AM-86-299

High-teperature structure and crystal chemistry of hydrous alkali-rich beryl from the Harding pegmatite, Toas County, New Mexico

Brown and Mills

To be deposited: Table 6

American Mineralogist: 71, 3-4, 547-556

TABLE 6.

*OBSERVED AND CALCULATED STRUCTURE FACTORS FOR THE HARDING BERYL AT 24°, 500°, 800°, and 24°C (after heating)*

Structure Factors for Beryl (24°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ | h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 0 | | | | | | | | | |
| 0 | 0 | 4 | 119 | 124 | 5 | 0 | 6 | 6 | 49 | 49 | 0 |
| 0 | 0 | 6 | 134 | 140 | 6 | 0 | 6 | 8 | 9 | 11 | 1 |
| 0 | 0 | 8 | 165 | 171 | 6 | 0 | 6 | 10 | 74 | 74 | 0 |
| 0 | 0 | 10 | 12 | 12 | 0 | 0 | 6 | 12 | 11 | 8 | 3 |
| 0 | 0 | 12 | 80 | 79 | 1 | 0 | 7 | 2 | 32 | 32 | 1 |
| 0 | 0 | 14 | 53 | 52 | 1 | 0 | 7 | 4 | 27 | 27 | 1 |
| 0 | 1 | 0 | 49 | 53 | 4 | 0 | 7 | 6 | 16 | 15 | 1 |
| 0 | 1 | 4 | 43 | 39 | 4 | 0 | 7 | 8 | 8 | 3 | 5 |
| 0 | 1 | 6 | 9 | 5 | 4 | 0 | 7 | 10 | 29 | 27 | 2 |
| 0 | 1 | 8 | 17 | 15 | 1 | 0 | 8 | 0 | 71 | 74 | 3 |
| 0 | 1 | 10 | 18 | 19 | 1 | 0 | 8 | 2 | 35 | 35 | 0 |
| 0 | 1 | 12 | 6 | 4 | 2 | 0 | 8 | 4 | 22 | 20 | 2 |
| 0 | 2 | 0 | 20 | 22 | 2 | 0 | 8 | 6 | 51 | 50 | 1 |
| 0 | 2 | 2 | 71 | 63 | 8 | 0 | 8 | 8 | 42 | 42 | 0 |
| 0 | 2 | 4 | 48 | 49 | 2 | 0 | 8 | 10 | 11 | 11 | 1 |
| 0 | 2 | 6 | 30 | 27 | 2 | 0 | 9 | 0 | 9 | 10 | 0 |
| 0 | 2 | 8 | 19 | 19 | 0 | 0 | 9 | 2 | 36 | 38 | 1 |
| 0 | 2 | 10 | 26 | 26 | 0 | 0 | 9 | 4 | 8 | 10 | 2 |
| 0 | 2 | 12 | 13 | 15 | 2 | 0 | 9 | 6 | 36 | 38 | 2 |
| 0 | 2 | 14 | 7 | 8 | 1 | 0 | 9 | 10 | 19 | 18 | 1 |
| 0 | 3 | 0 | 37 | 38 | 1 | 0 | 10 | 2 | 19 | 18 | 1 |
| 0 | 3 | 2 | 7 | 4 | 2 | 0 | 10 | 4 | 22 | 24 | 2 |
| 0 | 3 | 4 | 92 | 92 | 0 | 0 | 11 | 0 | 12 | 12 | 0 |
| 0 | 3 | 6 | 29 | 30 | 1 | 0 | 11 | 2 | 11 | 10 | 1 |
| 0 | 3 | 8 | 30 | 30 | 0 | 0 | 11 | 4 | 8 | 4 | 4 |
| 0 | 3 | 12 | 24 | 24 | 0 | 0 | 12 | 0 | 13 | 14 | 1 |
| 0 | 3 | 14 | 14 | 14 | 0 | 0 | 12 | 2 | 34 | 33 | 1 |
| 0 | 4 | 0 | 33 | 36 | 2 | | | | | | |
| 0 | 4 | 2 | 17 | 15 | 2 | | | H = 1 | | | |
| 0 | 4 | 6 | 30 | 30 | 0 | 1 | 1 | 0 | 4 | 0 | 4 |
| 0 | 4 | 8 | 20 | 21 | 0 | 1 | 1 | 2 | 116 | 116 | 1 |
| 0 | 4 | 10 | 9 | 8 | 1 | 1 | 1 | 4 | 17 | 17 | 0 |
| 0 | 4 | 12 | 13 | 11 | 1 | 1 | 1 | 6 | 71 | 72 | 2 |
| 0 | 4 | 14 | 14 | 15 | 1 | 1 | 1 | 10 | 47 | 49 | 2 |
| 0 | 5 | 0 | 66 | 65 | 1 | 1 | 1 | 14 | 25 | 25 | 0 |
| 0 | 5 | 2 | 16 | 12 | 4 | 1 | 2 | 0 | 48 | 48 | 0 |
| 0 | 5 | 4 | 12 | 10 | 2 | 1 | 2 | 1 | 89 | 91 | 2 |
| 0 | 5 | 6 | 26 | 26 | 0 | 1 | 2 | 3 | 17 | 13 | 3 |
| 0 | 5 | 8 | 29 | 29 | 0 | 1 | 2 | 4 | 17 | 17 | 0 |
| 0 | 5 | 12 | 17 | 15 | 2 | 1 | 2 | 5 | 31 | 32 | 1 |
| 0 | 6 | 0 | 47 | 47 | 0 | 1 | 2 | 6 | 39 | 40 | 1 |
| 0 | 6 | 2 | 104 | 106 | 2 | 1 | 2 | 7 | 65 | 66 | 1 |
| 0 | 6 | 4 | 50 | 51 | 1 | 1 | 2 | 8 | 20 | 19 | 1 |

Structure Factors for Beryl (24°C) h,k,l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ | h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 1 | | | | | | | | | |
| 1 | 2 | 9 | 23 | 23 | 0 | 1 | 6 | 4 | 14 | 13 | 1 |
| 1 | 2 | 10 | 22 | 21 | 1 | 1 | 6 | 5 | 7 | 2 | 5 |
| 1 | 2 | 11 | 11 | 11 | 1 | 1 | 6 | 6 | 14 | 14 | 0 |
| 1 | 2 | 12 | 10 | 10 | 0 | 1 | 6 | 7 | 10 | 7 | 3 |
| 1 | 2 | 13 | 30 | 30 | 0 | 1 | 6 | 8 | 26 | 26 | 0 |
| 1 | 2 | 14 | 18 | 18 | 0 | 1 | 6 | 12 | 13 | 12 | 1 |
| 1 | 3 | 0 | 44 | 42 | 2 | 1 | 7 | 0 | 28 | 29 | 1 |
| 1 | 3 | 1 | 40 | 36 | 4 | 1 | 7 | 1 | 29 | 29 | 1 |
| 1 | 3 | 2 | 16 | 16 | 1 | 1 | 7 | 2 | 12 | 12 | 0 |
| 1 | 3 | 3 | 50 | 50 | 0 | 1 | 7 | 3 | 35 | 35 | 0 |
| 1 | 3 | 4 | 18 | 18 | 0 | 1 | 7 | 4 | 36 | 38 | 2 |
| 1 | 3 | 5 | 16 | 16 | 0 | 1 | 7 | 5 | 29 | 29 | 0 |
| 1 | 3 | 6 | 25 | 23 | 1 | 1 | 7 | 6 | 17 | 17 | 0 |
| 1 | 3 | 7 | 16 | 17 | 1 | 1 | 7 | 7 | 18 | 19 | 1 |
| 1 | 3 | 8 | 19 | 18 | 1 | 1 | 7 | 8 | 23 | 23 | 0 |
| 1 | 3 | 11 | 24 | 24 | 0 | 1 | 7 | 9 | 21 | 20 | 1 |
| 1 | 3 | 12 | 9 | 6 | 2 | 1 | 7 | 11 | 20 | 18 | 1 |
| 1 | 3 | 14 | 9 | 10 | 1 | 1 | 7 | 12 | 11 | 13 | 2 |
| 1 | 4 | 0 | 82 | 85 | 3 | 1 | 8 | 0 | 29 | 29 | 0 |
| 1 | 4 | 1 | 55 | 55 | 0 | 1 | 8 | 1 | 6 | 6 | 0 |
| 1 | 4 | 2 | 31 | 30 | 1 | 1 | 8 | 2 | 9 | 9 | 0 |
| 1 | 4 | 3 | 77 | 79 | 2 | 1 | 8 | 3 | 18 | 17 | 2 |
| 1 | 4 | 4 | 30 | 30 | 0 | 1 | 8 | 4 | 16 | 17 | 1 |
| 1 | 4 | 5 | 56 | 57 | 1 | 1 | 8 | 6 | 10 | 11 | 1 |
| 1 | 4 | 6 | 9 | 4 | 5 | 1 | 8 | 7 | 9 | 8 | 2 |
| 1 | 4 | 7 | 35 | 35 | 1 | 1 | 8 | 8 | 21 | 20 | 1 |
| 1 | 4 | 8 | 38 | 39 | 1 | 1 | 8 | 9 | 8 | 7 | 2 |
| 1 | 4 | 9 | 39 | 40 | 0 | 1 | 9 | 0 | 1 | 2 | 1 |
| 1 | 4 | 10 | 20 | 20 | 0 | 1 | 9 | 1 | 16 | 16 | 0 |
| 1 | 4 | 11 | 35 | 35 | 1 | 1 | 9 | 3 | 35 | 34 | 1 |
| 1 | 4 | 12 | 22 | 21 | 1 | 1 | 9 | 4 | 19 | 20 | 0 |
| 1 | 4 | 13 | 19 | 19 | 0 | 1 | 9 | 5 | 23 | 23 | 1 |
| 1 | 5 | 1 | 14 | 15 | 1 | 1 | 9 | 9 | 17 | 17 | 0 |
| 1 | 5 | 2 | 34 | 36 | 1 | 1 | 10 | 0 | 39 | 39 | 1 |
| 1 | 5 | 3 | 9 | 8 | 1 | 1 | 10 | 1 | 45 | 45 | 0 |
| 1 | 5 | 4 | 26 | 28 | 2 | 1 | 10 | 3 | 24 | 23 | 0 |
| 1 | 5 | 6 | 18 | 18 | 0 | 1 | 10 | 4 | 18 | 18 | 0 |
| 1 | 5 | 7 | 14 | 15 | 1 | 1 | 10 | 5 | 31 | 31 | 1 |
| 1 | 5 | 10 | 27 | 26 | 1 | 1 | 10 | 7 | 39 | 40 | 1 |
| 1 | 5 | 13 | 9 | 7 | 2 | 1 | 10 | 8 | 22 | 23 | 1 |
| 1 | 6 | 0 | 39 | 38 | 1 | 1 | 11 | 0 | 20 | 19 | 1 |
| 1 | 6 | 1 | 8 | 8 | 0 | 1 | 11 | 3 | 11 | 12 | 1 |
| 1 | 6 | 2 | 7 | 7 | 0 | 1 | 11 | 4 | 15 | 14 | 1 |

Structure Factors for Beryl (24°C) h, k, l, $F_{obs}$, $F_{calc}$, and σ (F)

| h | k | l | $F_o$ | $F_c$ | σ (F) | h | k | l | $F_o$ | $F_c$ | σ (F) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 1 | | | | | | | | | |
| 1 | 12 | 0 | 13 | 13 | 0 | 2 | 5 | 7 | 51 | 51 | 0 |
| 1 | 12 | 1 | 11 | 10 | 1 | 2 | 5 | 8 | 43 | 43 | 0 |
| 1 | 12 | 2 | 19 | 20 | 1 | 2 | 5 | 9 | 29 | 30 | 1 |
| | | | | | | 2 | 5 | 12 | 24 | 23 | 2 |
| | | H = 2 | | | | 2 | 5 | 13 | 27 | 24 | 3 |
| 2 | 2 | 0 | 25 | 24 | 1 | 2 | 6 | 1 | 10 | 12 | 2 |
| 2 | 2 | 2 | 26 | 22 | 4 | 2 | 6 | 2 | 17 | 17 | 0 |
| 2 | 2 | 4 | 101 | 102 | 1 | 2 | 6 | 3 | 14 | 15 | 2 |
| 2 | 2 | 6 | 48 | 49 | 1 | 2 | 6 | 4 | 21 | 21 | 1 |
| 2 | 2 | 8 | 32 | 31 | 1 | 2 | 6 | 5 | 9 | 8 | 1 |
| 2 | 2 | 10 | 9 | 4 | 5 | 2 | 6 | 8 | 8 | 5 | 3 |
| 2 | 2 | 12 | 27 | 27 | 1 | 2 | 6 | 9 | 9 | 11 | 2 |
| 2 | 2 | 14 | 22 | 22 | 0 | 2 | 6 | 10 | 18 | 18 | 0 |
| 2 | 3 | 0 | 29 | 29 | 1 | 2 | 7 | 0 | 16 | 14 | 2 |
| 2 | 3 | 1 | 9 | 10 | 1 | 2 | 7 | 2 | 7 | 6 | 2 |
| 2 | 3 | 2 | 26 | 25 | 1 | 2 | 7 | 3 | 31 | 31 | 1 |
| 2 | 3 | 3 | 46 | 45 | 1 | 2 | 7 | 4 | 21 | 20 | 1 |
| 2 | 3 | 4 | 42 | 42 | 0 | 2 | 7 | 5 | 13 | 13 | 1 |
| 2 | 3 | 5 | 25 | 25 | 0 | 2 | 7 | 8 | 14 | 13 | 1 |
| 2 | 3 | 6 | 16 | 14 | 2 | 2 | 7 | 9 | 14 | 15 | 1 |
| 2 | 3 | 8 | 25 | 25 | 0 | 2 | 7 | 11 | 13 | 17 | 4 |
| 2 | 3 | 9 | 14 | 14 | 0 | 2 | 8 | 0 | 17 | 17 | 0 |
| 2 | 3 | 10 | 14 | 15 | 0 | 2 | 8 | 2 | 25 | 25 | 0 |
| 2 | 3 | 11 | 18 | 18 | 1 | 2 | 8 | 4 | 32 | 33 | 1 |
| 2 | 4 | 0 | 43 | 43 | 0 | 2 | 8 | 6 | 28 | 28 | 0 |
| 2 | 4 | 1 | 20 | 21 | 1 | 2 | 8 | 8 | 14 | 14 | 0 |
| 2 | 4 | 2 | 45 | 47 | 2 | 2 | 9 | 0 | 16 | 16 | 0 |
| 2 | 4 | 3 | 17 | 17 | 0 | 2 | 9 | 1 | 24 | 25 | 1 |
| 2 | 4 | 4 | 52 | 54 | 1 | 2 | 9 | 2 | 21 | 21 | 0 |
| 2 | 4 | 5 | 16 | 17 | 1 | 2 | 9 | 3 | 20 | 19 | 1 |
| 2 | 4 | 6 | 32 | 32 | 0 | 2 | 9 | 5 | 22 | 22 | 0 |
| 2 | 4 | 7 | 10 | 13 | 3 | 2 | 9 | 6 | 21 | 21 | 0 |
| 2 | 4 | 8 | 33 | 31 | 1 | 2 | 9 | 7 | 20 | 21 | 1 |
| 2 | 4 | 9 | 9 | 7 | 1 | 2 | 9 | 9 | 11 | 12 | 1 |
| 2 | 4 | 10 | 30 | 30 | 0 | 2 | 10 | 0 | 22 | 22 | 0 |
| 2 | 4 | 12 | 23 | 22 | 1 | 2 | 10 | 2 | 11 | 10 | 1 |
| 2 | 5 | 0 | 71 | 74 | 3 | 2 | 10 | 6 | 18 | 17 | 1 |
| 2 | 5 | 1 | 66 | 67 | 1 | 2 | 11 | 0 | 12 | 12 | 0 |
| 2 | 5 | 2 | 8 | 4 | 4 | 2 | 11 | 1 | 10 | 8 | 2 |
| 2 | 5 | 3 | 34 | 34 | 0 | 2 | 11 | 2 | 15 | 14 | 1 |
| 2 | 5 | 4 | 54 | 55 | 1 | 2 | 11 | 3 | 24 | 24 | 0 |
| 2 | 5 | 5 | 41 | 41 | 0 | 2 | 11 | 5 | 17 | 16 | 1 |
| 2 | 5 | 6 | 6 | 3 | 3 | | | | | | |

Structure Factors for Beryl (24°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ | h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 3 | | | | | | | | | |
| 3 | 3 | 0 | 29 | 26 | 3 | 3 | 9 | 1 | 14 | 13 | 2 |
| 3 | 3 | 2 | 68 | 68 | 0 | 3 | 9 | 3 | 21 | 19 | 1 |
| 3 | 3 | 4 | 10 | 12 | 3 | 3 | 9 | 4 | 22 | 23 | 1 |
| 3 | 3 | 6 | 65 | 67 | 2 | 3 | 9 | 5 | 17 | 14 | 3 |
| 3 | 3 | 10 | 30 | 29 | 1 | 3 | 9 | 7 | 9 | 8 | 1 |
| 3 | 4 | 1 | 14 | 12 | 2 | 3 | 9 | 8 | 16 | 16 | 0 |
| 3 | 4 | 2 | 9 | 11 | 2 | 3 | 10 | 3 | 20 | 20 | 0 |
| 3 | 4 | 3 | 68 | 71 | 3 | 3 | 10 | 4 | 19 | 19 | 0 |
| 3 | 4 | 4 | 33 | 34 | 1 | 3 | 10 | 5 | 11 | 10 | 1 |
| 3 | 4 | 5 | 35 | 36 | 1 | 3 | 11 | 0 | 25 | 24 | 1 |
| 3 | 4 | 8 | 13 | 11 | 1 | 3 | 11 | 2 | 6 | 6 | 0 |
| 3 | 4 | 9 | 30 | 29 | 1 | | | | | | |
| 3 | 4 | 10 | 13 | 12 | 1 | | | H = 4 | | | |
| 3 | 4 | 12 | 8 | 12 | 4 | 4 | 3 | 7 | 8 | 0 | 8 |
| 3 | 5 | 0 | 9 | 8 | 1 | 4 | 4 | 0 | 9 | 5 | 4 |
| 3 | 5 | 1 | 15 | 15 | 0 | 4 | 4 | 2 | 49 | 51 | 2 |
| 3 | 5 | 2 | 14 | 16 | 1 | 4 | 4 | 4 | 34 | 34 | 0 |
| 3 | 5 | 3 | 36 | 36 | 1 | 4 | 4 | 6 | 56 | 56 | 0 |
| 3 | 5 | 5 | 23 | 25 | 1 | 4 | 4 | 10 | 20 | 20 | 0 |
| 3 | 5 | 6 | 9 | 7 | 1 | 4 | 5 | 1 | 41 | 41 | 0 |
| 3 | 5 | 9 | 19 | 18 | 1 | 4 | 5 | 2 | 13 | 12 | 1 |
| 3 | 5 | 10 | 11 | 11 | 1 | 4 | 5 | 3 | 31 | 31 | 0 |
| 3 | 5 | 11 | 21 | 20 | 1 | 4 | 5 | 4 | 10 | 9 | 1 |
| 3 | 6 | 0 | 33 | 35 | 2 | 4 | 5 | 5 | 31 | 31 | 0 |
| 3 | 6 | 1 | 16 | 17 | 0 | 4 | 5 | 6 | 19 | 18 | 1 |
| 3 | 6 | 4 | 48 | 50 | 2 | 4 | 5 | 7 | 33 | 33 | 0 |
| 3 | 6 | 7 | 13 | 14 | 1 | 4 | 5 | 9 | 26 | 25 | 1 |
| 3 | 6 | 8 | 26 | 26 | 0 | 4 | 5 | 11 | 18 | 17 | 1 |
| 3 | 7 | 0 | 18 | 18 | 0 | 4 | 6 | 0 | 17 | 16 | 1 |
| 3 | 7 | 1 | 52 | 53 | 1 | 4 | 6 | 1 | 9 | 10 | 1 |
| 3 | 7 | 2 | 17 | 16 | 1 | 4 | 6 | 3 | 9 | 8 | 1 |
| 3 | 7 | 3 | 16 | 15 | 1 | 4 | 6 | 4 | 9 | 9 | 0 |
| 3 | 7 | 5 | 30 | 29 | 0 | 4 | 6 | 5 | 8 | 8 | 0 |
| 3 | 7 | 6 | 22 | 22 | 1 | 4 | 6 | 6 | 11 | 12 | 0 |
| 3 | 7 | 7 | 48 | 48 | 0 | 4 | 6 | 7 | 11 | 8 | 3 |
| 3 | 7 | 9 | 19 | 21 | 1 | 4 | 6 | 8 | 10 | 8 | 2 |
| 3 | 8 | 1 | 31 | 32 | 1 | 4 | 7 | 2 | 41 | 41 | 0 |
| 3 | 8 | 2 | 17 | 16 | 1 | 4 | 7 | 3 | 25 | 25 | 0 |
| 3 | 8 | 3 | 29 | 27 | 1 | 4 | 7 | 4 | 12 | 10 | 2 |
| 3 | 8 | 5 | 25 | 25 | 0 | 4 | 7 | 5 | 11 | 11 | 0 |
| 3 | 8 | 6 | 11 | 12 | 1 | 4 | 7 | 6 | 27 | 27 | 0 |
| 3 | 8 | 9 | 24 | 21 | 3 | 4 | 7 | 9 | 12 | 9 | 3 |
| 3 | 9 | 0 | 21 | 20 | 0 | 4 | 8 | 0 | 17 | 16 | 0 |

Structure Factors for Beryl (24°C) h, k, l, $F_{obs}$, $F_{calc}$, and σ(F)

| h | k | l | $F_o$ | $F_c$ | σ(F) | h | k | l | $F_o$ | $F_c$ | σ(F) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 4 | | | | 6 | 6 | 4 | 58 | 56 | 2 |
| 4 | 8 | 2 | 14 | 14 | 0 | 6 | 6 | 6 | 35 | 34 | 0 |
| 4 | 8 | 4 | 9 | 10 | 2 | 6 | 6 | 8 | 64 | 63 | 1 |
| 4 | 8 | 6 | 12 | 14 | 3 | 6 | 7 | 0 | 17 | 17 | 0 |
| 4 | 8 | 8 | 13 | 12 | 1 | 6 | 7 | 3 | 10 | 8 | 2 |
| 4 | 9 | 0 | 24 | 24 | 0 | 6 | 7 | 5 | 9 | 6 | 3 |
| 4 | 9 | 1 | 34 | 35 | 1 | 6 | 8 | 2 | 19 | 19 | 0 |
| 4 | 9 | 2 | 24 | 23 | 1 | 6 | 8 | 4 | 28 | 27 | 1 |
| 4 | 9 | 4 | 9 | 8 | 2 | | | | | | |
| 4 | 9 | 5 | 25 | 24 | 1 | | | H = 7 | | | |
| 4 | 9 | 6 | 27 | 27 | 1 | 7 | 7 | 2 | 16 | 19 | 2 |
| 4 | 10 | 0 | 20 | 21 | 1 | 7 | 7 | 4 | 9 | 8 | 1 |
| | | H = 5 | | | | | | H = 8 | | | |
| 5 | 1 | 8 | 8 | 5 | 3 | 8 | 3 | 4 | 10 | 7 | 3 |
| 5 | 4 | 0 | 13 | 13 | 1 | 8 | 3 | 7 | 24 | 25 | 2 |
| 5 | 5 | 0 | 20 | 20 | 0 | | | | | | |
| 5 | 5 | 2 | 43 | 43 | 1 | | | H = 9 | | | |
| 5 | 5 | 4 | 10 | 8 | 2 | 9 | 3 | 2 | 9 | 5 | 3 |
| 5 | 5 | 6 | 22 | 22 | 1 | 9 | 4 | 3 | 14 | 17 | 3 |
| 5 | 5 | 10 | 36 | 34 | 2 | | | | | | |
| 5 | 6 | 2 | 17 | 16 | 0 | | | H = 10 | | | |
| 5 | 6 | 3 | 9 | 7 | 2 | 10 | 2 | 1 | 10 | 5 | 4 |
| 5 | 6 | 10 | 15 | 14 | 1 | 10 | 2 | 5 | 3 | 4 | 0 |
| 5 | 7 | 0 | 8 | 7 | 0 | | | | | | |
| 5 | 7 | 3 | 18 | 19 | 1 | | | H = 11 | | | |
| 5 | 7 | 4 | 8 | 6 | 2 | 11 | 1 | 6 | 10 | 7 | 3 |
| 5 | 7 | 5 | 12 | 10 | 1 | 11 | 2 | 4 | 13 | 8 | 5 |
| 5 | 8 | 0 | 11 | 4 | 6 | | | | | | |
| 5 | 8 | 2 | 26 | 25 | 1 | | | | | | |
| 5 | 8 | 3 | 13 | 14 | 1 | | | | | | |
| 5 | 8 | 4 | 3 | 3 | 0 | | | | | | |
| 5 | 8 | 5 | 9 | 9 | 0 | | | | | | |
| 5 | 8 | 6 | 27 | 27 | 1 | | | | | | |
| 5 | 9 | 0 | 6 | 3 | 3 | | | | | | |
| 5 | 9 | 1 | 13 | 12 | 1 | | | | | | |
| 5 | 9 | 2 | 21 | 21 | 0 | | | | | | |
| 5 | 9 | 4 | 17 | 15 | 2 | | | | | | |
| | | H = 6 | | | | | | | | | |
| 6 | 2 | 0 | 10 | 7 | 2 | | | | | | |
| 6 | 5 | 7 | 10 | 3 | 7 | | | | | | |
| 6 | 6 | 0 | 93 | 93 | 1 | | | | | | |
| 6 | 6 | 2 | 29 | 27 | 2 | | | | | | |

Structure Factors for Beryl (500°C) h, k, l, $F_{obs}$, $F_{calc}$, and σ(F)

| h | k | l | $F_o$ | $F_c$ | σ(F) | h | k | l | $F_o$ | $F_c$ | σ(F) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 0 | | | | 2 | 1 | 0 | 49 | 46 | 3 |
| 0 | 0 | 4 | 109 | 117 | 9 | 2 | 2 | 0 | 19 | 20 | 1 |
| 0 | 0 | 6 | 123 | 127 | 4 | 2 | 2 | 2 | 23 | 22 | 1 |
| 0 | 0 | 8 | 146 | 152 | 7 | 2 | 2 | 4 | 96 | 96 | 0 |
| 0 | 0 | 10 | 12 | 10 | 2 | 2 | 2 | 6 | 44 | 44 | 0 |
| 0 | 0 | 12 | 64 | 59 | 5 | 2 | 2 | 8 | 26 | 25 | 0 |
| 0 | 0 | 14 | 38 | 37 | 1 | 2 | 2 | 12 | 20 | 21 | 1 |
| | | | | | | 2 | 2 | 14 | 13 | 15 | 2 |
| | | H = 1 | | | | | | | | | |
| 1 | 1 | 0 | 6 | 2 | 5 | | | H = 3 | | | |
| 1 | 1 | 2 | 115 | 115 | 0 | | | | | | |
| 1 | 1 | 4 | 19 | 15 | 4 | 3 | 3 | 0 | 33 | 30 | 3 |
| 1 | 1 | 6 | 65 | 65 | 0 | 3 | 3 | 2 | 65 | 66 | 1 |
| 1 | 1 | 10 | 39 | 39 | 0 | 3 | 3 | 4 | 9 | 12 | 3 |
| 1 | 1 | 14 | 20 | 16 | 4 | 3 | 3 | 6 | 58 | 61 | 3 |
| 1 | 0 | 10 | 20 | 16 | 4 | 3 | 3 | 8 | 12 | 8 | 4 |
| 1 | 0 | 8 | 16 | 16 | 0 | 3 | 3 | 10 | 21 | 22 | 1 |
| 1 | 0 | 6 | 8 | 4 | 4 | 3 | 3 | 12 | 11 | 2 | 9 |
| 1 | 0 | 4 | 39 | 37 | 2 | 3 | 2 | 12 | 17 | 16 | 1 |
| 1 | 0 | 2 | 33 | 39 | 6 | 3 | 2 | 11 | 10 | 12 | 2 |
| 1 | 0 | 0 | 49 | 52 | 3 | 3 | 2 | 10 | 9 | 12 | 2 |
| | | | | | | 3 | 2 | 9 | 10 | 11 | 2 |
| | | H = 2 | | | | 3 | 2 | 8 | 24 | 24 | 1 |
| 2 | 0 | 0 | 21 | 23 | 2 | 3 | 2 | 6 | 14 | 12 | 2 |
| 2 | 0 | 2 | 68 | 62 | 7 | 3 | 2 | 5 | 24 | 22 | 2 |
| 2 | 0 | 4 | 46 | 48 | 2 | 3 | 2 | 4 | 42 | 43 | 1 |
| 2 | 0 | 6 | 25 | 25 | 0 | 3 | 2 | 3 | 43 | 41 | 2 |
| 2 | 0 | 8 | 16 | 15 | 0 | 3 | 2 | 2 | 22 | 25 | 3 |
| 2 | 0 | 10 | 18 | 21 | 3 | 3 | 2 | 1 | 14 | 11 | 3 |
| 2 | 0 | 12 | 13 | 12 | 2 | 3 | 2 | 0 | 33 | 30 | 3 |
| 2 | 0 | 14 | 4 | 6 | 2 | 3 | 1 | 0 | 40 | 38 | 2 |
| 2 | 1 | 14 | 17 | 15 | 2 | 3 | 1 | 1 | 38 | 36 | 3 |
| 2 | 1 | 13 | 24 | 24 | 0 | 3 | 1 | 2 | 16 | 15 | 1 |
| 2 | 1 | 12 | 10 | 8 | 1 | 3 | 1 | 3 | 50 | 49 | 1 |
| 2 | 1 | 10 | 19 | 20 | 1 | 3 | 1 | 4 | 18 | 18 | 0 |
| 2 | 1 | 9 | 20 | 23 | 3 | 3 | 1 | 5 | 18 | 18 | 0 |
| 2 | 1 | 8 | 11 | 17 | 6 | 3 | 1 | 6 | 23 | 19 | 4 |
| 2 | 1 | 7 | 59 | 63 | 4 | 3 | 1 | 7 | 11 | 11 | 1 |
| 2 | 1 | 6 | 37 | 39 | 2 | 3 | 1 | 8 | 10 | 2 | 8 |
| 2 | 1 | 5 | 30 | 31 | 1 | 3 | 1 | 9 | 16 | 18 | 2 |
| 2 | 1 | 4 | 17 | 16 | 1 | 3 | 1 | 11 | 22 | 23 | 1 |
| 2 | 1 | 3 | 15 | 12 | 3 | 3 | 1 | 14 | 12 | 6 | 6 |
| 2 | 1 | 2 | 38 | 42 | 4 | 3 | 0 | 12 | 14 | 16 | 2 |
| 2 | 1 | 1 | 90 | 91 | 2 | 3 | 0 | 8 | 24 | 23 | 1 |

Structure Factors for Beryl (500°C) h, k, 1, $F_{obs}$, $F_{calc}$, and σ(F)

| h | k | 1 | $F_o$ | $F_c$ | σ(F) | h | k | 1 | $F_o$ | $F_c$ | σ(F) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 3 | | | | 4 | 3 | 4 | 32 | 36 | 4 |
| 3 | 0 | 6 | 26 | 26 | 1 | 4 | 3 | 3 | 65 | 66 | 2 |
| 3 | 0 | 4 | 85 | 83 | 1 | 4 | 3 | 1 | 10 | 13 | 3 |
| 3 | 0 | 0 | 34 | 35 | 2 | 4 | 4 | 2 | 47 | 47 | 0 |
| | | H = 4 | | | | 4 | 4 | 4 | 27 | 26 | 1 |
| 4 | 0 | 0 | 35 | 37 | 2 | 4 | 4 | 6 | 47 | 47 | 1 |
| 4 | 0 | 2 | 17 | 15 | 3 | 4 | 4 | 10 | 15 | 15 | 0 |
| 4 | 0 | 4 | 7 | 1 | 6 | | | | | | |
| 4 | 0 | 6 | 26 | 28 | 2 | | | H = 5 | | | |
| 4 | 0 | 8 | 19 | 21 | 2 | 5 | 5 | 0 | 14 | 17 | 3 |
| 4 | 0 | 14 | 13 | 12 | 1 | 5 | 5 | 2 | 39 | 42 | 3 |
| 4 | 1 | 13 | 13 | 16 | 3 | 5 | 5 | 4 | 12 | 10 | 1 |
| 4 | 1 | 12 | 15 | 15 | 0 | 5 | 5 | 6 | 18 | 21 | 4 |
| 4 | 1 | 11 | 28 | 29 | 1 | 5 | 5 | 10 | 26 | 28 | 2 |
| 4 | 1 | 10 | 15 | 14 | 1 | 5 | 4 | 11 | 18 | 14 | 4 |
| 4 | 1 | 9 | 32 | 33 | 1 | 5 | 4 | 9 | 26 | 20 | 6 |
| 4 | 1 | 8 | 31 | 34 | 3 | 5 | 4 | 7 | 26 | 29 | 3 |
| 4 | 1 | 7 | 32 | 31 | 0 | 5 | 4 | 6 | 17 | 17 | 0 |
| 4 | 1 | 6 | 10 | 2 | 8 | 5 | 4 | 5 | 27 | 28 | 1 |
| 4 | 1 | 5 | 52 | 55 | 4 | 5 | 4 | 4 | 9 | 10 | 1 |
| 4 | 1 | 4 | 25 | 25 | 0 | 5 | 4 | 3 | 28 | 28 | 0 |
| 4 | 1 | 3 | 73 | 77 | 4 | 5 | 4 | 2 | 14 | 14 | 0 |
| 4 | 1 | 2 | 27 | 26 | 0 | 5 | 4 | 1 | 40 | 38 | 2 |
| 4 | 1 | 1 | 53 | 54 | 0 | 5 | 3 | 0 | 10 | 7 | 4 |
| 4 | 1 | 0 | 78 | 81 | 3 | 5 | 3 | 1 | 13 | 13 | 1 |
| 4 | 2 | 0 | 41 | 39 | 1 | 5 | 3 | 2 | 15 | 12 | 3 |
| 4 | 2 | 1 | 19 | 20 | 1 | 5 | 3 | 3 | 32 | 33 | 1 |
| 4 | 2 | 2 | 46 | 45 | 1 | 5 | 3 | 5 | 20 | 22 | 2 |
| 4 | 2 | 3 | 12 | 15 | 3 | 5 | 3 | 6 | 13 | 5 | 8 |
| 4 | 2 | 4 | 48 | 49 | 2 | 5 | 3 | 9 | 14 | 16 | 2 |
| 4 | 2 | 5 | 18 | 15 | 3 | 5 | 3 | 11 | 16 | 16 | 0 |
| 4 | 2 | 6 | 30 | 31 | 1 | 5 | 2 | 13 | 18 | 16 | 1 |
| 4 | 2 | 7 | 9 | 11 | 1 | 5 | 2 | 12 | 13 | 14 | 1 |
| 4 | 2 | 8 | 23 | 27 | 4 | 5 | 2 | 11 | 14 | 14 | 1 |
| 4 | 2 | 9 | 9 | 5 | 4 | 5 | 2 | 9 | 26 | 26 | 0 |
| 4 | 2 | 10 | 28 | 25 | 3 | 5 | 2 | 8 | 36 | 31 | 5 |
| 4 | 2 | 11 | 12 | 5 | 7 | 5 | 2 | 7 | 45 | 44 | 1 |
| 4 | 2 | 12 | 19 | 19 | 1 | 5 | 2 | 6 | 8 | 4 | 4 |
| 4 | 3 | 12 | 13 | 11 | 2 | 5 | 2 | 5 | 38 | 37 | 1 |
| 4 | 3 | 11 | 24 | 24 | 0 | 5 | 2 | 4 | 46 | 46 | 0 |
| 4 | 3 | 9 | 26 | 23 | 3 | 5 | 2 | 3 | 33 | 33 | 0 |
| 4 | 3 | 8 | 12 | 10 | 2 | 5 | 2 | 1 | 64 | 64 | 0 |
| 4 | 3 | 5 | 33 | 34 | 2 | 5 | 2 | 0 | 66 | 63 | 3 |

Structure Factors for Beryl (500°C) h, k, l, $F_{obs}$, $F_{calc}$, and σ(F)

| h | k | l | $F_o$ | $F_c$ | σ(F) | h | k | l | $F_o$ | $F_c$ | σ(F) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 5 | | | | | | | | | |
| 5 | 1 | 1 | 14 | 16 | 2 | 6 | 4 | 8 | 11 | 7 | 4 |
| 5 | 1 | 2 | 35 | 33 | 3 | 6 | 4 | 9 | 12 | 5 | 8 |
| 5 | 1 | 4 | 24 | 27 | 2 | 6 | 4 | 10 | 10 | 3 | 7 |
| 5 | 1 | 6 | 19 | 16 | 3 | 6 | 5 | 10 | 10 | 10 | 0 |
| 5 | 1 | 8 | 9 | 5 | 4 | 6 | 5 | 9 | 9 | 2 | 7 |
| 5 | 1 | 10 | 24 | 22 | 2 | 6 | 5 | 3 | 11 | 6 | 5 |
| 5 | 0 | 12 | 16 | 11 | 5 | 6 | 5 | 2 | 17 | 15 | 1 |
| 5 | 0 | 8 | 25 | 26 | 1 | 6 | 5 | 0 | 10 | 12 | 1 |
| 5 | 0 | 6 | 20 | 20 | 0 | 6 | 6 | 0 | 80 | 81 | 1 |
| 5 | 0 | 4 | 9 | 10 | 1 | 6 | 6 | 2 | 25 | 28 | 2 |
| 5 | 0 | 2 | 14 | 9 | 5 | 6 | 6 | 4 | 49 | 49 | 0 |
| 5 | 0 | 0 | 68 | 66 | 2 | 6 | 6 | 6 | 33 | 32 | 0 |
| | | | | | | 6 | 6 | 8 | 49 | 48 | 1 |
| | | H = 6 | | | | | | H = 7 | | | |
| 6 | 0 | 0 | 41 | 38 | 3 | | | | | | |
| 6 | 0 | 2 | 98 | 100 | 2 | 7 | 7 | 2 | 16 | 19 | 3 |
| 6 | 0 | 4 | 47 | 51 | 4 | 7 | 6 | 5 | 10 | 5 | 5 |
| 6 | 0 | 6 | 42 | 44 | 2 | 7 | 6 | 4 | 10 | 4 | 6 |
| 6 | 0 | 8 | 13 | 6 | 7 | 7 | 6 | 0 | 14 | 19 | 5 |
| 6 | 0 | 10 | 57 | 57 | 0 | 7 | 5 | 3 | 16 | 17 | 1 |
| 6 | 1 | 12 | 15 | 11 | 3 | 7 | 5 | 8 | 0 | 1 | 0 |
| 6 | 1 | 8 | 25 | 23 | 2 | 7 | 4 | 9 | 11 | 6 | 5 |
| 6 | 1 | 6 | 15 | 14 | 1 | 7 | 4 | 6 | 19 | 21 | 2 |
| 6 | 1 | 4 | 14 | 16 | 1 | 7 | 4 | 5 | 10 | 11 | 1 |
| 6 | 1 | 2 | 11 | 9 | 2 | 7 | 4 | 3 | 22 | 22 | 0 |
| 6 | 1 | 1 | 9 | 8 | 0 | 7 | 4 | 2 | 36 | 32 | 4 |
| 6 | 2 | 2 | 16 | 15 | 1 | 7 | 4 | 0 | 9 | 4 | 5 |
| 6 | 2 | 3 | 14 | 16 | 2 | 7 | 3 | 0 | 15 | 18 | 4 |
| 6 | 2 | 4 | 23 | 22 | 0 | 7 | 3 | 1 | 48 | 48 | 1 |
| 6 | 2 | 5 | 10 | 8 | 2 | 7 | 3 | 2 | 16 | 11 | 5 |
| 6 | 2 | 6 | 8 | 6 | 2 | 7 | 3 | 3 | 18 | 16 | 2 |
| 6 | 2 | 8 | 13 | 6 | 7 | 7 | 3 | 5 | 28 | 26 | 2 |
| 6 | 2 | 10 | 15 | 16 | 1 | 7 | 3 | 6 | 21 | 17 | 4 |
| 6 | 3 | 9 | 11 | 4 | 7 | 7 | 3 | 7 | 42 | 40 | 2 |
| 6 | 3 | 8 | 21 | 21 | 1 | 7 | 3 | 8 | 11 | 11 | 0 |
| 6 | 3 | 7 | 16 | 13 | 3 | 7 | 3 | 9 | 16 | 19 | 3 |
| 6 | 3 | 4 | 42 | 42 | 0 | 7 | 2 | 11 | 15 | 14 | 2 |
| 6 | 3 | 1 | 16 | 15 | 1 | 7 | 2 | 9 | 4 | 12 | 8 |
| 6 | 3 | 0 | 30 | 30 | 0 | 7 | 2 | 8 | 15 | 14 | 1 |
| 6 | 4 | 0 | 18 | 16 | 1 | 7 | 2 | 5 | 16 | 12 | 4 |
| 6 | 4 | 1 | 11 | 12 | 1 | 7 | 2 | 4 | 21 | 21 | 0 |
| 6 | 4 | 4 | 9 | 7 | 2 | 7 | 2 | 3 | 27 | 28 | 2 |
| 6 | 4 | 6 | 11 | 9 | 1 | 7 | 2 | 2 | 9 | 3 | 5 |

Structure Factors for Beryl (500°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ | h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 7 | | | | 8 | 4 | 2 | 10 | 14 | 4 |
| 7 | 2 | 0 | 16 | 17 | 1 | 8 | 4 | 4 | 17 | 10 | 7 |
| 7 | 1 | 0 | 23 | 26 | 3 | 8 | 4 | 6 | 11 | 13 | 2 |
| 7 | 1 | 1 | 25 | 26 | 1 | 8 | 4 | 8 | 14 | 10 | 4 |
| 7 | 1 | 2 | 9 | 11 | 2 | 8 | 5 | 6 | 22 | 17 | 5 |
| 7 | 1 | 3 | 34 | 32 | 1 | 8 | 5 | 5 | 12 | 9 | 3 |
| 7 | 1 | 4 | 31 | 33 | 2 | 8 | 5 | 2 | 21 | 18 | 3 |
| 7 | 1 | 5 | 26 | 25 | 1 | 8 | 6 | 0 | 9 | 1 | 9 |
| 7 | 1 | 6 | 17 | 13 | 4 | 8 | 6 | 4 | 24 | 23 | 1 |
| 7 | 1 | 7 | 18 | 15 | 3 | | | | | | |
| 7 | 1 | 8 | 19 | 18 | 1 | | | H = 9 | | | |
| 7 | 1 | 9 | 13 | 15 | 2 | 9 | 5 | 1 | 13 | 9 | 4 |
| 7 | 1 | 11 | 15 | 13 | 2 | 9 | 5 | 2 | 19 | 12 | 7 |
| 7 | 1 | 12 | 15 | 10 | 4 | 9 | 5 | 4 | 11 | 16 | 6 |
| 7 | 0 | 10 | 20 | 25 | 5 | 9 | 4 | 6 | 21 | 23 | 3 |
| 7 | 0 | 6 | 15 | 16 | 1 | 9 | 4 | 5 | 21 | 21 | 0 |
| 7 | 0 | 4 | 20 | 23 | 4 | 9 | 4 | 3 | 12 | 15 | 3 |
| 7 | 0 | 2 | 31 | 32 | 1 | 9 | 4 | 2 | 19 | 22 | 3 |
| 7 | 0 | 0 | 10 | 10 | 1 | 9 | 4 | 1 | 30 | 31 | 1 |
| | | | | | | 9 | 4 | 0 | 17 | 17 | 0 |
| | | H = 8 | | | | 9 | 3 | 0 | 16 | 16 | 0 |
| 8 | 0 | 0 | 64 | 68 | 4 | 9 | 3 | 3 | 15 | 16 | 1 |
| 8 | 0 | 2 | 36 | 35 | 1 | 9 | 3 | 4 | 22 | 21 | 1 |
| 8 | 0 | 4 | 20 | 19 | 1 | 9 | 3 | 5 | 15 | 12 | 3 |
| 8 | 0 | 6 | 48 | 45 | 3 | 9 | 3 | 7 | 12 | 6 | 6 |
| 8 | 0 | 8 | 35 | 39 | 4 | 9 | 3 | 8 | 14 | 12 | 2 |
| 8 | 1 | 8 | 18 | 18 | 0 | 9 | 2 | 9 | 13 | 12 | 1 |
| 8 | 1 | 4 | 19 | 16 | 4 | 9 | 2 | 7 | 12 | 18 | 6 |
| 8 | 1 | 3 | 16 | 15 | 1 | 9 | 2 | 6 | 15 | 22 | 6 |
| 8 | 1 | 0 | 28 | 27 | 0 | 9 | 2 | 5 | 19 | 17 | 2 |
| 8 | 2 | 0 | 13 | 12 | 1 | 9 | 2 | 3 | 18 | 16 | 2 |
| 8 | 2 | 2 | 21 | 19 | 1 | 9 | 2 | 2 | 21 | 22 | 1 |
| 8 | 2 | 4 | 26 | 25 | 0 | 9 | 2 | 1 | 24 | 23 | 1 |
| 8 | 2 | 6 | 24 | 22 | 2 | 9 | 2 | 0 | 14 | 14 | 0 |
| 8 | 2 | 8 | 12 | 9 | 2 | 9 | 1 | 1 | 15 | 15 | 1 |
| 8 | 2 | 9 | 4 | 3 | 1 | 9 | 1 | 3 | 27 | 31 | 4 |
| 8 | 3 | 9 | 17 | 17 | 0 | 9 | 1 | 4 | 18 | 15 | 3 |
| 8 | 3 | 7 | 19 | 21 | 1 | 9 | 1 | 5 | 17 | 19 | 2 |
| 8 | 3 | 6 | 11 | 11 | 0 | 9 | 1 | 9 | 11 | 13 | 2 |
| 8 | 3 | 5 | 21 | 22 | 2 | 9 | 0 | 10 | 15 | 14 | 1 |
| 8 | 3 | 3 | 26 | 25 | 1 | 9 | 0 | 6 | 29 | 28 | 1 |
| 8 | 3 | 2 | 16 | 14 | 2 | 9 | 0 | 2 | 33 | 31 | 2 |
| 8 | 3 | 1 | 28 | 29 | 1 | | | | | | |
| 8 | 4 | 0 | 15 | 16 | 0 | | | | | | |

Structure Factors for Beryl (500°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|
| | H = 10 | | | | |
| 10 | 0 | 2 | 15 | 14 | 1 |
| 10 | 0 | 4 | 15 | 20 | 4 |
| 10 | 1 | 8 | 18 | 17 | 1 |
| 10 | 1 | 7 | 31 | 35 | 4 |
| 10 | 1 | 6 | 11 | 7 | 5 |
| 10 | 1 | 5 | 27 | 27 | 0 |
| 10 | 1 | 4 | 13 | 14 | 1 |
| 10 | 1 | 3 | 25 | 22 | 3 |
| 10 | 1 | 1 | 39 | 43 | 4 |
| 10 | 1 | 0 | 32 | 32 | 0 |
| 10 | 2 | 0 | 20 | 19 | 1 |
| 10 | 2 | 1 | 12 | 5 | 8 |
| 10 | 2 | 6 | 16 | 14 | 2 |
| 10 | 3 | 6 | 13 | 4 | 9 |
| 10 | 3 | 4 | 18 | 19 | 1 |
| 10 | 3 | 3 | 17 | 14 | 3 |
| 10 | 4 | 0 | 19 | 17 | 2 |
| | H = 11 | | | | |
| 11 | 3 | 0 | 22 | 18 | 4 |
| 11 | 2 | 5 | 13 | 14 | 1 |
| 11 | 2 | 3 | 20 | 20 | 0 |
| 11 | 1 | 0 | 16 | 16 | 0 |
| 11 | 1 | 3 | 13 | 9 | 4 |
| 11 | 1 | 4 | 17 | 10 | 7 |
| 11 | 0 | 0 | 10 | 11 | 1 |
| | H = 12 | | | | |
| 12 | 0 | 2 | 26 | 26 | 0 |
| 12 | 0 | 4 | 10 | 7 | 4 |
| 12 | 1 | 2 | 14 | 16 | 2 |

Structure Factors for Beryl (800°C) h, k, l, $F_{obs}$, $F_{calc}$, and σ(F)

| h | k | l | $F_o$ | $F_c$ | σ(F) | h | k | l | $F_o$ | $F_c$ | σ(F) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 0 | | | | 2 | 2 | 0 | 18 | 20 | 2 |
| 0 | 0 | 4 | 113 | 117 | 4 | 2 | 2 | 2 | 22 | 21 | 1 |
| 0 | 0 | 6 | 127 | 127 | 0 | 2 | 2 | 4 | 94 | 92 | 2 |
| 0 | 0 | 8 | 146 | 149 | 3 | 2 | 2 | 6 | 43 | 43 | 0 |
| 0 | 0 | 10 | 11 | 12 | 1 | 2 | 2 | 8 | 25 | 24 | 1 |
| 0 | 0 | 12 | 59 | 58 | 1 | 2 | 2 | 12 | 19 | 19 | 0 |
| 0 | 0 | 14 | 36 | 36 | 0 | 2 | 2 | 14 | 14 | 14 | 0 |
| | | H = 1 | | | | | | H = 3 | | | |
| 1 | 1 | 0 | 5 | 2 | 3 | 3 | 3 | 0 | 31 | 31 | 0 |
| 1 | 1 | 2 | 116 | 113 | 2 | 3 | 3 | 2 | 60 | 61 | 1 |
| 1 | 1 | 4 | 21 | 18 | 2 | 3 | 3 | 4 | 10 | 4 | 6 |
| 1 | 1 | 6 | 65 | 67 | 2 | 3 | 3 | 6 | 56 | 57 | 1 |
| 1 | 1 | 10 | 38 | 39 | 1 | 3 | 3 | 8 | 13 | 9 | 4 |
| 1 | 1 | 14 | 16 | 17 | 1 | 3 | 3 | 10 | 19 | 21 | 2 |
| 1 | 0 | 10 | 16 | 16 | 1 | 3 | 3 | 12 | 10 | 5 | 5 |
| 1 | 0 | 8 | 16 | 17 | 1 | 3 | 2 | 12 | 17 | 15 | 1 |
| 1 | 0 | 6 | 8 | 3 | 5 | 3 | 2 | 11 | 16 | 13 | 2 |
| 1 | 0 | 4 | 37 | 35 | 1 | 3 | 2 | 10 | 12 | 11 | 1 |
| 1 | 0 | 2 | 35 | 38 | 3 | 3 | 2 | 9 | 9 | 10 | 1 |
| 1 | 0 | 0 | 49 | 52 | 2 | 3 | 2 | 8 | 25 | 25 | 0 |
| | | H = 2 | | | | 3 | 2 | 6 | 12 | 11 | 1 |
| 2 | 0 | 0 | 24 | 24 | 0 | 3 | 2 | 5 | 24 | 24 | 1 |
| 2 | 0 | 2 | 66 | 60 | 6 | 3 | 2 | 3 | 41 | 41 | 1 |
| 2 | 0 | 4 | 48 | 50 | 2 | 3 | 2 | 2 | 21 | 23 | 3 |
| 2 | 0 | 6 | 24 | 25 | 1 | 3 | 2 | 1 | 12 | 11 | 2 |
| 2 | 0 | 8 | 19 | 18 | 1 | 3 | 2 | 0 | 33 | 32 | 0 |
| 2 | 0 | 10 | 19 | 18 | 0 | 3 | 1 | 0 | 37 | 36 | 1 |
| 2 | 0 | 12 | 14 | 14 | 0 | 3 | 1 | 1 | 37 | 34 | 3 |
| 2 | 1 | 14 | 11 | 14 | 3 | 3 | 1 | 2 | 19 | 19 | 0 |
| 2 | 1 | 13 | 24 | 23 | 1 | 3 | 1 | 3 | 49 | 47 | 1 |
| 2 | 1 | 11 | 12 | 11 | 1 | 3 | 1 | 4 | 21 | 22 | 1 |
| 2 | 1 | 10 | 18 | 19 | 1 | 3 | 1 | 5 | 18 | 17 | 0 |
| 2 | 1 | 9 | 20 | 21 | 2 | 3 | 1 | 6 | 20 | 20 | 0 |
| 2 | 1 | 8 | 12 | 14 | 2 | 3 | 1 | 7 | 9 | 11 | 2 |
| 2 | 1 | 7 | 61 | 61 | 0 | 3 | 1 | 9 | 19 | 16 | 3 |
| 2 | 1 | 6 | 40 | 40 | 0 | 3 | 1 | 11 | 20 | 21 | 1 |
| 2 | 1 | 5 | 32 | 32 | 0 | 3 | 1 | 13 | 12 | 3 | 9 |
| 2 | 1 | 4 | 14 | 13 | 1 | 3 | 0 | 12 | 19 | 17 | 2 |
| 2 | 1 | 3 | 17 | 12 | 4 | 3 | 0 | 8 | 24 | 22 | 2 |
| 2 | 1 | 2 | 38 | 41 | 2 | 3 | 0 | 6 | 26 | 26 | 0 |
| 2 | 1 | 1 | 88 | 89 | 2 | 3 | 0 | 4 | 82 | 83 | 1 |
| 2 | 1 | 0 | 44 | 45 | 0 | 3 | 0 | 0 | 30 | 34 | 4 |

Structure Factors for Beryl (800°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ | h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 4 | | | | 4 | 4 | 6 | 44 | 44 | 0 |
| 4 | 0 | 0 | 35 | 37 | 2 | 4 | 4 | 10 | 16 | 13 | 2 |
| 4 | 0 | 2 | 16 | 14 | 2 | | | | | | |
| 4 | 0 | 6 | 24 | 26 | 1 | | | H = 5 | | | |
| 4 | 0 | 8 | 22 | 23 | 0 | 5 | 5 | 0 | 13 | 9 | 4 |
| 4 | 0 | 10 | 9 | 7 | 2 | 5 | 5 | 2 | 33 | 34 | 0 |
| 4 | 0 | 12 | 10 | 11 | 1 | 5 | 5 | 4 | 13 | 13 | 0 |
| 4 | 1 | 13 | 11 | 15 | 4 | 5 | 5 | 10 | 23 | 24 | 1 |
| 4 | 1 | 12 | 12 | 16 | 4 | 5 | 4 | 11 | 14 | 13 | 1 |
| 4 | 1 | 11 | 26 | 28 | 1 | 5 | 4 | 9 | 22 | 19 | 3 |
| 4 | 1 | 10 | 15 | 15 | 1 | 5 | 4 | 7 | 27 | 26 | 1 |
| 4 | 1 | 9 | 31 | 30 | 0 | 5 | 4 | 6 | 16 | 15 | 1 |
| 4 | 1 | 8 | 29 | 29 | 0 | 5 | 4 | 5 | 26 | 26 | 0 |
| 4 | 1 | 7 | 32 | 31 | 1 | 5 | 4 | 3 | 27 | 27 | 1 |
| 4 | 1 | 5 | 51 | 54 | 2 | 5 | 4 | 2 | 15 | 14 | 1 |
| 4 | 1 | 4 | 24 | 24 | 0 | 5 | 4 | 1 | 36 | 35 | 1 |
| 4 | 1 | 3 | 71 | 71 | 1 | 5 | 3 | 0 | 8 | 11 | 3 |
| 4 | 1 | 2 | 25 | 26 | 1 | 5 | 3 | 1 | 14 | 13 | 1 |
| 4 | 1 | 1 | 52 | 53 | 1 | 5 | 3 | 2 | 13 | 16 | 3 |
| 4 | 1 | 0 | 74 | 76 | 2 | 5 | 3 | 3 | 30 | 30 | 0 |
| 4 | 2 | 0 | 39 | 38 | 1 | 5 | 3 | 5 | 21 | 20 | 1 |
| 4 | 2 | 1 | 18 | 18 | 1 | 5 | 3 | 7 | 13 | 8 | 5 |
| 4 | 2 | 2 | 46 | 44 | 2 | 5 | 3 | 9 | 11 | 14 | 4 |
| 4 | 2 | 3 | 16 | 11 | 4 | 5 | 3 | 10 | 12 | 8 | 4 |
| 4 | 2 | 4 | 43 | 45 | 2 | 5 | 3 | 11 | 12 | 15 | 3 |
| 4 | 2 | 5 | 13 | 15 | 2 | 5 | 3 | 12 | 3 | 2 | 2 |
| 4 | 2 | 6 | 33 | 32 | 1 | 5 | 2 | 13 | 13 | 14 | 1 |
| 4 | 2 | 7 | 12 | 10 | 3 | 5 | 2 | 12 | 14 | 14 | 1 |
| 4 | 2 | 8 | 25 | 24 | 1 | 5 | 2 | 11 | 11 | 12 | 1 |
| 4 | 2 | 10 | 25 | 25 | 1 | 5 | 2 | 9 | 23 | 27 | 3 |
| 4 | 2 | 12 | 12 | 16 | 4 | 5 | 2 | 8 | 33 | 33 | 1 |
| 4 | 3 | 12 | 10 | 10 | 0 | 5 | 2 | 7 | 42 | 42 | 0 |
| 4 | 3 | 11 | 24 | 22 | 2 | 5 | 2 | 5 | 34 | 34 | 0 |
| 4 | 3 | 10 | 12 | 8 | 4 | 5 | 2 | 4 | 44 | 44 | 0 |
| 4 | 3 | 9 | 22 | 22 | 0 | 5 | 2 | 3 | 33 | 32 | 1 |
| 4 | 3 | 8 | 15 | 12 | 3 | 5 | 2 | 1 | 59 | 62 | 2 |
| 4 | 3 | 5 | 31 | 31 | 0 | 5 | 2 | 0 | 62 | 62 | 1 |
| 4 | 3 | 4 | 34 | 34 | 0 | 5 | 1 | 0 | 8 | 6 | 2 |
| 4 | 3 | 3 | 62 | 63 | 1 | 5 | 1 | 1 | 14 | 14 | 1 |
| 4 | 3 | 1 | 11 | 11 | 0 | 5 | 1 | 2 | 37 | 37 | 0 |
| 4 | 4 | 0 | 10 | 7 | 3 | 5 | 1 | 4 | 20 | 22 | 1 |
| 4 | 4 | 2 | 42 | 43 | 1 | 5 | 1 | 5 | 1 | 2 | 1 |
| 4 | 4 | 4 | 23 | 25 | 2 | | | | | | |

Structure Factors for Beryl (800°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ | h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 5 | | | | | | H = 7 | | | |
| 5 | 1 | 6 | 20 | 19 | 2 | | | | | | |
| 5 | 1 | 7 | 13 | 13 | 0 | 7 | 7 | 0 | 13 | 9 | 4 |
| 5 | 1 | 10 | 21 | 23 | 2 | 7 | 6 | 4 | 10 | 3 | 7 |
| 5 | 1 | 13 | 11 | 4 | 7 | 7 | 5 | 0 | 10 | 10 | 1 |
| 5 | 0 | 12 | 10 | 13 | 2 | 7 | 5 | 3 | 15 | 13 | 2 |
| 5 | 0 | 8 | 25 | 25 | 0 | 7 | 5 | 4 | 9 | 8 | 1 |
| 5 | 0 | 6 | 19 | 22 | 3 | 7 | 5 | 5 | 11 | 8 | 2 |
| 5 | 0 | 4 | 15 | 13 | 2 | 7 | 4 | 6 | 19 | 20 | 2 |
| 5 | 0 | 2 | 10 | 8 | 2 | 7 | 4 | 5 | 12 | 10 | 2 |
| 5 | 0 | 0 | 65 | 64 | 1 | 7 | 4 | 3 | 16 | 17 | 2 |
| | | | | | | 7 | 4 | 2 | 32 | 31 | 1 |
| | | H = 6 | | | | 7 | 3 | 0 | 10 | 10 | 0 |
| 6 | 0 | 0 | 35 | 35 | 0 | 7 | 3 | 1 | 42 | 43 | 1 |
| 6 | 0 | 2 | 93 | 95 | 2 | 7 | 3 | 2 | 17 | 17 | 0 |
| 6 | 0 | 4 | 47 | 49 | 2 | 7 | 3 | 3 | 17 | 15 | 2 |
| 6 | 0 | 6 | 42 | 42 | 1 | 7 | 3 | 5 | 25 | 23 | 1 |
| 6 | 0 | 10 | 54 | 55 | 1 | 7 | 3 | 6 | 19 | 19 | 1 |
| 6 | 1 | 12 | 11 | 10 | 1 | 7 | 3 | 9 | 14 | 17 | 3 |
| 6 | 1 | 8 | 24 | 25 | 1 | 7 | 2 | 9 | 10 | 13 | 3 |
| 6 | 1 | 4 | 15 | 16 | 1 | 7 | 2 | 8 | 11 | 12 | 1 |
| 6 | 1 | 1 | 9 | 6 | 3 | 7 | 2 | 5 | 10 | 9 | 1 |
| 6 | 1 | 0 | 37 | 40 | 3 | 7 | 2 | 4 | 20 | 19 | 1 |
| 6 | 2 | 2 | 13 | 13 | 0 | 7 | 2 | 4 | 24 | 26 | 2 |
| 6 | 2 | 3 | 13 | 13 | 1 | 7 | 2 | 0 | 16 | 14 | 2 |
| 6 | 2 | 4 | 23 | 22 | 1 | 7 | 1 | 0 | 23 | 19 | 4 |
| 6 | 2 | 8 | 10 | 7 | 3 | 7 | 1 | 1 | 25 | 26 | 1 |
| 6 | 2 | 10 | 15 | 13 | 2 | 7 | 1 | 3 | 28 | 31 | 3 |
| 6 | 2 | 12 | 10 | 9 | 1 | 7 | 1 | 4 | 29 | 27 | 2 |
| 6 | 3 | 8 | 20 | 18 | 2 | 7 | 1 | 5 | 25 | 25 | 0 |
| 6 | 3 | 7 | 9 | 10 | 1 | 7 | 1 | 6 | 15 | 11 | 4 |
| 6 | 3 | 4 | 38 | 37 | 1 | 7 | 1 | 7 | 18 | 16 | 2 |
| 6 | 3 | 1 | 13 | 13 | 0 | 7 | 1 | 8 | 15 | 15 | 0 |
| 6 | 3 | 0 | 28 | 25 | 2 | 7 | 1 | 9 | 11 | 14 | 3 |
| 6 | 4 | 0 | 15 | 16 | 1 | 7 | 1 | 11 | 11 | 13 | 2 |
| 6 | 4 | 8 | 9 | 7 | 2 | 7 | 1 | 12 | 12 | 7 | 5 |
| 6 | 5 | 4 | 8 | 2 | 6 | 7 | 0 | 10 | 19 | 20 | 0 |
| 6 | 5 | 2 | 12 | 13 | 1 | 7 | 0 | 6 | 16 | 15 | 1 |
| 6 | 5 | 0 | 8 | 9 | 1 | 7 | 0 | 4 | 17 | 18 | 1 |
| 6 | 6 | 0 | 69 | 71 | 2 | 7 | 0 | 2 | 28 | 26 | 1 |
| 6 | 6 | 2 | 26 | 24 | 2 | | | | | | |
| 6 | 6 | 4 | 45 | 44 | 1 | | | H = 8 | | | |
| 6 | 6 | 6 | 30 | 27 | 2 | 8 | 0 | 0 | 57 | 60 | 3 |
| 6 | 6 | 8 | 41 | 43 | 2 | 8 | 0 | 2 | 36 | 34 | 2 |

Structure Factors for Beryl (800°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ | h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 8 | | | | 9 | 3 | 4 | 12 | 12 | 0 |
| 8 | 0 | 4 | 20 | 18 | 2 | 9 | 3 | 5 | 11 | 10 | 1 |
| 8 | 0 | 6 | 44 | 40 | 3 | 9 | 2 | 9 | 11 | 8 | 3 |
| 8 | 0 | 8 | 31 | 34 | 3 | 9 | 2 | 7 | 16 | 15 | 1 |
| 8 | 0 | 10 | 13 | 13 | 1 | 9 | 2 | 6 | 15 | 15 | 0 |
| 8 | 1 | 10 | 9 | 2 | 7 | 9 | 2 | 5 | 15 | 16 | 1 |
| 8 | 1 | 9 | 12 | 7 | 4 | 9 | 2 | 3 | 11 | 14 | 3 |
| 8 | 1 | 8 | 17 | 18 | 1 | 9 | 2 | 2 | 18 | 16 | 2 |
| 8 | 1 | 4 | 16 | 18 | 1 | 9 | 2 | 1 | 22 | 19 | 3 |
| 8 | 1 | 3 | 15 | 15 | 0 | 9 | 2 | 0 | 10 | 10 | 0 |
| 8 | 1 | 2 | 8 | 5 | 3 | 9 | 1 | 1 | 15 | 14 | 1 |
| 8 | 1 | 0 | 26 | 27 | 1 | 9 | 1 | 3 | 24 | 25 | 1 |
| 8 | 2 | 0 | 11 | 11 | 0 | 9 | 1 | 4 | 21 | 21 | 0 |
| 8 | 2 | 2 | 18 | 19 | 1 | 9 | 1 | 5 | 21 | 17 | 4 |
| 8 | 2 | 4 | 20 | 23 | 3 | 9 | 0 | 10 | 10 | 13 | 4 |
| 8 | 2 | 6 | 22 | 21 | 0 | 9 | 0 | 6 | 27 | 26 | 1 |
| 8 | 2 | 10 | 9 | 7 | 2 | 9 | 0 | 2 | 31 | 30 | 1 |
| 8 | 3 | 9 | 15 | 16 | 1 | | | | | | |
| 8 | 3 | 7 | 20 | 18 | 2 | | | H = 10 | | | |
| 8 | 3 | 5 | 17 | 19 | 2 | 10 | 0 | 2 | 14 | 14 | 0 |
| 8 | 3 | 3 | 21 | 24 | 2 | 10 | 0 | 4 | 14 | 18 | 4 |
| 8 | 3 | 2 | 17 | 15 | 2 | 10 | 1 | 8 | 16 | 12 | 4 |
| 8 | 3 | 1 | 23 | 25 | 2 | 10 | 1 | 7 | 28 | 28 | 0 |
| 8 | 4 | 0 | 14 | 13 | 1 | 10 | 1 | 5 | 24 | 23 | 1 |
| 8 | 4 | 2 | 11 | 13 | 2 | 10 | 1 | 4 | 9 | 10 | 0 |
| 8 | 4 | 6 | 9 | 10 | 1 | 10 | 1 | 3 | 22 | 21 | 2 |
| 8 | 5 | 6 | 18 | 18 | 1 | 10 | 1 | 1 | 34 | 35 | 1 |
| 8 | 5 | 5 | 9 | 7 | 2 | 10 | 1 | 0 | 28 | 26 | 2 |
| 8 | 5 | 4 | 9 | 3 | 6 | 10 | 2 | 0 | 19 | 15 | 4 |
| 8 | 5 | 3 | 9 | 9 | 0 | 10 | 2 | 4 | 2 | 2 | 1 |
| 8 | 5 | 2 | 17 | 18 | 1 | 10 | 2 | 6 | 9 | 11 | 2 |
| 8 | 6 | 2 | 12 | 15 | 3 | 10 | 3 | 5 | 11 | 7 | 3 |
| 8 | 6 | 4 | 19 | 18 | 1 | 10 | 3 | 4 | 11 | 14 | 3 |
| | | | | | | 10 | 3 | 3 | 12 | 14 | 3 |
| | | H = 9 | | | | 10 | 4 | 0 | 17 | 16 | 1 |
| 9 | 5 | 2 | 13 | 16 | 4 | | | | | | |
| 9 | 4 | 6 | 17 | 17 | 0 | | | H = 11 | | | |
| 9 | 4 | 5 | 19 | 18 | 1 | 11 | 3 | 0 | 14 | 18 | 4 |
| 9 | 4 | 2 | 11 | 16 | 5 | 11 | 2 | 5 | 13 | 13 | 0 |
| 9 | 4 | 1 | 27 | 26 | 0 | 11 | 2 | 3 | 17 | 17 | 0 |
| 9 | 4 | 0 | 14 | 15 | 1 | 11 | 2 | 0 | 9 | 7 | 3 |
| 9 | 3 | 0 | 14 | 12 | 2 | 11 | 1 | 0 | 13 | 17 | 4 |
| 9 | 3 | 1 | 13 | 10 | 3 | 11 | 1 | 2 | 2 | 2 | 0 |
| 9 | 3 | 3 | 10 | 13 | 3 | | | | | | |

Structure Factors for Beryl (800°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|
| | H = 11 | | | | |
| 11 | 1 | 4 | 14 | 14 | 1 |
| 11 | 0 | 2 | 12 | 8 | 4 |
| 11 | 0 | 0 | 3 | 8 | 5 |
| | H = 12 | | | | |
| 12 | 0 | 2 | 23 | 24 | 1 |
| 12 | 1 | 2 | 12 | 16 | 4 |

Structure Factors for Beryl (24°C after heating to 800°C) h, k, l, $F_{obs}$, $F_{calc}$, and σ(F)

| h | k | l | $F_o$ | $F_c$ | σ(F) |
|---|---|---|---|---|---|
| | | H = 0 | | | |
| 0 | 0 | 4 | 114 | 124 | 10 |
| 0 | 0 | 6 | 131 | 140 | 9 |
| 0 | 0 | 8 | 162 | 170 | 8 |
| 0 | 0 | 10 | 9 | 11 | 2 |
| 0 | 0 | 12 | 78 | 78 | 0 |
| 0 | 0 | 14 | 52 | 51 | 1 |
| | | H = 1 | | | |
| 1 | 1 | 0 | 5 | 1 | 4 |
| 1 | 1 | 2 | 119 | 116 | 2 |
| 1 | 1 | 4 | 18 | 17 | 1 |
| 1 | 1 | 6 | 69 | 71 | 2 |
| 1 | 1 | 10 | 47 | 47 | 0 |
| 1 | 1 | 12 | 9 | 5 | 4 |
| 1 | 1 | 14 | 20 | 22 | 3 |
| 1 | 0 | 10 | 18 | 19 | 1 |
| 1 | 0 | 8 | 13 | 15 | 2 |
| 1 | 0 | 6 | 7 | 4 | 2 |
| 1 | 0 | 4 | 40 | 39 | 1 |
| 1 | 0 | 0 | 50 | 53 | 2 |
| | | H = 2 | | | |
| 2 | 0 | 0 | 19 | 22 | 3 |
| 2 | 0 | 2 | 70 | 63 | 7 |
| 2 | 0 | 4 | 46 | 48 | 2 |
| 2 | 0 | 6 | 28 | 27 | 1 |
| 2 | 0 | 8 | 16 | 17 | 1 |
| 2 | 0 | 10 | 26 | 26 | 0 |
| 2 | 0 | 12 | 14 | 13 | 1 |
| 2 | 0 | 14 | 10 | 9 | 1 |
| 2 | 1 | 14 | 18 | 18 | 0 |
| 2 | 1 | 13 | 31 | 30 | 1 |
| 2 | 1 | 11 | 11 | 11 | 0 |
| 2 | 1 | 10 | 20 | 22 | 2 |
| 2 | 1 | 9 | 23 | 23 | 0 |
| 2 | 1 | 8 | 18 | 19 | 2 |
| 2 | 1 | 7 | 65 | 67 | 2 |
| 2 | 1 | 6 | 39 | 41 | 2 |
| 2 | 1 | 5 | 32 | 33 | 1 |
| 2 | 1 | 4 | 17 | 17 | 0 |
| 2 | 1 | 3 | 16 | 13 | 3 |
| 2 | 1 | 2 | 37 | 42 | 5 |
| 2 | 1 | 1 | 91 | 91 | 0 |
| 2 | 1 | 0 | 49 | 47 | 2 |
| 2 | 2 | 0 | 23 | 23 | 0 |
| 2 | 2 | 2 | 25 | 23 | 3 |
| 2 | 2 | 4 | 104 | 102 | 2 |
| 2 | 2 | 6 | 48 | 49 | 1 |
| 2 | 2 | 8 | 31 | 31 | 0 |
| 2 | 2 | 12 | 28 | 27 | 1 |
| 2 | 2 | 14 | 21 | 22 | 1 |
| | | H = 3 | | | |
| 3 | 3 | 0 | 30 | 28 | 2 |
| 3 | 3 | 2 | 70 | 69 | 0 |
| 3 | 3 | 4 | 11 | 11 | 0 |
| 3 | 3 | 6 | 65 | 67 | 2 |
| 3 | 3 | 8 | 9 | 9 | 0 |
| 3 | 3 | 10 | 26 | 28 | 2 |
| 3 | 3 | 12 | 8 | 4 | 4 |
| 3 | 2 | 12 | 18 | 18 | 0 |
| 3 | 2 | 11 | 16 | 17 | 1 |
| 3 | 2 | 10 | 9 | 14 | 5 |
| 3 | 2 | 9 | 13 | 13 | 0 |
| 3 | 2 | 8 | 27 | 25 | 2 |
| 3 | 2 | 6 | 13 | 14 | 0 |
| 3 | 2 | 5 | 24 | 25 | 1 |
| 3 | 2 | 4 | 43 | 42 | 1 |
| 3 | 2 | 3 | 46 | 45 | 1 |
| 3 | 2 | 2 | 27 | 26 | 1 |
| 3 | 2 | 1 | 11 | 10 | 1 |
| 3 | 2 | 0 | 30 | 30 | 1 |
| 3 | 1 | 0 | 44 | 41 | 3 |
| 3 | 1 | 1 | 41 | 36 | 5 |
| 3 | 1 | 2 | 15 | 16 | 1 |
| 3 | 1 | 3 | 50 | 50 | 0 |
| 3 | 1 | 4 | 17 | 17 | 0 |
| 3 | 1 | 5 | 13 | 16 | 3 |
| 3 | 1 | 6 | 24 | 24 | 1 |
| 3 | 1 | 7 | 15 | 16 | 0 |
| 3 | 1 | 9 | 20 | 18 | 1 |
| 3 | 1 | 11 | 24 | 24 | 0 |
| 3 | 1 | 12 | 11 | 6 | 4 |
| 3 | 1 | 14 | 12 | 10 | 2 |

Structure Factors forBeryl(24°C after heating to 800°C) h, k, l, $F_{obs}$, $F_{calc}$, and σ(F)

| h | k | l | $F_o$ | $F_c$ | σ(F) | h | k | l | $F_o$ | $F_c$ | σ(F) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 3 | | | | 4 | 3 | 9 | 27 | 28 | 1 |
| 3 | 0 | 14 | 11 | 12 | 1 | 4 | 3 | 8 | 11 | 11 | 0 |
| 3 | 0 | 12 | 25 | 23 | 2 | 4 | 3 | 6 | 7 | 4 | 3 |
| 3 | 0 | 8 | 30 | 29 | 1 | 4 | 3 | 5 | 35 | 36 | 1 |
| 3 | 0 | 6 | 28 | 29 | 0 | 4 | 3 | 4 | 33 | 34 | 1 |
| 3 | 0 | 4 | 91 | 91 | 0 | 4 | 3 | 3 | 69 | 71 | 2 |
| 3 | 0 | 2 | 4 | 4 | 0 | 4 | 3 | 2 | 10 | 12 | 2 |
| 3 | 0 | 0 | 36 | 38 | 2 | 4 | 3 | 1 | 11 | 12 | 1 |
| | | H = 4 | | | | 4 | 4 | 2 | 51 | 52 | 1 |
| 4 | 0 | 0 | 34 | 36 | 2 | 4 | 4 | 4 | 34 | 34 | 0 |
| 4 | 0 | 2 | 18 | 15 | 3 | 4 | 4 | 6 | 55 | 56 | 1 |
| 4 | 0 | 4 | 6 | 2 | 4 | 4 | 4 | 10 | 18 | 19 | 1 |
| 4 | 0 | 6 | 30 | 30 | 0 | 4 | 4 | 12 | 11 | 10 | 2 |
| 4 | 0 | 8 | 19 | 20 | 1 | | | | | | |
| 4 | 0 | 14 | 15 | 15 | 1 | | | H = 5 | | | |
| 4 | 1 | 13 | 20 | 19 | 2 | 5 | 5 | 0 | 20 | 19 | 1 |
| 4 | 1 | 12 | 23 | 21 | 2 | 5 | 5 | 2 | 42 | 44 | 2 |
| 4 | 1 | 11 | 34 | 34 | 0 | 5 | 5 | 4 | 12 | 9 | 3 |
| 4 | 1 | 10 | 19 | 19 | 0 | 5 | 5 | 6 | 22 | 22 | 0 |
| 4 | 1 | 9 | 39 | 39 | 0 | 5 | 5 | 10 | 34 | 33 | 1 |
| 4 | 1 | 8 | 37 | 38 | 1 | 5 | 4 | 11 | 18 | 17 | 1 |
| 4 | 1 | 7 | 35 | 34 | 1 | 5 | 4 | 9 | 26 | 26 | 1 |
| 4 | 1 | 5 | 55 | 56 | 2 | 5 | 4 | 8 | 8 | 6 | 2 |
| 4 | 1 | 4 | 29 | 29 | 0 | 5 | 4 | 7 | 33 | 33 | 0 |
| 4 | 1 | 3 | 77 | 78 | 1 | 5 | 4 | 6 | 18 | 17 | 0 |
| 4 | 1 | 2 | 30 | 30 | 0 | 5 | 4 | 5 | 31 | 31 | 0 |
| 4 | 1 | 1 | 56 | 55 | 1 | 5 | 4 | 4 | 12 | 10 | 2 |
| 4 | 1 | 0 | 83 | 83 | 0 | 5 | 4 | 3 | 31 | 31 | 0 |
| 4 | 2 | 0 | 44 | 42 | 2 | 5 | 4 | 2 | 10 | 11 | 1 |
| 4 | 2 | 1 | 21 | 21 | 0 | 5 | 4 | 1 | 42 | 42 | 0 |
| 4 | 2 | 2 | 45 | 46 | 1 | 5 | 4 | 0 | 13 | 11 | 1 |
| 4 | 2 | 3 | 16 | 16 | 0 | 5 | 3 | 1 | 13 | 15 | 2 |
| 4 | 2 | 4 | 52 | 53 | 1 | 5 | 3 | 2 | 15 | 15 | 0 |
| 4 | 2 | 5 | 16 | 17 | 1 | 5 | 3 | 3 | 36 | 36 | 0 |
| 4 | 2 | 6 | 31 | 32 | 0 | 5 | 3 | 5 | 26 | 24 | 1 |
| 4 | 2 | 7 | 13 | 13 | 0 | 5 | 3 | 6 | 10 | 7 | 3 |
| 4 | 2 | 8 | 32 | 32 | 0 | 5 | 3 | 7 | 8 | 9 | 1 |
| 4 | 2 | 10 | 29 | 29 | 1 | 5 | 3 | 8 | 9 | 5 | 4 |
| 4 | 2 | 11 | 11 | 8 | 3 | 5 | 3 | 9 | 20 | 18 | 2 |
| 4 | 2 | 12 | 23 | 22 | 1 | 5 | 3 | 10 | 13 | 10 | 3 |
| 4 | 3 | 12 | 13 | 12 | 2 | 5 | 3 | 11 | 22 | 20 | 2 |
| 4 | 3 | 11 | 31 | 31 | 1 | 5 | 2 | 13 | 25 | 24 | 2 |
| 4 | 3 | 10 | 11 | 12 | 1 | 5 | 2 | 12 | 24 | 21 | 3 |

Structure Factors for Beryl (24°C after heating to 800°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ | h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 5 | | | | 6 | 2 | 1 | 11 | 12 | 1 |
| 5 | 2 | 11 | 17 | 17 | 0 | 6 | 2 | 2 | 16 | 17 | 2 |
| 5 | 2 | 10 | 7 | 0 | 7 | 6 | 2 | 3 | 15 | 15 | 0 |
| 5 | 2 | 9 | 29 | 29 | 0 | 6 | 2 | 4 | 21 | 21 | 1 |
| 5 | 2 | 8 | 43 | 42 | 1 | 6 | 2 | 6 | 8 | 6 | 2 |
| 5 | 2 | 7 | 51 | 51 | 0 | 6 | 2 | 7 | 10 | 7 | 3 |
| 5 | 2 | 5 | 42 | 41 | 1 | 6 | 2 | 8 | 9 | 5 | 4 |
| 5 | 2 | 4 | 54 | 54 | 0 | 6 | 2 | 9 | 12 | 10 | 2 |
| 5 | 2 | 3 | 34 | 34 | 0 | 6 | 2 | 10 | 19 | 19 | 0 |
| 5 | 2 | 1 | 67 | 68 | 1 | 6 | 2 | 12 | 9 | 8 | 1 |
| 5 | 2 | 0 | 72 | 83 | 1 | 6 | 3 | 10 | 8 | 5 | 3 |
| 5 | 1 | 1 | 14 | 14 | 0 | 6 | 3 | 9 | 7 | 4 | 3 |
| 5 | 1 | 2 | 35 | 35 | 1 | 6 | 3 | 8 | 23 | 25 | 2 |
| 5 | 1 | 3 | 8 | 8 | 1 | 6 | 3 | 7 | 12 | 14 | 1 |
| 5 | 1 | 4 | 26 | 28 | 2 | 6 | 3 | 4 | 48 | 48 | 0 |
| 5 | 1 | 6 | 20 | 18 | 2 | 6 | 3 | 3 | 8 | 4 | 4 |
| 5 | 1 | 7 | 14 | 14 | 0 | 6 | 3 | 2 | 7 | 2 | 5 |
| 5 | 1 | 8 | 8 | 5 | 3 | 6 | 3 | 1 | 16 | 16 | 0 |
| 5 | 1 | 10 | 25 | 26 | 1 | 6 | 3 | 0 | 33 | 33 | 0 |
| 5 | 1 | 12 | 9 | 7 | 2 | 6 | 4 | 0 | 14 | 17 | 3 |
| 5 | 0 | 12 | 16 | 15 | 0 | 6 | 4 | 1 | 11 | 10 | 1 |
| 5 | 0 | 8 | 27 | 29 | 2 | 6 | 4 | 3 | 7 | 8 | 1 |
| 5 | 0 | 6 | 24 | 27 | 3 | 6 | 4 | 4 | 9 | 9 | 0 |
| 5 | 0 | 4 | 12 | 12 | 0 | 6 | 4 | 5 | 9 | 8 | 1 |
| 5 | 0 | 2 | 14 | 13 | 1 | 6 | 4 | 6 | 14 | 13 | 1 |
| 5 | 0 | 0 | 68 | 67 | 1 | 6 | 4 | 7 | 9 | 7 | 2 |
| | | H = 6 | | | | 6 | 4 | 9 | 8 | 5 | 3 |
| 6 | 0 | 0 | 48 | 45 | 3 | 6 | 5 | 10 | 15 | 14 | 1 |
| 6 | 0 | 2 | 105 | 107 | 2 | 6 | 5 | 4 | 10 | 9 | 2 |
| 6 | 0 | 4 | 50 | 51 | 1 | 6 | 5 | 3 | 9 | 7 | 2 |
| 6 | 0 | 6 | 48 | 49 | 1 | 6 | 5 | 2 | 18 | 17 | 1 |
| 6 | 0 | 8 | 12 | 11 | 1 | 6 | 5 | 0 | 9 | 7 | 2 |
| 6 | 0 | 10 | 72 | 73 | 1 | 6 | 6 | 0 | 92 | 94 | 2 |
| 6 | 0 | 12 | 10 | 8 | 2 | 6 | 6 | 2 | 29 | 27 | 2 |
| 6 | 1 | 12 | 13 | 12 | 2 | 6 | 6 | 4 | 58 | 57 | 1 |
| 6 | 1 | 8 | 24 | 26 | 1 | 6 | 6 | 6 | 37 | 34 | 2 |
| 6 | 1 | 7 | 10 | 7 | 3 | 6 | 6 | 8 | 62 | 63 | 1 |
| 6 | 1 | 6 | 14 | 14 | 0 | | | | | | |
| 6 | 1 | 4 | 13 | 13 | 0 | | | H = 7 | | | |
| 6 | 1 | 1 | 8 | 8 | 0 | 7 | 7 | 2 | 19 | 19 | 1 |
| 6 | 1 | 0 | 39 | 38 | 0 | 7 | 7 | 4 | 9 | 7 | 1 |
| 6 | 2 | 0 | 7 | 7 | 1 | 7 | 6 | 4 | 7 | 5 | 2 |

Structure Factors for Beryl (24°C after heating to 800°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ | h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | H = 7 | | | | | | | | | |
| 7 | 6 | 3 | 8 | 8 | 1 | 7 | 1 | 9 | 22 | 20 | 1 |
| 7 | 6 | 1 | 9 | 7 | 2 | 7 | 1 | 11 | 20 | 19 | 1 |
| 7 | 6 | 0 | 18 | 18 | 0 | 7 | 0 | 12 | 7 | 8 | 0 |
| 7 | 5 | 0 | 8 | 8 | 0 | 7 | 0 | 10 | 26 | 27 | 1 |
| 7 | 5 | 3 | 17 | 18 | 1 | 7 | 0 | 8 | 7 | 3 | 4 |
| 7 | 5 | 4 | 8 | 7 | 1 | 7 | 0 | 6 | 14 | 15 | 1 |
| 7 | 5 | 5 | 11 | 10 | 1 | 7 | 0 | 4 | 25 | 26 | 1 |
| 7 | 5 | 8 | 9 | 8 | 1 | 7 | 0 | 2 | 32 | 31 | 1 |
| 7 | 4 | 9 | 10 | 9 | 1 | 7 | 0 | 0 | 7 | 6 | 1 |
| 7 | 4 | 6 | 25 | 27 | 2 | | | | | | |
| 7 | 4 | 5 | 12 | 11 | 1 | | | H = 8 | | | |
| 7 | 4 | 4 | 9 | 11 | 2 | 8 | 0 | 0 | 71 | 72 | 1 |
| 7 | 4 | 3 | 25 | 25 | 0 | 8 | 0 | 2 | 34 | 34 | 1 |
| 7 | 4 | 2 | 42 | 41 | 1 | 8 | 0 | 4 | 22 | 21 | 0 |
| 7 | 4 | 0 | 9 | 5 | 4 | 8 | 0 | 6 | 49 | 49 | 0 |
| 7 | 3 | 0 | 18 | 17 | 1 | 8 | 0 | 8 | 41 | 42 | 1 |
| 7 | 3 | 1 | 52 | 53 | 1 | 8 | 0 | 10 | 12 | 11 | 1 |
| 7 | 3 | 2 | 14 | 15 | 1 | 8 | 1 | 11 | 11 | 10 | 2 |
| 7 | 3 | 3 | 17 | 16 | 1 | 8 | 1 | 9 | 8 | 7 | 1 |
| 7 | 3 | 4 | 7 | 5 | 2 | 8 | 1 | 8 | 17 | 20 | 4 |
| 7 | 3 | 5 | 31 | 30 | 1 | 8 | 1 | 6 | 9 | 11 | 2 |
| 7 | 3 | 6 | 21 | 21 | 0 | 8 | 1 | 4 | 19 | 18 | 1 |
| 7 | 3 | 7 | 46 | 48 | 2 | 8 | 1 | 3 | 17 | 17 | 0 |
| 7 | 3 | 8 | 9 | 10 | 0 | 8 | 1 | 2 | 10 | 10 | 1 |
| 7 | 3 | 9 | 20 | 21 | 1 | 8 | 1 | 0 | 31 | 29 | 1 |
| 7 | 2 | 11 | 17 | 17 | 0 | 8 | 2 | 0 | 17 | 16 | 1 |
| 7 | 2 | 10 | 8 | 5 | 2 | 8 | 2 | 2 | 26 | 26 | 0 |
| 7 | 2 | 9 | 13 | 15 | 2 | 8 | 2 | 4 | 33 | 33 | 0 |
| 7 | 2 | 8 | 15 | 13 | 1 | 8 | 2 | 5 | 7 | 0 | 7 |
| 7 | 2 | 5 | 14 | 13 | 1 | 8 | 2 | 6 | 27 | 29 | 1 |
| 7 | 2 | 4 | 20 | 21 | 1 | 8 | 2 | 8 | 11 | 13 | 2 |
| 7 | 2 | 3 | 32 | 31 | 1 | 8 | 2 | 10 | 12 | 11 | 1 |
| 7 | 2 | 2 | 9 | 7 | 2 | 8 | 3 | 9 | 21 | 21 | 0 |
| 7 | 2 | 0 | 17 | 15 | 2 | 8 | 3 | 7 | 25 | 25 | 0 |
| 7 | 1 | 0 | 29 | 28 | 1 | 8 | 3 | 6 | 14 | 12 | 2 |
| 7 | 1 | 1 | 30 | 30 | 0 | 8 | 3 | 5 | 22 | 24 | 3 |
| 7 | 1 | 2 | 13 | 13 | 0 | 8 | 3 | 4 | 8 | 7 | 1 |
| 7 | 1 | 3 | 34 | 37 | 3 | 8 | 3 | 3 | 27 | 28 | 1 |
| 7 | 1 | 4 | 35 | 37 | 1 | 8 | 3 | 2 | 15 | 16 | 1 |
| 7 | 1 | 5 | 28 | 30 | 1 | 8 | 3 | 1 | 32 | 31 | 0 |
| 7 | 1 | 6 | 16 | 17 | 1 | 8 | 4 | 0 | 15 | 17 | 1 |
| 7 | 1 | 7 | 18 | 20 | 2 | 8 | 4 | 2 | 15 | 16 | 1 |
| 7 | 1 | 8 | 23 | 22 | 1 | 8 | 4 | 3 | 8 | 4 | 4 |

Structure Factors for Beryl (24°C after heating to 800°C) h, k, l, $F_{obs}$, $F_{calc}$, and $\sigma(F)$

| h | k | l | $F_o$ | $F_c$ | $\sigma(F)$ |
|---|---|---|---|---|---|
| | H = 11 | | | | |
| 11 | 2 | 1 | 9 | 8 | 1 |
| 11 | 2 | 0 | 11 | 11 | 0 |
| 11 | 1 | 0 | 19 | 20 | 1 |
| 11 | 1 | 3 | 12 | 11 | 1 |
| 11 | 1 | 4 | 15 | 15 | 0 |
| 11 | 1 | 6 | 7 | 7 | 0 |
| 11 | 0 | 2 | 12 | 9 | 3 |
| 11 | 0 | 0 | 10 | 13 | 4 |
| | H = 12 | | | | |
| 12 | 0 | 0 | 13 | 13 | 0 |
| 12 | 0 | 2 | 33 | 34 | 1 |
| 12 | 1 | 2 | 19 | 20 | 1 |
| 12 | 1 | 1 | 10 | 10 | 0 |
| 12 | 1 | 0 | 13 | 13 | 0 |