Supplemental Information: A computationally guided investigation of the optical spectra of pure β-UO_3

Tyler L. Spano[1], Ashley E. Shields[1], Brianna S. Barth[1,2], Jeremiah D. Gruidl[1], Jennifer L. Niedziela[1], Roger J. Kapsimalis[1], Andrew Miskowiec[1]*

1. Nuclear Nonproliferation Division, Oak Ridge National Laboratory, 1 Bethel Valley Rd., Oak Ridge, TN, 37830
2. University of Texas at Austin, Department of Chemistry, 105 E. 24th St., Austin, TX, 78712
3. Materials Science and Technology Division, Oak Ridge National Laboratory, 1 Bethel Valley Rd., Oak Ridge, TN, 37830

*spanotl@ornl.gov

Figure S1. Diffractogram obtained (Cu-Kα, λ = 1.5406 Å) for ammonium uranyl carbonate heated to 500 °C compared with powder patterns for α- and β-UO_3 following the method of Sweet et al.[1]. α-UO_3 reflections are predominant with small intensity contributions from β-UO_3.

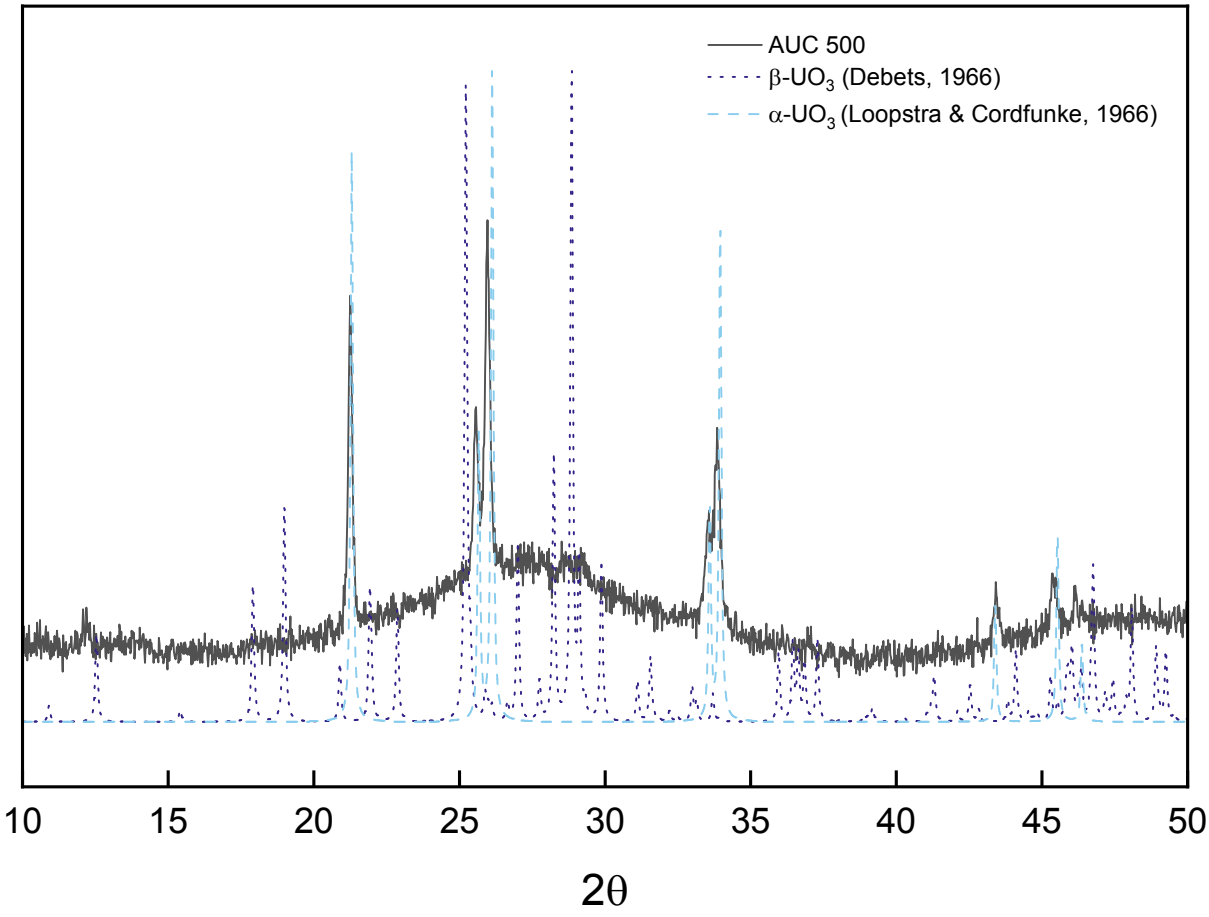

Table S1. Transformation matrix for converting the reported β-UO_3 unit cell [2] to a standard setting.

Reduced → Conventional		**Input → Reduced**		**T = Input → Conventional**
(100)		(001)		(001)
(00-1)	x	(100)	=	(0-10)
(010)		(010)		(100)

	a	***b***	***c***	**α**	**β**	**γ**	**Volume**	**Crystal System**	**Laue**
Input	10.34	14.33	3.91	90	99.03	90	572	monoclinic	*2/m*
Reduced	3.91	10.34	14.33	90	90	99.03	572		
Conventional	3.91	14.33	10.34	90	99.03	90	572	monoclinic	*2/m*

Figure S2. In-situ Raman spectroscopic data for UNH that was heated at a rate of ~35 °C/ minute to 450 °C, held at this temperature for ~5 minutes for data collection, and then heated to 500 °C and annealed for 72h. Results are compared with UNH that was flash heated to 450 °C as described in Section 2.1

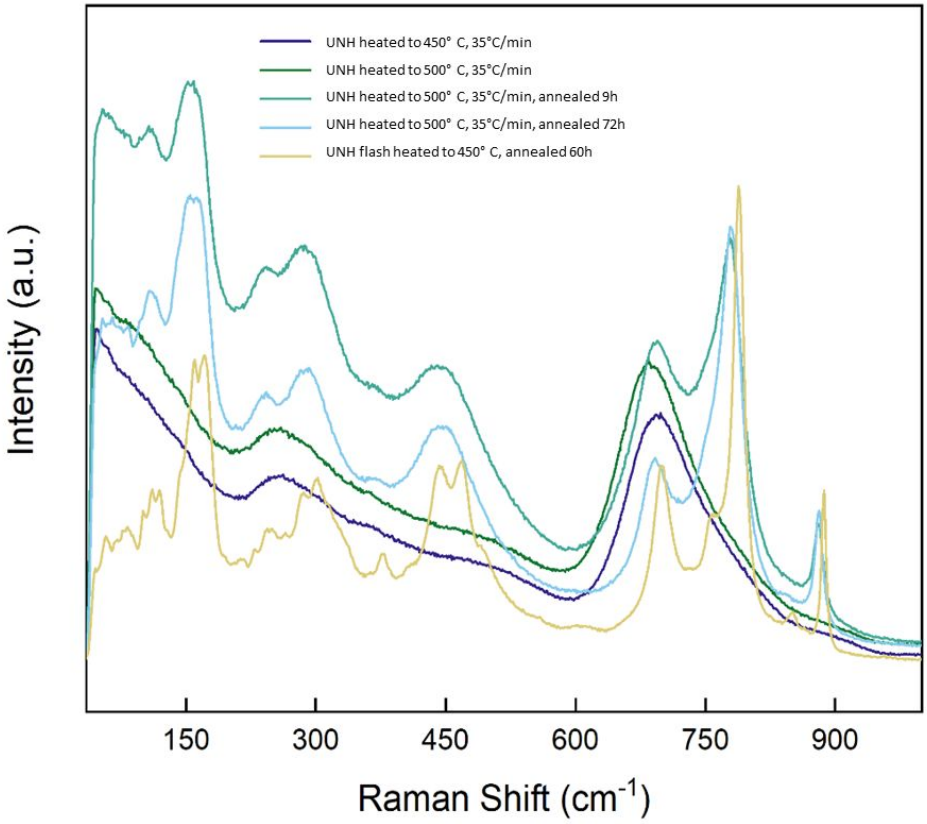

Figure S3. Secondary electron image of a β-UO_3 particle displaying botryoidal morphology and areas of voids and vesicles.

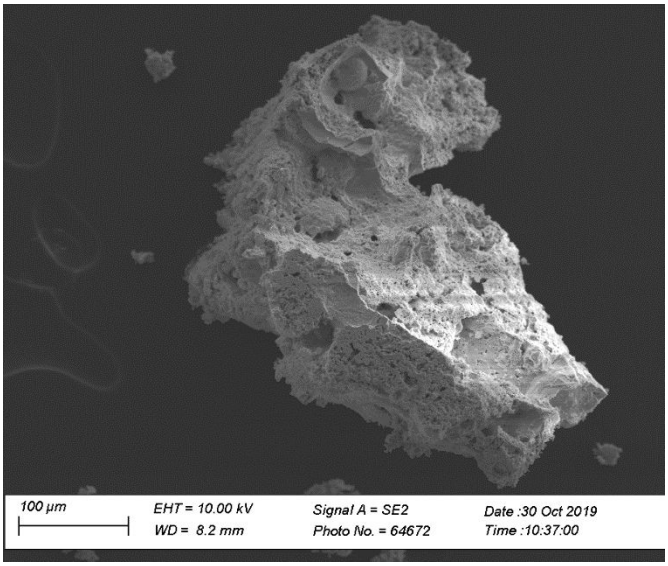

Figure S4. Energy dispersive X-ray spectra for β-UO_3. Only U and O are observed. C likely originates from GSR tab substrate.

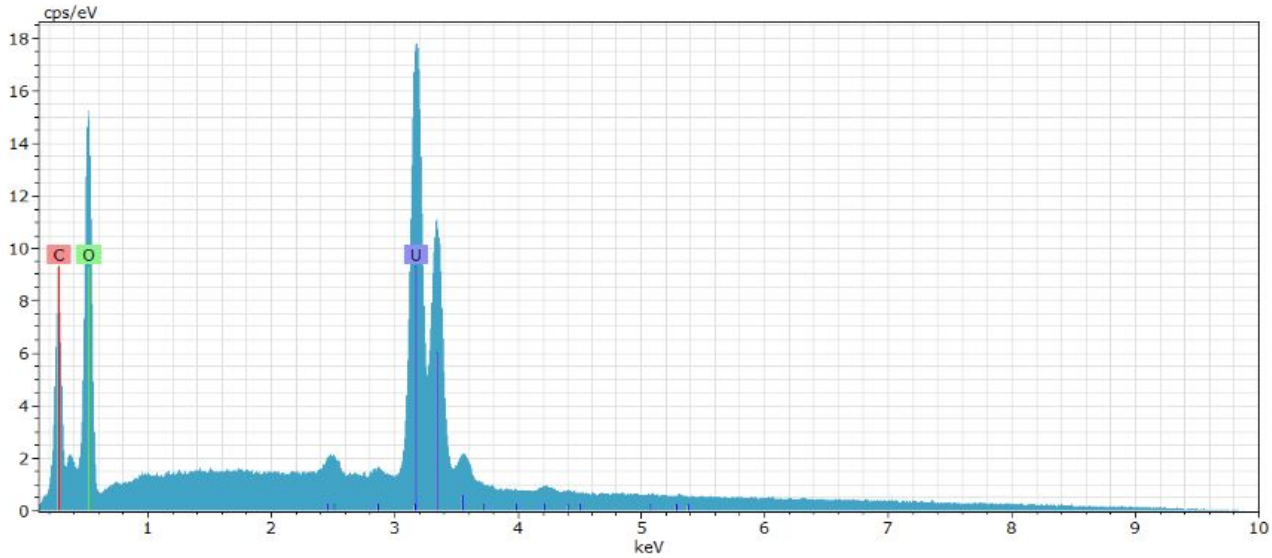

Table S2. DFPT predicted phonon modes, corresponding experimental modes from Raman spectroscopy (present work), and expected uranyl bond lengths calculated from predicted and experimental frequencies.

Frequency (THz)	Frequency (cm^{-1})	Irreducible Character	Corresponding Experimental Mode(s) (cm^{-1})	Uranyl bond length from DFPT (Å) (assuming ν_1)	Uranyl bond length from DFPT (Å) (assuming ν_3)	Uranyl bond length from experimental mode (Å) (assuming ν_1)	Uranyl bond length from experimental mode (Å) (assuming ν_3)
0.00	0.16	B	n/a	n/a	n/a	n/a	n/a
0.01	0.21	B	n/a	n/a	n/a	n/a	n/a
0.01	0.49	A	n/a	n/a	n/a	n/a	n/a
1.00	33.47	A	n/a	n/a	n/a	n/a	n/a
1.14	37.91	B	n/a	n/a	n/a	n/a	n/a
1.33	44.31	A	n/a	n/a	n/a	n/a	n/a
1.57	52.27	A	n/a	n/a	n/a	n/a	n/a
1.60	53.31	A	n/a	n/a	n/a	n/a	n/a
1.66	55.47	B	n/a	n/a	n/a	n/a	n/a
1.69	56.45	B	56.26	n/a	n/a	n/a	n/a
1.70	56.61	A	n/a	n/a	n/a	n/a	n/a
1.83	60.87	A	n/a	n/a	n/a	n/a	n/a
1.91	63.68	B	68.58	n/a	n/a	n/a	n/a
2.35	78.23	B	76.61	n/a	n/a	n/a	n/a
2.42	80.75	A	79.95	n/a	n/a	n/a	n/a
2.58	85.91	A	n/a	n/a	n/a	n/a	n/a
2.59	86.41	B	n/a	n/a	n/a	n/a	n/a
2.75	91.80	A	n/a	n/a	n/a	n/a	n/a
2.78	92.57	B	n/a	n/a	n/a	n/a	n/a
2.84	94.66	B	n/a	n/a	n/a	n/a	n/a
3.14	104.64	B	100.53	n/a	n/a	n/a	n/a
3.15	105.05	A	n/a	n/a	n/a	n/a	n/a

Frequency (THz)	Frequency (cm^{-1})	Irreducible Character	Corresponding Experimental Mode(s) (cm^{-1})	Uranyl bond length from DFPT (Å) (assuming ν_1)	Uranyl bond length from DFPT (Å) (assuming ν_3)	Uranyl bond length from experimental mode (Å) (assuming ν_1)	Uranyl bond length from experimental mode (Å) (assuming ν_3)
3.33	111.00	A	109.73	n/a	n/a	n/a	n/a
3.43	114.29	B	116.46	n/a	n/a	n/a	n/a
3.56	118.63	A	119.64	n/a	n/a	n/a	n/a
3.61	120.29	B	n/a	n/a	n/a	n/a	n/a
3.92	130.66	A	n/a	n/a	n/a	n/a	n/a
4.03	134.36	B	n/a	n/a	n/a	n/a	n/a
4.08	136.09	A	141.77	n/a	n/a	n/a	n/a
4.35	145.12	B	n/a	n/a	n/a	n/a	n/a
4.46	148.73	B	n/a	n/a	n/a	n/a	n/a
4.56	151.98	B	n/a	n/a	n/a	n/a	n/a
4.63	154.45	A	n/a	n/a	n/a	n/a	n/a
4.75	158.40	A	158.05/ 159.17	n/a	n/a	n/a	n/a
5.18	172.53	B	n/a	n/a	n/a	n/a	n/a
5.21	173.79	A	174.05	n/a	n/a	n/a	n/a
5.32	177.39	B	n/a	n/a	n/a	n/a	n/a
5.47	182.20	A	n/a	n/a	n/a	n/a	n/a
5.59	186.46	B	n/a	n/a	n/a	n/a	n/a
5.77	192.27	A	194.42	n/a	n/a	n/a	n/a
5.86	195.21	B	n/a	n/a	n/a	n/a	n/a
5.86	195.25	A	197.91	n/a	n/a	n/a	n/a
6.07	202.30	A	n/a	n/a	n/a	n/a	n/a
6.12	204.05	B	n/a	n/a	n/a	n/a	n/a
6.44	214.60	A	214.95	n/a	n/a	n/a	n/a
6.50	216.51	B	n/a	n/a	n/a	n/a	n/a
6.59	219.55	B	n/a	n/a	n/a	n/a	n/a
6.65	221.78	A	228.49	n/a	n/a	n/a	n/a
7.02	233.88	B	n/a	n/a	n/a	n/a	n/a

Frequency (THz)	Frequency (cm^{-1})	Irreducible Character	Corresponding Experimental Mode(s) (cm^{-1})	Uranyl bond length from DFPT (Å) (assuming ν_1)	Uranyl bond length from DFPT (Å) (assuming ν_3)	Uranyl bond length from experimental mode (Å) (assuming ν_1)	Uranyl bond length from experimental mode (Å) (assuming ν_3)
7.03	234.24	A	n/a	n/a	n/a	n/a	n/a
7.25	241.65	A	n/a	n/a	n/a	n/a	n/a
7.35	245.15	B	245.69	n/a	n/a	n/a	n/a
7.38	245.88	A	n/a	n/a	n/a	n/a	n/a
7.63	254.40	B	n/a	n/a	n/a	n/a	n/a
7.85	261.54	A	264.81	n/a	n/a	n/a	n/a
8.09	269.58	B	n/a	n/a	n/a	n/a	n/a
8.29	276.36	B	n/a	n/a	n/a	n/a	n/a
8.33	277.76	A	n/a	n/a	n/a	n/a	n/a
8.43	281.07	A	n/a	n/a	n/a	n/a	n/a
8.44	281.18	B	n/a	n/a	n/a	n/a	n/a
8.49	282.87	B	283.19	n/a	n/a	n/a	n/a
8.68	289.33	A	n/a	n/a	n/a	n/a	n/a
8.79	293.08	A	300.36	n/a	n/a	n/a	n/a
9.10	303.20	B	304.73	n/a	n/a	n/a	n/a
9.21	306.87	A	n/a	n/a	n/a	n/a	n/a
9.46	315.37	B	n/a	n/a	n/a	n/a	n/a
9.54	317.95	A	n/a	n/a	n/a	n/a	n/a
9.61	320.35	B	n/a	n/a	n/a	n/a	n/a
9.67	322.22	B	n/a	n/a	n/a	n/a	n/a
9.73	324.29	A	n/a	n/a	n/a	n/a	n/a
9.73	324.30	A	n/a	n/a	n/a	n/a	n/a
9.79	326.36	A	n/a	n/a	n/a	n/a	n/a
9.81	326.95	B	n/a	n/a	n/a	n/a	n/a
9.82	327.42	A	335.74	n/a	n/a	n/a	n/a
10.22	340.71	A	n/a	n/a	n/a	n/a	n/a
10.34	344.68	B	n/a	n/a	n/a	n/a	n/a

Frequency (THz)	Frequency (cm^{-1})	Irreducible Character	Corresponding Experimental Mode(s) (cm^{-1})	Uranyl bond length from DFPT (Å) (assuming ν_1)	Uranyl bond length from DFPT (Å) (assuming ν_3)	Uranyl bond length from experimental mode (Å) (assuming ν_1)	Uranyl bond length from experimental mode (Å) (assuming ν_3)
10.44	347.94	B	n/a	n/a	n/a	n/a	n/a
10.64	354.67	A	n/a	n/a	n/a	n/a	n/a
10.73	357.72	A	n/a	n/a	n/a	n/a	n/a
10.77	358.94	B	n/a	n/a	n/a	n/a	n/a
10.78	359.44	A	361.51	n/a	n/a	n/a	n/a
10.98	365.99	B	n/a	n/a	n/a	n/a	n/a
11.02	367.36	B	n/a	n/a	n/a	n/a	n/a
11.17	372.44	A	377.22	n/a	n/a	n/a	n/a
11.80	393.31	B	n/a	n/a	n/a	n/a	n/a
11.84	394.73	A	406.22	n/a	n/a	n/a	n/a
12.39	412.89	B	n/a	n/a	n/a	n/a	n/a
12.40	413.41	A	n/a	n/a	n/a	n/a	n/a
12.58	419.39	B	442.67	n/a	n/a	n/a	n/a
13.75	458.37	A	458.13	n/a	n/a	n/a	n/a
13.78	459.24	B	n/a	n/a	n/a	n/a	n/a
13.85	461.81	A	468.35	n/a	n/a	n/a	n/a
15.21	507.04	B	495.12	n/a	n/a	n/a	n/a
16.00	533.32	A	n/a	n/a	n/a	n/a	n/a
16.70	556.78	B	557.10	n/a	n/a	n/a	n/a
16.70	556.82	A	n/a	n/a	n/a	n/a	n/a
17.01	566.83	B	n/a	n/a	n/a	n/a	n/a
17.30	576.74	A	n/a	n/a	n/a	n/a	n/a
18.30	610.02	B	608.13	2.06	2.02	2.06	2.02
18.46	615.34	A	n/a	2.05	2.02	n/a	n/a
19.60	653.41	B	n/a	1.99	1.98	n/a	n/a
19.61	653.51	A	698.81	1.99	1.98	1.93	1.93
21.73	724.39	B	701.98	1.90	1.91	1.92	1.93

Frequency (THz)	Frequency (cm^{-1})	Irreducible Character	Corresponding Experimental Mode(s) (cm^{-1})	Uranyl bond length from DFPT (Å) (assuming ν_1)	Uranyl bond length from DFPT (Å) (assuming ν_3)	Uranyl bond length from experimental mode (Å) (assuming ν_1)	Uranyl bond length from experimental mode (Å) (assuming ν_3)
22.02	734.07	B	737.58	1.88	1.90	1.88	1.90
22.40	746.64	A	755.64	1.87	1.89	1.86	1.89
22.41	747.11	B	769.75	1.87	1.89	1.84	1.87
23.13	771.15	A	788.61	1.84	1.87	1.82	1.86
23.29	776.42	A	n/a	1.84	1.87	n/a	n/a
24.19	806.26	B	n/a	1.80	1.85	n/a	n/a
24.56	818.60	B	819.98	1.79	1.84	1.79	1.84
25.44	848.00	A	845.07	1.76	1.82	1.77	1.82
25.48	849.36	A	850.67	1.76	1.82	1.76	1.82
25.70	856.56	B	865.61	1.76	1.82	1.75	1.81
26.30	876.70	A	880.82, 886.68	1.74	1.80	1.73	1.80
26.70	890.13	B	n/a	1.73	1.79	n/a	n/a
28.45	948.44	A	958.61	1.68	1.76	1.67	1.76
29.83	994.19	B	1004.99	1.64	1.74	1.64	1.73
29.86	995.27	B	n/a	1.64	1.74	n/a	n/a
31.16	1038.66	A	1054.51	1.61	1.72	1.60	1.71

Table S3. Results of atom displacement and phase angle calculations from DFPT described in Section 3.2. Darker shading indicates larger U center contributions (s^n) and phase angles closer to 180°.

Contributing Center	U1		U2		U3		U4		U5	
Frequency	s^n	**Angle**	s^n	**Angle**	s^n	**Angle**	s^n	**Angle**	s^n	**Angle**
1038.93	0.02	121.17	0.03	122.13	0.02	10.01	0.44	1.51	0.45	2.16
1038.66	0.05	6.45	0.05	25.85	0.02	117.88	0.43	1.48	0.44	2.14
995.27	0.09	5.86	0.04	11.33	0.02	133.37	0.42	1.91	0.41	2.06
994.19	0.03	168.87	0.01	126.28	0.01	101.47	0.48	2.13	0.46	2.01
948.44	0.41	2.98	0.23	2.58	0.09	4.31	0.09	164.83	0.08	177.85
890.13	0.11	176.32	0.29	1.64	0.10	156.28	0.14	175.77	0.28	177.58
876.70	0.07	8.05	0.22	1.29	0.07	163.11	0.08	174.93	0.46	179.44
856.56	0.23	7.11	0.05	151.75	0.02	57.80	0.35	176.83	0.25	178.65
849.36	0.52	4.38	0.04	167.38	0.02	150.73	0.27	170.56	0.08	172.82
848.00	0.04	15.98	0.21	7.67	0.05	47.16	0.61	179.54	0.01	59.65
818.60	0.27	3.66	0.33	6.88	0.10	166.79	0.10	168.59	0.23	178.23
806.26	0.06	72.70	0.37	5.85	0.12	157.14	0.18	176.28	0.31	175.26
776.42	0.35	179.76	0.22	171.32	0.07	146.67	0.14	176.37	0.02	26.50
771.15	0.42	179.60	0.23	177.07	0.15	162.05	0.02	142.28	0.02	123.71
747.11	0.17	178.02	0.20	176.08	0.24	161.95	0.04	168.85	0.01	76.82
746.64	0.09	177.57	0.23	176.74	0.25	173.63	0.04	177.39	0.03	153.83
734.07	0.09	171.33	0.24	179.70	0.18	175.07	0.06	172.32	0.05	159.32
724.39	0.04	162.19	0.25	178.73	0.24	171.52	0.06	164.47	0.05	164.57
653.51	0.01	165.22	0.01	117.02	0.06	85.16	0.00	82.22	0.01	65.08
653.41	0.00	96.85	0.01	165.90	0.05	137.99	0.00	18.29	0.01	21.56
615.34	0.12	166.27	0.12	44.46	0.20	10.38	0.03	120.58	0.05	153.78
610.02	0.08	160.87	0.13	163.29	0.20	11.32	0.05	123.78	0.07	175.70
576.74	0.15	168.12	0.20	163.08	0.25	9.07	0.04	85.39	0.03	177.80
566.83	0.19	174.98	0.15	162.02	0.24	7.89	0.04	116.28	0.02	73.12
556.82	0.05	62.88	0.11	20.14	0.04	16.04	0.00	122.05	0.01	40.23
556.78	0.05	57.34	0.11	20.25	0.04	16.70	0.00	57.76	0.01	45.61
533.32	0.12	163.53	0.02	130.53	0.19	160.72	0.05	103.29	0.05	132.49
507.04	0.06	177.71	0.07	107.31	0.15	34.64	0.02	83.04	0.02	129.59
461.81	0.06	25.37	0.09	171.78	0.22	131.89	0.03	107.52	0.05	71.76
459.24	0.01	89.78	0.05	64.35	0.06	102.33	0.01	25.68	0.08	19.32
458.37	0.04	26.38	0.07	117.58	0.15	152.78	0.03	86.73	0.06	48.16
419.39	0.04	86.16	0.20	94.15	0.20	177.87	0.08	16.62	0.06	89.99
413.41	0.04	36.51	0.45	4.95	0.05	57.84	0.02	60.34	0.12	7.03
412.89	0.04	56.76	0.37	31.53	0.10	147.97	0.04	20.79	0.11	39.49
394.73	0.09	123.67	0.08	49.72	0.13	74.98	0.17	1.72	0.07	22.80
393.31	0.11	115.84	0.09	80.87	0.15	95.66	0.08	29.54	0.04	91.78
372.44	0.11	51.65	0.17	29.63	0.10	139.74	0.27	5.26	0.12	11.19

Contributing Center	U1		U2		U3		U4		U5	
Frequency	s^n	**Angle**	s^n	**Angle**	s^n	**Angle**	s^n	**Angle**	s^n	**Angle**
367.36	0.12	125.77	0.11	80.25	0.05	136.59	0.04	62.50	0.29	10.39
365.99	0.20	9.94	0.11	140.63	0.08	83.24	0.27	4.82	0.13	6.04
359.44	0.11	18.50	0.09	74.43	0.05	58.74	0.16	4.65	0.44	1.76
358.94	0.04	128.29	0.06	52.53	0.03	153.70	0.17	28.48	0.49	11.97
357.72	0.08	26.02	0.08	64.52	0.07	146.93	0.18	17.06	0.39	10.96
354.67	0.16	13.94	0.19	9.03	0.11	22.99	0.20	13.45	0.19	1.24
347.94	0.24	8.01	0.13	80.61	0.08	140.64	0.11	95.82	0.18	8.40
344.68	0.19	15.22	0.21	14.47	0.12	68.76	0.09	42.67	0.13	15.22
340.71	0.10	153.40	0.15	51.96	0.18	83.30	0.18	17.56	0.06	92.30
327.42	0.13	29.54	0.13	43.60	0.08	133.39	0.35	7.82	0.11	13.73
326.95	0.10	22.50	0.09	24.46	0.09	141.26	0.38	12.94	0.13	27.47
326.36	0.10	143.01	0.12	13.54	0.21	137.19	0.06	68.68	0.08	47.28
324.30	0.13	45.49	0.16	43.42	0.17	145.92	0.10	57.44	0.06	103.26
324.29	0.26	3.24	0.14	11.52	0.13	122.07	0.18	3.72	0.05	71.20
322.22	0.19	25.19	0.14	61.22	0.09	121.63	0.20	7.46	0.12	11.13
320.35	0.20	39.59	0.07	90.39	0.25	47.70	0.10	110.87	0.10	21.02
317.95	0.10	29.90	0.24	17.93	0.13	152.72	0.14	8.16	0.05	150.16
315.37	0.08	81.78	0.21	18.19	0.14	117.57	0.10	61.88	0.09	30.83
306.87	0.36	12.28	0.05	34.00	0.07	46.87	0.03	128.48	0.07	79.20
303.20	0.21	31.17	0.06	138.73	0.15	22.58	0.08	146.42	0.10	26.43
293.08	0.16	166.69	0.08	132.34	0.13	39.84	0.29	177.57	0.08	18.38
289.33	0.11	58.51	0.09	161.27	0.21	24.81	0.13	168.25	0.10	9.37
282.87	0.24	10.07	0.13	66.01	0.14	47.16	0.08	122.44	0.07	138.97
281.18	0.13	28.46	0.12	161.19	0.24	6.89	0.06	92.59	0.07	158.04
281.07	0.20	32.50	0.11	77.94	0.20	31.21	0.10	160.55	0.04	144.02
277.76	0.13	31.71	0.09	170.97	0.22	46.99	0.14	165.32	0.06	72.28
276.36	0.20	55.64	0.05	93.91	0.09	57.34	0.40	162.52	0.05	136.64
269.58	0.05	68.87	0.07	108.93	0.22	23.15	0.10	151.12	0.05	56.45
261.54	0.06	166.47	0.13	58.73	0.19	44.92	0.05	149.68	0.12	155.50
254.40	0.28	174.07	0.18	155.22	0.15	59.67	0.09	139.39	0.08	158.61
245.88	0.08	108.71	0.23	142.69	0.17	14.98	0.07	135.50	0.10	116.41
245.15	0.20	162.14	0.15	67.77	0.11	72.05	0.09	139.73	0.07	139.01
241.65	0.20	160.30	0.15	94.71	0.13	160.39	0.14	165.65	0.13	139.49
234.24	0.27	170.21	0.22	119.14	0.15	114.31	0.09	150.75	0.09	164.84
233.88	0.15	163.18	0.31	121.71	0.16	7.44	0.11	161.52	0.14	161.45
221.78	0.06	148.77	0.14	142.84	0.21	169.78	0.09	133.89	0.10	151.16
219.55	0.06	109.15	0.12	127.84	0.19	177.15	0.14	165.58	0.11	159.08
216.51	0.25	176.40	0.10	156.81	0.08	59.10	0.25	174.42	0.09	160.17
214.60	0.04	43.05	0.08	168.58	0.22	145.90	0.20	171.02	0.13	170.83
204.05	0.13	143.07	0.08	161.94	0.36	151.15	0.07	154.80	0.04	138.54

Contributing Center	U1		U2		U3		U4		U5	
Frequency	s^n	**Angle**	s^n	**Angle**	s^n	**Angle**	s^n	**Angle**	s^n	**Angle**
202.30	0.16	158.45	0.23	170.04	0.14	125.61	0.05	157.71	0.23	170.03
195.25	0.21	174.78	0.14	173.70	0.15	103.87	0.13	157.71	0.21	174.66
195.21	0.09	165.76	0.19	164.45	0.09	68.01	0.09	164.63	0.46	177.94
192.27	0.08	68.75	0.11	159.58	0.27	168.61	0.19	178.50	0.22	174.18
186.46	0.08	113.24	0.15	165.05	0.24	139.37	0.12	148.81	0.06	151.04
182.20	0.06	11.30	0.10	56.98	0.16	87.07	0.20	169.98	0.12	166.52
177.39	0.09	70.94	0.25	164.70	0.16	71.02	0.17	177.47	0.06	125.73
173.79	0.15	177.59	0.11	138.35	0.06	88.43	0.16	175.74	0.21	177.17
172.53	0.18	173.96	0.14	152.52	0.09	26.34	0.07	111.68	0.22	178.14
158.40	0.26	93.90	0.17	65.07	0.10	128.24	0.15	163.09	0.16	164.12
154.45	0.23	176.39	0.14	143.96	0.13	17.92	0.13	154.30	0.09	147.54
151.98	0.21	163.03	0.11	73.90	0.14	152.39	0.05	119.58	0.22	173.50
148.73	0.15	1.33	0.15	154.43	0.10	63.03	0.12	30.30	0.23	177.60
145.12	0.16	171.65	0.05	77.06	0.11	145.79	0.25	172.62	0.07	142.98
136.09	0.13	154.90	0.05	175.18	0.13	53.74	0.16	69.26	0.13	155.65
134.36	0.13	56.94	0.10	39.40	0.12	50.15	0.15	152.08	0.14	120.79
130.66	0.11	26.15	0.23	100.34	0.11	117.44	0.14	143.70	0.18	173.23
120.29	0.17	142.18	0.22	7.78	0.16	124.49	0.09	33.73	0.14	105.92
118.63	0.11	115.40	0.15	62.93	0.14	170.84	0.14	142.58	0.17	154.60
114.29	0.18	159.01	0.09	160.56	0.10	43.86	0.22	6.55	0.21	10.92
111.00	0.04	50.54	0.17	67.78	0.24	18.89	0.10	56.74	0.24	53.87
105.05	0.08	59.45	0.15	160.29	0.16	124.34	0.14	26.01	0.20	84.26
104.64	0.03	88.45	0.10	108.41	0.28	6.76	0.07	20.32	0.28	42.42
94.66	0.22	16.01	0.25	35.65	0.14	174.85	0.11	33.89	0.14	114.20
92.57	0.18	48.64	0.16	29.38	0.13	57.02	0.13	21.68	0.16	132.37
91.80	0.24	13.13	0.23	53.72	0.15	15.90	0.06	37.52	0.13	107.11
86.41	0.14	11.94	0.07	118.84	0.17	45.17	0.13	20.62	0.17	75.54
85.91	0.25	36.06	0.17	131.61	0.14	134.02	0.07	36.61	0.14	40.08
80.75	0.09	36.36	0.11	70.59	0.15	10.38	0.07	5.50	0.23	106.82
78.23	0.17	37.80	0.10	94.68	0.10	19.89	0.17	36.07	0.16	60.19
63.68	0.12	21.91	0.10	69.42	0.13	10.60	0.25	7.13	0.18	36.76
60.87	0.17	105.44	0.10	104.14	0.11	39.80	0.32	6.55	0.06	146.54
56.61	0.13	20.70	0.12	37.46	0.15	6.60	0.21	11.30	0.13	58.35
56.45	0.16	25.02	0.12	18.85	0.14	51.14	0.10	18.84	0.19	40.79
55.47	0.09	71.08	0.20	42.94	0.12	91.97	0.15	46.95	0.16	26.69
53.31	0.06	136.38	0.08	156.08	0.18	21.26	0.12	27.28	0.32	15.30
52.27	0.13	79.40	0.16	32.08	0.11	56.78	0.24	9.87	0.10	87.47
44.31	0.08	123.17	0.07	82.79	0.14	63.97	0.17	10.39	0.23	46.22
37.91	0.15	37.40	0.08	172.30	0.11	138.35	0.21	20.03	0.19	34.68
33.47	0.21	8.39	0.21	12.26	0.14	13.38	0.07	139.46	0.11	24.42

Contributing Center	U1		U2		U3		U4		U5	
Frequency	**s^n**	**Angle**	**s^n**	**Angle**	**s^n**	**Angle**	**s^n**	**Angle**	**s^n**	**Angle**
0.16	0.15	0.09	0.15	0.17	0.15	0.05	0.15	0.03	0.15	0.08
0.21	0.15	0.17	0.15	0.19	0.15	0.24	0.15	0.10	0.15	0.02
0.49	0.15	0.17	0.15	0.26	0.15	0.28	0.15	0.05	0.15	0.54

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2. Debets, P.C., *The structure of β-UO_3.* Acta Crystallographica, 1966. **21**(4): p. 589-593.