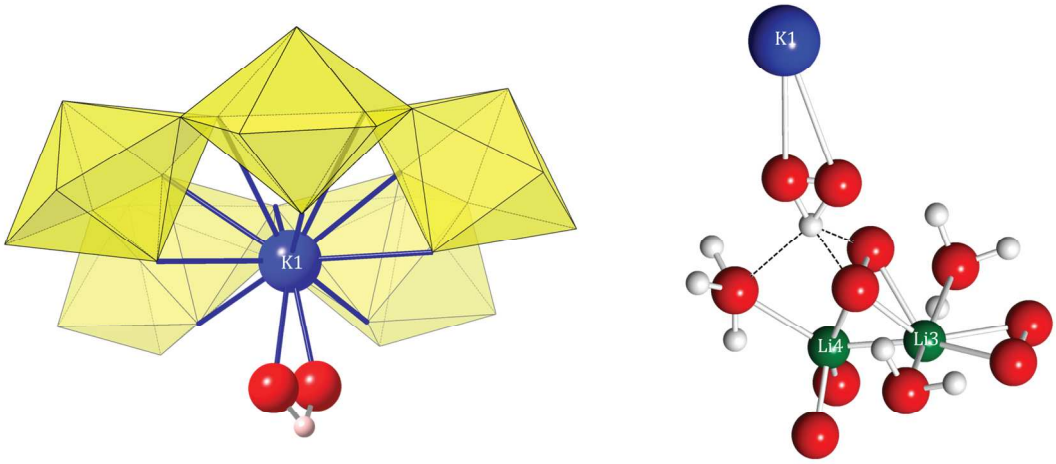

Figure S3. Left: a disordered, encapsulated water molecule binds to potassium beneath the pentagonal ring. Right: the coordination environment about internal Li atoms Li3 and Li4, with hydrogen bonds represented as dashed lines. Note: some H atoms positions were not located due to disorder. Color scheme: U (yellow), K (purple), O (red), H (white).

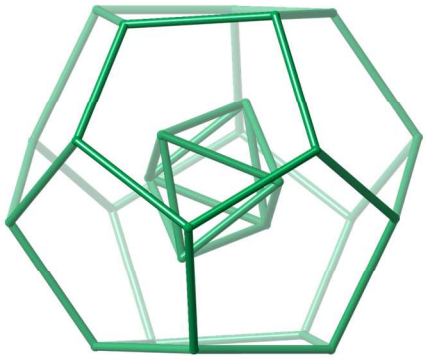

Fig S4. Lithium atom Li4 connects to itself taking the shape of an octahedron just below the dodecahedron formed by Li1 and Li2. It binds through disordered water that sits just below the pentagonal face of the Li-dodecahedron and assists in charge balance.

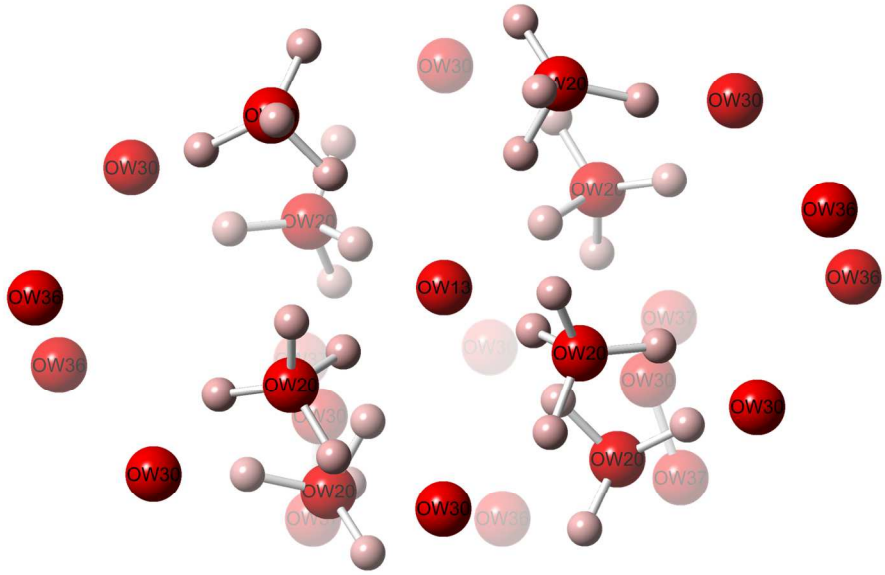

Figure S5. Disordered water molecules, and presumably Li cations, fill space external to cluster cages centered about water atom Ow13. Note: some hydrogen atom positions were not locatable due to disorder.

Table S2. Data collection and structure refinement details for U_{60}.

Diffractometer	TOPAZ
Wavelength	0.40 – 3.40 Å
Temperature	100(2) K
Structural Formula	$H_{403.32}K_{12}Li_{24}O_{554.71}U_{60}$
Space group	*Fm-3*
Unit cell dimensions	$a = b = c$ = 37.8411(9) Å
V (Å^3)	54186(2)
Z	4
$D_{calc.}$ (g.cm^{-3})	2.966 (for the above formula)
Absorption coefficient	0.2172 mm^{-1}
F(000)	42644
Crystal size	2.00 × 1.90 × 0.65 mm
θ range	7.429 to 79.091°
Index ranges	$-47 \le h \le 50$, $-47 \le k \le 40$, $-49 \le l \le 45$
Unique reflections	16718; R_{int} = 0.089
Reflections with $I_{obs} > 2\sigma(I)$	16718
Refinement method	Full-matrix least-squares on F^2
Parameters (restraints)	479(3187)
GoF (obs/all)	1.086/1.096
R (obs), wR (obs)	0.1050, 0.2616

R (all), *wR* (all)	0.1050, 0.2616
Largest diff. peak/hole	+1.14 /–0.76 e Å^{-3}

Table S3. Atomic coordinates and displacement parameters (U_{eq}/U_{iso}, in Å^2) for U_{60}.

Atom	Type	*x*	*y*	*z*	U_{eq}/U_{iso}	Site occ.
U1	U	0.3911(2)	0.4081(2)	0.2323(2)	0.037(2)	1
U2	U	0.4478(4)	0.5	0.2676(3)	0.046(3)	1
U3	U	0.4430(2)	0.3244(2)	0.2004(2)	0.040(2)	1
K1	K	0.3842(8)	0.5	0.1875(7)	0.037(6)	1
O1	O	0.5	0.5348(6)	0.2696(5)	0.051(5)	1
O2	O	0.4040(3)	0.2892(3)	0.1667(4)	0.041(3)	1
O3	O	0.5	0.3285(5)	0.2237(5)	0.041(4)	1
O4	O	0.3885(4)	0.3535(4)	0.2017(4)	0.043(3)	1
O5	O	0.4069(4)	0.4291(4)	0.1931(3)	0.038(3)	1
O6	O	0.4450(4)	0.3760(4)	0.2361(4)	0.049(4)	1
O7	O	0.3969(4)	0.5375(4)	0.2642(4)	0.054(4)	1
O8	O	0.4291(5)	0.4406(4)	0.2687(4)	0.057(4)	1
O9	O	0.3359(4)	0.4393(4)	0.2266(4)	0.050(4)	1
O10	O	0.4556(4)	0.3509(3)	0.1621(3)	0.038(3)	1
O11	O	0.4513(5)	0.5	0.2188(4)	0.038(4)	1
O12	O	0.3755(5)	0.3857(4)	0.2725(4)	0.056(4)	1
O13	O	0.5	0.2987(5)	0.2003(6)	0.047(5)	1
O14	O	0.4309(4)	0.2984(4)	0.2379(4)	0.062(5)	1
O15	O	0.4455(7)	0.5	0.3148(5)	0.064(7)	1
OW1	O	0.5	0.5805(6)	0.2144(6)	0.044(5)	1
OW2	O	0.3659(5)	0.3659(5)	0.1341(5)	0.060(8)	1
OW3	O	0.4394(8)	0.4148(8)	0.1272(8)	0.051(8)	0.5
OW4	O	0.4606(13)	0.4239(12)	0.1417(13)	0.061(12)	0.36
OW5	O	0	0.0162(12)	0.1653(14)	0.070(14)	0.5
OW6	O	0.3353(9)	0.3144(9)	0.2318(9)	0.114(11)	0.77
OW7	O	0.3828(12)	0.2398(12)	0.2117(12)	0.078(11)	0.5
OW8	O	0.5	0.5637(15)	0.3358(12)	0.053(12)	0.5
OW9	O	0.4239(7)	0.4202(7)	0.3376(8)	0.103(8)	1
OW10	O	0.3615(19)	0	0.1796(18)	0.06(2)	0.4
OW11	O	0.25	0.25	0.25	0.05(3)	0.384
OW12	O	0.0391(10)	0.3636(8)	0.1978(11)	0.105(10)	0.8
OW13	O	0.5	0	0	0.1(3)	0.18
OW14	O	0.434(3)	0.5	0.132(2)	0.06(2)	0.25
OW15	O	0.379(2)	0.053(3)	0.165(2)	0.02(2)	0.1
OW16	O	0.3228(11)	0.1142(11)	0.1638(11)	0.080(11)	0.5

OW17	O	0.087(2)	0	0.062(2)	0.05(3)	0.2
OW18	O	0.5	0.1379(15)	0.2137(14)	0.076(16)	0.5
OW19	O	0.3540(15)	0.0883(15)	0.1477(15)	0.055(16)	0.25
OW20	O	0.5434(15)	-0.0434(15)	0.0434(15)	0.08(4)	0.2631
OW21	O	0.3063(11)	0.4498(12)	0.2904(11)	0.058(9)	0.5
OW22	O	0.478(4)	0.25	0.25	0.07(4)	0.2
OW23	O	0.3159(13)	0.4675(13)	0.2904(12)	0.083(13)	0.5
OW24	O	0.3629(17)	0.2476(16)	0.2107(15)	0.024(13)	0.2
OW25	O	0.306(2)	0.1309(19)	0.178(3)	0.056(18)	0.25
OW26	O	0.25	0.312(5)	0.25	0.07(5)	0.12
OW27	O	0.288(3)	0.465(3)	0.280(3)	0.06(3)	0.2
OW28	O	0.3897(14)	-0.0155(12)	0.1246(13)	0.053(13)	0.3
OW29	O	0.5	0.241(2)	0.2393(18)	0.06(2)	0.3
OW30	O	0.5	-0.096(5)	0.049(4)	0.09(4)	0.2
OW31	O	0.289(2)	0.315(3)	0.286(2)	0.07(2)	0.2
OW32	O	0.413(3)	0.5	0.123(3)	0.08(3)	0.3
OW34	O	0.0234(16)	0.0234(16)	0.0234(16)	0.09(4)	0.3
OW35	O	0.099(4)	0.035(4)	0.019(4)	0.08(4)	0.15
OW36	O	0.5	0.472(6)	0.378(6)	0.11(6)	0.175
OW37	O	0.448(4)	0.522(3)	0.387(4)	0.11(4)	0.2
OW38	O	0.367(2)	-0.017(2)	0.183(3)	0.05(2)	0.25
OW39	O	0.5	0.580(2)	0.326(2)	0.068(19)	0.4
H1A	H	0.5	0.554(2)	0.253(2)	0.07(2)	0.5
H1B	H	0.5	0.545(2)	0.291(2)	0.059(19)	0.5
H1C	H	0.5	0.5631(19)	0.232(2)	0.042(18)	0.4
H4A	H	0.3785(14)	0.3591(15)	0.1769(18)	0.042(13)	0.4
H4B	H	0.3689(16)	0.3387(17)	0.2128(16)	0.099(17)	0.66
H4C	H	0.3608(12)	0.3441(15)	0.1236(13)	0.075(13)	0.66
H6A	H	0.4536(15)	0.3723(14)	0.2563(17)	0.058(14)	0.5
H6B	H	0.4659(15)	0.3910(16)	0.2253(14)	0.051(13)	0.5
H6C	H	0.4750(17)	0.4041(18)	0.2202(17)	0.070(19)	0.5
H4	H	0.5	0.573(2)	0.194(2)	0.08(2)	0.5
H5	H	0.3808(17)	0.3808(17)	0.1192(17)	0.09(7)	0.3
H6	H	0.4350(13)	0.4239(14)	0.1524(13)	0.062(13)	0.5
H7	H	0.4506(14)	0.3966(13)	0.1396(14)	0.064(14)	0.5
H8	H	0.356(2)	0.328(2)	0.226(2)	0.06(2)	0.33
H9	H	0.481(5)	0.557(7)	0.352(5)	0.10(7)	0.15
H10	H	-0.0173(16)	0	0.1802(17)	0.048(16)	0.5
H11	H	0.4294(17)	0.5	0.1077(15)	0.13(2)	1
H12	H	0.358(3)	0.065(3)	0.162(4)	0.05(4)	0.15

H13	H	0.423(3)	0.394(2)	0.344(3)	0.06(3)	0.25
H14	H	0.3871(9)	0.2566(10)	0.1984(9)	0.086(9)	1
H15	H	0.3163(10)	0.4484(10)	0.2692(11)	0.031(8)	0.5
H16	H	0.452(4)	0.5	0.371(4)	0.12(5)	0.4
H17	H	0.4257(10)	0.4279(9)	0.3187(10)	0.085(10)	1
H18	H	0.373(4)	0	0.157(3)	0.13(5)	0.5
H19	H	0.281(2)	0.437(2)	0.289(2)	0.08(2)	0.5
H20	H	0.3726(16)	0.0190(16)	0.1948(18)	0.055(19)	0.5
H21	H	0.5	0.236(8)	0.264(3)	0.12(8)	0.25
H22	H	0.413(2)	0.439(2)	0.353(2)	0.05(2)	0.25
H23	H	0.399(2)	0.227(2)	0.229(2)	0.05(2)	0.25
H24	H	0.1941(17)	0.3799(19)	0.196(2)	0.081(19)	0.5
H25	H	0.377(5)	0.25	0.25	0.01(4)	0.1
H26	H	0.018(6)	0	0.015(6)	0.05(6)	0.2
H27	H	0.4518(16)	0.3655(15)	0.283(2)	0.103(16)	0.75
H28	H	0.5	0.560(5)	0.312(3)	0.12(5)	0.4
H29	H	0.364(2)	0.092(3)	0.169(2)	0.04(2)	0.2
H30	H	0.395(3)	0.056(3)	0.185(3)	0.07(3)	0.25
H31	H	0.319(3)	0.332(3)	0.243(3)	0.09(4)	0.25
H32	H	0.327(3)	0.094(2)	0.180(2)	0.06(3)	0.25
H33	H	0.534(6)	-0.069(4)	0.038(6)	0.13(7)	0.2
H34	H	0.383(4)	0	0.142(3)	0.06(3)	0.3
H35	H	0.382(3)	0.087(6)	0.144(6)	0.05(6)	0.1
H36	H	0.295(3)	0.130(3)	0.160(4)	0.06(3)	0.25
H37	H	0.5	0.1235(19)	0.1975(19)	0.061(19)	0.5
H38	H	0.5285(17)	-0.0285(17)	0.0285(17)	0.09(5)	0.3
H39	H	0.522(2)	0.135(2)	0.227(2)	0.04(2)	0.25
H40	H	0.077(4)	0	0.038(3)	0.09(5)	0.3
H41	H	0.102(2)	0.017(2)	0.066(3)	0.05(2)	0.25
H42	H	0.3062(16)	0.1115(17)	0.1480(15)	0.068(15)	0.5
H43	H	0.037(3)	0.3369(17)	0.193(3)	0.06(2)	0.25
H44	H	0.281(2)	0.452(4)	0.290(3)	0.07(3)	0.33
Li1	Li	0.5	0.5644	0.169(5)	0.084	0.2
Li2	Li	0.391(4)	0.391(4)	0.109(4)	0.08(7)	0.45
Li3	Li	0.079(4)	0	0	0.05(4)	0.6
Li4	Li	0.040(5)	0	0.059(5)	0.07(5)	0.4
Li5	Li	0.5	0.208(3)	0.177(3)	0.07(3)	0.8

Table S4. Anisotropic displacement parameters (Å^2) for U_{60}.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
U1	0.048(5)	0.040(5)	0.022(4)	0.013(4)	0.023(4)	-0.006(4)
U2	0.078(9)	0.047(8)	0.013(5)	0	0.011(6)	0
U3	0.041(5)	0.039(5)	0.039(5)	0.023(4)	0.005(4)	0.002(4)
K1	0.055(16)	0.032(14)	0.023(13)	0	0.005(12)	0
O1	0.074(14)	0.059(14)	0.018(10)	-0.011(10)	0	0
O2	0.042(8)	0.036(7)	0.046(8)	0.024(6)	0.000(6)	-0.005(6)
O3	0.058(11)	0.034(9)	0.032(10)	0.022(7)	0	0
O4	0.053(8)	0.042(8)	0.033(8)	0.004(6)	0.007(7)	-0.007(6)
O5	0.054(8)	0.038(7)	0.023(7)	0.006(5)	0.014(6)	-0.004(6)
O6	0.061(10)	0.049(9)	0.038(9)	0.012(7)	0.002(8)	0.001(7)
O7	0.073(10)	0.058(9)	0.030(8)	-0.022(7)	0.025(7)	-0.002(8)
O8	0.090(11)	0.054(9)	0.027(7)	0.014(7)	0.008(7)	-0.007(8)
O9	0.047(8)	0.068(10)	0.035(8)	0.009(7)	0.026(6)	0.001(7)
O10	0.052(8)	0.028(7)	0.033(7)	0.018(5)	0.003(6)	-0.004(6)
O11	0.059(12)	0.042(10)	0.013(8)	0	0.015(7)	0
O12	0.088(12)	0.051(9)	0.031(7)	0.024(7)	0.017(7)	-0.008(8)
O13	0.052(11)	0.029(9)	0.060(12)	0.027(8)	0	0
O14	0.067(10)	0.075(11)	0.046(8)	0.048(8)	0.021(7)	-0.002(8)
O15	0.100(18)	0.086(17)	0.007(8)	0	0.000(9)	0

Table S5. Bond lengths (Å) for U_{60}.

U1-O5	1.787(15)	K1-O10	2.83(3)
U1-O12	1.840(14)	K1-O13	3.24(4)
U1-O2	2.340(18)	K1-O7	3.27(3)
U1-O8	2.341(19)	K1-O7	3.27(3)
U1-O4	2.376(18)	K1-O9	3.29(2)
U1-O6	2.378(19)	K1-O9	3.29(2)
U1-O7	2.396(19)	O1-H1B	0.89(8)
U1-O9	2.409(18)	O1-H1A	0.96(9)
U1-K1	3.879(15)	O1-U2	2.377(19)
U1-U3	3.919(13)	O2-O9	1.47(2)
U2-O15	1.79(2)	O2-U1	2.340(18)
U2-O11	1.85(2)	O3-O13	1.43(3)
U2-O8	2.358(16)	O3-U3	2.338(12)
U2-O8	2.359(16)	O4-H4B	1.02(7)
U2-O1	2.377(19)	O4-H4A	1.03(7)
U2-O1	2.377(19)	O6-H6A	0.84(7)
U2-O7	2.40(2)	O6-H6B	1.06(7)

U2-O7	2.40(2)	O7-O8	1.49(2)
U2-K1	3.87(3)	O7-U1	2.396(19)
U2-U2	3.95(3)	O8-O7	1.49(2)
U3-O14	1.789(14)	O9-O2	1.47(2)
U3-O10	1.826(14)	O9-U3	2.377(19)
U3-O4	2.337(18)	O10-K1	2.83(3)
U3-O3	2.338(12)	O13-U3	2.368(12)
U3-O2	2.366(18)	O13-K1	3.24(4)
U3-O13	2.368(12)	OW1-H4	0.84(9)
U3-O6	2.375(19)	OW1-H1C	0.93(8)
U3-O9	2.377(19)	OW1-H6C	1.13(7)
U3-K1	3.89(3)	OW1-H6C	1.13(7)
K1-OW32	2.68(9)	OW1-Li1	1.84(18)
K1-O11	2.80(4)	OW2-H4C	0.94(6)
K1-O5	2.826(17)	OW2-H4C	0.94(6)
K1-O5	2.826(17)	OW2-H4C	0.94(6)
K1-OW14	2.82(10)	OW2-H5	0.98(12)
K1-O10	2.83(3)	OW2-Li2	1.6(3)
OW3-H7	0.93(7)	OW15-H12	0.94(10)
OW3-H6	1.03(7)	OW15-H30	0.99(10)
OW3-OW4	1.03(5)	OW15-H22	1.46(13)
OW3-Li2	2.16(16)	OW15-OW38	1.59(14)
OW4-H6	1.05(7)	OW15-OW19	1.78(10)
OW4-H7	1.10(7)	OW16-H42	0.87(8)
OW4-Li1	1.86(12)	OW16-H32	0.98(9)
OW5-H10	1.06(7)	OW16-OW25	1.04(7)
OW5-H10	1.06(7)	OW16-H36	1.24(14)
OW5-OW5	1.23(9)	OW16-H24	1.39(9)
OW5-Li1	1.83(5)	OW16-OW19	1.65(8)
OW6-H8	0.97(9)	OW17-H41	0.87(10)
OW6-H31	0.99(10)	OW17-H41	0.87(10)
OW7-OW24	0.81(6)	OW17-H40	1.02(11)
OW7-H14	0.83(8)	OW17-Li4	1.8(2)
OW7-H23	1.03(9)	OW17-Li3	2.38(9)
OW8-OW39	0.72(7)	OW18-H37	0.82(9)
OW8-H28	0.90(11)	OW18-H39	0.99(7)
OW8-H9	0.99(8)	OW18-H39	0.99(7)
OW8-H9	0.99(8)	OW18-OW12	1.60(4)
OW9-H17	0.78(6)	OW18-OW12	1.60(4)
OW9-H13	1.03(9)	OW19-H29	0.89(10)

OW9-H22	1.00(9)	OW19-H12	1.04(10)
OW10-OW38	0.69(9)	OW19-H35	1.08(11)
OW10-OW38	0.69(9)	OW20-H38	0.97(11)
OW10-H18	0.97(11)	OW20-H33	1.07(11)
OW10-H20	1.01(9)	OW20-H33	1.07(11)
OW10-H20	1.01(9)	OW20-H33	1.07(11)
OW10-Li5	1.80(12)	OW21-OW23	0.76(5)
OW12-H27	0.81(11)	OW21-H15	0.89(7)
OW12-H43	1.03(7)	OW21-H44	0.98(9)
OW12-H39	1.28(11)	OW21-OW27	0.99(10)
OW12-OW18	1.60(4)	OW21-H19	1.07(10)
OW14-OW32	0.89(11)	OW21-Li5	2.01(6)
OW14-H11	0.95(10)	OW22-OW29	1.00(12)
OW22-OW29	1.00(12)	OW34-OW34	1.78(12)
OW22-H21	1.1(2)	OW34-OW34	1.78(12)
OW22-H21	1.1(2)	OW34-Li3	2.45(14)
OW22-OW22	1.7(3)	OW34-Li3	2.45(14)
OW23-H15	1.08(7)	OW34-Li3	2.45(14)
OW23-OW27	1.14(10)	OW35-OW35	1.4(3)
OW23-Li5	1.26(6)	OW35-Li3	1.69(16)
OW23-H44	1.46(12)	OW35-Li4	1.7(2)
OW24-H14	1.08(8)	OW37-H16	1.03(11)
OW25-H24	0.80(17)	OW37-OW30	1.06(15)
OW25-H36	0.8(2)	OW37-OW37	1.6(2)
OW25-H42	1.34(11)	OW38-H20	0.51(14)
OW27-H44	0.7(2)	OW38-H18	1.20(16)
OW27-H19	1.14(14)	OW38-OW38	1.29(18)
OW27-H15	1.31(11)	OW38-H20	1.46(13)
OW27-Li5	1.95(12)	OW38-OW15	1.59(14)
OW28-H34	0.92(10)	OW38-Li5	2.01(12)
OW28-OW28	1.17(9)	OW39-H28	0.9(2)
OW29-H21	0.9(4)	H1A-H1C	0.88(9)
OW29-H21	0.97(11)	H1B-H28	1.00(13)
OW29-OW22	1.00(12)	H1C-H1A	0.88(9)
OW29-OW29	1.06(15)	H4A-H4C	0.80(6)
OW29-Li5	2.68(13)	H4B-H8	0.79(8)
OW30-OW37	1.06(15)	H4C-Li2	2.2(3)
OW30-OW37	1.06(15)	H6A-H27	1.04(7)
OW30-H16	1.3(3)	H6B-H6C	0.63(7)
OW31-OW31	1.47(16)	H6C-H6B	0.63(7)

OW31-OW31	1.47(16)	H4-Li1	1.00(19)
OW32-H11	0.85(10)	H5-Li2	0.7(3)
OW34-H26	0.96(10)	H8-H4B	0.79(8)
OW34-H26	0.96(10)	H10-OW5	1.06(7)
OW34-H26	0.96(10)	H12-H29	1.08(15)
OW34-Li4	1.73(18)	H15-Li5	2.15(6)
OW34-Li4	1.73(18)	H16-OW37	1.03(11)
OW34-Li4	1.73(18)	H16-OW30	1.3(3)
H18-H34	0.68(14)	Li2-H4C	2.2(3)
H18-OW38	1.20(16)	Li3-H40	1.43(12)
H19-H44	0.59(14)	Li3-H40	1.43(12)
H20-OW38	0.51(14)	Li3-OW35	1.69(16)
H20-Li5	2.06(12)	Li3-OW35	1.69(16)
H21-OW29	0.9(4)	Li3-OW35	1.69(16)
H21-OW22	1.1(2)	Li3-Li4	1.7(2)
H26-H26	0.91(14)	Li3-Li4	1.7(2)
H26-H26	0.91(14)	Li3-OW17	2.38(9)
H26-H26	0.91(14)	Li3-OW34	2.45(14)
H26-OW34	0.96(10)	Li4-H40	1.6(3)
H26-Li4	1.9(3)	Li4-Li3	1.7(2)
H26-Li4	2.2(3)	Li4-OW35	1.7(2)
H26-Li4	2.2(3)	Li4-OW35	1.7(2)
H27-H6A	1.04(7)	Li4-OW34	1.73(18)
H28-H1B	1.00(13)	Li4-H26	1.9(3)
H29-H12	1.08(15)	Li4-H11	2.2(2)
H34-H18	0.68(14)	Li4-H40	2.19(18)
H34-OW28	0.92(10)	Li4-H40	2.19(18)
H36-H42	0.94(11)	Li4-H26	2.2(3)
H39-OW12	1.28(11)	Li5-OW23	1.26(6)
H40-Li3	1.43(12)	Li5-OW23	1.26(6)
H40-Li4	1.6(3)	Li5-OW10	1.80(12)
H40-Li4	2.19(18)	Li5-OW27	1.95(12)
H40-Li4	2.19(18)	Li5-OW27	1.95(12)
H42-H36	0.94(11)	Li5-OW21	2.01(6)
H44-H19	0.59(14)	Li5-OW21	2.01(6)
Li1-H4	1.00(19)	Li5-OW38	2.01(12)
Li1-OW5	1.83(5)	Li5-OW38	2.01(12)
Li1-OW4	1.86(12)	Li5-H20	2.06(12)
Li1-OW4	1.86(12)	Li5-H20	2.06(12)
Li2-H5	0.7(3)	Li5-H15	2.15(6)

Li2-OW3	2.16(16)
Li2-OW3	2.16(16)
Li2-H4C	2.2(3)
Li2-H4C	2.2(3)

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