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The crystal chemistry of the uranyl silicate minerals

FRANCES V. STOHL[1] AND DEANE K. SMITH

Department of Geosciences, The Pennsylvania State University
University Park, Pennsylvania 16802

Abstract

The uranyl silicate minerals have been divided into three groups on the basis of their uranium to silicon ratios. The 1:1 group includes uranophane, beta-uranophane, boltwoodite, sodium boltwoodite, kasolite, sklodowskite, and cuprosklodowskite. A structure refinement of uranophane, a structure determination of boltwoodite, and previously reported structure determinations of most of these minerals indicate that they are composed of uranyl silicate chains made of edge-shared uranium pentagonal bipyramidal groups and silicate tetrahedra. These chains have the composition $[(UO_2)(SiO_4)]_n^{-2n}$ and are crosslinked by a bridging oxygen atom to form a uranyl silicate sheet. These sheets are crossbonded by the additional cations in the structure. The uranyl minerals with a uranium to silicon ratio of 1:3 include weeksite and haiweeite. A partial structure analysis of weeksite suggests that the structure type for this group consists of uranyl silicate chains, similar to those found in the 1:1 group, that are crosslinked by the additional silicate tetrahedra in the structure. The uranyl mineral group with a uranium to silicon ratio of 2:1 contains only the mineral soddyite. This structure is composed of uranyl silicate chains that are crossbonded by sharing a common silicon to give a three-dimensional framework structure. A new triclinic uranyl silicate mineral was discovered during this study, although there is not enough sample to describe it adequately. The locations of the uranium atoms in this structure indicate that it may not be composed of uranyl silicate chains such as those found in all the other uranyl silicate minerals.

Introduction

The known uranyl silicate minerals can be divided into several categories on the basis of their uranium to silicon ratios (Table 1). Three categories, with uranium to silicon ratios of 1:1, 1:3, and 2:1, are well defined as reported by Stohl (1974) and Stohl and Smith (1974). The minerals listed in Table 1 are the only accepted uranyl silicates as indicated by Fleischer (1980).

1:1 Uranyl silicate group

Structure determinations were carried out for six of the members of the group with a uranium to silicon ratio of 1:1. The structure of uranophane was originally determined by Smith *et al.* (1957), and is revised in this study. The structure of beta-uranophane was determined by Smith and Stohl (1972). A structure analysis of boltwoodite was carried out during this study. The structure of kasolite was originally determined by Huynen *et al.* (1963), and was revised by Mokeeva (1965), and by Rosenzweig and Ryan (1977). The sklodowskite structure was analyzed by Mokeeva (1959), and refined by Huynen and Van Meerssche (1962), by Mokeeva (1964), and by Ryan and Rosenzweig (1977). The cuprosklodowskite structure was originally determined by Piret-Meunier and Van Meerssche (1963), and was revised by Rosenzweig and Ryan (1975). The formulas listed in Table 1 for uranophane and boltwoodite are based on this work whereas the other formulas come from the most recent structural papers for each mineral.

The description, properties, and cell constants of sodium boltwoodite were reported by Chernikov *et al.* (1975). There has not been any structure work on this mineral. Its cells constants, however, are very similar to those of the other 1:1 uranyl silicate minerals, indicating that it probably contains the same uranyl silicate sheets.

[1]Present address: Organization 4731, Sandia National Laboratories, Albuquerque, New Mexico 87185.

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Table 3. Observed and calculated structure factors for uranophane.

h	k	ℓ	Fo	Fc	h	k	ℓ	Fo	Fc
0	0	1	181	178	1	1	5	42	43
0	0	2	88	66	1	2	-5	41	42
0	0	3	263	246	1	2	-4	73	80
0	0	4	247	237	1	2	-3	71	88
0	0	5	100	100	1	2	-2	19	16
0	1	1	211	210	1	2	-1	48	71
0	1	2	361	347	1	2	0	166	154
0	1	3	128	127	1	2	1	17	20
0	1	4	49	49	1	2	2	19	13
0	1	5	146	142	1	2	3	39	55
0	2	0	359	356	1	2	4	78	94
0	2	1	9º	106	1	2	5	37	42
0	2	2	11	16	1	3	-4	58	54
0	2	3	158	155	1	3	-3	65	79
0	2	4	222	210	1	3	-2	173	207
0	2	5	118	116	1	3	-1	95	112
0	3	1	179	190	1	3	0	58	44
0	3	2	256	266	1	3	1	88	103
0	3	3	98	103	1	3	2	113	140
0	3	4	77	73	1	3	3	48	60
0	4	0	209	210	1	3	4	41	46
0	4	1	93	102	1	4	-4	131	133
0	4	2	0	18	1	4	-3	99	110
0	4	3	102	112	1	4	-2	20	13
0	4	4	129	137	1	4	-1	98	111
0	5	1	39	50	1	4	0	227	209
0	5	2	100	117	1	4	1	48	55
1	0	-5	0	3	1	4	2	11	10
1	0	-4	0	8	1	4	3	94	110
1	0	-3	24	44	1	4	4	134	140
1	0	-2	13	6	1	5	-3	85	91
1	0	-1	16	50	1	5	-2	168	180
1	0	0	0	3	1	5	-1	79	83
1	0	1	17	49	1	5	0	10	12
1	0	2	19	21	1	5	1	101	115
1	0	3	11	29	1	5	2	145	171
1	0	4	16	6	2	0	-5	109	106
1	0	5	11	6	2	0	-4	275	256
1	1	-5	21	20	2	0	-3	227	220
1	1	-4	16	21	2	0	-2	22	29
1	1	-3	14	15	2	0	-1	209	222
1	1	-2	32	59	2	0	0	322	360
1	1	-1	19	35	2	0	1	146	145
1	1	0	32	46	2	0	2	37	44
1	1	1	15	30	2	0	3	263	248
1	1	2	61	83	2	0	4	231	210
1	1	3	37	45	2	0	5	61	68
1	1	4	23	20	2	1	-5	141	135

Table 3, continued

h	k	ℓ	Fo	Fc
2	1	-4	86	76
2	1	-3	219	199
2	1	-2	289	276
2	1	-1	131	129
2	1	0	11	14
2	1	1	174	178
2	1	2	274	274
2	1	3	148	140
2	1	4	87	84
2	1	5	150	136
2	2	-5	111	103
2	2	-4	211	204
2	2	-3	132	131
2	2	-2	26	17
2	2	-1	162	164
2	2	0	323	293
2	2	1	114	119
2	2	2	21	23
2	2	3	177	176
2	2	4	174	182
2	2	5	80	82
2	3	-4	84	76
2	3	-3	109	119
2	3	-2	225	247
2	3	-1	116	132
2	3	0	27	22
2	3	1	172	188
2	3	2	207	220
2	3	3	66	74
2	3	4	68	69
2	4	-4	126	133
2	4	-3	71	79
2	4	-2	34	41
2	4	-1	72	91
2	4	0	173	178
2	4	1	42	47
2	4	2	0	16
2	4	3	85	99
2	5	-3	44	53
2	5	-2	84	108
2	5	-1	51	59
2	5	0	20	20
2	5	1	69	75
2	5	2	80	101
3	0	-5	0	5
3	0	-4	19	3
3	0	-3	27	49
3	0	-2	0	10
3	0	-1	11	41
3	0	0	0	7
3	0	1	16	38
3	0	2	23	27
3	0	3	10	15
3	0	4	0	0
3	0	5	18	4
3	1	-5	21	29
3	1	-4	16	14
3	1	-3	48	61
3	1	-2	38	45
3	1	-1	34	46
3	1	0	25	33
3	1	1	38	56
3	1	2	25	40
3	1	3	15	15
3	1	4	16	26
3	1	5	26	23
3	2	-5	63	63
3	2	-4	70	78
3	2	-3	23	30
3	2	-2	10	7
3	2	-1	55	69
3	2	0	95	93
3	2	1	49	53
3	2	2	19	26
3	2	3	68	83
3	2	4	44	56
3	3	-4	35	30
3	3	-3	81	99
3	3	-2	82	95
3	3	-1	79	80
3	3	0	15	9
3	3	1	137	143
3	3	2	140	150
3	3	3	33	35
3	3	4	60	57
3	4	-4	122	123
3	4	-3	64	74
3	4	-2	16	10
3	4	-1	88	95
3	4	0	191	175
3	4	1	70	66
3	4	2	31	28
3	4	3	117	121
3	5	-2	144	146
3	5	-1	80	80
3	5	0	16	10

Table 3, continued

h	k	ℓ	Fo	Fc	h	k	ℓ	Fo	Fc
3	5	1	116	114	4	4	2	31	28
3	5	2	162	157	4	4	3	86	93
4	0	-5	130	121	4	5	-2	65	73
4	0	-4	165	166	4	5	-1	36	37
4	0	-3	171	164	4	5	0	16	9
4	0	-2	109	91	4	5	1	45	48
4	0	-1	265	266	4	5	2	87	94
4	0	0	373	359	5	0	-5	23	12
4	0	1	90	8	5	0	-4	10	8
4	0	2	89	74	5	0	-3	20	41
4	0	3	200	191	5	0	-2	13	17
4	0	4	175	168	5	0	-1	10	30
4	0	5	53	48	5	0	0	0	9
4	1	-5	96	95	5	0	1	10	23
4	1	-4	65	63	5	0	2	23	24
4	1	-3	182	174	5	0	3	0	7
4	1	-2	187	179	5	0	4	0	3
4	1	-1	138	137	5	1	-5	28	16
4	1	0	15	7	5	1	-4	11	20
4	1	1	190	187	5	1	-3	18	20
4	1	2	196	197	5	1	-2	26	42
4	1	3	71	68	5	1	-1	0	10
4	1	4	55	54	5	1	0	28	22
4	1	5	122	116	5	1	1	18	28
4	2	-5	139	132	5	1	2	60	68
4	2	-4	150	141	5	1	3	29	33
4	2	-3	103	103	5	1	4	0	10
4	2	-2	30	39	5	2	-5	37	45
4	2	-1	145	140	5	2	-4	59	67
4	2	0	189	188	5	2	-3	51	62
4	2	1	54	56	5	2	-2	0	6
4	2	2	26	25	5	2	-1	68	78
4	2	3	125	123	5	2	0	102	97
4	2	4	173	165	5	2	1	0	5
4	3	-4	75	69	5	2	2	11	17
4	3	-3	137	138	5	2	3	45	57
4	3	-2	170	172	5	2	4	72	80
4	3	-1	138	137	5	3	-4	52	51
4	3	0	35	32	5	3	-3	95	108
4	3	1	152	158	5	3	-2	146	150
4	3	2	183	186	5	3	-1	74	73
4	3	3	43	41	5	3	0	45	33
4	3	4	76	73	5	3	1	91	86
4	4	-3	70	81	5	3	2	107	117
4	4	-2	0	12	5	3	3	26	26
4	4	-1	100	104	5	3	4	42	38
4	4	0	152	142	5	4	-3	91	94
4	4	1	66	69	5	4	-2	0	11

Table 3, continued

h	k	ℓ	Fo	Fc	h	k	ℓ	Fo	Fc
5	4	-1	123	119	6	4	-1	116	118
5	4	0	153	144	6	4	0	117	124
5	4	1	44	42	6	4	1	26	28
5	4	2	16	10	6	4	2	27	32
5	4	3	99	103	6	5	-2	74	72
5	5	-2	124	120	6	5	-1	49	50
5	5	-1	76	75	6	5	0	24	20
5	5	0	22	22	6	5	1	83	81
5	5	1	111	102	7	0	-5	0	15
6	0	-5	132	136	7	0	-4	0	17
6	0	-4	209	197	7	0	-3	15	27
6	0	-3	181	182	7	0	-2	17	14
6	0	-2	49	41	7	0	-1	13	23
6	0	-1	176	183	7	0	0	51	9
6	0	0	275	285	7	0	1	17	11
6	0	1	61	64	7	0	2	10	17
6	0	2	61	70	7	0	3	11	5
6	0	3	221	208	7	0	4	17	2
6	0	4	202	187	7	1	-5	22	30
6	1	-5	140	129	7	1	-4	0	9
6	1	-4	23	25	7	1	-3	31	42
6	1	-3	212	202	7	1	-2	43	46
6	1	-2	181	175	7	1	-1	63	66
6	1	-1	106	114	7	1	0	21	15
6	1	0	45	39	7	1	1	42	44
6	1	1	134	140	7	1	2	50	57
6	1	2	270	269	7	1	3	16	18
6	1	3	48	43	7	1	4	11	16
6	1	4	74	73	7	2	-4	59	62
6	2	-4	144	139	7	2	-3	44	47
6	2	-3	112	112	7	2	-2	10	11
6	2	-2	27	31	7	2	-1	58	55
6	2	-1	155	153	7	2	0	115	106
6	2	0	237	222	7	2	1	47	41
6	2	1	91	86	7	2	2	29	31
6	2	2	28	26	7	2	3	63	68
6	2	3	169	169	7	3	-4	22	7
6	2	4	177	173	7	3	-3	91	93
6	3	-4	33	36	7	3	-2	91	89
6	3	-3	150	154	7	3	-1	98	90
6	3	-2	164	165	7	3	0	22	22
6	3	-1	108	109	7	3	1	133	122
6	3	0	45	45	7	3	2	143	138
6	3	1	163	167	7	3	3	17	10
6	3	2	183	182	7	4	-3	76	81
6	3	3	17	17	7	4	-2	16	5
6	4	-3	72	75	7	4	-1	110	106
6	4	-2	16	10	7	4	0	186	166

Table 3, continued

h	k	ℓ	Fo	Fc	h	k	ℓ	Fo	Fc
7	4	1	65	55	9	0	3	16	4
7	4	2	30	30	9	1	-4	21	14
7	5	-1	91	84	9	1	-3	37	36
7	5	0	18	15	9	1	-2	36	35
8	0	-4	184	179	9	1	-1	28	21
8	0	-3	172	175	9	1	0	15	7
8	0	-2	20	9	9	1	1	52	49
8	0	-1	297	298	9	1	2	48	48
8	0	0	322	312	9	1	3	33	25
8	0	1	66	55	9	2	-4	75	73
8	0	2	82	78	9	2	-3	45	51
8	0	3	231	225	9	2	-2	19	19
8	0	4	179	165	9	2	-1	110	106
8	1	-4	11	6	9	2	0	71	61
8	1	-3	195	193	9	2	1	19	13
8	1	-2	216	208	9	2	2	0	8
8	1	-1	138	137	9	2	3	77	81
8	1	0	62	63	9	3	-3	124	126
8	1	1	233	228	9	3	-2	138	124
8	1	2	210	211	9	3	-1	62	55
8	1	3	42	35	9	3	0	46	39
8	2	-4	165	153	9	3	1	131	116
8	2	-3	121	118	9	3	2	95	96
8	2	-2	22	26	9	4	-2	28	18
8	2	-1	194	191	9	4	-1	157	140
8	2	0	211	213	9	4	0	139	121
8	2	1	37	39	9	4	1	44	36
8	2	2	25	30	10	0	-4	218	207
8	2	3	183	181	10	0	-3	123	123
8	3	-3	151	154	10	0	-2	36	37
8	3	-2	192	186	10	0	-1	242	245
8	3	-1	94	95	10	0	0	199	200
8	3	0	50	51	10	0	1	57	50
8	3	1	190	190	10	0	2	69	66
8	3	2	183	178	10	0	3	232	223
8	3	3	17	6	10	1	-4	25	17
8	4	-2	27	25	10	1	-3	216	208
8	4	-1	123	126	10	1	-2	161	160
8	4	0	148	150	10	1	-1	88	91
8	4	1	39	38	10	1	0	25	28
8	4	2	25	23	10	1	1	205	215
9	0	-4	17	19	10	1	2	190	188
9	0	-3	16	16	10	1	3	31	26
9	0	-2	0	9	10	2	-3	84	91
9	0	-1	15	19	10	2	-2	26	25
9	0	0	0	9	10	2	-1	190	194
9	0	1	0	4	10	2	0	178	171
9	0	2	19	12	10	2	1	86	78

Table 3, continued

h	k	ℓ	Fo	Fc	h	k	ℓ	Fo	Fc
10	2	2	45	38	11	3	-2	80	69
10	3	-2	140	144	11	3	-1	59	54
10	3	-1	91	89	11	3	0	47	41
10	3	0	50	51	12	0	-3	129	126
10	3	1	170	177	12	0	-2	41	46
11	0	-3	0	10	12	0	-1	218	220
11	0	-2	11	6	12	0	0	154	151
11	0	-1	19	16	12	0	1	43	46
11	0	0	0	9	12	1	-3	160	158
11	0	1	0	0	12	1	-2	127	123
11	0	2	17	9	12	1	-1	102	105
11	1	-3	35	34	12	1	0	90	80
11	1	-2	43	39	12	1	1	156	161
11	1	-1	42	41	12	2	-2	31	31
11	1	0	23	10	12	2	-1	167	164
11	1	1	50	49	12	2	0	101	108
11	1	2	38	38	12	2	1	41	48
11	2	-3	25	26	13	0	-2	0	6
11	2	-2	0	16	13	0	-1	21	11
11	2	-1	68	68	13	0	0	0	7
11	2	0	79	70	13	1	-1	25	22
11	2	1	0	10	13	1	0	11	15
11	2	2	39	31					

Table 7. Observed and calculated structure factors for boltwoodite.

h	k	ℓ	Fo	Fc	h	k	ℓ	Fo	Fc
0	0	1	95	98	1	2	0	207	174
0	0	2	39	40	1	2	1	48	43
0	0	3	142	148	1	2	2	26	30
0	0	4	113	123	1	2	3	100	102
0	0	5	23	36	1	2	4	97	95
0	1	1	98	93	1	3	-4	39	32
0	1	2	169	167	1	3	-3	63	66
0	1	3	65	68	1	3	-2	131	132
0	1	4	40	42	1	3	0	0	4
0	1	5	72	75	1	3	1	122	97
0	2	1	60	55	1	3	2	137	116
0	2	2	0	11	1	3	3	22	19
0	2	3	94	97	1	3	4	58	49
0	2	4	96	102	1	4	-4	86	93
0	2	5	42	38	1	4	-3	57	58
0	3	1	166	134	1	4	-2	0	5
0	3	2	191	162	1	4	0	154	122
0	3	3	53	49	1	4	1	38	29
0	3	4	53	46	1	4	2	25	21
0	4	1	85	60	1	4	3	87	76
0	4	2	0	6	1	5	-3	62	61
0	4	3	103	93	1	5	-2	103	112
0	4	4	103	96	1	5	0	0	14
0	5	1	66	57	1	5	1	111	84
0	5	2	122	103	1	5	2	127	97
1	0	-5	38	41	2	0	-5	58	59
1	0	-4	115	111	2	0	-4	101	111
1	0	-3	99	87	2	0	-3	75	84
1	0	-2	0	5	2	0	-1	140	150
1	0	0	157	165	2	0	0	166	173
1	0	1	51	51	2	0	1	0	17
1	0	2	34	29	2	0	2	70	61
1	0	3	104	104	2	0	3	106	108
1	0	4	78	79	2	0	4	83	83
1	0	5	0	6	2	1	-5	45	47
1	1	-5	72	70	2	1	-4	22	25
1	1	-4	25	24	2	1	-3	87	97
1	1	-3	80	82	2	1	-1	41	44
1	1	-2	153	160	2	1	0	0	21
1	1	0	0	11	2	1	1	72	77
1	1	1	121	120	2	1	2	115	111
1	1	2	120	125	2	1	3	0	7
1	1	3	37	35	2	1	4	45	39
1	1	4	50	50	2	2	-5	56	54
1	2	-5	57	56	2	2	-4	75	90
1	2	-4	116	122	2	2	-3	33	36
1	2	-3	76	83	2	2	-1	60	68
1	2	-2	0	9	2	2	0	80	88

Table 7, continued

h	k	ℓ	Fo	Fc	h	k	ℓ	Fo	Fc
2	2	1	24	26	3	3	0	40	36
2	2	2	26	23	3	3	1	108	103
2	2	3	83	77	3	3	2	105	95
2	2	4	81	72	3	3	3	0	15
2	3	-4	29	31	3	4	-2	0	17
2	3	-3	76	82	3	4	-1	93	90
2	3	-1	66	72	3	4	0	97	93
2	3	0	50	47	3	4	1	0	5
2	3	1	125	107	3	4	2	38	32
2	3	2	119	105	3	5	-1	31	32
2	3	3	0	2	3	5	0	51	40
2	4	-4	76	90	4	0	-5	78	91
2	4	-3	40	45	4	0	-3	48	55
2	4	-1	81	80	4	0	-2	44	52
2	4	0	119	99	4	0	-1	153	166
2	4	1	24	23	4	0	0	103	111
2	4	2	44	33	4	0	1	0	16
2	4	3	94	81	4	0	2	71	72
2	5	-1	30	30	4	1	-3	106	119
2	5	0	0	14	4	1	-2	84	90
2	5	1	69	59	4	1	-1	0	19
3	0	-5	60	66	4	1	0	43	53
3	0	-4	78	91	4	1	1	108	119
3	0	-2	0	16	4	1	2	71	72
3	0	-1	88	98	4	2	-3	27	26
3	0	0	125	135	4	2	-2	29	36
3	0	1	0	12	4	2	-1	101	108
3	0	2	51	48	4	2	0	80	86
3	0	3	113	106	4	2	1	0	2
3	1	-5	41	46	4	2	2	44	49
3	1	-4	0	10	4	3	-3	107	115
3	1	-2	88	107	4	3	-2	108	107
3	1	-1	40	46	4	3	-1	0	19
3	1	0	57	61	4	3	0	70	68
3	1	1	104	109	4	3	1	119	117
3	1	2	106	106	4	4	-2	40	36
3	1	3	0	13	4	4	-1	113	105
3	2	-5	77	80	4	4	0	82	79
3	2	-4	78	98	5	0	-4	68	71
3	2	-2	34	32	5	0	-3	0	16
3	2	-1	119	122	5	0	-2	22	27
3	2	0	121	124	5	0	-1	97	111
3	2	1	0	3	5	0	0	52	59
3	2	2	50	46	5	0	1	0	7
3	2	3	111	110	5	1	-4	28	31
3	3	-4	20	15	5	1	-3	98	112
3	3	-2	88	88	5	1	-2	55	63
3	3	-1	52	47	5	1	-1	0	3

Table 7, continued

h	k	ℓ	Fo	Fc	h	k	ℓ	Fo	Fc
5	1	0	55	61	5	2	0	39	48
5	1	1	80	92	5	2	1	0	13
5	2	-3	0	13	5	3	-2	58	56
5	2	-2	47	47	5	3	-1	21	15
5	2	-1	109	116					