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# Preisingerite, $Bi_3O(OH)(AsO_4)_2$, a new species from San Juan Province, Argentina: its description and crystal structure[1]

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**Abstract**

Preisingerite, ideally $Bi_3O(OH)(AsO_4)_2$, triclinic, $P\bar{1}$, $a$ = 9.993(3), $b$ = 7.404(3), $c$ = 6.937(3)Å, $\alpha$ = 87.82(2), $\beta$ = 115.01(2), $\gamma$ = 111.07(2)°, Z = 2, was heretofore known as an unnamed species, for which only qualitative chemical composition and unindexed X-ray powder patterns had been reported. The mineral described here occurs in the weathering zones of the Bi–As–Cu deposits of San Francisco de Los Andes and Cerro Negro de la Aguadita, Department of Calingasta, San Juan Province, Argentina, as poorly developed tiny translucent grayish white crystals which are tabular parallel to (010) with a rhomboidal shape. Electron microprobe analysis yields Bi 68%, As 15%, P 0.3% and Pb < 0.5%. The calculated density is 7.24 g/cm³. The crystals are biaxial with $\alpha$ = 2.130, $\beta$ = 2.16 and $\gamma$ = 2.195 ($\lambda$ = 589 nm) derived from reflectivity measurements and from 2V, which is close to 90° as determined with a polarizing microscope.

The structure analysis, which converged to R = 0.046 for 1440 observed reflections, reveals clusters of six Bi atoms which are connected by two oxygens and two OH groups. These $Bi_6O_2(OH)_2$ groups are linked into a framework via the $AsO_4$ tetrahedra. The three different Bi atoms have one-sided coordinations, each with four oxygens at distances of 2.11–2.46Å (average 2.28Å). These coordinations are supplemented by five additional oxygens at distances of 2.57–3.36Å. Bonds within the $AsO_4$ tetrahedra measure 1.66–1.71Å (average 1.682Å). A hydrogen bond between the OH oxygen and an arsenate oxygen is indicated by O · · · O = 2.72Å.

## Introduction

In the late 1960's Dr. E. J. Llambías and Dr. L. Malvicini studied two Bi–As–Cu mineralized deposits in the San Juan Province, Argentina and observed two bismuth arsenate minerals, one of which was later identified as rooseveltite, $BiAsO_4$ (Bedlivy *et al.*, 1969, 1972). The second unnamed mineral was considered to be a new species because the X-ray powder pattern (Bedlivy *et al.*, 1969) did not match those of other bismuth arsenate minerals (atelestite, arsenobismite, walpurgite, mixite), although a powder pattern of an unnamed bismuth arsenate mentioned by Frondel (1943) showed some resemblance. The problem of better characterizing the mineral from Argentina remained unresolved until recently, when samples were first studied by modern X-ray single crystal methods. These allowed the successful solution of the structure and also revealed the chemical formula. Then, with calculated and measured powder diagrams at hand, it became apparent that the new mineral was most likely identical to the unnamed bismuth arsenate of unknown composition detected by Frondel (1943) in samples from Utah (USA), Bolivia and Germany.

The mineral was named in honor of Anton Preisinger, professor of Mineralogy, Crystallography and Structural Chemistry at the University of Technology in Vienna. The mineral and its name have been approved by the Commission on New Minerals and Mineral Names of the International Mineralogical Association. Holotype material from Argentina is deposited at the Museum of Natural History in Vienna.

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Table 3. Observed and calculated structure factors for preisingerite, $Bi_3O(OH)(AsO_4)_2$



Observed and calculated structure factors for preisingerite, $Bi_3O(OH)(AsO_4)_2$

| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 26 | -25 | 3 | 2 | 0 | 229 | -208 | 7 | 4 | 0 | 93 | 93 | -8 | 8 | 0 | 53 | -54 | 4 | -7 | 1 | 110 | -114 |
| 2 | 0 | 0 | 64 | 65 | 5 | 2 | 0 | 60 | -58 | 9 | 4 | 0 | 99 | -103 | -6 | 8 | 0 | 101 | 106 | 5 | -7 | 1 | 89 | -96 |
| 3 | 0 | 0 | 53 | 47 | 6 | 2 | 0 | 85 | 81 | -12 | 5 | 0 | 74 | 74 | -5 | 8 | 0 | 56 | -60 | 6 | -7 | 1 | 80 | 83 |
| 4 | 0 | 0 | 72 | 71 | 7 | 2 | 0 | 100 | -104 | -10 | 5 | 0 | 101 | 104 | -3 | 8 | 0 | 133 | 124 | 7 | -7 | 1 | 132 | -137 |
| 5 | 0 | 0 | 354 | -335 | 8 | 2 | 0 | 125 | 124 | -9 | 5 | 0 | 110 | 109 | 0 | 8 | 0 | 70 | 61 | 8 | -7 | 1 | 74 | 70 |
| 7 | 0 | 0 | 37 | -41 | -10 | 3 | 0 | 81 | 81 | -7 | 5 | 0 | 115 | -120 | 2 | 8 | 0 | 154 | -144 | 9 | -7 | 1 | 74 | 70 |
| 8 | 0 | 0 | 100 | -100 | -9 | 3 | 0 | 118 | -120 | -6 | 5 | 0 | 133 | 140 | -10 | 9 | 0 | 92 | -84 | -4 | -6 | 1 | 178 | 177 |
| 9 | 0 | 0 | 56 | -54 | -8 | 3 | 0 | 118 | 115 | -5 | 5 | 0 | 184 | -193 | -9 | 9 | 0 | 94 | 90 | -2 | -6 | 1 | 61 | -63 |
| 10 | 0 | 0 | 110 | 109 | -7 | 3 | 0 | 53 | 57 | -4 | 5 | 0 | 157 | -172 | -8 | 9 | 0 | 69 | -65 | 1 | -6 | 1 | 174 | -163 |
| -11 | 1 | 0 | 130 | -125 | -6 | 3 | 0 | 80 | 80 | -3 | 5 | 0 | 146 | -155 | -6 | 9 | 0 | 71 | 61 | 2 | -6 | 1 | 107 | -108 |
| -8 | 1 | 0 | 161 | -159 | -5 | 3 | 0 | 85 | -88 | -2 | 5 | 0 | 83 | 88 | -5 | 9 | 0 | 118 | 117 | 3 | -6 | 1 | 82 | 85 |
| -7 | 1 | 0 | 80 | -82 | -4 | 3 | 0 | 206 | 209 | -1 | 5 | 0 | 251 | -231 | -3 | 9 | 0 | 77 | 73 | 4 | -6 | 1 | 125 | -135 |
| -6 | 1 | 0 | 72 | 73 | -3 | 3 | 0 | 97 | -97 | 0 | 5 | 0 | 148 | 139 | -1 | 9 | 0 | 84 | -75 | 6 | -6 | 1 | 46 | 54 |
| -5 | 1 | 0 | 49 | 45 | -2 | 3 | 0 | 83 | -88 | 1 | 5 | 0 | 139 | 133 | 0 | 9 | 0 | 88 | -80 | 7 | -6 | 1 | 115 | 124 |
| -4 | 1 | 0 | 51 | -49 | 0 | 3 | 0 | 67 | -59 | 2 | 5 | 0 | 129 | 127 | -6 | 10 | 0 | 61 | 53 | 8 | -6 | 1 | 103 | -101 |
| -3 | 1 | 0 | 375 | 361 | 1 | 3 | 0 | 199 | -177 | 4 | 5 | 0 | 167 | 160 | -3 | 10 | 0 | 130 | -123 | 9 | -6 | 1 | 112 | 119 |
| -2 | 1 | 0 | 125 | 124 | 2 | 3 | 0 | 121 | -116 | 6 | 5 | 0 | 65 | -68 | 3 | -10 | 1 | 108 | 100 | -7 | -5 | 1 | 123 | 122 |
| -1 | 1 | 0 | 66 | 72 | 3 | 3 | 0 | 61 | 61 | -12 | 6 | 0 | 96 | 97 | 6 | -10 | 1 | 83 | 75 | -4 | -5 | 1 | 85 | -85 |
| 0 | 1 | 0 | 47 | -39 | 4 | 3 | 0 | 138 | -135 | -7 | 6 | 0 | 90 | -95 | -1 | -9 | 1 | 97 | -84 | -3 | -5 | 1 | 118 | 118 |
| 1 | 1 | 0 | 235 | 210 | 6 | 3 | 0 | 90 | 94 | -6 | 6 | 0 | 136 | -140 | 0 | -9 | 1 | 98 | 92 | -2 | -5 | 1 | 116 | -117 |
| 2 | 1 | 0 | 383 | -355 | 7 | 3 | 0 | 117 | 118 | -5 | 6 | 0 | 54 | 54 | 4 | -9 | 1 | 108 | 107 | -1 | -5 | 1 | 67 | -67 |
| 3 | 1 | 0 | 57 | -51 | 9 | 3 | 0 | 120 | 132 | -4 | 6 | 0 | 106 | -113 | 5 | -9 | 1 | 61 | -58 | 2 | -5 | 1 | 133 | -147 |
| 4 | 1 | 0 | 107 | -105 | -12 | 4 | 0 | 92 | -93 | -3 | 6 | 0 | 55 | 58 | 9 | -9 | 1 | 76 | -70 | 4 | -5 | 1 | 90 | 98 |
| 6 | 1 | 0 | 176 | -171 | -9 | 4 | 0 | 104 | 107 | -1 | 6 | 0 | 212 | 199 | -4 | -8 | 1 | 99 | -88 | 5 | -5 | 1 | 55 | -55 |
| 7 | 1 | 0 | 135 | 129 | -8 | 4 | 0 | 104 | -102 | 1 | 6 | 0 | 141 | 127 | -1 | -8 | 1 | 81 | 78 | 6 | -5 | 1 | 63 | 65 |
| 11 | 1 | 0 | 88 | 87 | -7 | 4 | 0 | 227 | 227 | 4 | 6 | 0 | 101 | -102 | 1 | -8 | 1 | 174 | 165 | 7 | -5 | 1 | 79 | 82 |
| -12 | 2 | 0 | 68 | -59 | -6 | 4 | 0 | 56 | 59 | 6 | 6 | 0 | 68 | -71 | 4 | -8 | 1 | 65 | -64 | 8 | -5 | 1 | 75 | 77 |
| -10 | 2 | 0 | 156 | -149 | -4 | 4 | 0 | 107 | -111 | -12 | 7 | 0 | 79 | -70 | 5 | -8 | 1 | 55 | 62 | 9 | -5 | 1 | 63 | -62 |
| -7 | 2 | 0 | 51 | 48 | -3 | 4 | 0 | 154 | 165 | -9 | 7 | 0 | 89 | -82 | 6 | -8 | 1 | 138 | -146 | 10 | -5 | 1 | 90 | 98 |
| -5 | 2 | 0 | 223 | 209 | -2 | 4 | 0 | 280 | -303 | -8 | 7 | 0 | 59 | -66 | 7 | -8 | 1 | 57 | -57 | -8 | -4 | 1 | 87 | 87 |
| -4 | 2 | 0 | 76 | 74 | -1 | 4 | 0 | 161 | -155 | -4 | 7 | 0 | 108 | 117 | -4 | -7 | 1 | 77 | 82 | -7 | -4 | 1 | 51 | -61 |
| -2 | 2 | 0 | 76 | 79 | 0 | 4 | 0 | 41 | -27 | 0 | 7 | 0 | 145 | 128 | -2 | -7 | 1 | 102 | 97 | -6 | -4 | 1 | 105 | 110 |
| -1 | 2 | 0 | 34 | -39 | 2 | 4 | 0 | 137 | -132 | 1 | 7 | 0 | 106 | -98 | -1 | -7 | 1 | 130 | 128 | -4 | -4 | 1 | 41 | 33 |
| 0 | 2 | 0 | 63 | -56 | 3 | 4 | 0 | 154 | 148 | 5 | 7 | 0 | 120 | -112 | 1 | -7 | 1 | 123 | -118 | -3 | -4 | 1 | 126 | -125 |
| 1 | 2 | 0 | 120 | -108 | 4 | 4 | 0 | 157 | 158 | -11 | 8 | 0 | 106 | -104 | 2 | -7 | 1 | 92 | 94 | -2 | -4 | 1 | 107 | 105 |
| 2 | 2 | 0 | 80 | 77 | 6 | 4 | 0 | 80 | 80 | -10 | 8 | 0 | 68 | 70 | 3 | -7 | 1 | 116 | -126 | -1 | -4 | 1 | 184 | -171 |

Observed and calculated structure factors for preisingerite, $Bi_3O(OH)(AsO_4)_2$



| h | k | l | Fo | Fc | h | k | l | Fo | Fc | h | k | l | Fo | Fc | h | k | l | Fo | Fc | h | k | l | Fo | Fc |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | -4 | 1 | 48 | -47 | 0 | -2 | 1 | 482 | 449 | 0 | 0 | 1 | 113 | -102 | -9 | 3 | 1 | 129 | 133 | 2 | 5 | 1 | 110 | 113 |
| 1 | -4 | 1 | 84 | -90 | 1 | -2 | 1 | 104 | -111 | 3 | 0 | 1 | 301 | -280 | -6 | 3 | 1 | 142 | 146 | 5 | 5 | 1 | 131 | -122 |
| 2 | -4 | 1 | 86 | 96 | 2 | -2 | 1 | 107 | 117 | 5 | 0 | 1 | 41 | -41 | -5 | 3 | 1 | 265 | -268 | 7 | 5 | 1 | 98 | -97 |
| 3 | -4 | 1 | 78 | -83 | 5 | -2 | 1 | 323 | -311 | 7 | 0 | 1 | 100 | -104 | -4 | 3 | 1 | 154 | -162 | -11 | 6 | 1 | 98 | -100 |
| 4 | -4 | 1 | 113 | 122 | 6 | -2 | 1 | 57 | 61 | 8 | 0 | 1 | 126 | 125 | -3 | 3 | 1 | 135 | -142 | -10 | 6 | 1 | 106 | 104 |
| 5 | -4 | 1 | 122 | 131 | 7 | -2 | 1 | 124 | -127 | -9 | 1 | 1 | 153 | -154 | -2 | 3 | 1 | 56 | 53 | -9 | 6 | 1 | 135 | -134 |
| 6 | -4 | 1 | 59 | 63 | 8 | -2 | 1 | 107 | -107 | -8 | 1 | 1 | 152 | 156 | -1 | 3 | 1 | 261 | -256 | -8 | 6 | 1 | 67 | -58 |
| 8 | -4 | 1 | 59 | 59 | 10 | -2 | 1 | 109 | 105 | -6 | 1 | 1 | 53 | 54 | 0 | 3 | 1 | 280 | 267 | -6 | 6 | 1 | 90 | 89 |
| 10 | -4 | 1 | 120 | -120 | 11 | -2 | 1 | 44 | -46 | -5 | 1 | 1 | 31 | -33 | 1 | 3 | 1 | 82 | 73 | -5 | 6 | 1 | 157 | -161 |
| 12 | -4 | 1 | 62 | -57 | -11 | -1 | 1 | 116 | -114 | -4 | 1 | 1 | 288 | 281 | 2 | 3 | 1 | 124 | 123 | -4 | 6 | 1 | 107 | 121 |
| -8 | -3 | 1 | 72 | 75 | -9 | -1 | 1 | 87 | -91 | -3 | 1 | 1 | 93 | -85 | 4 | 3 | 1 | 210 | 215 | -3 | 6 | 1 | 108 | 122 |
| -7 | -3 | 1 | 93 | 94 | -8 | -1 | 1 | 129 | -130 | -2 | 1 | 1 | 37 | 34 | 5 | 3 | 1 | 69 | -70 | 0 | 6 | 1 | 133 | 136 |
| -6 | -3 | 1 | 159 | -158 | -7 | -1 | 1 | 103 | -108 | 1 | 1 | 1 | 354 | -336 | 9 | 3 | 1 | 101 | -104 | 2 | 6 | 1 | 143 | -147 |
| -4 | -3 | 1 | 91 | -91 | -6 | -1 | 1 | 61 | 64 | 4 | 1 | 1 | 148 | -151 | -12 | 4 | 1 | 135 | 138 | 4 | 6 | 1 | 62 | -67 |
| -3 | -3 | 1 | 145 | -138 | -5 | -1 | 1 | 75 | -81 | 6 | 1 | 1 | 138 | 138 | -7 | 4 | 1 | 114 | -119 | 5 | 6 | 1 | 90 | -95 |
| -2 | -3 | 1 | 300 | -280 | -4 | -1 | 1 | 42 | 45 | 7 | 1 | 1 | 78 | 79 | -6 | 4 | 1 | 104 | -114 | -11 | 7 | 1 | 94 | -86 |
| -1 | -3 | 1 | 240 | 212 | -3 | -1 | 1 | 255 | 241 | 9 | 1 | 1 | 156 | 153 | -4 | 4 | 1 | 111 | -113 | -10 | 7 | 1 | 94 | -90 |
| 0 | -3 | 1 | 126 | -113 | -2 | -1 | 1 | 67 | 62 | -12 | 2 | 1 | 116 | -119 | -2 | 4 | 1 | 57 | 57 | [illegible] | 7 | 1 | 88 | 87 |
| 1 | -3 | 1 | 80 | 81 | -1 | -1 | 1 | 37 | 35 | -10 | 2 | 1 | 68 | 68 | -1 | 4 | 1 | 165 | 160 | [illegible] | 7 | 1 | 126 | -125 |
| 2 | -3 | 1 | 90 | 96 | 0 | -1 | 1 | 90 | 93 | -9 | 2 | 1 | 35 | 39 | 0 | 4 | 1 | 76 | -77 | [illegible] | 7 | 1 | 51 | 51 |
| 3 | -3 | 1 | 324 | 343 | 1 | -1 | 1 | 115 | 119 | -8 | 2 | 1 | 49 | -55 | 1 | 4 | 1 | 186 | 182 | -6 | 7 | 1 | 99 | 99 |
| 4 | -3 | 1 | 99 | -100 | 2 | -1 | 1 | 295 | -284 | -7 | 2 | 1 | 342 | 333 | 3 | 4 | 1 | 48 | 49 | -5 | 7 | 1 | 136 | 144 |
| 5 | -3 | 1 | 144 | 147 | 4 | -1 | 1 | 106 | -106 | -6 | 2 | 1 | 41 | 42 | 4 | 4 | 1 | 101 | -102 | -4 | 7 | 1 | 54 | -61 |
| 6 | -3 | 1 | 60 | 65 | 6 | -1 | 1 | 177 | -172 | -4 | 2 | 1 | 38 | -37 | 5 | 4 | 1 | 76 | 74 | -3 | 7 | 1 | 168 | 184 |
| 7 | -3 | 1 | 99 | -95 | 7 | -1 | 1 | 142 | 142 | -3 | 2 | 1 | 182 | 189 | 6 | 4 | 1 | 96 | -95 | -1 | 7 | 1 | 62 | -68 |
| 8 | -3 | 1 | 146 | -145 | 8 | -1 | 1 | 68 | -67 | -2 | 2 | 1 | 415 | -460 | -12 | 5 | 1 | 75 | -73 | 0 | 7 | 1 | 85 | -89 |
| 10 | -3 | 1 | 84 | -88 | 11 | -1 | 1 | 86 | 86 | -1 | 2 | 1 | 91 | -95 | -11 | 5 | 1 | 78 | 84 | 2 | 7 | 1 | 128 | -132 |
| 11 | -3 | 1 | 90 | -91 | -10 | 0 | 1 | 152 | -156 | 0 | 2 | 1 | 95 | -87 | -10 | 5 | 1 | 71 | -79 | 3 | 7 | 1 | 54 | -56 |
| -11 | -2 | 1 | 91 | 89 | -9 | 0 | 1 | 67 | 70 | 2 | 2 | 1 | 208 | -201 | -9 | 5 | 1 | 53 | -59 | -8 | 8 | 1 | 153 | 143 |
| -10 | -2 | 1 | 90 | 86 | -8 | 0 | 1 | 64 | -60 | 3 | 2 | 1 | 267 | 258 | -8 | 5 | 1 | 76 | -80 | -6 | 8 | 1 | 102 | 100 |
| -8 | -2 | 1 | 82 | -79 | -7 | 0 | 1 | 51 | 52 | 4 | 2 | 1 | 72 | 68 | -7 | 5 | 1 | 57 | 57 | -3 | 8 | 1 | 148 | -155 |
| -6 | -2 | 1 | 121 | -124 | -5 | 0 | 1 | 203 | 195 | 6 | 2 | 1 | 134 | 143 | -6 | 5 | 1 | 133 | -133 | -1 | 8 | 1 | 114 | -120 |
| -5 | -2 | 1 | 306 | -294 | -4 | 0 | 1 | 54 | -52 | 7 | 2 | 1 | 107 | 114 | -4 | 5 | 1 | 88 | 91 | 2 | 8 | 1 | 68 | 70 |
| -4 | -2 | 1 | 107 | 103 | -3 | 0 | 1 | 81 | 84 | 8 | 2 | 1 | 43 | -60 | -1 | 5 | 1 | 131 | 134 | -10 | 9 | 1 | 63 | 58 |
| -3 | -2 | 1 | 26 | -29 | -2 | 0 | 1 | 87 | 80 | -13 | 3 | 1 | 68 | 69 | 0 | 5 | 1 | 133 | 128 | -7 | 9 | 1 | 74 | 68 |
| -1 | -2 | 1 | 121 | 114 | -1 | 0 | 1 | 49 | 46 | -10 | 3 | 1 | 128 | 136 | 1 | 5 | 1 | 103 | -105 | -6 | 9 | 1 | 82 | -84 |

Observed and calculated structure factors for preisingerite, $Bi_3O(OH)(AsO_4)_2$



| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -2 | 9 | 1 | 113 | -113 | 10 | -6 | 2 | 70 | -72 | -6 | -3 | 2 | 67 | 65 | -3 | -1 | 2 | 126 | -116 | 2 | 1 | 2 | 110 | 107 |
| -1 | 9 | 1 | 71 | 74 | -8 | -5 | 2 | 111 | 110 | -5 | -3 | 2 | 140 | -139 | -2 | -1 | 2 | 179 | 165 | 4 | 1 | 2 | 230 | 227 |
| -8 | 10 | 1 | 88 | -75 | -6 | -5 | 2 | 86 | -91 | -4 | -3 | 2 | 100 | 104 | 1 | -1 | 2 | 328 | -321 | 5 | 1 | 2 | 121 | -119 |
| -5 | 10 | 1 | 97 | -93 | -4 | -5 | 2 | 76 | -76 | -3 | -3 | 2 | 145 | 142 | 2 | -1 | 2 | 60 | 56 | 9 | 1 | 2 | 104 | -107 |
| -2 | -9 | 2 | 81 | 73 | -3 | -5 | 2 | 143 | -145 | -2 | -3 | 2 | 46 | 49 | 3 | -1 | 2 | 170 | -161 | -12 | 2 | 2 | 143 | 142 |
| -1 | -9 | 2 | 101 | 93 | -2 | -5 | 2 | 166 | -161 | 0 | -3 | 2 | 189 | 178 | 4 | -1 | 2 | 123 | -125 | -10 | 2 | 2 | 62 | 60 |
| 2 | -9 | 2 | 83 | 76 | -1 | -5 | 2 | 140 | 136 | 1 | -3 | 2 | 65 | 66 | 6 | -1 | 2 | 141 | 143 | -7 | 2 | 2 | 214 | -209 |
| 3 | -9 | 2 | 99 | -93 | 0 | -5 | 2 | 172 | -164 | 2 | -3 | 2 | 152 | -162 | 9 | -1 | 2 | 147 | 148 | -5 | 2 | 2 | 71 | -70 |
| 4 | -9 | 2 | 67 | -67 | 1 | -5 | 2 | 65 | 62 | 3 | -3 | 2 | 57 | 61 | -12 | 0 | 2 | 110 | -109 | -4 | 2 | 2 | 169 | -162 |
| 7 | -9 | 2 | 110 | -112 | 2 | -5 | 2 | 112 | 128 | 4 | -3 | 2 | 43 | -44 | -10 | 0 | 2 | 66 | 61 | -3 | 2 | 2 | 67 | -70 |
| 8 | -9 | 2 | 83 | 81 | 3 | -5 | 2 | 164 | 181 | 6 | -3 | 2 | 121 | -120 | -7 | 0 | 2 | 329 | 320 | -2 | 2 | 2 | 61 | 63 |
| -4 | -8 | 2 | 157 | 148 | 4 | -5 | 2 | 69 | -68 | 7 | -3 | 2 | 92 | 93 | -5 | 0 | 2 | 48 | 47 | -1 | 2 | 2 | 83 | 81 |
| 1 | -8 | 2 | 131 | -131 | 5 | -5 | 2 | 198 | 208 | 8 | -3 | 2 | 95 | -97 | -4 | 0 | 2 | 25 | 32 | 0 | 2 | 2 | 87 | -75 |
| 4 | -8 | 2 | 98 | -105 | 7 | -5 | 2 | 71 | -74 | -10 | -2 | 2 | 107 | -107 | -3 | 0 | 2 | 88 | 84 | 1 | 2 | 2 | 188 | 172 |
| 6 | -8 | 2 | 68 | 59 | 8 | -5 | 2 | 95 | -99 | -9 | -2 | 2 | 77 | 74 | -2 | 0 | 2 | 488 | -473 | 3 | 2 | 2 | 53 | 54 |
| 8 | -8 | 2 | 68 | -67 | 10 | -5 | 2 | 126 | -122 | -8 | -2 | 2 | 84 | -84 | -1 | 0 | 2 | 51 | 45 | 4 | 2 | 2 | 81 | -79 |
| 9 | -8 | 2 | 103 | 103 | 11 | -5 | 2 | 59 | -44 | -6 | -2 | 2 | 52 | -54 | 0 | 0 | 2 | 198 | -186 | 5 | 2 | 2 | 130 | 133 |
| -3 | -7 | 2 | 115 | 116 | -6 | -4 | 2 | 186 | -189 | -5 | -2 | 2 | 172 | 170 | 1 | 0 | 2 | 157 | -153 | 6 | 2 | 2 | 100 | -103 |
| -2 | -7 | 2 | 108 | -105 | -5 | -4 | 2 | 133 | -136 | -4 | -2 | 2 | 113 | -110 | 2 | 0 | 2 | 174 | -165 | -12 | 3 | 2 | 57 | -57 |
| 2 | -7 | 2 | 126 | -133 | -3 | -4 | 2 | 64 | -59 | -3 | -2 | 2 | 153 | 147 | 3 | 0 | 2 | 293 | 282 | -11 | 3 | 2 | 124 | 126 |
| 3 | -7 | 2 | 47 | 53 | -2 | -4 | 2 | 60 | -57 | -2 | -2 | 2 | 131 | 114 | 4 | 0 | 2 | 43 | -46 | -10 | 3 | 2 | 109 | -111 |
| 5 | -7 | 2 | 40 | -39 | -1 | -4 | 2 | 141 | 136 | -1 | -2 | 2 | 79 | 73 | 5 | 0 | 2 | 96 | 96 | -8 | 3 | 2 | 49 | -52 |
| 7 | -7 | 2 | 77 | 75 | 0 | -4 | 2 | 238 | 223 | 0 | -2 | 2 | 85 | -84 | 6 | 0 | 2 | 160 | 160 | -7 | 3 | 2 | 72 | 71 |
| 10 | -7 | 2 | 75 | 75 | 1 | -4 | 2 | 108 | -11[illegible] | 1 | -2 | 2 | 90 | 94 | 7 | 0 | 2 | 101 | 100 | -6 | 3 | 2 | 248 | -248 |
| -6 | -6 | 2 | 90 | 99 | 2 | -4 | 2 | 154 | 172 | 2 | -2 | 2 | 58 | -57 | 8 | 0 | 2 | 96 | -99 | -5 | 3 | 2 | 51 | 50 |
| -3 | -6 | 2 | 99 | -95 | 3 | -4 | 2 | 57 | 64 | 3 | -2 | 2 | 135 | -129 | -13 | 1 | 2 | 63 | 65 | -3 | 3 | 2 | 55 | -56 |
| -2 | -6 | 2 | 79 | 79 | 5 | -4 | 2 | 172 | -187 | 4 | -2 | 2 | 53 | -56 | -10 | 1 | 2 | 124 | 130 | -1 | 3 | 2 | 244 | 230 |
| -1 | -6 | 2 | 189 | -171 | 6 | -4 | 2 | 114 | 112 | 6 | -2 | 2 | [illegible]0 | -46 | -9 | 1 | 2 | 137 | 139 | 0 | 3 | 2 | 73 | 75 |
| 0 | -6 | 2 | 60 | -53 | 7 | -4 | 2 | 148 | -150 | 7 | -2 | 2 | 82 | -84 | -7 | 1 | 2 | 83 | 87 | 1 | 3 | 2 | 47 | -46 |
| 1 | -6 | 2 | 97 | -101 | 8 | -4 | 2 | 57 | -48 | 8 | -2 | 2 | 107 | 108 | -6 | 1 | 2 | 67 | 66 | 2 | 3 | 2 | 146 | 144 |
| 2 | -6 | 2 | 53 | 52 | 10 | -4 | 2 | 81 | 79 | 10 | -2 | 2 | 68 | 61 | -5 | 1 | 2 | 303 | -284 | 4 | 3 | 2 | 63 | -63 |
| 3 | -6 | 2 | 105 | -119 | 11 | -4 | 2 | 77 | -72 | -9 | -1 | 2 | 125 | -129 | -4 | 1 | 2 | 101 | -95 | 5 | 3 | 2 | 77 | -76 |
| 4 | -6 | 2 | 118 | 124 | -10 | -3 | 2 | 55 | 59 | -8 | -1 | 2 | 121 | 125 | -3 | 1 | 2 | 84 | -82 | 7 | 3 | 2 | 143 | -147 |
| 5 | -6 | 2 | 49 | 63 | -9 | -3 | 2 | 119 | -121 | -6 | -1 | 2 | 40 | 38 | -2 | 1 | 2 | 90 | -93 | -11 | 4 | 2 | 54 | -56 |
| 6 | -6 | 2 | 73 | 72 | -8 | -3 | 2 | 67 | -73 | -5 | -1 | 2 | 34 | 37 | -1 | 1 | 2 | 205 | -211 | -10 | 4 | 2 | 105 | 112 |
| 8 | -6 | 2 | 81 | 81 | -7 | -3 | 2 | 87 | -83 | -4 | -1 | 2 | 387 | 369 | 0 | 1 | 2 | 229 | 210 | -9 | 4 | 2 | 206 | -207 |

Observed and calculated structure factors for preisingerite, $Bi_3O(OH)(AsO_4)_2$



| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -8 | 4 | 2 | 48 | -54 | -7 | 7 | 2 | 65 | 58 | -6 | -6 | 3 | 169 | -174 | -4 | -3 | 3 | 242 | 230 | -5 | -1 | 3 | 146 | -138 |
| -7 | 4 | 2 | 49 | -51 | -6 | 7 | 2 | 90 | -86 | -3 | -6 | 3 | 65 | -63 | -3 | -3 | 3 | 116 | -110 | -4 | -1 | 3 | 107 | -100 |
| -5 | 4 | 2 | 201 | -208 | -3 | 7 | 2 | 53 | -57 | -2 | -6 | 3 | 52 | -57 | -2 | -3 | 3 | 223 | 207 | -3 | -1 | 3 | 33 | -29 |
| -4 | 4 | 2 | 218 | 228 | -2 | 7 | 2 | 127 | -135 | -1 | -6 | 3 | 152 | 145 | 0 | -3 | 3 | 65 | -66 | -2 | -1 | 3 | 135 | -133 |
| -3 | 4 | 2 | 86 | 89 | -1 | 7 | 2 | 85 | 87 | 0 | -6 | 3 | 87 | 82 | 1 | -3 | 3 | 234 | -261 | -1 | -1 | 3 | 205 | -187 |
| -2 | 4 | 2 | 77 | 78 | 0 | 7 | 2 | 57 | -57 | 2 | -6 | 3 | 128 | 145 | 2 | -3 | 3 | 70 | 76 | 0 | -1 | 3 | 148 | 155 |
| -1 | 4 | 2 | 60 | 59 | 3 | 7 | 2 | 98 | 100 | 5 | -6 | 3 | 66 | -69 | 3 | -3 | 3 | 231 | -243 | 1 | -1 | 3 | 54 | -55 |
| 0 | 4 | 2 | 241 | 242 | 4 | 7 | 2 | 74 | -67 | 6 | -6 | 3 | 93 | 92 | 4 | -3 | 3 | 93 | -102 | 2 | -1 | 3 | 78 | 77 |
| 1 | 4 | 2 | 124 | -122 | -12 | 8 | 2 | 82 | -77 | 7 | -6 | 3 | 119 | -122 | 5 | -3 | 3 | 41 | 35 | 3 | -1 | 3 | 37 | 41 |
| 2 | 4 | 2 | 72 | -71 | -11 | 8 | 2 | 73 | 66 | -9 | -5 | 3 | 102 | -99 | 6 | -3 | 3 | 110 | 105 | 4 | -1 | 3 | 168 | 162 |
| 4 | 4 | 2 | 102 | -107 | -8 | 8 | 2 | 87 | -83 | -5 | -5 | 3 | 128 | -134 | 7 | -3 | 3 | 59 | -56 | 5 | -1 | 3 | 96 | -93 |
| 5 | 4 | 2 | 133 | -131 | -7 | 8 | 2 | 107 | 104 | -4 | -5 | 3 | 107 | 114 | 8 | -3 | 3 | 111 | 106 | 6 | -1 | 3 | 107 | 103 |
| 7 | 4 | 2 | 55 | 51 | -5 | 8 | 2 | 106 | -110 | 0 | -5 | 3 | 148 | 145 | 9 | -3 | 3 | 107 | 102 | 9 | -1 | 3 | 86 | -86 |
| -12 | 5 | 2 | 65 | -69 | -2 | 8 | 2 | 98 | -103 | 2 | -5 | 3 | 36 | -43 | -9 | -2 | 3 | 73 | -77 | -12 | 0 | 3 | 130 | 134 |
| -11 | 5 | 2 | 117 | -124 | 0 | 8 | 2 | 105 | 105 | 3 | -5 | 3 | 52 | 53 | -8 | -2 | 3 | 113 | 114 | -10 | 0 | 3 | 80 | 83 |
| -10 | 5 | 2 | 49 | -50 | -10 | 9 | 2 | 90 | 86 | 5 | -5 | 3 | 64 | -68 | -7 | -2 | 3 | 189 | 191 | -8 | 0 | 3 | 52 | 52 |
| -8 | 5 | 2 | 158 | -166 | -7 | 9 | 2 | 102 | -100 | 6 | -5 | 3 | 47 | -52 | -6 | -2 | 3 | 34 | -34 | -7 | 0 | 3 | 184 | -180 |
| -7 | 5 | 2 | 138 | 142 | -5 | 9 | 2 | 113 | -118 | 8 | -5 | 3 | 102 | -104 | -5 | -2 | 3 | 74 | 73 | -6 | 0 | 3 | 53 | 53 |
| -6 | 5 | 2 | 104 | 104 | -4 | 9 | 2 | 64 | -53 | -9 | -4 | 3 | 58 | 56 | -4 | -2 | 3 | 115 | 115 | -5 | 0 | 3 | 107 | -101 |
| -5 | 5 | 2 | 152 | 154 | 0 | 9 | 2 | 76 | 82 | -8 | -4 | 3 | 87 | -91 | -2 | -2 | 3 | 333 | -310 | -4 | 0 | 3 | 104 | -91 |
| -3 | 5 | 2 | 252 | 274 | -8 | 10 | 2 | 82 | -77 | -5 | -4 | 3 | 91 | 94 | -1 | -2 | 3 | 94 | 85 | -3 | 0 | 3 | 104 | -102 |
| -2 | 5 | 2 | 84 | -79 | -5 | 10 | 2 | 89 | 92 | -4 | -4 | 3 | 97 | -98 | 0 | -2 | 3 | 205 | -215 | -2 | 0 | 3 | 137 | 125 |
| 0 | 5 | 2 | 80 | -81 | -2 | -9 | 3 | 83 | -72 | -3 | -4 | 3 | 156 | 153 | 1 | -2 | 3 | 154 | -171 | 0 | 0 | 3 | 42 | -38 |
| 2 | 5 | 2 | 227 | -233 | 2 | -9 | 3 | 101 | -96 | -1 | -4 | 3 | 123 | 118 | 2 | -2 | 3 | 57 | -62 | 1 | 0 | 3 | 171 | 154 |
| -9 | 6 | 2 | 83 | 85 | -1 | -8 | 3 | 148 | -134 | 0 | -4 | 3 | 88 | -72 | 3 | -2 | 3 | 236 | 231 | 2 | 0 | 3 | 38 | 41 |
| -8 | 6 | 2 | 129 | 127 | 1 | -8 | 3 | 70 | -69 | 1 | -4 | 3 | 138 | 151 | 4 | -2 | 3 | 112 | -110 | 3 | 0 | 3 | 47 | 50 |
| -6 | 6 | 2 | 141 | 140 | 3 | -8 | 3 | 79 | -88 | 2 | -4 | 3 | 69 | -72 | 5 | -2 | 3 | 148 | 150 | 5 | 0 | 3 | 125 | 123 |
| -3 | 6 | 2 | 140 | -146 | 4 | -8 | 3 | 112 | 120 | 3 | -4 | 3 | 71 | -72 | 6 | -2 | 3 | 106 | 103 | 6 | 0 | 3 | 85 | -83 |
| -1 | 6 | 2 | 136 | -142 | 8 | -8 | 3 | 100 | 97 | 4 | -4 | 3 | 56 | -63 | 7 | -2 | 3 | 77 | 75 | -11 | 1 | 3 | 135 | 141 |
| 1 | 6 | 2 | 63 | -66 | -4 | -7 | 3 | 58 | -57 | 6 | -4 | 3 | 110 | -118 | 8 | -2 | 3 | 90 | -84 | -10 | 1 | 3 | 89 | -88 |
| 2 | 6 | 2 | 87 | 84 | -3 | -7 | 3 | 127 | -129 | 8 | -4 | 3 | 64 | 61 | 9 | -2 | 3 | 83 | 74 | -7 | 1 | 3 | 43 | 38 |
| 3 | 6 | 2 | 68 | -65 | 0 | -7 | 3 | 142 | -138 | -10 | -3 | 3 | 77 | -86 | -12 | -1 | 3 | 84 | -82 | -6 | 1 | 3 | 288 | -276 |
| 4 | 6 | 2 | 76 | 77 | 1 | -7 | 3 | 82 | 82 | -9 | -3 | 3 | 91 | -87 | -11 | -1 | 3 | 83 | 79 | -5 | 1 | 3 | 103 | 96 |
| -11 | 7 | 2 | 64 | 59 | 2 | -7 | 3 | 85 | 94 | -8 | -3 | 3 | 85 | 83 | -10 | -1 | 3 | 102 | 102 | -4 | 1 | 3 | 106 | -99 |
| -10 | 7 | 2 | 77 | 74 | 3 | -7 | 3 | 79 | 85 | -7 | -3 | 3 | 66 | -66 | -9 | -1 | 3 | 101 | 104 | -3 | 1 | 3 | 37 | -41 |
| -8 | 7 | 2 | 103 | 96 | 5 | -7 | 3 | 161 | 177 | -5 | -3 | 3 | 94 | 92 | -7 | -1 | 3 | 150 | 153 | -1 | 1 | 3 | 261 | 263 |

Observed and calculated structure factors for preisingerite, $Bi_3O(OH)(AsO_4)_2$



| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 1 | 3 | 53 | -50 | -5 | 4 | 3 | 72 | 74 | 1 | 7 | 3 | 68 | 72 | 8 | -5 | 4 | 138 | 136 | -3 | -2 | 4 | 86 | -80 |
| 1 | 1 | 3 | 88 | 83 | -3 | 4 | 3 | 102 | -106 | -10 | 8 | 3 | 102 | -95 | -9 | -4 | 4 | 82 | -84 | -2 | -2 | 4 | 96 | 92 |
| 2 | 1 | 3 | 166 | 164 | -2 | 4 | 3 | 54 | 52 | -8 | 8 | 3 | 111 | -106 | -8 | -4 | 4 | 140 | 143 | -1 | -2 | 4 | 158 | -150 |
| 3 | 1 | 3 | 53 | 53 | -1 | 4 | 3 | 152 | -153 | -6 | 8 | 3 | 59 | -56 | -7 | -4 | 4 | 89 | 87 | 1 | -2 | 4 | 56 | 59 |
| 4 | 1 | 3 | 89 | -86 | 1 | 4 | 3 | 85 | -86 | -5 | 8 | 3 | 99 | 100 | -5 | -4 | 4 | 95 | 95 | 2 | -2 | 4 | 50 | 50 |
| 7 | 1 | 3 | 169 | -165 | 2 | 4 | 3 | 76 | 71 | -3 | 8 | 3 | 102 | 107 | -4 | -4 | 4 | 136 | 138 | 4 | -2 | 4 | 104 | 98 |
| -10 | 2 | 3 | 63 | 63 | 3 | 4 | 3 | 106 | -108 | -1 | 8 | 3 | 86 | 92 | -3 | -4 | 4 | 90 | -84 | 5 | -2 | 4 | 79 | 77 |
| -9 | 2 | 3 | 217 | -222 | 4 | 4 | 3 | 82 | 86 | -10 | 9 | 3 | 68 | -55 | -2 | -4 | 4 | 127 | -119 | 6 | -2 | 4 | 65 | -68 |
| -7 | 2 | 3 | 61 | -65 | -13 | 5 | 3 | 105 | -106 | -9 | 9 | 3 | 82 | -73 | -1 | -4 | 4 | 58 | 54 | -11 | -1 | 4 | 107 | 111 |
| -6 | 2 | 3 | 45 | -48 | -10 | 5 | 3 | 65 | 62 | -4 | 9 | 3 | 109 | 117 | 0 | -4 | 4 | 175 | -178 | -10 | -1 | 4 | 62 | -70 |
| -5 | 2 | 3 | 210 | -207 | -9 | 5 | 3 | 63 | -69 | -7 | 10 | 3 | 90 | 77 | 1 | -4 | 4 | 58 | -74 | -9 | -1 | 4 | 68 | 70 |
| -4 | 2 | 3 | 357 | 356 | -8 | 5 | 3 | 178 | 181 | 0 | -9 | 4 | 80 | -85 | 3 | -4 | 4 | 116 | 120 | -6 | -1 | 4 | 233 | -224 |
| -2 | 2 | 3 | 122 | 129 | -6 | 5 | 3 | 56 | -56 | 1 | -9 | 4 | 56 | 59 | 4 | -4 | 4 | 105 | -113 | -5 | -1 | 4 | 117 | 112 |
| -1 | 2 | 3 | 171 | 168 | -3 | 5 | 3 | 122 | -125 | -1 | -8 | 4 | 118 | 110 | 5 | -4 | 4 | 132 | 139 | -4 | -1 | 4 | 206 | -200 |
| 0 | 2 | 3 | 274 | 266 | -2 | 5 | 3 | 98 | -98 | 2 | -8 | 4 | 89 | 87 | 6 | -4 | 4 | 48 | 52 | -3 | -1 | 4 | 65 | -65 |
| 1 | 2 | 3 | 199 | -190 | -1 | 5 | 3 | 66 | 64 | -5 | -7 | 4 | 108 | -99 | 9 | -4 | 4 | 97 | 94 | -2 | -1 | 4 | 57 | -58 |
| 4 | 2 | 3 | 128 | -127 | 0 | 5 | 3 | 102 | -106 | -4 | -7 | 4 | 81 | 80 | -11 | -3 | 4 | 85 | 87 | -1 | -1 | 4 | 255 | 239 |
| 5 | 2 | 3 | 155 | -158 | 3 | 5 | 3 | 61 | 71 | 0 | -7 | 4 | 118 | 116 | -9 | -3 | 4 | 86 | 86 | 0 | -1 | 4 | 119 | -127 |
| -12 | 3 | 3 | 96 | -89 | 4 | 5 | 3 | 73 | -77 | 1 | -7 | 4 | 60 | -60 | -7 | -3 | 4 | 154 | 161 | 1 | -1 | 4 | 170 | 160 |
| -11 | 3 | 3 | 112 | -118 | 5 | 5 | 3 | 122 | 117 | 5 | -7 | 4 | 57 | -59 | -6 | -3 | 4 | 42 | -45 | 2 | -1 | 4 | 170 | 162 |
| -9 | 3 | 3 | 51 | -52 | -13 | 6 | 3 | 60 | 62 | -4 | -6 | 4 | 93 | -91 | -5 | -3 | 4 | 55 | -56 | 4 | -1 | 4 | 91 | -87 |
| -8 | 3 | 3 | 144 | -147 | -12 | 6 | 3 | 108 | -107 | -3 | -6 | 4 | 123 | 121 | -4 | -3 | 4 | 49 | -52 | 5 | -1 | 4 | 59 | 57 |
| -7 | 3 | 3 | 156 | 150 | -11 | 6 | 3 | 104 | 106 | -1 | -6 | 4 | 80 | 76 | -2 | -3 | 4 | 162 | -152 | 6 | -1 | 4 | 62 | -61 |
| -6 | 3 | 3 | 88 | 86 | -8 | 6 | 3 | 51 | -42 | 1 | -6 | 4 | 155 | 159 | 0 | -3 | 4 | 44 | 47 | 7 | -1 | 4 | 136 | -133 |
| -5 | 3 | 3 | 86 | 89 | -7 | 6 | 3 | 189 | 185 | 2 | -6 | 4 | 80 | -91 | 1 | -3 | 4 | 59 | -59 | -11 | 0 | 4 | 93 | 93 |
| -3 | 3 | 3 | 285 | 314 | -6 | 6 | 3 | 124 | -124 | 6 | -6 | 4 | 124 | -125 | 3 | -3 | 4 | 47 | 48 | -9 | 0 | 4 | 198 | -204 |
| -2 | 3 | 3 | 131 | -137 | -5 | 6 | 3 | 68 | -68 | -7 | -5 | 4 | 75 | -79 | 4 | -3 | 4 | 95 | 97 | -7 | 0 | 4 | 87 | -87 |
| 0 | 3 | 3 | 85 | -80 | -2 | 6 | 3 | 166 | -170 | -5 | -5 | 4 | 112 | 118 | 5 | -3 | 4 | 57 | -56 | -6 | 0 | 4 | 153 | -150 |
| 1 | 3 | 3 | 51 | -47 | 0 | 6 | 3 | 67 | 63 | -4 | -5 | 4 | 99 | 97 | 6 | -3 | 4 | 107 | 103 | -5 | 0 | 4 | 101 | -109 |
| 2 | 3 | 3 | 262 | -258 | -13 | 7 | 3 | 62 | 63 | -2 | -5 | 4 | 196 | 196 | 9 | -3 | 4 | 62 | -54 | -4 | 0 | 4 | 280 | 270 |
| 7 | 3 | 3 | 101 | 103 | -12 | 7 | 3 | 63 | 64 | 0 | -5 | 4 | 84 | -81 | -10 | -2 | 4 | 87 | 88 | -3 | 0 | 4 | 86 | -80 |
| -12 | 4 | 3 | 62 | -65 | -10 | 7 | 3 | 149 | 144 | 1 | -5 | 4 | 113 | -125 | -8 | -2 | 4 | 62 | 61 | -2 | 0 | 4 | 171 | 159 |
| -10 | 4 | 3 | 51 | -52 | -7 | 7 | 3 | 105 | -97 | 2 | -5 | 4 | 66 | 73 | -7 | -2 | 4 | 114 | -119 | -1 | 0 | 4 | 155 | 166 |
| -9 | 4 | 3 | 124 | 123 | -5 | 7 | 3 | 208 | -221 | 3 | -5 | 4 | 195 | -221 | -6 | -2 | 4 | 107 | 108 | 0 | 0 | 4 | 204 | 202 |
| -8 | 4 | 3 | 72 | 73 | -2 | 7 | 3 | 51 | 53 | 6 | -5 | 4 | 45 | 58 | -5 | -2 | 4 | 114 | -111 | 1 | 0 | 4 | 222 | -212 |
| -6 | 4 | 3 | 108 | 110 | 0 | 7 | 3 | 156 | 158 | 7 | -5 | 4 | 60 | -62 | -4 | -2 | 4 | 31 | -29 | 2 | 0 | 4 | 100 | 97 |

Observed and calculated structure factors for preisingerite, $Bi_3O(OH)(AsO_4)_2$



| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 3 | 0 | 4 | 70 | -71 |
| 4 | 0 | 4 | 127 | -125 |
| 5 | 0 | 4 | 127 | -127 |
| 7 | 0 | 4 | 87 | -86 |
| -12 | 1 | 4 | 75 | -76 |
| -11 | 1 | 4 | 107 | -118 |
| -9 | 1 | 4 | 126 | -136 |
| -8 | 1 | 4 | 104 | -103 |
| -7 | 1 | 4 | 88 | 82 |
| -6 | 1 | 4 | 47 | 43 |
| -5 | 1 | 4 | 48 | 48 |
| -4 | 1 | 4 | 128 | 128 |
| -3 | 1 | 4 | 214 | 215 |
| -2 | 1 | 4 | 91 | -97 |
| -1 | 1 | 4 | 66 | 64 |
| 0 | 1 | 4 | 85 | -83 |
| 1 | 1 | 4 | 36 | -33 |
| 2 | 1 | 4 | 216 | -211 |
| 3 | 1 | 4 | 85 | 81 |
| 4 | 1 | 4 | 87 | -88 |
| 5 | 1 | 4 | 41 | 14 |
| 7 | 1 | 4 | 99 | 97 |
| -12 | 2 | 4 | 74 | -81 |
| -10 | 2 | 4 | 72 | -79 |
| -9 | 2 | 4 | 135 | 138 |
| -7 | 2 | 4 | 75 | 71 |
| -6 | 2 | 4 | 87 | 81 |
| -5 | 2 | 4 | 126 | 127 |
| -4 | 2 | 4 | 30 | -30 |
| -2 | 2 | 4 | 58 | 60 |
| -1 | 2 | 4 | 141 | -139 |
| 0 | 2 | 4 | 37 | -25 |
| 3 | 2 | 4 | 133 | -128 |
| 4 | 2 | 4 | 93 | 88 |
| -13 | 3 | 4 | 133 | -129 |
| -12 | 3 | 4 | 77 | 77 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -9 | 3 | 4 | 44 | -46 |
| -8 | 3 | 4 | 210 | 210 |
| -7 | 3 | 4 | 61 | -59 |
| -5 | 3 | 4 | 42 | 43 |
| -4 | 3 | 4 | 81 | 90 |
| -3 | 3 | 4 | 164 | -176 |
| 0 | 3 | 4 | 154 | -154 |
| 1 | 3 | 4 | 55 | -57 |
| 2 | 3 | 4 | 54 | 46 |
| 5 | 3 | 4 | 148 | 139 |
| -12 | 4 | 4 | 92 | -95 |
| -11 | 4 | 4 | 154 | 160 |
| -9 | 4 | 4 | 51 | 50 |
| -7 | 4 | 4 | 213 | 220 |
| -6 | 4 | 4 | 177 | -177 |
| -3 | 4 | 4 | 40 | -39 |
| -2 | 4 | 4 | 256 | -262 |
| -1 | 4 | 4 | 77 | 78 |
| 2 | 4 | 4 | 87 | 71 |
| 3 | 4 | 4 | 139 | 138 |
| -13 | 5 | 4 | 81 | 85 |
| -10 | 5 | 4 | 165 | 172 |
| -9 | 5 | 4 | 47 | -45 |
| -7 | 5 | 4 | 90 | -72 |
| -5 | 5 | 4 | 270 | -283 |
| -2 | 5 | 4 | 45 | 43 |
| 0 | 5 | 4 | 194 | 206 |
| -12 | 6 | 4 | 61 | 68 |
| -10 | 6 | 4 | 61 | -62 |
| -8 | 6 | 4 | 104 | -100 |
| -7 | 6 | 4 | 80 | -78 |
| -6 | 6 | 4 | 57 | -58 |
| -5 | 6 | 4 | 61 | 65 |
| -4 | 6 | 4 | 58 | -67 |
| -3 | 6 | 4 | 120 | 132 |
| -1 | 6 | 4 | 86 | 87 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 0 | 6 | 4 | 53 | -52 |
| 1 | 6 | 4 | 79 | 80 |
| 2 | 6 | 4 | 66 | -64 |
| -12 | 7 | 4 | 65 | -66 |
| -10 | 7 | 4 | 117 | -108 |
| -9 | 7 | 4 | 53 | -57 |
| -5 | 7 | 4 | 53 | 64 |
| -4 | 7 | 4 | 95 | 96 |
| -3 | 7 | 4 | 63 | -66 |
| -2 | 7 | 4 | 49 | 76 |
| 1 | 7 | 4 | 80 | -80 |
| -10 | 8 | 4 | 71 | 58 |
| -9 | 8 | 4 | 140 | -122 |
| -8 | 8 | 4 | 52 | 42 |
| -7 | 8 | 4 | 52 | 61 |
| -4 | 8 | 4 | 104 | 109 |
| -9 | 9 | 4 | 76 | 67 |
| -8 | 9 | 4 | 71 | -63 |
| -7 | 9 | 4 | 136 | 122 |
| -3 | -8 | 5 | 93 | 89 |
| 1 | -8 | 5 | 119 | 117 |
| 2 | -8 | 5 | 82 | -76 |
| -5 | -7 | 5 | 106 | 101 |
| -2 | -7 | 5 | 139 | 135 |
| 3 | -7 | 5 | 160 | -169 |
| -4 | -6 | 5 | 76 | 81 |
| -3 | -6 | 5 | 77 | 86 |
| 0 | -6 | 5 | 123 | -120 |
| 1 | -6 | 5 | 58 | -58 |
| 4 | -6 | 5 | 82 | -87 |
| 5 | -6 | 5 | 101 | 107 |
| -7 | -5 | 5 | 126 | 126 |
| -6 | -5 | 5 | 72 | -75 |
| -2 | -5 | 5 | 137 | -135 |
| 3 | -5 | 5 | 59 | 64 |
| 6 | -5 | 5 | 80 | 77 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| -10 | -4 | 5 | 66 | 72 |
| -7 | -4 | 5 | 65 | -63 |
| -6 | -4 | 5 | 117 | 120 |
| -5 | -4 | 5 | 100 | -100 |
| -3 | -4 | 5 | 90 | -83 |
| -1 | -4 | 5 | 204 | -193 |
| 2 | -4 | 5 | 53 | 45 |
| 4 | -4 | 5 | 110 | 114 |
| -9 | -3 | 5 | 77 | 76 |
| -7 | -3 | 5 | 59 | -61 |
| -6 | -3 | 5 | 145 | -141 |
| -5 | -3 | 5 | 93 | 91 |
| -4 | -3 | 5 | 216 | -205 |
| -3 | -3 | 5 | 65 | -70 |
| -1 | -3 | 5 | 145 | 141 |
| 0 | -3 | 5 | 103 | -113 |
| 1 | -3 | 5 | 192 | 212 |
| 2 | -3 | 5 | 76 | 87 |
| 3 | -3 | 5 | 51 | 47 |
| 5 | -3 | 5 | 88 | 87 |
| 6 | -3 | 5 | 100 | -100 |
| 7 | -3 | 5 | 79 | -79 |
| -11 | -2 | 5 | 113 | 116 |
| -10 | -2 | 5 | 71 | -67 |
| -9 | -2 | 5 | 93 | -97 |
| -7 | -2 | 5 | 89 | -89 |
| -6 | -2 | 5 | 157 | -158 |
| -4 | -2 | 5 | 160 | 151 |
| -3 | -2 | 5 | 102 | -89 |
| -2 | -2 | 5 | 175 | 160 |
| -1 | -2 | 5 | 147 | 142 |
| 0 | -2 | 5 | 72 | 82 |
| 1 | -2 | 5 | 113 | -116 |
| 2 | -2 | 5 | 165 | 161 |
| 3 | -2 | 5 | 117 | -112 |
| 4 | -2 | 5 | 69 | -66 |

| h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|
| 5 | -2 | 5 | 85 | -83 |
| 7 | -2 | 5 | 116 | -106 |
| -11 | -1 | 5 | 80 | -89 |
| -9 | -1 | 5 | 161 | -165 |
| -6 | -1 | 5 | 50 | 48 |
| -4 | -1 | 5 | 166 | 164 |
| -3 | -1 | 5 | 124 | 118 |
| -2 | -1 | 5 | 47 | -50 |
| -1 | -1 | 5 | 91 | 90 |
| 2 | -1 | 5 | 144 | -133 |
| 3 | -1 | 5 | 76 | 75 |
| 4 | -1 | 5 | 99 | -94 |
| 7 | -1 | 5 | 77 | 73 |
| -12 | 0 | 5 | 74 | -78 |
| -10 | 0 | 5 | 75 | -77 |
| -9 | 0 | 5 | 130 | 134 |
| -8 | 0 | 5 | 77 | -73 |
| -7 | 0 | 5 | 79 | 80 |
| -6 | 0 | 5 | 65 | 67 |
| -5 | 0 | 5 | 100 | 101 |
| -4 | 0 | 5 | 70 | -69 |
| -3 | 0 | 5 | 104 | 100 |
| -1 | 0 | 5 | 79 | -74 |
| 0 | 0 | 5 | 42 | -47 |
| 2 | 0 | 5 | 55 | -47 |
| 3 | 0 | 5 | 113 | -115 |
| 4 | 0 | 5 | 68 | 68 |
| -13 | 1 | 5 | 99 | -102 |
| -12 | 1 | 5 | 63 | 68 |
| -11 | 1 | 5 | 36 | -41 |
| -8 | 1 | 5 | 214 | 208 |
| -7 | 1 | 5 | 127 | -123 |
| -6 | 1 | 5 | 105 | 103 |
| -5 | 1 | 5 | 96 | 91 |
| -4 | 1 | 5 | 102 | 104 |
| -3 | 1 | 5 | 170 | -171 |

Observed and calculated structure factors for preisingerite, $Bi_3O(OH)(AsO_4)_2$



| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -2 | 1 | 5 | 91 | 104 | -9 | 4 | 5 | 42 | -43 | -5 | -6 | 6 | 59 | -74 | 0 | -1 | 6 | 100 | -101 | -3 | 2 | 6 | 78 | 87 |
| -1 | 1 | 5 | 95 | -92 | -8 | 4 | 5 | 102 | -103 | -1 | -6 | 6 | 149 | -143 | 1 | -1 | 6 | 69 | -63 | -2 | 2 | 6 | 48 | 49 |
| 0 | 1 | 5 | 140 | -131 | -7 | 4 | 5 | 102 | -107 | -7 | -5 | 6 | 70 | -73 | 3 | -1 | 6 | 126 | -116 | 1 | 2 | 6 | 119 | 119 |
| 1 | 1 | 5 | 87 | -87 | -4 | 4 | 5 | 53 | -59 | -4 | -5 | 6 | 160 | -163 | 5 | -1 | 6 | 84 | 83 | -11 | 3 | 6 | 58 | 60 |
| 2 | 1 | 5 | 49 | 49 | -3 | 4 | 5 | 107 | 111 | 0 | -5 | 6 | 68 | -72 | -11 | 0 | 6 | 75 | 83 | -10 | 3 | 6 | 162 | -164 |
| 3 | 1 | 5 | 62 | -54 | -1 | 4 | 5 | 65 | 66 | 1 | -5 | 6 | 167 | 190 | -9 | 0 | 6 | 37 | 48 | -9 | 3 | 6 | 69 | 72 |
| 5 | 1 | 5 | 131 | 124 | 1 | 4 | 5 | 131 | 130 | 5 | -5 | 6 | 77 | 80 | -8 | 0 | 6 | 140 | 135 | -7 | 3 | 6 | 32 | -45 |
| -13 | 2 | 5 | 61 | -64 | 2 | 4 | 5 | 60 | -63 | -7 | -4 | 6 | 83 | -80 | -7 | 0 | 6 | 101 | 100 | -6 | 3 | 6 | 89 | -94 |
| -12 | 2 | 5 | 56 | -55 | -11 | 5 | 5 | 64 | 59 | -6 | -4 | 6 | 122 | -123 | -6 | 0 | 6 | 130 | -130 | -5 | 3 | 6 | 127 | 133 |
| -11 | 2 | 5 | 142 | 149 | -10 | 5 | 5 | 162 | -166 | -3 | -4 | 6 | 65 | -66 | -5 | 0 | 6 | 121 | 118 | -4 | 3 | 6 | 52 | -61 |
| -9 | 2 | 5 | 41 | 41 | -6 | 5 | 5 | 71 | -65 | -2 | -4 | 6 | 134 | 126 | -4 | 0 | 6 | 86 | -83 | -2 | 3 | 6 | 101 | 100 |
| -8 | 2 | 5 | 89 | 87 | -5 | 5 | 5 | 111 | 116 | -1 | -4 | 6 | 92 | 89 | -3 | 0 | 6 | 128 | -125 | -1 | 3 | 6 | 64 | 63 |
| -7 | 2 | 5 | 195 | 195 | -2 | 5 | 5 | 104 | 107 | 2 | -4 | 6 | 121 | 129 | -2 | 0 | 6 | 154 | -159 | 2 | 3 | 6 | 64 | 57 |
| -6 | 2 | 5 | 204 | -198 | -1 | 5 | 5 | 64 | 65 | 3 | -4 | 6 | 96 | -98 | -1 | 0 | 6 | 103 | 94 | 3 | 3 | 6 | 91 | -92 |
| -5 | 2 | 5 | 74 | 75 | 2 | 5 | 5 | 84 | 84 | -9 | -3 | 6 | 136 | -149 | 0 | 0 | 6 | 175 | -170 | -13 | 4 | 6 | 89 | -93 |
| -4 | 2 | 5 | 71 | -73 | 3 | 5 | 5 | 84 | -89 | -4 | -3 | 6 | 135 | 135 | 2 | 0 | 6 | 65 | 68 | -9 | 4 | 6 | 186 | -191 |
| -3 | 2 | 5 | 98 | -107 | -13 | 6 | 5 | 101 | -98 | 1 | -3 | 6 | 47 | -51 | 3 | 0 | 6 | 113 | 113 | -8 | 4 | 6 | 105 | 103 |
| -2 | 2 | 5 | 237 | -257 | -9 | 6 | 5 | 171 | -168 | 2 | -3 | 6 | 56 | -60 | 5 | 0 | 6 | 122 | 116 | -7 | 4 | 6 | 72 | -74 |
| -1 | 2 | 5 | 99 | 95 | -8 | 6 | 5 | 90 | 83 | 4 | -3 | 6 | 82 | -80 | -11 | 1 | 6 | 139 | 143 | -4 | 4 | 6 | 179 | 197 |
| 0 | 2 | 5 | 113 | -114 | -4 | 6 | 5 | 173 | 180 | -9 | -2 | 6 | 79 | 79 | -10 | 1 | 6 | 71 | 73 | -3 | 4 | 6 | 49 | -54 |
| 2 | 2 | 5 | 74 | 73 | -1 | 6 | 5 | 63 | 61 | -8 | -2 | 6 | 110 | -116 | -7 | 1 | 6 | 38 | 12 | -2 | 4 | 6 | 83 | 89 |
| 3 | 2 | 5 | 133 | 133 | 1 | 6 | 5 | 83 | -93 | -7 | -2 | 6 | 66 | 70 | -6 | 1 | 6 | 103 | -99 | 1 | 4 | 6 | 101 | -107 |
| 5 | 2 | 5 | 80 | 73 | -12 | 7 | 5 | 144 | -131 | -5 | -2 | 6 | 91 | 92 | -5 | 1 | 6 | 166 | -164 | -12 | 5 | 6 | 122 | -126 |
| -13 | 3 | 5 | 75 | 82 | -9 | 7 | 5 | 51 | 52 | -4 | -2 | 6 | 83 | -82 | -4 | 1 | 6 | 48 | 48 | -7 | 5 | 6 | 201 | 201 |
| -11 | 3 | 5 | 82 | 80 | -7 | 7 | 5 | 183 | 175 | -3 | -2 | 6 | 146 | 139 | -3 | 1 | 6 | 79 | -85 | -5 | 5 | 6 | 69 | 76 |
| -10 | 3 | 5 | 143 | 143 | -3 | 7 | 5 | 73 | 78 | 2 | -2 | 6 | 103 | -95 | 0 | 1 | 6 | 159 | 154 | -3 | 5 | 6 | 74 | 62 |
| -9 | 3 | 5 | 42 | -42 | -2 | 7 | 5 | 116 | -124 | -11 | -1 | 6 | 66 | -65 | 1 | 1 | 6 | 47 | -44 | -2 | 5 | 6 | 147 | -150 |
| -6 | 3 | 5 | 71 | -74 | -10 | 8 | 5 | 92 | 79 | -10 | -1 | 6 | 45 | -44 | 2 | 1 | 6 | 112 | 110 | 0 | 5 | 6 | 69 | -75 |
| -5 | 3 | 5 | 232 | -245 | -9 | 8 | 5 | 57 | 60 | -8 | -1 | 6 | 127 | 129 | -12 | 2 | 6 | 103 | 101 | -10 | 6 | 6 | 71 | 68 |
| -4 | 3 | 5 | 37 | 40 | -8 | 8 | 5 | 79 | 77 | -7 | -1 | 6 | 107 | -109 | -11 | 2 | 6 | 75 | -79 | -9 | 6 | 6 | 88 | 87 |
| -3 | 3 | 5 | 69 | -77 | -6 | 8 | 5 | 68 | 71 | -6 | -1 | 6 | 148 | 153 | -10 | 2 | 6 | 50 | 49 | -8 | 6 | 6 | 48 | 45 |
| 0 | 3 | 5 | 204 | 204 | -5 | 8 | 5 | 72 | -72 | -5 | -1 | 6 | 74 | 73 | -9 | 2 | 6 | 55 | -57 | -6 | 6 | 6 | 82 | 82 |
| 2 | 3 | 5 | 87 | 85 | -3 | 8 | 5 | 88 | -90 | -4 | -1 | 6 | 81 | 81 | -8 | 2 | 6 | 60 | -56 | -5 | 6 | 6 | 67 | -69 |
| 5 | 3 | 5 | 91 | -89 | -6 | 9 | 5 | 100 | -101 | -3 | -1 | 6 | 138 | -136 | -7 | 2 | 6 | 121 | -120 | -3 | 6 | 6 | 80 | -78 |
| -12 | 4 | 5 | 100 | 99 | -2 | -7 | 6 | 107 | -98 | -2 | -1 | 6 | 136 | 127 | -5 | 2 | 6 | 43 | -36 | -1 | 6 | 6 | 103 | -107 |
| -11 | 4 | 5 | 61 | -65 | -6 | -6 | 6 | 100 | 96 | -1 | -1 | 6 | 130 | -142 | -4 | 2 | 6 | 56 | -60 | -12 | 7 | 6 | 117 | 112 |

Observed and calculated structure factors for preisingerite, $Bi_3O(OH)(AsO_4)_2$



| h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ | h | k | l | $F_o$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -8 | 7 | 6 | 61 | 56 | -3 | -1 | 7 | 77 | -74 | -12 | 3 | 7 | 105 | -102 | -5 | -2 | 8 | 130 | -130 | -11 | 4 | 8 | 119 | 124 |
| -7 | 7 | 6 | 65 | -64 | 0 | -1 | 7 | 95 | 88 | -9 | 3 | 7 | 48 | -44 | 0 | -2 | 8 | 68 | 78 | -9 | 4 | 8 | 84 | 79 |
| -6 | 7 | 6 | 70 | -65 | 2 | -1 | 7 | 86 | 78 | -7 | 3 | 7 | 146 | 150 | -10 | -1 | 8 | 50 | -68 | -6 | 4 | 8 | 128 | -132 |
| -6 | 8 | 6 | 106 | -100 | -12 | 0 | 7 | 76 | 80 | -5 | 3 | 7 | 87 | 92 | -9 | -1 | 8 | 90 | 91 | -5 | 4 | 8 | 70 | 61 |
| -5 | -6 | 7 | 55 | 58 | -11 | 0 | 7 | 82 | -82 | -3 | 3 | 7 | 55 | 63 | -8 | -1 | 8 | 96 | -104 | -4 | 4 | 8 | 90 | -93 |
| -2 | -6 | 7 | 83 | 73 | -10 | 0 | 7 | 81 | 82 | -2 | 3 | 7 | 120 | -133 | -5 | -1 | 8 | 60 | 59 | -3 | 4 | 8 | 64 | -58 |
| -1 | -6 | 7 | 58 | 58 | -9 | 0 | 7 | 49 | -51 | 0 | 3 | 7 | 79 | -91 | -4 | -1 | 8 | 155 | -152 | -9 | 5 | 8 | 110 | -110 |
| 2 | -6 | 7 | 53 | 65 | -7 | 0 | 7 | 94 | -92 | -9 | 4 | 7 | 103 | 106 | -3 | -1 | 8 | 93 | 94 | -7 | 5 | 8 | 78 | -71 |
| -4 | -5 | 7 | 116 | 107 | -6 | 0 | 7 | 67 | 66 | -6 | 4 | 7 | 81 | 84 | 1 | -1 | 8 | 139 | 131 | -5 | 5 | 8 | 85 | -89 |
| -8 | -4 | 7 | 103 | -104 | -5 | 0 | 7 | 107 | -105 | -3 | 4 | 7 | 49 | -45 | -10 | 0 | 8 | 101 | -102 | -4 | 5 | 8 | 80 | 86 |
| -5 | -4 | 7 | 54 | 54 | 1 | 0 | 7 | 79 | 75 | -1 | 4 | 7 | 114 | -108 | -9 | 0 | 8 | 69 | -66 | -8 | 6 | 8 | 90 | -78 |
| -3 | -4 | 7 | 153 | 145 | -10 | 1 | 7 | 124 | -124 | -12 | 5 | 7 | 121 | 127 | -7 | 0 | 8 | 118 | -113 | -4 | -3 | 9 | 121 | -113 |
| 2 | -4 | 7 | 89 | -99 | -9 | 1 | 7 | 95 | 92 | -8 | 5 | 7 | 84 | 83 | -5 | 0 | 8 | 63 | 63 | -3 | -3 | 9 | 91 | 91 |
| -10 | -3 | 7 | 51 | -47 | -8 | 1 | 7 | 97 | -100 | -7 | 5 | 7 | 99 | -95 | -4 | 0 | 8 | 102 | 98 | -7 | -2 | 9 | 102 | -90 |
| -7 | -3 | 7 | 69 | -68 | -7 | 1 | 7 | 52 | -50 | -4 | 5 | 7 | 66 | -73 | -3 | 0 | 8 | 45 | -51 | -2 | -2 | 9 | 132 | 127 |
| -6 | -3 | 7 | 150 | 152 | -6 | 1 | 7 | 92 | -91 | -11 | 6 | 7 | 138 | 134 | -2 | 0 | 8 | 151 | 164 | -9 | -1 | 9 | 67 | -66 |
| -5 | -3 | 7 | 59 | 55 | -5 | 1 | 7 | 109 | 107 | -10 | 6 | 7 | 58 | -58 | 1 | 0 | 8 | 64 | -65 | -8 | -1 | 9 | 60 | 64 |
| -2 | -3 | 7 | 132 | 125 | -4 | 1 | 7 | 133 | -138 | -9 | 6 | 7 | 50 | 42 | -9 | 1 | 8 | 58 | -62 | -5 | -1 | 9 | 44 | 46 |
| -1 | -3 | 7 | 143 | -154 | -3 | 1 | 7 | 46 | 57 | -6 | 6 | 7 | 139 | -139 | -7 | 1 | 8 | 90 | 86 | -8 | 0 | 9 | 60 | -66 |
| 3 | -3 | 7 | 119 | -121 | -2 | 1 | 7 | 75 | 72 | -3 | 6 | 7 | 71 | -65 | -5 | 1 | 8 | 94 | 89 | -7 | 0 | 9 | 94 | 95 |
| 4 | -3 | 7 | 83 | 82 | -1 | 1 | 7 | 58 | 50 | -10 | 7 | 7 | 67 | 67 | -2 | 1 | 8 | 85 | -83 | -10 | 1 | 9 | 62 | 63 |
| -9 | -2 | 7 | 48 | 53 | 1 | 1 | 7 | 111 | 109 | -9 | 7 | 7 | 130 | -125 | 0 | 1 | 8 | 88 | -84 | -8 | 1 | 9 | 64 | 58 |
| -8 | -2 | 7 | 149 | 149 | 3 | 1 | 7 | 75 | -71 | -7 | 7 | 7 | 70 | -62 | -12 | 2 | 8 | 61 | -66 | -7 | 1 | 9 | 73 | -74 |
| -5 | -2 | 7 | 116 | 116 | -13 | 2 | 7 | 71 | -73 | -5 | 7 | 7 | 98 | -97 | -9 | 2 | 8 | 94 | 90 | -6 | 1 | 9 | 134 | 132 |
| -4 | -2 | 7 | 75 | -76 | -10 | 2 | 7 | 89 | -84 | -2 | -5 | 8 | 89 | 78 | -8 | 2 | 8 | 41 | -33 | -10 | 2 | 9 | 60 | -52 |
| -3 | -2 | 7 | 89 | -90 | -9 | 2 | 7 | 133 | -138 | -1 | -5 | 8 | 135 | -129 | -7 | 2 | 8 | 78 | 75 | -9 | 2 | 9 | 112 | 99 |
| -2 | -2 | 7 | 85 | -83 | -8 | 2 | 7 | 82 | 86 | -5 | -4 | 8 | 74 | 60 | -6 | 2 | 8 | 44 | 45 | -6 | 2 | 9 | 105 | -88 |
| 0 | -2 | 7 | 143 | -152 | -7 | 2 | 7 | 118 | -114 | -3 | -4 | 8 | 78 | -71 | -1 | 2 | 8 | 90 | -90 | -5 | 2 | 9 | 60 | 63 |
| 1 | -2 | 7 | 64 | 65 | -5 | 2 | 7 | 43 | 48 | 0 | -4 | 8 | 97 | -104 | -12 | 3 | 8 | 111 | 112 | -4 | 2 | 9 | 120 | -126 |
| 3 | -2 | 7 | 65 | 64 | -4 | 2 | 7 | 159 | 173 | 1 | -4 | 8 | 61 | 60 | -11 | 3 | 8 | 68 | -76 | -9 | 3 | 9 | 63 | -65 |
| -11 | -1 | 7 | 146 | 142 | -3 | 2 | 7 | 71 | -76 | -7 | -3 | 8 | 50 | 48 | -8 | 3 | 8 | 67 | 68 | -6 | 3 | 9 | 53 | -46 |
| -7 | -1 | 7 | 48 | 45 | -2 | 2 | 7 | 146 | 141 | -6 | -3 | 8 | 110 | -98 | -7 | 3 | 8 | 99 | -102 | -4 | 3 | 9 | 60 | 70 |
| -6 | -1 | 7 | 112 | -110 | 1 | 2 | 7 | 92 | -97 | -10 | -2 | 8 | 94 | 92 | -6 | 3 | 8 | 89 | 95 | -8 | 4 | 9 | 69 | -69 |
| -5 | -1 | 7 | 59 | -68 | -13 | 3 | 7 | 76 | -74 | -6 | -2 | 8 | 69 | 68 | -1 | 3 | 8 | 55 | -62 | | | | | |

Table 4. X-ray powder diffraction data for preisingerite

| h | k | l | 1 $d_{cal}$ | 1 $I_{cal}$ | 2 $d_{obs}$ | 2 $I_{obs}$ | 3 $d_{obs}$ | 3 $I_{obs}$ | 4 $d_{obs}$ | 4 $I_{obs}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0 | 0 | 8.379 | 2 | 8.402 | 1 | | | 8.488 | 10 |
| 0 | 1 | 0 | 6.846 | 3 | 6.835 | 4 | 6.80 | 10 | | |
| -1 | 1 | 0 | 6.688 | 10 | 6.691 | 8 | 6.66 | 14 | | |
| -1 | 0 | 1 | 6.565 | 4 | 6.567 | 4 | | | | |
| 0 | 0 | 1 | 6.229 | 17 | 6.231 | 17 | 6.21 | 15 | 6.226 | 10 |
| 0 | -1 | 1 | 4.951 | 9 | 4.955 | 6 | 4.92 | 7 | | |
| 1 | 1 | 0 | 4.527 | 38 } | 4.524 | 35 | 4.50 | 50 | 4.545 | 20 |
| -2 | 0 | 1 | 4.512 | 5 } | | | | | | |
| -2 | 1 | 0 | 4.391 | 12 | 4.395 | 10 | 4.38 | 13 | | |
| 2 | 0 | 0 | 4.190 | 3 | 4.190 | 3 | | | 4.191 | 10 |
| 1 | -1 | 1 | 4.130 | 10 | 4.128 | 8 | 4.12 | 8 | | |
| -1 | 2 | 0 | 3.698 | 1 | 3.693 | 1 | | | | |
| 0 | 2 | 0 | 3.423 | 1 | 3.436 | 6 | 3.41 | 10 | | |
| -2 | 2 | 0 | 3.344 | 3 | 3.344 | 3 | | | | |
| -2 | 0 | 2 | 3.283 | 100 | 3.281 | 100 | 3.28 | 72 | 3.280 | 100 |
| -2 | 2 | 1 | 3.258 | 93 } | 3.263 | 97 | 3.25 | 90 | | |
| -1 | 2 | 1 | 3.249 | 4 } | | | | | | |
| 1 | 1 | 1 | 3.199 | 47 } | | | | | | |
| 0 | -2 | 1 | 3.187 | 85 } | 3.194 | 87 | 3.18 | 100 | 3.200 | 90 |
| -2 | 1 | 2 | 3.157 | 4 } | | | | | | |
| 1 | -2 | 1 | 3.115 | 5 } | 3.113 | 13 | | | | |
| 0 | 0 | 2 | 3.115 | 14 } | | | | | | |
| -1 | 1 | 2 | 3.094 | 17 } | | | | | | |
| 2 | 1 | 0 | 3.090 | 49 } | 3.091 | 74 | 3.08 | 76 | 3.108 | 90 |
| 2 | -1 | 1 | 3.087 | 32 } | | | | | | |
| -3 | 1 | 0 | 3.017 | 49 | 3.016 | 38 | 3.01 | 37 | 3.026 | 40 |
| -3 | 2 | 1 | 2.861 | 12 } | 2.859 | 13 | 2.85 | 16 | 2.866 | 20 |
| -1 | -2 | 1 | 2.859 | 5 } | | | | | | |
| 0 | 2 | 1 | 2.843 | 2 } | 2.843 | 3 | | | | |
| -3 | 1 | 2 | 2.832 | 2 } | | | | | | |
| 1 | 2 | 0 | 2.817 | 4 | 2.817 | 3 | | | 2.825 | 10 |
| -2 | -1 | 2 | 2.796 | 8 | 2.796 | 4 | | | | |
| -3 | 0 | 2 | 2.769 | 2 | 2.768 | 1 | | | | |
| 2 | -2 | 1 | 2.710 | 4 } | 2.703 | 15 | 2.69 | 14 | 2.717 | 20 |
| 0 | 1 | 2 | 2.701 | 13 } | | | | | | |
| 1 | -1 | 2 | 2.613 | 28 | 2.612 | 18 | 2.61 | 18 | 2.621 | 40 |
| 1 | 0 | 2 | 2.574 | 6 | 2.575 | 8 | 2.57 | 6 | 2.591 | 10 |
| -3 | -1 | 1 | 2.514 | 14 | 2.512 | 9 | 2.51 | 10 | | |
| -4 | 1 | 1 | 2.491 | 19 | 2.489 | 15 | 2.49 | 13 | 2.500 | 30 |
| -1 | 2 | 2 | 2.441 | 2 | 2.440 | 1 | | | | |
| -2 | 3 | 0 | 2.428 | 2 | 2.428 | 3 | | | | |
| -3 | -1 | 2 | 2.365 | 3 | 2.368 | 4 | | | 2.392 | 10 |
| -2 | 0 | 3 | 2.306 | 3 | 2.305 | 3 | | | | |
| -1 | 3 | 1 | 2.267 | 13 } | 2.265 | 15 | | | 2.282 | 20 |
| -3 | 3 | 1 | 2.262 | 4 } | | | | | | |
| -4 | 2 | 2 | 2.229 | 5 | 2.229 | 3 | | | | |
| 3 | 0 | 1 | 2.212 | 14 | 2.211 | 14 | | | 2.223 | 30 |
| -1 | -1 | 3 | 2.175 | 6 | 2.176 | 5 | | | 2.191 | 10 |
| -2 | -1 | 3 | 2.147 | 3 | 2.147 | 1 | | | | |
| -1 | 1 | 3 | 2.118 | 12 | 2.118 | 9 | | | 2.128 | 20 |
| 2 | 0 | 2 | 2.097 | 4 | 2.096 | 4 | | | | |
| 0 | -1 | 3 | 2.066 | 4 } | | | | | | |
| -1 | -3 | 1 | 2.059 | 7 } | 2.057 | 15 | | | 2.073 | 30 |
| 0 | 3 | 1 | 2.055 | 11 } | | | | | | |

Table 4, continued

| h | k | l | 1 $d_{cal}$ | 1 $I_{cal}$ | 2 $d_{obs}$ | 2 $I_{obs}$ | 3 $d_{obs}$ | 3 $I_{obs}$ | 4 $d_{obs}$ | 4 $I_{obs}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| -4 | 3 | 1 | 2.047 | 4 } | 2.035 | 8 | | | | |
| -3 | 3 | 2 | 2.036 | 1 } | | | | | | |
| 1 | 3 | 0 | 2.016 | 4 | 2.016 | 4 | | | | |
| 0 | -3 | 2 | 1.9718 | 4 } | | | | | | |
| -4 | -1 | 2 | 1.9685 | 19 } | | | | | | |
| 3 | -3 | 1 | 1.9670 | 17 } | 1.967 | 31 | | | 1.983 | 80 |
| -5 | 1 | 2 | 1.9654 | 11 } | | | | | | |
| -4 | 3 | 0 | 1.9565 | 6 } | | | | | | |
| 2 | 2 | 1 | 1.9343 | 5 | 1.935 | 3 | | | | |
| -3 | -2 | 2 | 1.9252 | 3 | 1.928 | 3 | | | | |
| -1 | 3 | 2 | 1.9104 | 7 } | 1.906 | 13 | | | 1.913 | 50 |
| -4 | 2 | 3 | 1.9050 | 16 } | | | | | | |
| 0 | -2 | 3 | 1.8919 | 6 | 1.892 | 3 | | | | |
| 1 | 2 | 2 | 1.8632 | 3 } | 1.863 | 9 | | | 1.874 | 20 |
| -2 | -2 | 3 | 1.8622 | 12 } | | | | | | |
| -2 | 4 | 0 | 1.8487 | 11 } | | | | | | |
| -1 | 2 | 3 | 1.8487 | 4 } | 1.849 | 14 | | | | |
| 3 | 2 | 0 | 1.8478 | 5 } | | | | | | |
| 1 | 0 | 3 | 1.8360 | 3 } | 1.834 | 4 | | | 1.842 | 20 |
| -5 | 0 | 1 | 1.8325 | 4 } | | | | | | |
| -2 | -3 | 1 | 1.8211 | 9 | 1.820 | 13 | | | | |
| -5 | 2 | 0 | 1.7984 | 5 } | 1.794 | 10 | | | 1.804 | 50 |
| -5 | 3 | 1 | 1.7948 | 8 } | | | | | | |
| -5 | 2 | 3 | 1.7491 | 4 | 1.750 | 4 | | | 1.754 | 20 |
| 3 | 0 | 2 | 1.7351 | 8 | 1.735 | 3 | | | | |
| -3 | 3 | 3 | 1.7182 | 10 | 1.719 | 13 | | | 1.722 | 20 |
| -3 | 1 | 4 | 1.7007 | 4 | 1.701 | 3 | | | | |
| 0 | 2 | 3 | 1.6778 | 7 } | 1.676 | 9 | | | 1.682 | 50 |
| 5 | 0 | 0 | 1.6758 | 11 } | | | | | | |
| -1 | -1 | 4 | 1.6471 | 5 | 1.647 | 1 | | | 1.654 | 10 |
| -4 | 0 | 4 | 1.6413 | 6 | 1.642 | 4 | | | | |
| -4 | 4 | 2 | 1.6290 | 5 | 1.629 | 2 | | | 1.632 | 10 |
| 3 | 2 | 1 | 1.6185 | 6 | 1.619 | 3 | | | | |
| 1 | -3 | 3 | 1.5970 | 6 } | 1.596 | 6 | | | 1.610 | 20 |
| 0 | -4 | 2 | 1.5933 | 4 } | | | | | | |
| -6 | 1 | 3 | 1.5752 | 6 | 1.575 | 4 | | | 1.576 | 70 |
| -6 | 3 | 2 | 1.5694 | 5 } | 1.570 | 9 | | | | |
| 5 | -2 | 1 | 1.5687 | 8 } | | | | | | |
| 2 | -4 | 2 | 1.5573 | 2 | 1.558 | 4 | | | | |
| -5 | 4 | 2 | 1.5457 | 3 } | 1.542 | 5 | | | 1.545 | 20 |
| -4 | -1 | 4 | 1.5427 | 3 } | | | | | | |

1 Calculated pattern. Integrated intensities evaluated with isotropic temperature factors and complex neutral atom scattering factors for all atoms. Lp-corrections for Cu/Ni radiation. 163 reflections with $I_{cal}<3$ and $d_{cal}>1.5418$ Å were omitted.

2 Pattern measured on a PHILIPS powder diffractometer with graphite monochromatized Cu Kα radiation and a beam divergence angle of 1°; scanned at 1/8° 2θ per minute. The intensities refer to peak heights.

3 Pattern reported by Bedlivy, Llambías and Astarloa (1969); $d_{obs}$ and peak heights obtained by diffractometry with Cu/Ni radiation.

4 Pattern of the unnamed bismuth arsenate mineral recorded by Frondel (1943) with film methods and Cu/Ni radiation; a correction for absorption apparently has not been applied to the intensities.

Table 5. X-ray powder patterns for heated preisingerite.

| 1 | | | 2 | |
|---|---|---|---|---|
| $d_{obs}$ | $I_{obs}$ | h k l | $d_{obs}$ | $I_{obs}$ |
| 8.346 | 1 | 1 0 0 | 6.758 | 13 |
| 6.652 | 3 | 0 1 0 | 6.417 | 8 |
| 6.632 | 2 | -1 0 1 | 6.046 | 5 |
| 6.482 | 3 | -1 1 0 | 5.772 | 5 |
| 6.246 | 11 | 0 0 1 | 5.454 | 1 |
| 4.885 | 6 | 0 -1 1 | 5.372 | 1 |
| 4.541 | 4 | -2 0 1 | 5.277 | 1 |
| 4.473 | 16 | 1 1 0 | 4.861 | 5 |
| 4.402 | 3 | -2 1 1 | 4.809 | 11 |
| 4.318 | 7 | -2 1 0, 0 1 1 | 4.720 | 3 |
| 4.175 | 2 | 1 0 1, 2 0 0 | 4.301 | 9 |
| 4.080 | 11 | 1 -1 1 | 4.152 | 3 |
| 3.590 | 19 | -1 2 0 | 4.095 | 10 |
| 3.473 | 1 | -1 0 2 | 3.746 | 3 |
| 3.290 | 63 | -2 0 2 + | 3.678 | 7 |
| 3.243 | 3 | -2 2 0 | 3.583 | 10 |
| 3.179 | 100 | 1 1 1 + | 3.376 | 8 |
| 3.125 | 63 | 0 0 2 + | 3.320 | 100 |
| 3.077 | 48 | -1 -1 2 + | 3.255 | 48 |
| 2.994 | 36 | -3 1 0, 0 -1 2 | 3.220 | 37 |
| 2.823 | 2 | -3 1 2 | 3.143 | 34 |
| 2.791 | 11 | 0 2 1 + | 3.089 | 8 |
| 2.768 | 2 | 1 2 0 + | 3.008 | 19 |
| 2.700 | 17 | 0 1 2 | 2.964 | 21 |
| 2.654 | 3 | 2 -2 1, -3 2 0 | 2.894 | 2 |
| 2.603 | 21 | 1 -1 2 | 2.823 | 52 |
| 2.579 | 5 | 1 0 2 | 2.743 | 23 |
| 2.501 | 5 | -3 -1 1 | 2.694 | 8 |
| 2.471 | 6 | -4 1 1 | 2.633 | 9 |
| 2.444 | 1 | -3 2 2, 0 -2 2 | 2.600 | 3 |
| 2.414 | 1 | -1 2 2, 2 1 1 | 2.522 | 10 |
| 2.394 | 4 | -1 -2 2 | 2.498 | 2 |
| 2.362 | 3 | -4 1 2 + | 2.465 | 10 |
| 2.318 | 3 | -2 0 3 + | 2.411 | 3 |
| 2.294 | 1 | 1 -2 2 + | 2.356 | 2 |
| 2.221 | 7 | 1 -3 1 + | 2.332 | 2 |
| 2.205 | 19 | 3 0 1 + | 2.276 | 5 |
| 2.181 | 5 | -2 -2 2 + | 2.233 | 7 |
| 2.177 | 2 | -1 -1 3 + | 2.196 | 5 |
| 2.166 | 1 | -3 3 0 | 2.176 | 7 |
| 2.149 | 2 | -2 -1 3 + | 2.141 | 7 |
| 2.125 | 5 | -1 1 3 + | 2.080 | 3 |
| 2.095 | 2 | 2 0 2 + | 2.019 | 12 |
| 2.067 | 2 | 0 -1 3 + | 1.965 | 1 |
| 2.014 | 24 | -4 1 3 + | 1.953 | 1 |
| 1.959 | 24 | -3 -2 1 + | 1.924 | 10 |
| 1.920 | 15 | 3 -3 1 + | 1.882 | 10 |
| 1.894 | 9 | -4 3 2 + | 1.857 | 1 |
| 1.879 | 2 | 0 -2 3, -1 3 2 | 1.841 | 3 |
| 1.852 | 8 | 1 2 2 + | 1.838 | 3 |

Table 5 (cont'd)

| 1 | | | 2 | |
|---|---|---|---|---|
| $d_{obs}$ | $I_{obs}$ | h k l | $d_{obs}$ | $I_{obs}$ |
| 1.841 | 5 | -1 2 3 + | 1.811 | 5 |
| 1.831 | 4 | 3 2 0, -5 0 1 | 1.789 | 7 |
| 1.816 | 1 | 3 -1 2, 4 1 0 | 1.776 | 11 |
| 1.790 | 15 | -2 -3 1 + | 1.740 | 4 |
| 1.775 | 1 | 1 3 1 + | 1.734 | 5 |
| 1.758 | 8 | -5 3 1 + | 1.728 | 5 |
| 1.734 | 12 | -2 0 4 + | 1.722 | 6 |
| 1.717 | 5 | 2 3 0 + | 1.692 | 5 |
| 1.707 | 1 | 0 3 2 + | 1.684 | 3 |
| 1.697 | 3 | 2 -4 1 + | 1.661 | 8 |
| 1.678 | 12 | -2 -1 4 + | 1.657 | 6 |
| 1.653 | 10 | -2 3 3 + | 1.626 | 4 |
| 1.618 | 1 | -5 -1 1 + | 1.622 | 3 |
| 1.609 | 2 | 3 2 1 + | 1.608 | 1 |
| 1.604 | 1 | 2 -2 3 + | 1.590 | 2 |
| 1.590 | 4 | 2 2 2 | 1.570 | 6 |
| 1.573 | 9 | 4 -1 1 + | 1.544 | 5 |
| 1.554 | 11 | 0 -4 2 + | | |

[1] After heating to 540°C for 30 minutes. The indices are based on a triclinic cell with a=9.92(1), b=7.16(1), c=6.97(1) Å, α=87.79(5), β=115.25(5), γ=110.29(5)° and V=416 $Å^3$. "+" indicates that additional indices are possible.

[2] After heating to 800°C for 30 minutes.