

Observed and calculated structure factors for biotite-1M crystals: A4

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
1	1	1	40.4	-40.9	-1	9	8	17.7	18.9	1	1	6	28.8	-29.5
1	1	0	28.4	31.7	-1	9	9	49.3	-48.9	1	1	4	10.0	9.8
-1	1	1	12.8	13.9	-1	9	11	13.3	-13.8	1	1	3	41.2	-40.6
-1	1	2	60.3	-63.6	1	11	0	19.3	20.6	1	1	2	79.8	-83.5
-1	1	3	77.1	-77.6	-1	11	2	26.4	-27.9	0	12	7	35.0	-37.3
-1	1	4	17.8	-17.2	-1	11	3	24.2	-25.0	0	12	4	39.8	41.4
-1	1	5	10.5	10.7	-1	11	5	18.3	18.0	0	12	3	34.1	-34.9
-1	1	7	37.3	-37.8	-1	11	7	20.1	-21.7	0	12	2	7.6	8.2
-1	1	8	15.7	-16.4	1	13	1	12.4	-11.5	0	12	1	26.8	-28.5
-1	1	11	17.2	-17.8	1	13	0	9.2	8.7	0	12	0	76.5	79.0
-1	1	12	12.8	-12.1	-1	13	3	13.9	-14.5	0	10	9	10.3	-9.9
-1	1	15	12.6	-11.5	1	13	4	11.4	11.1	0	10	7	16.8	16.6
1	3	1	9.0	9.1	1	13	2	17.9	-18.0	0	10	6	16.6	17.6
1	3	0	25.2	-22.5	1	11	6	10.1	-10.1	0	10	4	7.9	-7.7
-1	3	1	146.7	-146.0	1	11	3	14.3	-14.6	0	10	3	8.3	8.3
-1	3	2	122.0	122.0	1	11	2	18.4	-18.1	0	10	2	22.0	22.8
-1	3	3	130.7	-130.7	1	9	11	7.6	6.9	0	8	12	12.7	12.8
-1	3	4	73.4	73.3	1	9	10	24.6	25.9	0	8	11	18.2	18.2
-1	3	5	149.0	-148.5	1	9	9	42.7	-43.1	0	8	9	16.0	-16.0
-1	3	6	71.2	70.1	1	9	7	35.7	-36.2	0	8	7	26.7	27.2
-1	3	9	84.9	-82.7	1	9	6	70.4	72.8	0	8	6	29.9	31.3
-1	3	10	9.6	10.4	1	9	5	57.3	-57.6	0	8	4	11.8	-12.0
-1	3	11	10.1	-10.2	1	9	3	43.2	-43.6	0	8	2	27.4	26.1
-1	3	12	59.3	59.1	1	9	2	48.4	48.1	0	8	1	16.0	15.2
-1	3	13	62.7	-59.6	1	7	11	11.4	-12.3	0	6	13	10.9	8.0
-1	3	15	20.8	-18.7	1	7	10	17.0	-17.6	0	6	12	19.5	20.4
1	5	1	45.8	-43.4	1	7	6	12.1	-12.4	0	6	11	58.1	-56.1
1	5	0	21.3	20.1	1	7	3	24.9	-25.9	0	6	10	51.3	49.1
-1	5	1	19.5	19.3	1	7	2	35.2	-34.4	0	6	9	9.4	-10.4
-1	5	2	30.9	-30.5	1	5	11	13.5	-13.4	0	6	8	75.5	73.2
-1	5	3	45.3	-45.6	1	5	7	28.2	-28.7	0	6	7	70.2	-72.1
-1	5	4	16.4	-16.1	1	5	6	29.9	-30.9	0	6	6	11.6	11.9
-1	5	7	27.6	-27.8	1	5	5	8.5	8.6	0	6	5	20.8	18.5
-1	5	11	18.2	-18.6	1	5	4	21.7	22.7	0	6	4	88.3	87.4
-1	5	12	13.7	-12.3	1	5	3	19.2	-19.8	0	6	3	52.9	-53.7
1	7	0	28.1	28.3	1	5	2	60.0	-61.5	0	6	2	36.3	33.7

-1 7 2 49.1 -48.1 1 3 14 20.8 21.1 0 6 1 73.9 -74.0
-1 7 3 47.3 -47.4 1 3 13 50.8 -46.4 0 6 0 177.8 177.3
-1 7 5 22.0 23.6 1 3 12 12.5 12.6 0 4 12 21.7 19.0
-1 7 7 30.5 -31.3 1 3 10 25.5 24.9 0 4 11 26.3 26.2
-1 7 8 18.4 -18.7 1 3 9 77.2 -76.9 0 4 9 27.1 -27.4
1 9 1 28.3 -27.1 1 3 7 51.0 -48.9 0 4 8 10.8 -11.9
1 9 0 14.0 -13.4 1 3 6 143.8 143.0 0 4 7 42.5 42.4
-1 9 1 68.4 -65.0 1 3 5 123.9 -124.2 0 4 6 56.9 56.6
-1 9 2 84.1 82.7 1 3 4 13.3 -12.9 0 4 5 16.5 16.3
-1 9 3 38.5 -37.9 1 3 3 103.9 -103.4 0 4 4 22.4 -24.1
-1 9 4 21.4 22.2 1 3 2 69.8 68.8 0 4 3 14.6 -14.7
-1 9 5 94.4 -93.6 1 1 11 16.8 -15.5 0 4 2 28.2 29.2
-1 9 6 35.5 35.9 1 1 10 15.4 -15.9 0 4 1 41.4 41.1
-1 9 7 12.0 10.2 1 1 7 29.0 -28.4 0 4 0 47.9 46.5

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H K L /FO/ /FC/ H K L /FO/ /FC/ H K L /FO/ /FC/

0 2 15 13.5 12.7 -2 8 1 15.5 -15.8 -2 0 8 48.6 48.8
0 2 13 12.0 -10.0 2 6 12 54.7 52.3 -2 0 10 77.4 78.4
0 2 11 17.8 18.5 2 6 11 36.0 -38.0 -2 0 11 24.4 -24.5
0 2 10 12.5 12.2 2 6 10 14.2 15.3 -2 0 13 12.7 -12.9
0 2 7 34.9 34.7 2 6 9 16.6 -15.9 -2 0 14 48.3 46.2
0 2 6 21.0 21.3 2 6 8 49.3 48.5 -2 0 15 21.5 -21.1
0 2 5 11.9 -12.4 2 6 7 18.2 -18.2 -2 2 2 40.6 44.5
0 2 3 59.3 59.8 2 6 5 27.4 -27.9 -2 2 3 14.0 14.9
0 2 2 82.3 82.3 2 6 4 118.8 118.7 -2 2 4 22.7 -22.8
0 2 1 11.0 10.1 2 6 3 56.9 -58.8 -2 2 5 13.5 -14.8
0 2 0 43.5 -42.7 2 6 2 35.3 36.0 -2 2 6 29.9 31.5
0 0 15 33.1 -29.6 2 6 1 108.3 -103.3 -2 2 7 57.9 60.3
0 0 14 18.9 18.7 2 6 0 121.1 120.4 -2 2 8 25.6 27.3
0 0 13 15.3 15.1 -2 6 1 45.0 44.0 -2 2 9 25.6 -26.0
0 0 12 41.2 38.5 2 4 10 13.2 12.5 -2 2 10 17.1 -17.4
0 0 11 59.7 -59.8 2 4 7 16.8 17.7 -2 2 11 11.6 13.5
0 0 10 61.1 58.0 2 4 6 34.2 34.9 -2 2 12 27.7 29.2
0 0 9 40.3 -39.2 2 4 5 7.4 7.0 -2 2 13 11.8 10.6
0 0 8 83.8 83.2 2 4 4 19.2 -20.7 -2 4 2 11.8 12.6
0 0 7 80.1 -79.2 2 4 2 50.3 54.9 -2 4 3 47.1 47.8
0 0 6 59.9 60.3 2 4 1 49.6 52.9 -2 4 4 26.6 27.4
0 0 5 76.7 75.7 -2 4 1 27.0 -27.6 -2 4 7 19.9 20.8

0	0	4	77.7	76.7	2	2	11	27.2	25.7	-2	4	8	15.4	16.2
0	0	3	140.1	-140.2	2	2	10	22.1	22.2	-2	4	9	8.7	-8.6
0	0	2	19.6	20.3	2	2	8	28.6	-29.6	-2	4	11	15.7	17.4
0	0	1	87.8	-88.7	2	2	6	56.6	56.7	-2	4	12	15.2	15.7
0	12	6	10.6	11.0	2	2	5	44.6	46.5	-2	4	14	10.6	-10.8
1	1	13	9.3	9.1	2	2	3	25.1	-27.9	-2	6	2	26.0	24.4
1	7	7	8.6	-8.3	2	2	1	33.8	36.7	-2	6	3	91.6	-87.8
-1	11	8	10.2	-10.1	2	2	0	43.8	46.0	-2	6	4	42.1	39.2
-1	5	6	7.6	-8.1	-2	2	1	38.4	39.7	-2	6	6	104.5	101.6
2	12	5	20.8	-21.3	2	0	14	19.9	18.0	-2	6	7	79.7	-81.5
2	12	4	51.7	55.5	2	0	12	60.3	59.9	-2	6	8	39.1	39.7
2	12	3	24.4	-24.2	2	0	11	59.7	-58.8	-2	6	9	15.2	-15.7
2	12	2	18.1	18.5	2	0	10	12.1	11.4	-2	6	10	45.9	46.5
2	12	1	46.0	-48.1	2	0	9	10.5	-10.7	-2	6	11	23.5	-24.6
2	12	0	51.2	50.9	2	0	8	82.5	81.8	-2	8	2	14.4	14.5
-2	12	1	11.6	9.7	2	0	5	67.7	-69.2	-2	8	3	25.2	25.4
2	10	8	12.7	-11.0	2	0	4	150.1	149.7	-2	8	4	12.1	10.7
2	10	6	20.3	22.7	2	0	3	71.3	-72.5	-2	8	7	20.7	21.7
2	10	5	12.1	11.4	2	0	2	130.6	132.0	-2	8	8	11.4	12.4
2	10	3	10.0	-9.5	2	0	1	126.3	-124.9	-2	8	11	10.5	9.6
2	10	2	15.1	14.6	2	0	0	145.9	145.6	-2	8	12	14.7	15.4
2	10	1	18.5	17.9	-2	0	1	22.9	20.7	-2	10	2	12.0	10.7
2	8	11	12.4	11.3	-2	0	2	9.5	-8.6	-2	10	3	14.3	14.7
2	8	10	10.7	10.3	-2	0	3	66.3	-67.2	-2	10	5	7.9	-7.7
2	8	6	25.2	28.1	-2	0	4	106.2	104.3	-2	10	6	8.6	8.1
2	8	4	15.0	-14.7	-2	0	5	16.9	14.3	-2	10	7	18.0	18.6
2	8	2	26.0	25.7	-2	0	6	124.5	124.9	-2	10	8	10.8	10.3
2	8	1	29.8	30.2	-2	0	7	141.6	-144.3	-2	10	9	12.0	-11.2
1														
H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-2	12	2	11.9	12.1	3	9	9	37.7	-38.8	4	10	5	13.5	13.7
-2	12	3	45.8	-43.2	-3	11	1	12.0	11.6	4	10	3	11.8	-11.7
-2	12	4	24.7	24.8	3	11	1	21.2	-21.1	4	10	1	17.1	18.5
-2	12	6	44.2	45.4	3	11	2	9.5	-9.0	4	10	0	12.9	12.4
-2	12	7	46.2	-46.8	3	11	5	11.8	-11.6	4	8	7	8.4	-8.3
-3	1	1	21.9	24.3	3	11	6	12.3	-14.7	4	8	6	13.5	13.7
3	1	1	38.2	-41.7	-3	13	1	9.7	9.4	4	8	5	22.9	24.3

Observed and calculated structure factors for biotite-1M crystals: A4

3	1	2	37.0	-39.2	-3	11	8	11.5	-11.2	4	8	3	15.0	-13.9
3	1	5	16.2	-17.7	-3	11	3	17.3	-16.5	4	8	1	17.9	18.6
3	1	6	20.9	-21.4	-3	9	11	26.1	-27.4	4	8	0	19.5	18.4
3	1	9	12.1	-13.8	-3	9	9	55.2	-54.6	4	6	9	26.2	-26.2
3	1	10	17.1	-18.6	-3	9	8	41.7	40.6	4	6	8	44.3	43.1
3	1	12	11.6	10.4	-3	9	5	47.4	-47.1	4	6	6	37.1	37.2
-3	3	1	187.8	-180.3	-3	9	4	30.6	31.9	4	6	5	70.3	-74.3
3	3	0	75.1	75.2	-3	9	3	27.0	-27.2	4	6	4	56.8	60.1
3	3	1	34.8	-34.2	-3	9	2	33.2	31.1	4	6	3	10.3	-7.3
3	3	2	48.2	53.0	-3	7	12	13.1	-13.2	4	6	2	45.1	44.5
3	3	3	88.1	-88.1	-3	7	8	15.2	-17.2	4	6	1	49.3	-49.7
3	3	4	19.0	-18.1	-3	7	7	17.3	-17.2	4	6	0	27.3	27.1
3	3	5	11.6	-11.0	-3	7	4	17.1	-15.1	-4	6	1	17.5	14.4
3	3	6	72.3	73.4	-3	7	3	26.6	-27.5	4	4	10	16.2	17.0
3	3	7	72.1	-75.5	-3	5	8	32.3	-33.7	4	4	9	10.7	10.6
3	3	9	49.0	-49.9	-3	5	7	14.7	-15.5	4	4	8	12.4	-11.9
3	3	10	58.2	57.6	-3	5	6	23.3	24.2	4	4	7	13.1	-13.7
3	3	11	18.8	-19.8	-3	5	5	14.2	15.4	4	4	6	18.7	17.4
-3	5	1	26.5	27.6	-3	5	4	28.0	-29.1	4	4	5	32.6	33.3
3	5	0	12.2	11.6	-3	5	3	59.0	-59.7	4	4	4	11.3	12.9
3	5	1	28.3	-29.0	-3	5	2	17.1	-17.7	4	4	3	14.1	-14.5
3	5	2	32.8	-32.6	-3	3	13	20.5	-20.9	4	4	1	20.2	21.4
3	5	3	9.4	-9.3	-3	3	12	57.0	57.4	4	4	0	20.8	20.9
3	5	5	11.5	-12.6	-3	3	11	51.5	-50.0	4	2	6	25.7	27.1
3	5	6	12.5	-13.2	-3	3	9	72.9	-74.4	4	2	5	24.5	25.9
3	5	9	13.8	-13.7	-3	3	8	71.3	72.6	4	2	3	22.9	-26.0
3	5	10	16.6	-17.5	-3	3	7	13.3	-12.1	4	2	2	15.0	14.3
3	5	12	12.3	12.2	-3	3	6	19.2	-19.2	4	2	1	55.0	55.3
-3	7	1	10.4	10.7	-3	3	5	89.3	-88.7	4	2	0	34.4	37.0
3	7	0	11.1	-8.9	-3	3	4	55.9	55.1	-4	2	1	15.7	-17.2
3	7	1	33.8	-33.7	-3	3	3	36.6	-35.1	4	0	9	25.8	-25.5
3	7	2	15.3	-16.8	-3	3	2	77.7	75.5	4	0	8	46.1	46.0
3	7	3	11.3	11.4	-3	1	12	11.4	-12.2	4	0	7	13.8	-15.2
3	7	5	18.0	-17.0	-3	1	8	33.7	-36.0	4	0	6	39.9	41.5
3	7	6	21.4	-22.0	-3	1	7	19.5	-20.3	4	0	5	84.3	-83.5
3	7	10	12.9	-10.9	-3	1	6	17.0	17.5	4	0	4	102.0	103.2
-3	9	1	91.6	-89.3	-3	1	5	12.7	12.7	4	0	2	38.7	40.7
3	9	0	55.7	52.1	-3	1	4	32.5	-34.5	4	0	1	86.6	-88.8
3	9	2	30.7	29.9	-3	1	3	64.9	-67.5	4	0	0	23.8	24.3

Observed and calculated structure factors for biotite-1M crystals: A4

3	9	3	65.6	-66.0	-3	1	2	16.4	-17.7	-4	0	1	47.6	45.6
3	9	4	12.8	-11.9	-3	1	13	8.2	-8.3	-4	0	2	121.0	121.9
3	9	6	54.2	56.4	4	12	0	14.3	14.9	-4	0	3	104.4	-104.5
3	9	7	38.5	-43.1	4	10	6	11.1	11.2	-4	0	4	35.4	36.9
1														
H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-4	0	5	58.1	-60.4	-5	3	1	71.6	-68.6	-5	1	13	12.8	-12.9
-4	0	6	122.1	122.5	5	3	0	91.1	87.1	-5	1	9	20.0	-19.6
-4	0	7	29.5	-29.0	5	3	1	40.0	-39.8	-5	1	8	22.8	-23.8
-4	0	9	18.0	-18.7	5	3	2	22.6	23.5	-5	1	6	14.3	14.2
-4	0	10	49.3	50.0	5	3	3	98.8	-97.2	-5	1	4	32.7	-33.5
-4	0	11	15.5	-15.2	5	3	4	39.2	36.8	-5	1	3	22.1	-21.8
-4	0	12	13.4	15.3	5	3	5	11.7	11.3	-5	1	2	10.6	10.5
-4	0	13	36.4	-38.8	5	3	6	18.7	19.1	6	8	3	9.9	-9.9
-4	0	14	52.3	53.2	5	3	7	49.9	-50.1	6	8	1	11.5	10.8
-4	2	2	22.5	-25.1	5	3	9	14.3	-14.9	6	8	0	21.9	20.6
-4	2	3	15.9	18.6	5	5	0	21.7	-20.7	6	6	5	36.9	-39.4
-4	2	4	37.1	38.7	5	5	1	17.6	-18.3	6	6	4	12.3	10.9
-4	2	5	17.1	16.7	5	5	4	14.4	-11.2	6	6	2	43.9	43.4
-4	2	8	16.7	17.9	5	5	5	20.9	-22.1	6	6	1	37.2	-35.8
-4	2	11	9.8	9.9	5	5	7	12.8	10.4	-6	6	1	30.5	-30.8
-4	2	12	16.5	18.3	-5	7	1	13.4	12.4	6	4	5	19.2	19.2
-4	2	13	8.9	8.8	5	7	1	22.5	-21.2	6	4	4	9.0	8.9
-4	4	2	8.0	8.2	-5	9	1	54.8	-52.3	6	4	3	13.1	-13.1
-4	4	3	24.1	24.8	5	9	0	53.0	50.1	6	4	2	11.7	-12.6
-4	4	4	14.2	15.3	5	9	1	18.8	-20.1	6	4	1	18.0	17.7
-4	4	5	11.6	-13.2	5	9	2	25.3	24.4	6	4	0	30.9	31.3
-4	4	7	18.6	20.2	5	9	3	59.0	-57.5	-6	4	1	10.9	8.3
-4	4	8	33.4	34.8	5	9	4	23.3	22.7	6	2	5	15.5	17.4
-4	4	10	15.6	-17.1	-5	11	2	12.6	10.5	6	2	4	19.2	18.8
-4	4	12	13.9	15.2	-5	9	8	49.6	48.5	6	2	1	7.9	7.9
-4	4	13	14.9	15.4	-5	9	7	47.7	-47.1	6	2	0	17.4	17.7
-4	6	2	70.4	66.9	-5	9	5	26.1	-25.6	6	0	8	29.3	29.3
-4	6	3	88.0	-84.4	-5	9	4	44.9	44.2	6	0	6	59.0	57.1
-4	6	4	39.3	38.9	-5	9	3	15.4	-12.5	6	0	5	44.0	-43.5
-4	6	5	22.9	-23.1	-5	7	9	17.7	-18.2	6	0	2	49.3	49.5
-4	6	6	95.6	96.6	-5	7	8	15.2	-14.3	6	0	1	31.6	-32.0
-4	6	7	34.6	-37.0	-5	7	6	17.5	16.4	6	0	0	27.5	26.8

-4	6	8	12.1	-10.5	-5	7	4	31.5	-30.6	-6	0	1	35.8	-34.0
-4	6	9	19.7	-19.4	-5	7	3	20.1	-20.0	-6	0	2	93.7	93.8
-4	6	10	47.6	50.3	-5	7	2	11.4	11.4	-6	0	3	54.2	-54.0
-4	6	12	14.5	14.3	-5	5	10	10.2	10.1	-6	0	4	10.1	9.4
-4	8	3	15.5	16.2	-5	5	9	14.3	-13.8	-6	0	5	32.1	-31.9
-4	8	4	12.3	13.0	-5	5	8	23.8	-22.1	-6	0	6	73.5	68.8
-4	8	8	22.8	23.4	-5	5	6	9.8	9.7	-6	0	7	15.3	12.6
-4	8	10	11.8	-10.6	-5	5	4	21.9	-22.1	-6	0	9	56.3	-58.2
-4	10	3	11.6	10.4	-5	5	3	16.4	-15.3	-6	0	10	42.0	45.2
-4	10	4	15.7	14.5	-5	3	12	27.8	26.7	-6	0	12	39.1	41.2
-4	12	2	37.5	38.4	-5	3	11	45.7	-45.2	-6	2	3	8.7	8.7
-4	12	3	45.3	-45.0	-5	3	9	37.2	-37.9	-6	2	4	23.4	24.7
5	1	0	18.1	-19.9	-5	3	8	77.4	75.2	-6	2	6	11.0	-11.2
5	1	1	24.9	-25.5	-5	3	7	62.7	-61.3	-6	2	8	20.2	19.5
5	1	4	11.0	-11.7	-5	3	5	46.3	-43.9	-6	2	9	21.6	22.3
5	1	5	19.1	-20.6	-5	3	4	51.7	50.2	-6	2	11	12.2	-11.8
5	1	9	14.4	-14.4	-5	3	3	29.6	-28.3	-6	4	2	15.0	-15.8
5	1	10	9.5	-9.9	-5	3	2	18.1	-14.8	-6	4	4	19.3	19.3

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-6	4	5	16.9	16.7	7	3	0	47.3	45.3	-7	3	4	53.7	51.8
-6	6	2	86.3	84.0	7	3	1	27.1	-27.5	-7	3	3	51.5	-53.9
-6	6	3	31.8	-30.5	7	3	3	47.3	-48.6	-7	3	2	11.8	-10.9
-6	6	4	11.1	9.7	7	3	4	47.0	51.4	-7	1	9	16.6	-18.7
-6	6	5	36.6	-37.0	7	5	0	13.1	-15.0	-7	1	5	15.5	-17.0
-6	6	6	43.9	43.8	-7	5	7	10.8	10.8	-7	1	4	17.4	-18.9
-6	6	8	12.0	11.2	-7	5	5	17.1	-17.4	-7	1	7	8.8	8.7
-6	6	9	37.1	-39.0	-7	5	4	17.3	-18.6	-8	0	1	47.1	-49.5
-6	8	2	11.9	-12.9	-7	5	2	12.5	11.9	-8	0	2	44.5	42.2
-6	8	4	13.8	15.2	-7	3	8	22.5	23.3	-8	0	3	15.9	7.9
-6	8	5	10.3	10.4	-7	3	7	57.1	-61.4	-8	0	4	18.9	16.3
7	1	0	17.1	-16.7	-7	3	6	25.6	25.9	-8	0	5	35.1	-35.5
7	1	4	12.1	-13.3	-7	3	5	21.3	-20.4	-8	2	3	13.9	-14.1
-7	3	1	15.0	-12.6										