

Observed and calculated structure factors for biotite-1M crystals: CC1

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
1	1	1	38.4	-38.4	-1	9	3	35.5	-35.5	1	3	7	50.6	-50.9
1	1	0	29.5	31.9	-1	9	4	19.0	20.5	1	3	6	143.5	146.9
-1	1	1	13.9	15.3	-1	9	5	98.0	-92.8	1	3	5	121.1	-124.0
-1	1	2	62.6	-65.0	-1	9	6	35.6	35.6	1	3	4	15.2	-14.5
-1	1	3	79.1	-82.3	-1	9	7	13.0	12.8	1	3	3	103.7	-102.3
-1	1	4	16.8	-15.6	-1	9	8	15.7	17.3	1	3	2	66.9	65.3
-1	1	5	10.2	10.6	-1	9	9	50.3	-49.3	1	1	14	8.4	-7.4
-1	1	7	37.3	-39.0	-1	9	11	11.2	-11.4	1	1	13	9.6	10.7
-1	1	8	16.5	-16.3	1	11	0	20.7	21.0	1	1	11	16.4	-16.6
-1	1	11	17.6	-18.3	-1	11	2	26.1	-27.2	1	1	10	16.0	-16.0
-1	1	12	12.7	-13.0	-1	11	3	24.4	-25.1	1	1	7	28.4	-29.2
-1	1	13	6.9	6.9	-1	11	5	16.9	17.2	1	1	6	28.8	-30.1
-1	1	15	13.9	-12.2	-1	11	7	22.3	-22.6	1	1	4	10.7	10.6
-1	1	9	6.8	6.8	1	13	1	11.7	-10.9	1	1	3	41.4	-42.0
1	3	1	9.1	9.0	1	13	0	8.4	9.1	1	1	2	84.5	-87.7
1	3	0	28.3	-25.9	-1	13	1	7.8	7.0	0	12	7	36.9	-36.7
-1	3	1	146.8	-143.4	-1	13	3	15.7	-15.6	0	12	4	40.8	40.3
-1	3	2	125.6	121.8	1	13	4	12.0	11.6	0	12	3	34.7	-34.0
-1	3	3	131.0	-129.0	1	13	2	17.5	-18.6	0	12	1	24.3	-26.1
-1	3	4	71.2	71.4	1	11	6	11.1	-10.8	0	12	0	79.3	78.4
-1	3	5	149.0	-150.0	1	11	3	13.6	-14.3	0	10	9	11.9	-10.8
-1	3	6	68.8	70.8	1	11	2	17.3	-18.2	0	10	7	15.4	16.9
-1	3	7	9.2	7.4	1	9	11	10.2	10.6	0	10	6	16.9	16.9
-1	3	9	86.3	-83.8	1	9	10	28.1	26.4	0	10	2	22.3	23.5
-1	3	12	64.8	62.8	1	9	9	46.1	-43.6	0	8	12	14.1	13.1
-1	3	13	67.1	-64.6	1	9	7	35.9	-35.5	0	8	11	19.6	19.3
-1	3	15	20.4	-18.4	1	9	6	75.3	74.1	0	8	9	16.7	-17.5
1	5	1	41.6	-43.1	1	9	5	56.8	-56.8	0	8	8	8.5	-8.2
1	5	0	18.5	20.6	1	9	3	41.9	-42.1	0	8	7	27.0	27.5
-1	5	1	17.0	17.6	1	9	2	46.6	47.2	0	8	6	33.4	33.6
-1	5	2	29.4	-31.7	1	7	11	12.5	-13.2	0	8	4	11.1	-12.4
-1	5	3	44.9	-46.4	1	7	10	17.3	-17.6	0	8	2	26.1	27.0
-1	5	4	14.7	-14.5	1	7	7	9.5	-9.6	0	8	1	14.6	15.2
-1	5	6	9.3	-8.3	1	7	6	12.1	-12.7	0	6	13	10.5	10.3
-1	5	7	27.8	-29.2	1	7	3	24.7	-26.2	0	6	12	21.0	19.8
-1	5	9	7.9	8.1	1	7	2	34.2	-35.8	0	6	11	60.2	-60.2

-1	5	11	18.9	-19.8	1	5	11	15.3	-14.4	0	6	10	51.5	50.8
-1	5	12	11.2	-12.5	1	5	10	8.1	-8.2	0	6	8	75.4	74.4
-1	5	13	11.2	9.7	1	5	7	28.0	-28.7	0	6	7	70.5	-73.3
1	7	0	25.4	27.6	1	5	6	31.5	-32.0	0	6	6	9.6	8.4
-1	7	2	45.3	-46.9	1	5	5	7.6	7.7	0	6	5	22.9	21.1
-1	7	3	45.8	-48.0	1	5	4	22.2	23.0	0	6	4	88.2	87.4
-1	7	5	23.4	23.6	1	5	3	19.2	-20.6	0	6	3	50.7	-51.5
-1	7	7	30.6	-32.0	1	5	2	56.8	-60.5	0	6	2	32.6	31.8
-1	7	8	17.6	-19.6	1	3	14	23.1	23.1	0	6	1	70.4	-72.0
-1	7	11	6.8	-6.6	1	3	13	50.5	-49.5	0	6	0	176.6	175.0
1	9	1	25.4	-24.2	1	3	12	11.1	11.2	0	4	12	22.0	20.8
1	9	0	18.1	-15.7	1	3	11	14.7	13.5	0	4	11	27.0	28.2
-1	9	1	64.7	-63.9	1	3	10	26.3	25.7	0	4	9	27.6	-30.0
-1	9	2	81.9	80.4	1	3	9	81.9	-79.1	0	4	8	11.8	-12.7

1														
H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
0	4	7	43.1	44.2	2	10	2	13.8	14.9	2	0	3	72.6	-72.0
0	4	6	53.9	58.3	2	10	1	16.4	17.8	2	0	2	131.3	129.5
0	4	5	16.1	16.5	2	8	11	12.6	11.3	2	0	1	127.0	-124.2
0	4	4	23.3	-24.8	2	8	10	11.4	12.0	2	0	0	151.4	146.0
0	4	3	15.7	-14.1	2	8	6	29.9	28.8	-2	0	1	27.9	25.9
0	4	2	27.8	30.5	2	8	4	12.3	-14.1	-2	0	2	10.6	-9.3
0	4	1	40.1	39.9	2	8	2	23.8	26.5	-2	0	3	65.6	-67.1
0	4	0	48.3	47.5	2	8	1	28.8	29.4	-2	0	4	109.2	103.0
0	2	15	14.9	14.8	-2	8	1	16.4	-16.8	-2	0	5	18.4	17.1
0	2	13	13.3	-13.1	2	6	12	59.6	57.4	-2	0	6	124.4	124.4
0	2	11	19.8	19.6	2	6	11	40.2	-39.8	-2	0	7	151.5	-148.2
0	2	10	13.6	13.6	2	6	10	13.2	13.5	-2	0	8	48.7	48.8
0	2	7	32.5	34.1	2	6	9	16.2	-15.6	-2	0	10	81.2	81.6
0	2	6	19.9	21.8	2	6	8	47.2	47.7	-2	0	11	23.7	-25.5
0	2	5	12.0	-11.7	2	6	7	14.6	-16.4	-2	0	12	12.4	-12.8
0	2	3	57.0	58.9	2	6	5	25.5	-26.8	-2	0	13	11.8	-13.0
0	2	2	81.8	83.6	2	6	4	120.4	119.3	-2	0	14	49.0	48.3
0	2	1	9.0	9.3	2	6	3	57.6	-58.1	-2	0	15	22.3	-22.4
0	2	0	33.2	-35.5	2	6	2	32.5	33.5	-2	2	2	43.2	44.6
0	0	15	34.8	-32.7	2	6	1	107.6	-101.4	-2	2	3	13.8	15.9
0	0	14	19.9	17.3	2	6	0	117.3	118.8	-2	2	4	24.1	-24.2
0	0	13	19.5	18.9	-2	6	1	49.2	46.5	-2	2	5	15.3	-15.6

0	0	12	43.5	41.0	2	4	11	10.3	10.9	-2	2	6	33.9	32.6
0	0	11	65.8	-64.5	2	4	10	13.5	13.5	-2	2	7	61.0	62.4
0	0	10	61.3	59.7	2	4	8	7.3	-7.4	-2	2	8	26.0	28.0
0	0	9	39.7	-42.1	2	4	7	17.8	17.8	-2	2	9	27.8	-28.7
0	0	8	80.9	85.0	2	4	6	33.3	35.2	-2	2	10	18.5	-19.1
0	0	7	76.6	-78.8	2	4	5	7.3	7.2	-2	2	11	13.7	13.5
0	0	6	58.6	59.1	2	4	4	18.7	-20.6	-2	2	12	29.1	30.9
0	0	5	82.5	80.5	2	4	2	54.0	55.6	-2	2	13	12.8	10.8
0	0	4	76.0	76.8	2	4	1	51.0	51.7	-2	2	14	11.8	-11.3
0	0	3	137.7	-139.1	-2	4	1	25.1	-27.0	-2	4	2	10.9	12.4
0	0	2	14.6	15.9	2	2	13	10.7	-10.9	-2	4	3	47.5	48.8
0	0	1	83.3	-86.7	2	2	11	28.2	28.2	-2	4	4	27.2	27.8
0	4	14	7.8	-8.2	2	2	10	23.4	24.2	-2	4	7	19.5	20.0
1	1	8	3.0	3.1	2	2	9	11.4	-9.5	-2	4	8	15.2	16.4
1	13	3	5.5	-5.1	2	2	8	28.8	-32.0	-2	4	11	17.0	18.1
-1	3	11	7.6	-7.6	2	2	6	57.3	59.3	-2	4	12	17.5	16.2
-1	3	8	3.2	3.4	2	2	5	45.6	49.0	-2	4	14	13.4	-13.4
2	12	5	20.2	-20.8	2	2	3	27.7	-29.1	-2	6	2	21.9	22.9
2	12	4	52.8	55.5	2	2	1	34.0	35.9	-2	6	3	87.8	-86.6
2	12	3	20.4	-21.5	2	2	0	49.3	47.1	-2	6	4	38.5	37.1
2	12	2	15.3	16.4	-2	2	1	39.9	39.4	-2	6	6	104.0	100.7
2	12	1	44.6	-47.0	2	0	14	21.1	18.5	-2	6	7	78.7	-82.0
2	12	0	50.6	48.8	2	0	12	65.1	65.3	-2	6	8	39.0	39.6
-2	12	1	14.3	11.8	2	0	11	63.1	-63.7	-2	6	9	13.7	-14.7
2	10	8	12.9	-12.4	2	0	9	8.9	-9.2	-2	6	10	45.9	46.6
2	10	7	5.4	5.7	2	0	8	82.0	83.0	-2	6	11	26.2	-26.2
2	10	6	23.8	24.0	2	0	5	69.6	-69.9	-2	8	2	14.6	15.8
2	10	5	11.3	12.0	2	0	4	148.8	152.1	-2	8	3	26.3	25.5
1														
H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
-2	8	5	7.4	-7.9	3	7	10	12.2	-12.0	-3	1	12	11.9	-12.8
-2	8	7	21.5	21.7	-3	9	1	87.8	-87.5	-3	1	8	35.1	-36.6
-2	8	8	11.0	11.7	3	9	0	52.1	49.5	-3	1	7	18.9	-19.8
-2	8	12	16.1	15.8	3	9	2	28.2	28.4	-3	1	6	17.4	17.6
-2	10	2	10.3	10.3	3	9	3	65.3	-64.9	-3	1	5	11.3	12.5
-2	10	3	14.9	15.3	3	9	4	14.6	-13.7	-3	1	4	33.5	-34.4
-2	10	7	18.6	19.0	3	9	6	57.2	56.3	-3	1	3	66.0	-68.3

Observed and calculated structure factors for biotite-1M crystals: CC1

-2	10	8	12.3	11.8	3	9	7	42.8	-43.9	-3	1	2	16.0	-15.9
-2	10	9	12.0	-11.7	3	9	9	39.4	-39.5	4	12	0	15.9	13.1
-2	12	3	42.9	-41.8	-3	11	1	12.3	11.6	-4	12	1	10.7	9.8
-2	12	4	24.1	23.6	3	11	1	21.0	-21.5	4	10	5	11.7	13.5
-2	12	6	42.8	43.5	3	11	2	9.0	-8.9	4	10	1	18.5	19.1
-2	12	7	44.9	-47.3	3	11	5	12.1	-12.7	4	10	0	11.6	12.0
-3	1	1	22.5	23.8	3	11	6	12.0	-14.2	4	8	6	13.6	14.1
3	1	1	41.6	-42.5	-3	11	8	10.9	-11.0	4	8	5	26.0	26.0
3	1	2	40.5	-40.8	-3	11	7	13.0	-12.6	4	8	3	14.8	-15.4
3	1	5	17.5	-18.0	-3	11	3	17.3	-17.9	4	8	1	18.5	17.7
3	1	6	21.9	-21.3	-3	9	11	25.7	-26.5	4	8	0	19.5	19.0
3	1	9	14.1	-14.2	-3	9	9	51.8	-54.2	4	6	10	11.4	-10.1
3	1	10	18.7	-19.6	-3	9	8	40.3	40.8	4	6	9	25.6	-26.3
3	1	12	12.7	12.4	-3	9	5	47.7	-47.0	4	6	8	47.3	43.9
-3	3	1	179.3	-177.4	-3	9	4	29.4	30.6	4	6	6	36.3	37.2
3	3	0	78.6	73.7	-3	9	3	23.7	-23.9	4	6	5	77.0	-75.8
3	3	1	31.8	-32.9	-3	9	2	29.4	29.8	4	6	4	60.2	59.4
3	3	2	51.2	51.2	-3	7	12	13.1	-14.2	4	6	2	43.1	43.1
3	3	3	90.7	-87.8	-3	7	11	8.5	-8.6	4	6	1	45.7	-48.4
3	3	4	22.5	-20.5	-3	7	8	18.9	-18.3	4	6	0	25.8	25.3
3	3	5	8.1	-8.1	-3	7	7	15.9	-16.6	-4	6	1	16.1	15.8
3	3	6	71.7	73.9	-3	7	4	15.9	-15.6	4	4	10	19.0	19.3
3	3	7	77.4	-77.5	-3	7	3	27.3	-28.5	4	4	9	11.8	10.7
3	3	9	52.0	-51.9	-3	5	9	9.1	-8.5	4	4	8	14.8	-14.3
3	3	10	62.7	62.3	-3	5	8	33.1	-33.4	4	4	7	13.3	-15.0
3	3	11	22.0	-20.1	-3	5	7	15.4	-16.1	4	4	6	17.3	18.1
3	3	12	11.3	-11.5	-3	5	6	23.0	23.9	4	4	5	34.4	35.1
-3	5	1	25.0	27.4	-3	5	5	13.9	15.0	4	4	4	14.9	14.1
3	5	0	11.5	11.2	-3	5	4	27.9	-28.0	4	4	3	16.0	-15.6
3	5	1	30.4	-30.4	-3	5	3	58.8	-60.1	4	4	1	21.1	20.6
3	5	2	31.6	-33.2	-3	5	2	15.1	-16.2	4	4	0	20.7	20.9
3	5	3	8.8	-9.3	-3	3	14	10.8	-10.3	4	2	10	10.3	9.7
3	5	5	12.3	-13.3	-3	3	13	20.5	-21.2	4	2	6	26.3	27.5
3	5	6	12.8	-12.8	-3	3	12	60.2	60.9	4	2	5	26.3	26.7
3	5	9	15.0	-14.8	-3	3	11	48.8	-50.0	4	2	4	9.9	-10.2
3	5	10	17.5	-18.2	-3	3	9	72.0	-74.9	4	2	3	25.8	-27.1
-3	7	1	9.4	10.6	-3	3	8	74.2	73.1	4	2	2	13.6	14.9
3	7	0	8.4	-8.3	-3	3	7	10.6	-9.9	4	2	1	54.5	54.7
3	7	1	35.0	-33.5	-3	3	6	23.2	-20.0	4	2	0	35.7	37.1

Observed and calculated structure factors for biotite-1M crystals: CC1

3	7	2	18.0	-17.7	-3	3	5	88.5	-88.2	-4	2	1	15.1	-16.6
3	7	3	12.5	11.5	-3	3	4	55.3	53.7	4	0	9	25.2	-25.7
3	7	5	16.7	-17.3	-3	3	3	36.7	-33.8	4	0	8	42.8	45.7
3	7	6	22.2	-22.3	-3	3	2	72.4	73.0	4	0	7	14.6	-15.7
1														
H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
4	0	6	42.0	42.7	-4	10	8	12.4	13.3	-5	3	13	10.3	9.0
4	0	5	84.7	-84.1	-4	12	2	37.7	37.5	-5	3	12	27.9	28.3
4	0	4	105.7	104.2	-4	12	3	43.8	-43.8	-5	3	11	46.5	-45.9
4	0	2	38.6	38.3	5	1	0	18.1	-18.9	-5	3	9	36.4	-36.3
4	0	1	90.6	-87.9	5	1	1	24.9	-26.3	-5	3	8	76.5	75.6
4	0	0	22.0	23.3	5	1	4	11.9	-11.9	-5	3	7	57.7	-58.8
-4	0	1	50.1	47.1	5	1	5	19.5	-20.3	-5	3	5	42.8	-43.3
-4	0	2	121.7	120.7	5	1	7	10.1	10.4	-5	3	4	49.8	49.3
-4	0	3	105.8	-102.2	5	1	9	14.5	-15.8	-5	3	3	25.8	-26.7
-4	0	4	34.0	34.1	5	1	10	10.9	-10.2	-5	3	2	15.4	-15.0
-4	0	5	57.4	-59.5	-5	3	1	65.3	-66.5	-5	1	13	13.5	-13.1
-4	0	6	120.6	120.9	5	3	0	87.3	84.9	-5	1	10	8.9	9.0
-4	0	7	29.0	-28.8	5	3	1	39.6	-38.9	-5	1	9	20.0	-19.8
-4	0	9	17.9	-17.9	5	3	2	19.8	21.8	-5	1	8	22.5	-23.4
-4	0	10	49.7	50.1	5	3	3	100.8	-97.1	-5	1	6	12.5	14.5
-4	0	11	16.1	-16.3	5	3	4	36.6	37.5	-5	1	4	33.6	-34.0
-4	0	12	11.0	12.2	5	3	5	14.8	13.9	-5	1	3	21.2	-21.6
-4	0	13	39.9	-39.8	5	3	6	17.5	17.4	6	8	3	12.3	-10.8
-4	0	14	56.9	56.8	5	3	7	52.1	-50.9	6	8	2	8.4	-8.2
-4	2	2	23.4	-25.0	5	3	9	11.6	-13.6	6	8	1	10.8	11.1
-4	2	3	18.3	18.4	5	5	0	18.8	-19.2	6	8	0	19.5	21.0
-4	2	4	37.6	38.6	5	5	1	18.8	-18.9	6	6	5	37.9	-38.3
-4	2	5	15.0	15.9	5	5	4	12.7	-11.6	6	6	4	10.8	9.8
-4	2	8	18.5	17.4	5	5	5	22.6	-22.2	6	6	3	10.5	8.3
-4	2	11	10.9	11.2	-5	7	1	12.0	12.1	6	6	2	43.1	41.9
-4	2	12	16.2	19.1	5	7	1	21.7	-22.4	6	6	1	35.7	-35.7
-4	2	13	8.6	8.2	-5	9	1	51.3	-50.3	-6	6	1	27.8	-28.4
-4	4	3	24.8	24.7	5	9	0	49.6	49.2	6	4	5	20.7	19.7
-4	4	4	15.5	15.1	5	9	1	17.4	-18.0	6	4	3	13.7	-13.8
-4	4	5	14.7	-14.6	5	9	2	23.0	22.4	6	4	1	16.9	18.2
-4	4	7	18.9	19.9	5	9	3	55.6	-57.6	6	4	0	29.6	31.5
-4	4	8	38.5	36.0	5	9	4	22.8	22.2	-6	4	1	8.6	8.5

-4	4	10	18.6	-19.3	-5	9	8	48.9	47.9	6	2	7	12.1	-12.4
-4	4	12	14.9	14.7	-5	9	7	46.3	-45.0	6	2	5	16.4	17.7
-4	4	13	16.1	16.9	-5	9	5	26.1	-24.0	6	2	4	21.6	20.5
-4	6	2	66.3	65.1	-5	9	4	43.4	43.3	6	2	2	9.3	-9.7
-4	6	3	81.8	-82.6	-5	9	3	12.9	-11.2	6	2	1	7.0	7.5
-4	6	4	36.5	36.7	-5	9	2	13.9	-11.6	6	2	0	16.0	17.2
-4	6	5	18.8	-20.6	-5	7	9	17.8	-18.8	6	0	8	27.8	29.6
-4	6	6	93.5	95.6	-5	7	8	14.9	-13.5	6	0	6	58.7	58.5
-4	6	7	37.7	-37.3	-5	7	6	17.0	16.4	6	0	5	42.0	-42.6
-4	6	8	13.1	-13.1	-5	7	4	29.5	-31.3	6	0	2	49.2	48.1
-4	6	9	19.4	-19.0	-5	7	3	19.1	-18.6	6	0	1	29.0	-31.2
-4	6	10	52.4	51.3	-5	5	10	13.5	12.1	6	0	0	26.5	25.9
-4	6	12	13.2	11.9	-5	5	9	14.1	-13.6	-6	0	1	31.8	-31.7
-4	8	3	15.7	16.2	-5	5	8	22.8	-22.2	-6	0	2	91.0	91.3
-4	8	4	12.3	12.4	-5	5	6	11.2	10.5	-6	0	3	52.5	-52.6
-4	8	8	23.3	24.5	-5	5	4	22.2	-22.3	-6	0	5	30.5	-31.0
-4	10	3	9.8	10.4	-5	5	3	17.4	-16.2	-6	0	6	72.7	69.0
-4	10	4	15.3	15.7	-5	5	2	9.0	9.4	-6	0	7	13.4	13.1

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-6	0	9	58.3	-58.9	-6	6	9	37.4	-38.1	-7	5	2	11.5	12.3
-6	0	10	43.2	43.8	-6	8	2	12.4	-12.9	-7	3	8	23.1	23.1
-6	0	12	40.6	40.6	-6	8	4	15.6	16.0	-7	3	7	61.6	-59.4
-6	2	4	23.3	25.0	-6	8	5	9.1	9.6	-7	3	6	23.1	24.1
-6	2	8	18.7	19.8	7	1	0	15.1	-16.5	-7	3	5	16.7	-18.0
-6	2	9	22.1	23.1	7	1	4	12.0	-12.8	-7	3	4	48.8	49.8
-6	2	11	13.5	-13.6	-7	3	1	13.8	-11.0	-7	3	3	49.6	-52.5
-6	4	2	13.6	-15.7	7	3	0	45.5	44.8	-7	3	2	11.1	-11.5
-6	4	4	17.9	19.3	7	3	1	26.8	-26.4	-7	1	9	17.4	-18.3
-6	4	5	16.0	16.8	7	3	3	47.4	-48.2	-7	1	5	16.4	-17.3
-6	6	2	83.6	82.6	7	3	4	51.5	52.1	-7	1	4	16.9	-18.8
-6	6	3	28.0	-28.4	7	5	0	15.0	-15.1	-8	0	1	45.2	-48.0
-6	6	5	35.7	-36.7	-7	5	7	10.9	10.4	-8	0	2	42.5	40.8
-6	6	6	43.3	42.8	-7	5	5	16.8	-17.7	-8	0	4	15.0	15.6
-6	6	8	10.0	10.0	-7	5	4	18.2	-18.4					