

Observed and calculated structure factors for biotite-1M crystals: C3-31

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
1	1	1	38.5	-39.3	-1	11	3	26.7	-27.3	0	12	3	35.7	-38.1
1	1	0	34.9	34.4	-1	11	7	22.2	-23.3	0	12	1	29.7	-29.2
-1	1	1	14.2	17.2	1	11	6	10.3	-10.6	0	12	0	88.1	86.7
-1	1	2	64.6	-64.9	1	11	3	14.9	-15.4	0	10	9	9.2	-10.2
-1	1	3	82.7	-84.9	1	11	2	19.4	-19.4	0	10	7	16.9	16.9
-1	1	4	17.6	-18.5	1	9	9	44.9	-44.3	0	10	6	16.3	17.1
-1	1	5	10.6	9.7	1	9	7	34.1	-36.1	0	10	4	7.1	-6.7
-1	1	7	36.9	-38.1	1	9	6	74.6	75.8	0	10	3	10.4	10.5
-1	1	8	16.7	-15.9	1	9	5	58.0	-60.4	0	10	2	24.0	25.2
-1	1	9	5.5	6.1	1	9	4	5.8	5.9	0	10	1	4.1	3.9
-1	1	11	17.9	-17.2	1	9	3	42.9	-44.4	0	8	11	17.1	18.2
-1	1	12	13.4	-12.9	1	9	2	49.4	49.4	0	8	9	17.8	-18.0
-1	1	13	5.9	6.1	1	7	11	12.6	-13.8	0	8	8	7.3	-7.4
1	3	0	21.6	-20.5	1	7	10	16.7	-16.4	0	8	7	29.2	29.3
-1	3	4	70.7	73.0	1	7	8	6.7	7.1	0	8	6	33.3	33.7
-1	3	6	69.5	68.7	1	7	7	9.5	-9.6	0	8	4	13.0	-13.3
-1	3	7	7.9	6.6	1	7	6	12.9	-13.2	0	8	2	26.7	27.5
-1	3	8	8.2	7.5	1	7	3	27.5	-27.4	0	8	1	15.3	16.4
-1	3	9	79.1	-81.8	1	7	2	36.9	-36.3	0	6	12	16.9	16.8
-1	3	10	6.9	8.8	1	5	11	14.0	-14.0	0	6	11	54.4	-57.6
-1	3	11	9.8	-9.7	1	5	10	7.5	-7.2	0	6	10	52.4	51.0
-1	3	12	61.6	60.2	1	5	7	29.2	-28.8	0	6	9	8.0	-8.2
-1	3	13	60.8	-57.9	1	5	6	31.4	-31.3	0	6	8	70.7	73.3
1	5	1	41.5	-43.5	1	5	5	6.9	7.9	0	6	7	73.9	-75.2
-1	5	1	18.6	18.3	1	5	4	21.3	21.8	0	6	6	10.5	10.6
-1	5	2	31.0	-31.9	1	5	3	22.1	-21.1	0	6	5	19.0	20.2
-1	5	3	47.3	-48.1	1	5	2	60.7	-62.7	0	6	2	33.6	35.7
-1	5	4	16.1	-15.8	1	3	13	50.0	-46.3	0	6	1	74.6	-76.0
-1	5	6	7.7	-7.6	1	3	12	13.0	13.2	0	4	12	21.7	20.4
-1	5	7	28.4	-28.8	1	3	11	10.7	11.0	0	4	11	25.1	26.0
-1	5	9	7.1	7.8	1	3	10	24.9	24.3	0	4	9	27.4	-28.8
-1	5	11	16.6	-18.5	1	3	9	75.5	-76.7	0	4	8	11.9	-10.9
-1	5	12	11.9	-12.7	1	3	8	6.4	4.4	0	4	7	44.7	44.6
-1	5	13	8.6	8.6	1	3	7	47.0	-48.3	0	4	6	59.0	57.9
-1	7	4	4.6	4.9	1	3	6	141.1	142.2	0	4	5	15.4	15.2
-1	7	5	21.2	23.4	1	3	5	126.3	-125.6	0	4	4	23.4	-25.0
-1	7	7	33.0	-32.1	1	3	4	11.2	-11.8	0	4	3	14.1	-17.0

-1	7	8	18.5	-19.0	1	3	3	107.9	-105.5	0	4	1	43.4	44.4
-1	7	11	7.1	-6.3	1	3	2	68.2	67.3	0	4	0	55.6	55.3
-1	7	12	6.6	-6.8	1	1	13	9.6	10.1	0	2	13	12.2	-12.2
1	9	1	25.4	-26.9	1	1	11	16.9	-16.5	0	2	12	7.9	6.3
1	9	0	14.0	-15.2	1	1	10	15.4	-14.3	0	2	11	18.1	18.1
-1	9	1	66.7	-67.9	1	1	8	3.1	3.1	0	2	10	12.7	12.2
-1	9	4	21.8	23.0	1	1	7	30.0	-28.7	0	2	7	32.2	33.8
-1	9	5	97.4	-97.3	1	1	6	28.7	-30.0	0	2	6	19.5	19.9
-1	9	6	34.5	35.9	1	1	4	10.0	9.2	0	2	5	12.5	-12.0
-1	9	7	11.2	12.7	1	1	3	41.2	-44.0	0	2	4	6.4	7.9
-1	9	8	18.5	19.7	1	1	2	91.9	-89.9	0	2	1	7.6	5.2
-1	9	9	49.4	-49.6	0	12	5	7.6	9.4	0	2	0	43.5	-42.4
1	11	0	21.9	22.2	0	12	4	41.5	42.4	0	0	14	19.9	18.6
H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
0	0	13	17.0	16.7	2	6	7	19.7	-18.7	-2	0	12	11.9	-11.2
0	0	12	36.8	36.2	2	6	6	6.8	6.0	-2	0	13	13.5	-14.7
0	0	11	56.0	-60.5	2	6	5	26.5	-26.2	-2	0	14	46.0	45.0
0	0	10	55.2	56.8	2	6	4	120.6	120.6	-2	2	2	44.0	45.7
0	0	9	40.2	-38.7	2	6	3	64.4	-61.0	-2	2	3	14.7	13.7
0	0	8	82.4	82.5	2	6	2	37.5	35.2	-2	2	4	26.6	-25.5
0	0	7	81.1	-78.7	2	6	1	104.4	-104.1	-2	2	5	16.0	-15.6
0	0	6	64.7	63.6	2	6	0	124.1	123.7	-2	2	6	32.8	31.6
0	0	5	77.2	76.9	-2	6	1	47.8	47.1	-2	2	7	59.6	61.1
0	0	4	72.9	74.4	2	4	11	10.6	10.0	-2	2	8	27.7	28.8
0	2	2	88.4	87.6	2	4	10	13.1	12.5	-2	2	9	26.9	-26.3
0	2	3	62.7	64.5	2	4	7	17.4	17.1	-2	2	10	19.1	-19.0
0	2	8	5.2	4.4	2	4	6	33.4	33.7	-2	2	11	12.2	11.1
0	4	2	28.8	29.4	2	4	4	20.1	-19.5	-2	2	12	31.5	29.2
0	6	3	50.7	-53.1	2	4	2	57.3	56.7	-2	2	13	11.2	11.3
0	6	4	87.9	89.8	2	4	1	49.8	52.1	-2	2	14	9.4	-9.7
-1	3	1	143.8	-147.3	-2	4	1	30.0	-27.5	-2	4	2	14.4	13.7
1	5	0	21.0	20.1	2	2	11	29.7	26.6	-2	4	3	51.1	49.4
1	7	0	29.4	28.5	2	2	10	22.3	21.3	-2	4	4	30.4	28.9
-1	11	5	17.2	18.5	2	2	9	10.2	-9.6	-2	4	7	20.6	20.3
-1	11	2	29.2	-29.1	2	2	8	30.8	-30.0	-2	4	8	16.8	16.7
-1	9	3	39.4	-38.8	2	2	7	6.2	6.0	-2	4	9	8.8	-8.3
-1	9	2	88.2	85.2	2	2	6	56.9	57.9	-2	4	11	15.0	16.2
-1	7	3	46.9	-49.1	2	2	5	44.8	47.0	-2	4	12	17.2	15.9
-1	7	2	47.9	-48.0	2	2	3	29.6	-29.8	-2	6	2	28.2	26.1

-1	3	5	151.1	-150.8	2	2	1	33.5	35.9	-2	6	3	90.1	-89.5
-1	3	3	135.2	-134.5	2	2	0	53.4	52.3	-2	6	4	39.3	37.6
-1	3	2	122.3	123.2	-2	2	1	50.4	47.2	-2	6	6	101.8	103.9
2	12	3	24.5	-24.4	2	0	12	53.4	56.7	-2	6	7	79.3	-80.4
2	12	2	19.8	19.5	2	0	11	62.8	-60.6	-2	6	8	38.1	39.2
2	12	1	53.5	-51.4	2	0	10	11.7	11.2	-2	6	9	16.7	-15.9
2	12	0	55.2	52.8	2	0	8	83.5	81.8	-2	6	10	46.1	45.2
2	10	7	6.2	5.6	2	0	7	9.3	-8.9	-2	6	11	25.7	-24.8
2	10	6	23.9	25.4	2	0	6	7.1	-7.6	-2	8	2	16.3	15.6
2	10	5	13.0	12.3	2	0	5	65.5	-68.5	-2	8	3	28.3	27.2
2	10	4	8.8	-8.8	2	0	4	155.0	151.7	-2	8	4	12.8	11.8
2	10	3	11.6	-11.0	2	0	3	70.0	-71.3	-2	8	7	21.0	21.1
2	10	2	14.9	14.7	2	0	2	134.8	134.2	-2	8	8	12.3	12.6
2	10	1	19.8	18.3	2	0	1	124.5	-124.6	-2	8	9	11.0	-10.1
2	10	0	7.4	6.7	-2	0	1	20.8	19.4	-2	8	11	8.7	9.8
2	8	8	8.3	-8.2	-2	0	2	6.2	-6.1	-2	10	2	13.7	12.0
2	8	6	27.8	27.7	-2	0	3	69.2	-67.3	-2	10	3	14.9	14.5
2	8	4	13.7	-13.8	-2	0	4	108.1	105.6	-2	10	5	9.3	-9.2
2	8	2	29.8	28.0	-2	0	5	13.7	13.6	-2	10	7	18.7	20.5
2	8	1	32.6	30.3	-2	0	6	129.1	125.4	-2	10	8	12.3	12.4
-2	8	1	17.5	-16.9	-2	0	7	146.5	-142.2	-2	12	2	11.1	11.5
2	6	11	36.3	-38.8	-2	0	8	46.9	46.2	-2	12	3	46.9	-44.7
2	6	10	11.9	14.3	-2	0	9	4.7	-4.6	-2	12	4	23.4	25.8
2	6	9	14.9	-15.7	-2	0	10	77.8	78.1	-3	1	1	24.5	23.7
2	6	8	45.7	47.7	-2	0	11	24.9	-23.0	3	1	0	5.9	4.6
H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
3	1	1	43.1	-43.3	3	11	3	7.3	7.6	-4	10	1	8.1	-7.5
3	1	2	41.2	-40.8	3	11	4	9.4	10.5	4	8	6	13.6	14.4
3	1	3	5.3	-5.3	-3	11	4	9.5	-8.9	4	8	5	25.5	25.9
3	1	5	16.6	-17.3	-3	11	3	18.0	-18.1	4	8	3	15.7	-14.7
3	1	6	21.7	-22.0	-3	9	9	54.9	-54.8	4	8	1	17.6	17.6
3	1	9	12.5	-11.9	-3	9	8	43.7	42.6	4	8	0	21.1	19.3
3	1	10	18.8	-18.1	-3	9	5	48.6	-48.2	4	6	8	42.0	44.3
3	1	11	4.7	-4.5	-3	9	4	29.5	31.8	4	6	6	36.7	35.0
-3	3	1	175.4	-177.5	-3	9	3	27.2	-26.9	4	6	5	75.3	-74.5
3	3	0	71.7	75.4	-3	9	2	33.3	32.0	4	6	4	56.8	60.0
3	3	1	38.9	-36.3	-3	7	11	7.4	-8.2	4	6	2	45.5	44.8
3	3	2	53.1	52.4	-3	7	8	18.6	-17.8	4	6	1	50.7	-49.4

Observed and calculated structure factors for biotite-1M crystals: C3-31

3	3	3	87.6	-88.7	-3	7	7	16.3	-16.4	4	6	0	27.9	27.0
3	3	4	18.3	-17.9	-3	7	4	17.4	-16.2	-4	6	1	9.4	13.7
3	3	5	9.7	-11.7	-3	7	3	30.8	-29.4	4	4	9	9.5	9.2
3	3	6	72.0	73.1	-3	5	12	8.1	-7.1	4	4	8	12.8	-13.8
3	3	7	72.2	-73.7	-3	5	9	7.9	-9.5	4	4	7	12.3	-14.0
3	3	8	9.6	9.4	-3	5	8	32.1	-32.5	4	4	6	16.9	17.9
3	3	9	49.3	-49.2	-3	5	7	14.1	-14.5	4	4	5	32.9	34.3
3	3	10	59.6	57.6	-3	5	6	22.8	23.4	4	4	4	13.9	13.4
3	3	11	20.4	-18.0	-3	5	5	13.3	13.5	4	4	3	15.5	-14.9
-3	5	1	28.5	26.8	-3	5	4	30.2	-29.8	4	4	1	21.1	20.1
3	5	0	11.2	10.5	-3	5	3	60.9	-59.5	4	4	0	21.8	21.6
3	5	1	32.9	-31.4	-3	5	2	16.2	-15.7	4	2	10	8.3	8.6
3	5	2	35.2	-33.2	-3	3	13	19.7	-17.8	4	2	6	25.1	25.6
3	5	3	9.1	-8.8	-3	3	12	56.3	56.5	4	2	5	24.7	24.5
3	5	5	12.4	-12.5	-3	3	11	50.1	-49.2	4	2	4	10.7	-9.6
3	5	6	14.8	-13.9	-3	3	10	9.7	8.9	4	2	3	23.4	-23.8
3	5	9	12.5	-13.0	-3	3	9	70.5	-72.1	4	2	2	15.2	14.9
3	5	10	18.0	-17.0	-3	3	8	73.6	72.8	4	2	1	53.4	53.4
-3	7	1	11.6	11.1	-3	3	7	11.2	-12.3	4	2	0	36.4	35.5
3	7	0	9.1	-8.4	-3	3	6	19.0	-18.6	-4	2	1	14.6	-15.3
3	7	1	37.3	-34.4	-3	3	5	89.4	-88.1	4	0	9	26.2	-24.9
3	7	2	19.1	-18.3	-3	3	4	54.4	53.8	4	0	8	44.4	44.5
3	7	3	10.0	10.7	-3	3	3	37.3	-37.2	4	0	7	16.2	-16.2
3	7	4	9.3	8.9	-3	1	13	8.2	-8.1	4	0	6	39.8	40.1
3	7	5	17.1	-17.0	-3	1	12	10.9	-11.6	4	0	5	84.7	-79.4
3	7	6	22.7	-22.6	-3	1	10	7.0	7.4	4	0	4	101.2	101.9
-3	9	1	94.0	-91.3	-3	1	9	6.9	-7.2	4	0	2	39.1	38.9
3	9	0	53.9	52.8	-3	1	8	34.5	-34.9	4	0	1	82.7	-87.7
3	9	1	7.9	-7.5	-3	1	7	18.8	-18.6	4	0	0	30.2	27.3
3	9	2	32.5	30.2	-3	1	6	17.1	17.4	-4	0	1	42.4	44.8
3	9	3	68.9	-67.1	-3	1	5	9.8	10.3	-4	0	2	119.4	121.4
3	9	4	13.6	-13.1	-3	1	4	35.3	-36.0	-4	0	3	100.2	-101.8
3	9	6	57.1	58.1	-3	1	3	67.5	-68.0	-4	0	4	32.5	34.7
3	9	7	41.8	-43.5	-3	1	2	14.9	-15.8	-4	0	5	60.5	-59.9
-3	11	1	12.9	11.9	4	10	3	10.3	-12.0	-4	0	6	121.7	118.9
3	11	0	5.7	-5.6	4	10	2	5.0	4.9	-4	0	7	26.2	-26.0
3	11	1	24.8	-23.1	4	10	1	20.8	19.3	-4	0	8	7.1	7.0
3	11	2	9.0	-9.3	4	10	0	12.1	12.5	-4	0	9	17.3	-19.4
H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/

Observed and calculated structure factors for biotite-1M crystals: C3-31

-4	0	10	47.0	47.2	5	5	1	18.8	-19.1	6	6	2	41.1	41.0
-4	0	11	14.8	-15.3	5	5	3	9.9	8.6	6	6	1	35.6	-36.6
-4	0	12	13.0	13.7	5	5	4	10.1	-10.4	6	6	0	9.8	8.7
-4	0	13	37.2	-37.7	5	5	5	19.7	-21.1	-6	6	1	30.9	-28.0
-4	2	2	23.5	-22.8	5	5	7	9.7	10.1	6	4	5	17.0	18.0
-4	2	3	16.9	18.5	-5	7	1	12.8	12.1	6	4	3	13.2	-12.6
-4	2	4	40.7	38.0	5	7	0	8.0	-7.8	6	4	2	11.0	-11.7
-4	2	5	14.2	15.5	5	7	1	23.1	-22.4	6	4	1	16.0	17.5
-4	2	8	17.8	17.6	5	7	2	7.4	-7.2	6	4	0	30.0	30.0
-4	2	11	9.6	9.4	5	7	5	9.5	-8.0	-6	4	1	7.8	7.9
-4	2	12	17.7	17.7	-5	9	1	48.8	-51.4	6	2	5	17.6	17.4
-4	2	13	9.7	8.4	5	9	0	47.9	49.9	6	2	4	19.0	19.0
-4	4	2	8.6	9.5	5	9	1	18.4	-19.9	6	2	2	8.0	-9.6
-4	4	3	23.8	23.9	5	9	2	24.4	23.9	6	2	0	16.0	16.9
-4	4	4	13.1	14.2	-5	9	5	25.2	-25.2	6	0	6	53.5	53.0
-4	4	5	14.1	-14.0	-5	9	4	44.3	43.5	6	0	5	40.6	-41.7
-4	4	7	21.0	19.9	-5	9	3	14.1	-12.8	6	0	4	5.6	5.3
-4	4	8	34.4	35.6	-5	9	2	12.8	-10.0	6	0	2	48.1	47.9
-4	4	10	16.9	-18.1	-5	7	9	18.7	-18.6	6	0	1	32.4	-31.3
-4	4	12	13.7	13.8	-5	7	8	12.5	-12.7	6	0	0	26.2	26.5
-4	6	2	64.3	67.2	-5	7	6	15.6	16.1	-6	0	1	33.1	-31.7
-4	6	3	82.2	-82.9	-5	7	5	6.2	-6.8	-6	0	2	88.3	88.2
-4	6	4	40.5	38.4	-5	7	4	32.4	-30.9	-6	0	3	50.7	-50.2
-4	6	5	22.8	-22.7	-5	7	3	19.7	-19.3	-6	0	4	8.4	9.0
-4	6	6	96.7	95.5	-5	7	2	13.5	12.3	-6	0	5	31.1	-31.0
-4	6	7	35.6	-35.6	-5	5	10	8.9	10.0	-6	0	6	66.1	65.3
-4	6	8	12.7	-11.8	-5	5	9	13.7	-14.2	-6	0	7	11.1	11.9
-4	6	9	20.5	-20.3	-5	5	8	19.9	-20.4	-6	0	9	54.5	-55.9
-4	6	10	48.4	49.3	-5	5	6	10.5	10.2	-6	0	10	38.4	40.4
-4	8	3	16.5	15.4	-5	5	5	3.9	-3.9	-6	2	3	8.0	7.6
-4	8	4	12.8	11.9	-5	5	4	21.8	-22.9	-6	2	4	22.2	22.4
-4	8	7	11.4	11.4	-5	5	3	16.1	-15.5	-6	2	6	10.8	-10.5
-4	8	8	24.8	24.8	-5	5	2	10.6	8.9	-6	2	8	16.5	18.8
-4	10	3	9.1	10.7	-5	3	11	44.4	-43.8	-6	2	9	20.5	21.1
-4	10	4	16.9	16.1	-5	3	9	34.4	-34.6	-6	4	2	15.5	-14.3
5	1	0	19.4	-18.8	-5	3	8	72.5	72.2	-6	4	3	8.9	-8.9
5	1	1	26.2	-26.1	-5	3	7	57.9	-58.6	-6	4	4	17.1	18.4
5	1	4	10.2	-10.5	-5	3	5	45.7	-43.5	-6	4	5	15.8	16.0
5	1	5	18.9	-19.4	-5	3	4	48.2	48.3	-6	6	2	81.8	81.8

Observed and calculated structure factors for biotite-1M crystals: C3-31

5	1	7	10.0	9.4	-5	3	3	30.5	-28.6	-6	6	3	28.8	-28.4
-5	3	1	66.8	-66.1	-5	3	2	15.3	-12.6	-6	6	4	9.1	8.1
5	3	0	85.9	82.7	-5	1	12	5.7	-5.5	-6	6	5	37.2	-37.2
5	3	1	43.1	-39.6	-5	1	10	8.0	7.1	-6	6	6	41.8	41.5
5	3	2	19.0	22.4	-5	1	9	17.2	-19.6	-6	6	7	7.0	7.5
5	3	3	93.9	-93.7	-5	1	8	21.1	-21.5	-7	1	1	5.9	-5.2
5	3	4	35.6	36.3	-5	1	6	13.1	13.8	7	1	0	16.1	-15.6
5	3	5	12.9	10.4	-5	1	5	6.4	-6.3	7	1	1	6.8	-6.0
5	3	6	20.5	19.2	-5	1	4	32.7	-33.7	7	1	2	5.7	5.5
5	3	7	50.6	-49.2	-5	1	3	20.9	-21.2	-7	3	1	11.1	-12.2
5	5	0	19.7	-19.2	-5	1	2	12.1	10.5	7	3	0	42.4	42.7

H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/	H	K	L	/FO/	/FC/
7	3	1	26.5	-26.7	-7	3	3	48.4	-50.8	-7	1	5	16.9	-16.8
-7	3	6	22.3	24.3	-7	3	2	9.3	-8.0	-7	1	4	18.7	-17.6
-7	3	5	19.0	-19.2	-7	1	7	8.3	8.1	-7	1	2	7.5	8.1
-7	3	4	44.5	46.6	-7	1	6	4.9	4.8					