

The crystal chemistry of the uranyl silicate minerals

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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 $[(\text{UO}_2)(\text{SiO}_4)]_n^{2-}$ 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 cell 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.

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Table 3. Observed and calculated structure factors for uranophane.

| h | k | l | F _o | F _c | h | k | l | F _o | F _c |
|---|---|----|----------------|----------------|---|---|----|----------------|----------------|
| 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 | 90 | 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 | Po | Pc | h | k | l | Po | Pc |
|---|---|----|-----|-----|---|---|----|-----|-----|
| 2 | 1 | -4 | 86 | 76 | 3 | 0 | -1 | 11 | 41 |
| 2 | 1 | -3 | 219 | 199 | 3 | 0 | 0 | 0 | 7 |
| 2 | 1 | -2 | 289 | 276 | 3 | 0 | 1 | 16 | 38 |
| 2 | 1 | -1 | 131 | 129 | 3 | 0 | 2 | 23 | 27 |
| 2 | 1 | 0 | 11 | 14 | 3 | 0 | 3 | 10 | 15 |
| 2 | 1 | 1 | 174 | 178 | 3 | 0 | 4 | 0 | 0 |
| 2 | 1 | 2 | 274 | 274 | 3 | 0 | 5 | 18 | 4 |
| 2 | 1 | 3 | 148 | 140 | 3 | 1 | -5 | 21 | 29 |
| 2 | 1 | 4 | 87 | 84 | 3 | 1 | -4 | 16 | 14 |
| 2 | 1 | 5 | 150 | 136 | 3 | 1 | -3 | 48 | 61 |
| 2 | 2 | -5 | 111 | 103 | 3 | 1 | -2 | 38 | 45 |
| 2 | 2 | -4 | 211 | 204 | 3 | 1 | -1 | 34 | 46 |
| 2 | 2 | -3 | 132 | 131 | 3 | 1 | 0 | 25 | 33 |
| 2 | 2 | -2 | 26 | 17 | 3 | 1 | 1 | 38 | 56 |
| 2 | 2 | -1 | 162 | 164 | 3 | 1 | 2 | 25 | 40 |
| 2 | 2 | 0 | 323 | 293 | 3 | 1 | 3 | 15 | 15 |
| 2 | 2 | 1 | 114 | 119 | 3 | 1 | 4 | 16 | 26 |
| 2 | 2 | 2 | 21 | 23 | 3 | 1 | 5 | 26 | 23 |
| 2 | 2 | 3 | 177 | 176 | 3 | 2 | -5 | 63 | 63 |
| 2 | 2 | 4 | 174 | 182 | 3 | 2 | -4 | 70 | 78 |
| 2 | 2 | 5 | 80 | 82 | 3 | 2 | -3 | 23 | 30 |
| 2 | 3 | -4 | 84 | 76 | 3 | 2 | -2 | 10 | 7 |
| 2 | 3 | -3 | 109 | 119 | 3 | 2 | -1 | 55 | 69 |
| 2 | 3 | -2 | 225 | 247 | 3 | 2 | 0 | 95 | 93 |
| 2 | 3 | -1 | 116 | 132 | 3 | 2 | 1 | 49 | 53 |
| 2 | 3 | 0 | 27 | 22 | 3 | 2 | 2 | 19 | 26 |
| 2 | 3 | 1 | 172 | 188 | 3 | 2 | 3 | 68 | 83 |
| 2 | 3 | 2 | 207 | 220 | 3 | 2 | 4 | 44 | 56 |
| 2 | 3 | 3 | 66 | 74 | 3 | 3 | -4 | 35 | 30 |
| 2 | 3 | 4 | 68 | 69 | 3 | 3 | -3 | 81 | 99 |
| 2 | 4 | -4 | 126 | 133 | 3 | 3 | -2 | 82 | 95 |
| 2 | 4 | -3 | 71 | 79 | 3 | 3 | -1 | 79 | 80 |
| 2 | 4 | -2 | 34 | 41 | 3 | 3 | 0 | 15 | 9 |
| 2 | 4 | -1 | 72 | 91 | 3 | 3 | 1 | 137 | 143 |
| 2 | 4 | 0 | 173 | 178 | 3 | 3 | 2 | 140 | 150 |
| 2 | 4 | 1 | 42 | 47 | 3 | 3 | 3 | 33 | 35 |
| 2 | 4 | 2 | 0 | 16 | 3 | 3 | 4 | 60 | 57 |
| 2 | 4 | 3 | 85 | 99 | 3 | 4 | -4 | 122 | 123 |
| 2 | 5 | -3 | 44 | 53 | 3 | 4 | -3 | 64 | 74 |
| 2 | 5 | -2 | 84 | 108 | 3 | 4 | -2 | 16 | 10 |
| 2 | 5 | -1 | 51 | 59 | 3 | 4 | -1 | 88 | 95 |
| 2 | 5 | 0 | 20 | 20 | 3 | 4 | 0 | 191 | 175 |
| 2 | 5 | 1 | 69 | 75 | 3 | 4 | 1 | 70 | 66 |
| 2 | 5 | 2 | 80 | 101 | 3 | 4 | 2 | 31 | 28 |
| 3 | 0 | -5 | 0 | 5 | 3 | 4 | 3 | 117 | 121 |
| 3 | 0 | -4 | 19 | 3 | 3 | 5 | -2 | 144 | 146 |
| 3 | 0 | -3 | 27 | 49 | 3 | 5 | -1 | 80 | 80 |
| 3 | 0 | -2 | 0 | 10 | 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 | F _o | F _c | h | k | l | F _o | F _c |
|---|---|----|----------------|----------------|---|---|----|----------------|----------------|
| 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 | | | | | |