AM-95-593

Crystal structure and twinning of $Sb_2AsS_2$, the synthetic analogue of paakkonenite

P. Bonazzi, D. Borrini, F. Mazzi, F. Olmi

For deposit: Table 4

American Mineralogist, 80, 9-10, 1054-1058.

Table 4. List of observed and calculated structure factors for synthetic $Sb_2AsS_2$.

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| -2 | 0 | 1 | 66.0 | 61.1 |
| -4 | 0 | 2 | 470.8 | 468.8 |
| -6 | 0 | 3 | 102.9 | 102.3 |
| -8 | 0 | 4 | 244.4 | 235.6 |
| -10 | 0 | 5 | 86.1 | 83.5 |
| -12 | 0 | 6 | 96.6 | 90.5 |
| -14 | 0 | 7 | 44.2 | 47.4 |
| 0 | 0 | 1 | 21.1 | 24.4 |
| 2 | 0 | 0* | .7 | 50.4 |
| -2 | 0 | 2* | 25.1 | 46.4 |
| -4 | 0 | 1 | 58.4 | 72.7 |
| -4 | 0 | 3 | 79.1 | 77.2 |
| -6 | 0 | 4 | 45.9 | 55.9 |
| -6 | 0 | 2 | 53.1 | 62.4 |
| -8 | 0 | 3 | 80.9 | 73.4 |
| -8 | 0 | 5 | 78.5 | 76.2 |
| -10 | 0 | 6 | 43.2 | 49.2 |
| -10 | 0 | 4 | 58.0 | 55.1 |
| -12 | 0 | 7 | 57.1 | 47.0 |
| -12 | 0 | 5 | 48.9 | 45.7 |
| -14 | 0 | 8* | .0 | 32.7 |
| -14 | 0 | 6* | 44.3 | 36.6 |
| 0 | 0 | 2 | 38.6 | 38.0 |
| -2 | 0 | 3 | 267.9 | 271.7 |
| 2 | 0 | 1 | 260.5 | 267.6 |
| 4 | 0 | 0 | 39.1 | 40.6 |
| -4 | 0 | 4 | 37.6 | 39.6 |
| -6 | 0 | 5 | 189.5 | 189.1 |
| -6 | 0 | 1 | 173.3 | 178.9 |
| -8 | 0 | 6* | 42.3 | 34.3 |
| -8 | 0 | 2* | 44.4 | 36.3 |
| -10 | 0 | 3 | 96.7 | 99.7 |
| -10 | 0 | 7 | 112.7 | 110.0 |
| -12 | 0 | 4* | 29.7 | 22.7 |
| -12 | 0 | 8* | 30.1 | 20.8 |
| -14 | 0 | 5 | 57.9 | 52.7 |
| -14 | 0 | 9 | 58.1 | 59.0 |
| 0 | 0 | 3* | 8.1 | 3.3 |
| 2 | 0 | 2 | 58.2 | 63.4 |
| -2 | 0 | 4 | 55.7 | 57.0 |
| -4 | 0 | 5* | 14.8 | 13.6 |
| 4 | 0 | 1* | 15.7 | 14.6 |
| -6 | 0 | 6 | 80.6 | 85.8 |
| 6 | 0 | 0 | 92.1 | 95.6 |
| -8 | 0 | 1* | .0 | 8.3 |
| -8 | 0 | 7* | 15.7 | 7.4 |
| -10 | 0 | 2 | 92.4 | 85.7 |
| -10 | 0 | 8 | 78.3 | 77.7 |
| -12 | 0 | 3* | 20.0 | 5.4 |
| -12 | 0 | 9* | 17.4 | 5.9 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| 0 | 0 | 4 | 51.7 | 43.7 |
| -2 | 0 | 5 | 45.7 | 41.8 |
| 2 | 0 | 3 | 50.1 | 45.0 |
| -4 | 0 | 6 | 74.7 | 74.7 |
| 4 | 0 | 2 | 67.4 | 66.8 |
| -6 | 0 | 7 | 42.5 | 39.9 |
| 6 | 0 | 1 | 48.1 | 44.4 |
| 8 | 0 | 0 | 65.4 | 70.9 |
| -8 | 0 | 8 | 77.8 | 78.6 |
| -10 | 0 | 9* | 15.4 | 26.8 |
| -10 | 0 | 1* | 30.5 | 29.2 |
| -12 | 0 | 10 | 51.1 | 54.2 |
| -12 | 0 | 2 | 45.5 | 48.9 |
| 0 | 0 | 5 | 363.5 | 365.8 |
| 2 | 0 | 4 | 66.5 | 74.3 |
| -2 | 0 | 6 | 61.5 | 67.4 |
| 4 | 0 | 3 | 296.6 | 292.3 |
| -4 | 0 | 7 | 295.1 | 289.8 |
| -6 | 0 | 8 | 75.6 | 73.2 |
| 6 | 0 | 2 | 85.3 | 79.3 |
| -8 | 0 | 9 | 152.9 | 161.0 |
| 8 | 0 | 1 | 169.8 | 165.7 |
| 10 | 0 | 0 | 66.5 | 63.1 |
| -10 | 0 | 10 | 64.3 | 62.2 |
| -12 | 0 | 11 | 55.3 | 69.5 |
| -12 | 0 | 1 | 80.9 | 74.6 |
| 0 | 0 | 6 | 51.9 | 56.9 |
| -2 | 0 | 7 | 47.5 | 33.6 |
| 2 | 0 | 5 | 43.9 | 37.1 |
| -4 | 0 | 8 | 61.9 | 60.1 |
| 4 | 0 | 4 | 59.7 | 56.6 |
| -6 | 0 | 9 | 59.4 | 62.8 |
| 6 | 0 | 3 | 59.6 | 67.3 |
| 8 | 0 | 2 | 49.9 | 48.1 |
| -8 | 0 | 10 | 55.6 | 51.5 |
| 10 | 0 | 1* | 47.8 | 58.0 |
| -10 | 0 | 11* | 44.5 | 54.1 |
| 12 | 0 | 0* | 23.3 | 32.4 |
| -12 | 0 | 12* | 23.3 | 34.1 |
| 0 | 0 | 7 | 99.2 | 100.1 |
| 2 | 0 | 6 | 249.7 | 247.7 |
| -2 | 0 | 8 | 249.7 | 248.9 |
| -4 | 0 | 9 | 89.0 | 88.7 |
| 4 | 0 | 5 | 98.0 | 95.3 |
| -6 | 0 | 10 | 162.8 | 167.5 |
| 6 | 0 | 4 | 163.4 | 164.0 |
| -8 | 0 | 11 | 57.4 | 63.0 |
| 8 | 0 | 3 | 71.7 | 69.7 |
| 10 | 0 | 2 | 74.9 | 78.0 |
| -10 | 0 | 12 | 77.3 | 82.7 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| 12 | 0 | 1 | 37.0 | 35.2 |
| -12 | 0 | 13 | 22.9 | 31.5 |
| 0 | 0 | 8* | 2.7 | 33.1 |
| 2 | 0 | 7 | 77.9 | 79.8 |
| -2 | 0 | 9 | 80.7 | 85.4 |
| 4 | 0 | 6* | 21.5 | 23.0 |
| -4 | 0 | 10* | 10.7 | 22.2 |
| -6 | 0 | 11 | 69.3 | 76.0 |
| 6 | 0 | 5 | 61.8 | 68.0 |
| 8 | 0 | 4* | 15.7 | 3.5 |
| -8 | 0 | 12* | 7.4 | 3.8 |
| -10 | 0 | 13* | 48.6 | 53.5 |
| 10 | 0 | 3* | 42.2 | 50.1 |
| 12 | 0 | 2s | 23.6 | 2.1 |
| 0 | 0 | 9 | 68.3 | 63.7 |
| -2 | 0 | 10* | 17.0 | 18.7 |
| 2 | 0 | 8* | 8.1 | 16.9 |
| 4 | 0 | 7 | 61.9 | 60.4 |
| -4 | 0 | 11 | 65.5 | 62.3 |
| 6 | 0 | 6* | 29.9 | 29.9 |
| -6 | 0 | 12* | 34.1 | 32.2 |
| -8 | 0 | 13* | 48.9 | 53.4 |
| 8 | 0 | 5* | 47.5 | 50.2 |
| 10 | 0 | 4* | 18.4 | 21.4 |
| -10 | 0 | 14* | 13.5 | 23.3 |
| 0 | 0 | 10 | 77.7 | 76.2 |
| 2 | 0 | 9* | 27.1 | 22.2 |
| -2 | 0 | 11* | 29.5 | 20.5 |
| -4 | 0 | 12 | 66.3 | 68.5 |
| 4 | 0 | 8 | 72.4 | 71.8 |
| 6 | 0 | 7* | 36.1 | 22.6 |
| -6 | 0 | 13* | 32.4 | 21.3 |
| -8 | 0 | 14* | 31.8 | 54.1 |
| 8 | 0 | 6* | 53.9 | 59.4 |
| 10 | 0 | 5* | 32.8 | 25.0 |
| -10 | 0 | 15* | 30.9 | 25.7 |
| 0 | 0 | 11 | 29.3 | 28.5 |
| -2 | 0 | 12 | 46.6 | 23.3 |
| 2 | 0 | 10 | 44.0 | 26.0 |
| -4 | 0 | 13* | 17.9 | 37.7 |
| 4 | 0 | 9* | 32.8 | 42.1 |
| 6 | 0 | 8 | 40.4 | 33.9 |
| -6 | 0 | 14 | 43.5 | 32.0 |
| 8 | 0 | 7* | 27.2 | 47.5 |
| -8 | 0 | 15* | 20.5 | 42.4 |
| 0 | 0 | 12 | 89.6 | 86.7 |
| -2 | 0 | 13 | 122.2 | 119.0 |
| 2 | 0 | 11 | 122.6 | 117.8 |
| -4 | 0 | 14 | 70.7 | 74.7 |
| 4 | 0 | 10 | 77.7 | 80.9 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| -6 | 0 | 15 | 72.5 | 80.4 |
| 6 | 0 | 9 | 79.9 | 78.0 |
| 8 | 0 | 8 | 52.5 | 55.9 |
| -8 | 0 | 16 | 32.7 | 50.0 |
| 0 | 0 | 13 | 42.6 | 33.0 |
| -2 | 0 | 14 | 61.5 | 64.4 |
| 2 | 0 | 12 | 62.3 | 62.2 |
| 4 | 0 | 11* | .0 | 22.6 |
| -4 | 0 | 15* | 32.3 | 24.0 |
| -6 | 0 | 16 | 46.6 | 54.5 |
| 6 | 0 | 10 | 51.0 | 50.4 |
| 0 | 0 | 14* | .0 | 50.8 |
| -2 | 0 | 15 | 35.1 | 36.3 |
| 2 | 0 | 13 | 41.6 | 36.3 |
| -4 | 0 | 16* | .0 | 44.0 |
| 4 | 0 | 12* | 34.9 | 45.3 |
| 1 | 1 | 0 | 115.1 | 119.8 |
| -1 | 1 | 1 | 114.9 | 116.5 |
| -3 | 1 | 1 | 101.0 | 104.2 |
| -3 | 1 | 2 | 96.1 | 99.8 |
| -5 | 1 | 2 | 110.7 | 113.5 |
| -5 | 1 | 3 | 97.7 | 103.5 |
| -7 | 1 | 4 | 71.8 | 75.6 |
| -7 | 1 | 3 | 83.4 | 82.6 |
| -9 | 1 | 5 | 75.4 | 75.4 |
| -9 | 1 | 4 | 86.8 | 84.5 |
| -11 | 1 | 6 | 54.0 | 51.8 |
| -11 | 1 | 5 | 60.0 | 57.9 |
| -13 | 1 | 7 | 51.7 | 46.2 |
| -13 | 1 | 6 | 53.7 | 50.9 |
| -1 | 1 | 2 | 47.2 | 51.3 |
| 1 | 1 | 1 | 47.0 | 50.1 |
| 3 | 1 | 0* | 3.2 | 9.4 |
| -3 | 1 | 3* | 18.6 | 10.4 |
| -5 | 1 | 4 | 86.9 | 88.1 |
| -5 | 1 | 1 | 85.0 | 85.8 |
| -7 | 1 | 5* | 22.1 | 25.1 |
| -7 | 1 | 2* | 16.6 | 23.4 |
| -9 | 1 | 6 | 83.3 | 80.1 |
| -9 | 1 | 3 | 75.1 | 76.5 |
| -11 | 1 | 4* | 17.9 | 16.5 |
| -11 | 1 | 7* | 16.4 | 16.8 |
| -13 | 1 | 8 | 51.7 | 51.5 |
| -13 | 1 | 5 | 48.6 | 47.9 |
| -1 | 1 | 3 | 367.3 | 360.9 |
| 1 | 1 | 2 | 365.7 | 368.4 |
| -3 | 1 | 4 | 264.3 | 260.6 |
| 3 | 1 | 1 | 259.7 | 255.2 |
| -5 | 1 | 5 | 301.6 | 294.3 |
| 5 | 1 | 0 | 306.4 | 299.6 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| -7 | 1 | 6 | 114.4 | 111.8 |
| -7 | 1 | 1 | 115.6 | 111.1 |
| -9 | 1 | 7 | 175.9 | 173.0 |
| -9 | 1 | 2 | 184.4 | 176.0 |
| -11 | 1 | 8 | 34.1 | 27.4 |
| -11 | 1 | 3 | 36.4 | 29.2 |
| -13 | 1 | 4 | 83.3 | 80.4 |
| -13 | 1 | 9 | 70.2 | 78.5 |
| 1 | 1 | 3* | 16.5 | 36.5 |
| -1 | 1 | 4* | 24.4 | 40.8 |
| 3 | 1 | 2 | 68.0 | 61.0 |
| -3 | 1 | 5 | 71.4 | 62.1 |
| -5 | 1 | 6 | 49.5 | 57.0 |
| 5 | 1 | 1 | 47.9 | 58.0 |
| 7 | 1 | 0 | 71.1 | 66.6 |
| -7 | 1 | 7 | 77.9 | 69.0 |
| -9 | 1 | 8 | 55.0 | 52.9 |
| -9 | 1 | 1 | 62.2 | 56.0 |
| -11 | 1 | 2 | 48.8 | 49.6 |
| -11 | 1 | 9 | 50.9 | 50.6 |
| -13 | 1 | 10* | 34.7 | 32.2 |
| -13 | 1 | 3* | 47.2 | 34.6 |
| 1 | 1 | 4 | 194.4 | 194.3 |
| -1 | 1 | 5 | 202.5 | 206.0 |
| 3 | 1 | 3 | 196.2 | 195.4 |
| -3 | 1 | 6 | 192.5 | 187.0 |
| 5 | 1 | 2 | 137.7 | 136.6 |
| -5 | 1 | 7 | 151.1 | 149.0 |
| 7 | 1 | 1 | 128.5 | 127.3 |
| -7 | 1 | 8 | 124.1 | 123.6 |
| -9 | 1 | 9 | 90.8 | 85.7 |
| 9 | 1 | 0 | 80.2 | 76.6 |
| -11 | 1 | 10 | 54.1 | 61.7 |
| -11 | 1 | 1 | 58.7 | 61.1 |
| -13 | 1 | 2* | 38.7 | 39.8 |
| -13 | 1 | 11* | 48.1 | 44.0 |
| -1 | 1 | 6 | 28.2 | 35.2 |
| 1 | 1 | 5 | 26.8 | 31.4 |
| -3 | 1 | 7 | 40.4 | 36.4 |
| 3 | 1 | 4 | 36.9 | 32.5 |
| -5 | 1 | 8 | 42.0 | 50.1 |
| 5 | 1 | 3 | 39.1 | 48.8 |
| 7 | 1 | 2 | 48.9 | 44.9 |
| -7 | 1 | 9 | 48.7 | 46.5 |
| -9 | 1 | 10* | 36.3 | 46.0 |
| 9 | 1 | 1* | 30.9 | 46.9 |
| -11 | 1 | 11 | 46.3 | 42.3 |
| 11 | 1 | 0 | 45.4 | 44.4 |
| -1 | 1 | 7 | 44.9 | 38.9 |
| 1 | 1 | 6 | 44.2 | 35.6 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| 3 | 1 | 5 | 63.8 | 57.1 |
| -3 | 1 | 8 | 65.4 | 58.5 |
| -5 | 1 | 9 | 35.3 | 36.7 |
| 5 | 1 | 4 | 32.9 | 33.6 |
| 7 | 1 | 3 | 58.8 | 59.9 |
| -7 | 1 | 10 | 64.4 | 63.7 |
| -9 | 1 | 11* | 28.2 | 35.1 |
| 9 | 1 | 2* | 21.2 | 32.3 |
| 11 | 1 | 1 | 39.1 | 40.2 |
| -11 | 1 | 12 | 39.0 | 43.7 |
| -1 | 1 | 8 | 144.7 | 137.5 |
| 1 | 1 | 7 | 147.3 | 145.5 |
| -3 | 1 | 9 | 100.2 | 104.7 |
| 3 | 1 | 6 | 98.2 | 99.9 |
| 5 | 1 | 5 | 140.5 | 134.8 |
| -5 | 1 | 10 | 131.2 | 128.0 |
| -7 | 1 | 11 | 35.9 | 47.7 |
| 7 | 1 | 4 | 39.8 | 48.8 |
| 9 | 1 | 3 | 94.4 | 93.3 |
| -9 | 1 | 12 | 81.9 | 88.6 |
| 11 | 1 | 2* | 22.2 | 25.3 |
| -11 | 1 | 13* | 21.5 | 22.8 |
| -1 | 1 | 9 | 36.9 | 26.0 |
| 1 | 1 | 8 | 39.0 | 24.0 |
| -3 | 1 | 10 | 61.5 | 55.4 |
| 3 | 1 | 7 | 56.7 | 58.9 |
| -5 | 1 | 11* | 19.4 | 1.9 |
| 5 | 1 | 6* | 22.0 | 1.8 |
| 7 | 1 | 5 | 57.9 | 69.6 |
| -7 | 1 | 12 | 60.1 | 65.8 |
| 9 | 1 | 4* | 9.8 | 4.1 |
| -9 | 1 | 13* | 13.7 | 4.6 |
| -11 | 1 | 14 | 35.7 | 50.0 |
| 11 | 1 | 3 | 38.7 | 52.7 |
| -1 | 1 | 10 | 147.7 | 146.9 |
| 1 | 1 | 9 | 141.2 | 133.2 |
| 3 | 1 | 8 | 152.4 | 152.7 |
| -3 | 1 | 11 | 142.7 | 140.6 |
| 5 | 1 | 7 | 83.3 | 86.3 |
| -5 | 1 | 12 | 92.5 | 96.6 |
| -7 | 1 | 13 | 87.8 | 99.3 |
| 7 | 1 | 6 | 104.7 | 106.5 |
| -9 | 1 | 14* | 39.7 | 48.1 |
| 9 | 1 | 5* | 35.4 | 43.5 |
| -1 | 1 | 11 | 69.4 | 69.1 |
| 1 | 1 | 10 | 63.5 | 62.8 |
| 3 | 1 | 9 | 47.5 | 52.0 |
| -3 | 1 | 12 | 44.8 | 51.0 |
| -5 | 1 | 13 | 61.0 | 62.3 |
| 5 | 1 | 8 | 57.1 | 55.7 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| 7 | 1 | 7* | 30.8 | 33.4 |
| -7 | 1 | 14* | 33.9 | 37.0 |
| 9 | 1 | 6 | 34.8 | 34.6 |
| -9 | 1 | 15 | 38.6 | 38.6 |
| -1 | 1 | 12* | 36.9 | 39.4 |
| 1 | 1 | 11* | 38.3 | 43.1 |
| -3 | 1 | 13* | 48.9 | 49.5 |
| 3 | 1 | 10* | 44.6 | 46.0 |
| 5 | 1 | 9* | 31.5 | 34.1 |
| -5 | 1 | 14* | 26.2 | 30.5 |
| 7 | 1 | 8 | 44.2 | 41.7 |
| -7 | 1 | 15 | 38.1 | 45.3 |
| 1 | 1 | 12* | 12.9 | 5.4 |
| -1 | 1 | 13* | 6.0 | 6.0 |
| 3 | 1 | 11* | 16.7 | 15.9 |
| -3 | 1 | 14* | 13.1 | 14.8 |
| -5 | 1 | 15* | 13.1 | 12.7 |
| 5 | 1 | 10* | 14.5 | 14.0 |
| 7 | 1 | 9* | 10.2 | 24.4 |
| -7 | 1 | 16* | 23.0 | 23.0 |
| -1 | 1 | 14* | 29.5 | 14.0 |
| 1 | 1 | 13* | 32.9 | 12.5 |
| -3 | 1 | 15* | 19.3 | 32.1 |
| 3 | 1 | 12* | 17.3 | 35.6 |
| 5 | 1 | 11* | 10.2 | 15.1 |
| -5 | 1 | 16* | 34.0 | 14.2 |
| -1 | 1 | 15 | 64.3 | 63.9 |
| 1 | 1 | 14 | 63.4 | 57.1 |
| 0 | 2 | 0 | 400.3 | 437.3 |
| -2 | 2 | 1* | 40.7 | 38.8 |
| -4 | 2 | 2 | 353.0 | 348.7 |
| -6 | 2 | 3 | 79.1 | 78.7 |
| -8 | 2 | 4 | 195.8 | 191.3 |
| -10 | 2 | 5 | 68.1 | 67.9 |
| -12 | 2 | 6 | 74.9 | 76.6 |
| 0 | 2 | 1* | 21.8 | 29.1 |
| 2 | 2 | 0* | 29.7 | 42.4 |
| -2 | 2 | 2* | 25.7 | 39.8 |
| -4 | 2 | 1 | 61.5 | 55.4 |
| -4 | 2 | 3 | 63.0 | 60.4 |
| -6 | 2 | 2 | 46.6 | 51.3 |
| -6 | 2 | 4 | 41.3 | 46.3 |
| -8 | 2 | 5 | 68.6 | 62.5 |
| -8 | 2 | 3 | 64.6 | 59.5 |
| -10 | 2 | 4 | 44.8 | 46.6 |
| -10 | 2 | 6 | 39.3 | 41.7 |
| -12 | 2 | 7* | 41.8 | 39.8 |
| -12 | 2 | 5* | 43.7 | 38.4 |
| 0 | 2 | 2 | 31.2 | 28.9 |
| -2 | 2 | 3 | 197.4 | 198.8 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| 2 | 2 | 1 | 194.8 | 195.5 |
| 4 | 2 | 0 | 33.2 | 30.8 |
| -4 | 2 | 4 | 35.4 | 30.3 |
| -6 | 2 | 5 | 147.0 | 148.4 |
| -6 | 2 | 1 | 141.3 | 140.2 |
| -8 | 2 | 2 | 38.8 | 28.3 |
| -8 | 2 | 6 | 35.1 | 27.1 |
| -10 | 2 | 7 | 93.9 | 90.9 |
| -10 | 2 | 3 | 85.5 | 82.3 |
| -12 | 2 | 8* | 7.8 | 16.7 |
| -12 | 2 | 4* | 28.5 | 18.0 |
| 0 | 2 | 3* | 17.3 | .5 |
| -2 | 2 | 4 | 44.2 | 43.6 |
| 2 | 2 | 2 | 47.0 | 48.5 |
| -4 | 2 | 5* | 2.6 | 10.3 |
| 4 | 2 | 1* | 11.5 | 10.9 |
| -6 | 2 | 6 | 68.6 | 67.2 |
| 6 | 2 | 0 | 72.9 | 74.6 |
| -8 | 2 | 1* | 15.6 | 7.8 |
| -8 | 2 | 7* | 4.1 | 7.2 |
| -10 | 2 | 2 | 72.4 | 71.0 |
| -10 | 2 | 8 | 65.0 | 64.6 |
| -12 | 2 | 9* | 8.1 | 3.4 |
| -12 | 2 | 3* | 8.8 | 3.1 |
| 0 | 2 | 4 | 38.2 | 28.7 |
| -2 | 2 | 5* | 39.7 | 34.5 |
| 2 | 2 | 3* | 37.4 | 37.1 |
| 4 | 2 | 2 | 54.3 | 49.7 |
| -4 | 2 | 6 | 57.0 | 55.4 |
| -6 | 2 | 7 | 41.1 | 35.3 |
| 6 | 2 | 1 | 41.1 | 39.2 |
| 8 | 2 | 0 | 57.9 | 57.0 |
| -8 | 2 | 8 | 63.6 | 63.0 |
| -10 | 2 | 1* | 23.7 | 26.8 |
| -10 | 2 | 9* | 26.9 | 24.5 |
| -12 | 2 | 2* | 30.4 | 41.2 |
| -12 | 2 | 10* | 44.7 | 45.6 |
| 0 | 2 | 5 | 279.9 | 278.8 |
| 2 | 2 | 4 | 55.1 | 57.2 |
| -2 | 2 | 6 | 52.4 | 52.0 |
| 4 | 2 | 3 | 237.0 | 230.7 |
| -4 | 2 | 7 | 231.1 | 228.6 |
| -6 | 2 | 8 | 61.5 | 58.6 |
| 6 | 2 | 2 | 65.8 | 63.7 |
| -8 | 2 | 9 | 127.2 | 132.5 |
| 8 | 2 | 1 | 137.1 | 136.5 |
| 10 | 2 | 0 | 53.4 | 52.0 |
| -10 | 2 | 10 | 51.1 | 51.1 |
| -12 | 2 | 1 | 68.9 | 63.8 |
| -12 | 2 | 11 | 53.5 | 59.3 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| 0 | 2 | 6 | 49.9 | 51.5 |
| 2 | 2 | 5* | 34.0 | 31.3 |
| -2 | 2 | 7* | 36.8 | 28.0 |
| 4 | 2 | 4 | 53.3 | 49.7 |
| -4 | 2 | 8 | 52.7 | 52.4 |
| 6 | 2 | 3 | 48.0 | 55.7 |
| -6 | 2 | 9 | 48.3 | 51.5 |
| 8 | 2 | 2 | 44.3 | 42.3 |
| -8 | 2 | 10 | 49.7 | 44.9 |
| 10 | 2 | 1* | 44.9 | 49.0 |
| -10 | 2 | 11* | 40.4 | 45.5 |
| 0 | 2 | 7 | 84.7 | 80.7 |
| 2 | 2 | 6 | 199.7 | 198.2 |
| -2 | 2 | 8 | 201.5 | 199.2 |
| 4 | 2 | 5 | 82.7 | 77.5 |
| -4 | 2 | 9 | 75.7 | 72.4 |
| -6 | 2 | 10 | 133.3 | 137.4 |
| 6 | 2 | 4 | 134.2 | 134.5 |
| -8 | 2 | 11 | 50.6 | 52.4 |
| 8 | 2 | 3 | 61.5 | 57.8 |
| -10 | 2 | 12 | 59.5 | 70.0 |
| 10 | 2 | 2 | 64.8 | 66.0 |
| 0 | 2 | 8* | 23.1 | 25.7 |
| 2 | 2 | 7 | 68.2 | 68.9 |
| -2 | 2 | 9 | 72.0 | 73.5 |
| 4 | 2 | 6* | 3.4 | 18.0 |
| -4 | 2 | 10* | 13.1 | 17.2 |
| -6 | 2 | 11 | 59.4 | 65.3 |
| 6 | 2 | 5 | 54.9 | 58.3 |
| -8 | 2 | 12* | 12.8 | 1.9 |
| 8 | 2 | 4* | 6.5 | 1.8 |
| -10 | 2 | 13 | 39.8 | 46.2 |
| 10 | 2 | 3 | 37.0 | 43.1 |
| 0 | 2 | 9 | 54.6 | 50.7 |
| -2 | 2 | 10* | 16.5 | 15.1 |
| 2 | 2 | 8* | 10.7 | 13.8 |
| -4 | 2 | 11 | 50.8 | 50.4 |
| 4 | 2 | 7 | 49.0 | 48.9 |
| 6 | 2 | 6* | 29.6 | 25.9 |
| -6 | 2 | 12* | 29.1 | 27.6 |
| -8 | 2 | 13 | 32.7 | 44.7 |
| 8 | 2 | 5 | 39.7 | 42.1 |
| 0 | 2 | 10 | 68.1 | 61.9 |
| 2 | 2 | 9* | 26.4 | 19.1 |
| -2 | 2 | 11* | 19.7 | 17.7 |
| 4 | 2 | 8 | 60.9 | 59.1 |
| -4 | 2 | 12 | 53.9 | 56.3 |
| 6 | 2 | 7* | 30.9 | 18.9 |
| -6 | 2 | 13* | 21.9 | 17.7 |
| 8 | 2 | 6 | 43.7 | 50.3 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| -8 | 2 | 14 | 30.5 | 45.8 |
| 0 | 2 | 11 | 30.8 | 25.7 |
| 2 | 2 | 10* | 38.4 | 22.6 |
| -2 | 2 | 12* | 42.8 | 20.3 |
| 4 | 2 | 9* | 9.8 | 37.2 |
| -4 | 2 | 13* | 23.9 | 33.3 |
| 6 | 2 | 8 | 35.8 | 28.8 |
| -6 | 2 | 14 | 36.4 | 27.0 |
| 0 | 2 | 12 | 78.0 | 74.0 |
| -2 | 2 | 13 | 102.1 | 100.6 |
| 2 | 2 | 11 | 105.3 | 99.7 |
| -4 | 2 | 14 | 56.4 | 64.0 |
| 4 | 2 | 10 | 69.6 | 69.2 |
| -6 | 2 | 15 | 59.4 | 68.7 |
| 6 | 2 | 9 | 64.6 | 66.7 |
| 0 | 2 | 13* | 25.2 | 27.6 |
| -2 | 2 | 14 | 53.6 | 56.6 |
| 2 | 2 | 12 | 59.1 | 54.7 |
| -4 | 2 | 15* | 5.8 | 20.0 |
| 4 | 2 | 11* | 25.3 | 18.9 |
| 1 | 3 | 0 | 66.5 | 68.7 |
| -1 | 3 | 1 | 66.9 | 66.9 |
| -3 | 3 | 1 | 60.1 | 61.0 |
| -3 | 3 | 2 | 58.3 | 57.9 |
| -5 | 3 | 2 | 67.9 | 70.7 |
| -5 | 3 | 3 | 65.9 | 64.5 |
| -7 | 3 | 3 | 50.6 | 51.0 |
| -7 | 3 | 4 | 47.1 | 46.2 |
| -9 | 3 | 5 | 55.7 | 52.2 |
| -9 | 3 | 4 | 60.1 | 58.5 |
| -11 | 3 | 5 | 43.0 | 40.2 |
| -11 | 3 | 6 | 32.4 | 35.9 |
| -1 | 3 | 2 | 32.2 | 34.8 |
| 1 | 3 | 1 | 33.5 | 35.8 |
| -3 | 3 | 3* | 6.9 | 2.6 |
| 3 | 3 | 0* | 9.5 | 2.6 |
| -5 | 3 | 4 | 59.8 | 59.1 |
| -5 | 3 | 1 | 58.2 | 59.3 |
| -7 | 3 | 2* | 5.3 | 11.6 |
| -7 | 3 | 5* | 17.0 | 12.3 |
| -9 | 3 | 6 | 57.6 | 56.8 |
| -9 | 3 | 3 | 57.7 | 55.2 |
| -11 | 3 | 4* | 11.9 | 9.7 |
| -11 | 3 | 7* | 9.7 | 9.9 |
| 1 | 3 | 2 | 213.6 | 215.4 |
| -1 | 3 | 3 | 211.6 | 210.9 |
| -3 | 3 | 4 | 160.7 | 160.6 |
| 3 | 3 | 1 | 159.9 | 157.3 |
| -5 | 3 | 5 | 193.0 | 188.1 |
| 5 | 3 | 0 | 195.2 | 191.7 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| -7 | 3 | 6 | 75.6 | 76.2 |
| -7 | 3 | 1 | 77.8 | 75.7 |
| -9 | 3 | 2 | 122.6 | 120.9 |
| -9 | 3 | 7 | 118.2 | 118.6 |
| -11 | 3 | 3* | 23.5 | 22.6 |
| -11 | 3 | 8* | 27.9 | 21.3 |
| -1 | 3 | 4* | 12.3 | 36.2 |
| 1 | 3 | 3* | 23.6 | 32.3 |
| 3 | 3 | 2 | 42.7 | 45.3 |
| -3 | 3 | 5 | 47.7 | 44.6 |
| -5 | 3 | 6* | 33.9 | 41.6 |
| 5 | 3 | 1* | 35.0 | 40.7 |
| 7 | 3 | 0 | 48.2 | 48.1 |
| -7 | 3 | 7 | 55.0 | 48.8 |
| -9 | 3 | 1* | 44.4 | 39.8 |
| -9 | 3 | 8* | 36.4 | 38.5 |
| -11 | 3 | 9* | 36.4 | 37.2 |
| -11 | 3 | 2* | 40.4 | 37.0 |
| -1 | 3 | 5 | 127.2 | 128.5 |
| 1 | 3 | 4 | 123.0 | 121.1 |
| -3 | 3 | 6 | 116.4 | 117.4 |
| 3 | 3 | 3 | 124.5 | 122.9 |
| 5 | 3 | 2 | 94.0 | 90.5 |
| -5 | 3 | 7 | 97.7 | 98.6 |
| 7 | 3 | 1 | 84.6 | 84.1 |
| -7 | 3 | 8 | 79.9 | 81.6 |
| 9 | 3 | 0 | 58.4 | 54.9 |
| -9 | 3 | 9 | 59.7 | 61.3 |
| 1 | 3 | 5* | 18.8 | 23.2 |
| -1 | 3 | 6* | 19.0 | 25.6 |
| -3 | 3 | 7 | 31.0 | 30.3 |
| 3 | 3 | 4 | 32.6 | 27.3 |
| 5 | 3 | 3* | 28.2 | 31.6 |
| -5 | 3 | 8* | 25.0 | 33.0 |
| -7 | 3 | 9* | 35.5 | 35.9 |
| 7 | 3 | 2* | 35.1 | 33.7 |
| 9 | 3 | 1 | 28.0 | 32.2 |
| -9 | 3 | 10 | 25.0 | 31.6 |
| -1 | 3 | 7* | 26.1 | 23.9 |
| 1 | 3 | 6* | 25.0 | 21.5 |
| -3 | 3 | 8 | 38.3 | 36.8 |
| 3 | 3 | 5 | 44.5 | 36.6 |
| 5 | 3 | 4* | 23.8 | 23.6 |
| -5 | 3 | 9* | 20.5 | 25.1 |
| 7 | 3 | 3* | 44.2 | 41.8 |
| -7 | 3 | 10* | 39.8 | 44.0 |
| 9 | 3 | 2* | 20.0 | 23.6 |
| -9 | 3 | 11* | 23.1 | 25.2 |
| -1 | 3 | 8 | 92.7 | 91.3 |
| 1 | 3 | 7 | 100.8 | 96.9 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| 3 | 3 | 6 | 66.9 | 67.3 |
| -3 | 3 | 9 | 65.8 | 70.8 |
| -5 | 3 | 10 | 85.5 | 87.1 |
| 5 | 3 | 5 | 95.8 | 92.1 |
| 7 | 3 | 4* | 30.7 | 34.5 |
| -7 | 3 | 11* | .0 | 33.8 |
| 9 | 3 | 3 | 65.8 | 66.7 |
| -9 | 3 | 12 | 49.6 | 62.9 |
| 1 | 3 | 8* | 31.9 | 20.2 |
| -1 | 3 | 9* | 25.0 | 22.1 |
| 3 | 3 | 7* | 42.5 | 44.8 |
| -3 | 3 | 10* | 45.9 | 41.8 |
| -5 | 3 | 11* | 27.4 | 4.4 |
| 5 | 3 | 6* | 14.1 | 3.9 |
| 7 | 3 | 5* | 44.9 | 52.6 |
| -7 | 3 | 12* | 43.7 | 49.4 |
| 1 | 3 | 9 | 100.7 | 93.3 |
| -1 | 3 | 10 | 107.4 | 102.9 |
| -3 | 3 | 11 | 100.3 | 98.7 |
| 3 | 3 | 8 | 109.7 | 107.4 |
| -5 | 3 | 12 | 65.8 | 69.5 |
| 5 | 3 | 7 | 60.4 | 62.1 |
| 7 | 3 | 6* | 75.7 | 76.8 |
| -7 | 3 | 13* | 52.5 | 71.4 |
| -1 | 3 | 11 | 52.8 | 51.1 |
| 1 | 3 | 10 | 53.6 | 46.7 |
| 3 | 3 | 9 | 39.2 | 40.0 |
| -3 | 3 | 12 | 36.1 | 39.5 |
| 5 | 3 | 8 | 45.2 | 41.1 |
| -5 | 3 | 13 | 42.6 | 45.9 |
| -1 | 3 | 12* | 24.5 | 28.0 |
| 1 | 3 | 11* | 9.7 | 30.7 |
| -3 | 3 | 13* | 20.4 | 36.0 |
| 3 | 3 | 10* | 29.1 | 33.5 |
| 0 | 4 | 0 | 223.9 | 227.9 |
| -2 | 4 | 1* | 25.1 | 19.5 |
| -4 | 4 | 2 | 193.8 | 190.5 |
| -6 | 4 | 3 | 45.2 | 42.5 |
| -8 | 4 | 4 | 112.0 | 113.0 |
| 0 | 4 | 1* | 31.3 | 26.6 |
| -2 | 4 | 2* | 3.3 | 29.4 |
| 2 | 4 | 0* | 20.2 | 30.5 |
| -4 | 4 | 3* | 42.0 | 38.0 |
| -4 | 4 | 1* | 39.3 | 34.0 |
| -6 | 4 | 4* | 25.5 | 31.2 |
| -6 | 4 | 2* | 29.2 | 33.9 |
| -8 | 4 | 3 | 42.2 | 35.7 |
| -8 | 4 | 5 | 42.4 | 38.5 |
| 0 | 4 | 2* | 17.1 | 13.5 |
| 2 | 4 | 1 | 101.5 | 100.5 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| -2 | 4 | 3 | 101.9 | 102.3 |
| 4 | 4 | 0* | 14.3 | 14.7 |
| -4 | 4 | 4* | 24.2 | 15.0 |
| -6 | 4 | 1 | 79.9 | 77.4 |
| -6 | 4 | 5 | 79.9 | 82.1 |
| -8 | 4 | 6* | 4.6 | 14.6 |
| -8 | 4 | 2* | 22.9 | 14.5 |
| 0 | 4 | 3* | 21.7 | 3.5 |
| -2 | 4 | 4* | 17.2 | 18.2 |
| 2 | 4 | 2* | 21.4 | 20.4 |
| 4 | 4 | 1* | 2.6 | 8.6 |
| -4 | 4 | 5* | 17.2 | 9.1 |
| -6 | 4 | 6 | 39.4 | 37.1 |
| 6 | 4 | 0 | 38.2 | 40.6 |
| -8 | 4 | 1* | 15.8 | 7.0 |
| -8 | 4 | 7* | 4.3 | 7.2 |
| 0 | 4 | 4* | 9.6 | 8.5 |
| -2 | 4 | 5* | 28.0 | 25.4 |
| 2 | 4 | 3* | 25.0 | 27.2 |
| 4 | 4 | 2* | 31.1 | 25.2 |
| -4 | 4 | 6* | 32.5 | 27.6 |
| -6 | 4 | 7 | 25.1 | 26.1 |
| 6 | 4 | 1 | 34.0 | 29.0 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| -8 | 4 | 8* | 22.7 | 36.0 |
| 8 | 4 | 0* | 35.0 | 32.8 |
| 0 | 4 | 5 | 151.2 | 153.9 |
| -2 | 4 | 6 | 26.9 | 30.8 |
| 2 | 4 | 4 | 32.7 | 33.6 |
| -4 | 4 | 7 | 127.0 | 129.8 |
| 4 | 4 | 3 | 130.9 | 131.1 |
| -6 | 4 | 8* | 24.3 | 33.5 |
| 6 | 4 | 2* | 40.6 | 36.7 |
| 0 | 4 | 6* | 26.9 | 37.1 |
| -2 | 4 | 7* | 22.8 | 19.4 |
| 2 | 4 | 5* | 22.1 | 21.7 |
| -4 | 4 | 8 | 31.6 | 37.0 |
| 4 | 4 | 4 | 34.4 | 35.6 |
| -6 | 4 | 9* | 21.2 | 31.4 |
| 6 | 4 | 3* | 29.3 | 34.5 |
| 0 | 4 | 7 | 54.3 | 47.3 |
| 2 | 4 | 6 | 119.6 | 114.9 |
| -2 | 4 | 8 | 113.3 | 115.4 |
| -4 | 4 | 9 | 43.5 | 43.1 |
| 4 | 4 | 5 | 48.2 | 45.9 |
| -6 | 4 | 10 | 73.3 | 83.0 |
| 6 | 4 | 4 | 81.2 | 81.3 |

| h | k | l | /Fo/ | /Fc/ |
|---|---|---|---|---|
| 0 | 4 | 8* | 3.0 | 12.4 |
| 2 | 4 | 7* | 49.7 | 47.0 |
| -2 | 4 | 9* | 50.4 | 49.8 |
| -4 | 4 | 10* | .0 | 7.9 |
| 4 | 4 | 6* | 20.7 | 8.5 |
| 0 | 4 | 9 | 34.8 | 29.3 |
| -2 | 4 | 10* | .0 | 9.0 |
| 2 | 4 | 8* | 6.0 | 8.5 |
| 1 | 5 | 0* | 30.5 | 29.9 |
| -1 | 5 | 1* | 28.5 | 29.6 |
| -3 | 5 | 1* | 25.8 | 27.0 |
| -3 | 5 | 2* | 33.2 | 25.0 |
| -1 | 5 | 2* | 6.9 | 23.0 |
| 1 | 5 | 1* | 1.1 | 24.7 |
| 3 | 5 | 0* | 8.4 | 7.3 |
| -3 | 5 | 3* | 16.6 | 8.0 |
| 1 | 5 | 2 | 107.4 | 105.8 |
| -1 | 5 | 3 | 105.8 | 103.3 |
| -3 | 5 | 4 | 81.3 | 81.1 |
| 3 | 5 | 1 | 81.0 | 79.3 |
| -1 | 5 | 4* | 26.4 | 26.3 |
| 1 | 5 | 3* | 26.4 | 23.5 |
| 0 | 0 | 0 | .0 | .0 |

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*Notes*:

1) both $F_o$ and $F_c$ value are referred to a twinned crystal (two components of 45% and 55% respectively).

2) reflections are sorted in order to point out the couples of twin-related indices.

3) reflections flagged with (*) are those with $I<2\sigma(I)$.