

AM-95-593

Crystal structure and twinning of Sb_2AsS_2 , the synthetic analogue of paak-
konenite

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For deposit: Table 4

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

h	k	l	/Fo/	/Fc/	h	k	l	/Fo/	/Fc/	h	k	l	/Fo/	/Fc/
-2	0	1	66.0	61.1	0	0	4	51.7	43.7	12	0	1	37.0	35.2
-4	0	2	470.8	468.8	-2	0	5	45.7	41.8	-12	0	13	22.9	31.5
-6	0	3	102.9	102.3	2	0	3	50.1	45.0	0	0	8x	2.7	33.1
-8	0	4	244.4	235.6	-4	0	6	74.7	74.7	2	0	7	77.9	79.8
-10	0	5	86.1	83.5	4	0	2	67.4	66.8	-2	0	9	80.7	85.4
-12	0	6	96.6	90.5	-6	0	7	42.5	39.9	4	0	6x	21.5	23.0
-14	0	7	44.2	47.4	6	0	1	48.1	44.4	-4	0	10x	10.7	22.2
0	0	1	21.1	24.4	8	0	0	65.4	70.9	-6	0	11	69.3	76.0
2	0	0x	.7	50.4	-8	0	8	77.8	78.6	6	0	5	61.8	68.0
-2	0	2x	25.1	46.4	-10	0	9x	15.4	26.8	8	0	4x	15.7	3.5
-4	0	1	58.4	72.7	-10	0	1x	30.5	29.2	-8	0	12x	7.4	3.0
-4	0	3	79.1	77.2	-12	0	10	51.1	54.2	-10	0	13x	48.6	53.5
-6	0	4	45.9	55.9	-12	0	2	45.5	48.9	10	0	3x	42.2	50.1
-6	0	2	53.1	62.4	0	0	5	363.5	365.8	12	0	2s	23.6	2.1
-8	0	3	80.9	73.4	2	0	4	66.5	74.3	0	0	9	68.3	63.7
-8	0	5	78.5	76.2	-2	0	6	61.5	67.4	-2	0	10x	17.0	18.7
-10	0	6	43.2	49.2	4	0	3	296.6	292.3	2	0	8x	8.1	16.9
-10	0	4	58.0	55.1	-4	0	7	295.1	289.8	4	0	7	61.9	60.4
-12	0	7	57.1	47.0	-6	0	8	75.6	73.2	-4	0	11	65.5	62.3
-12	0	5	48.9	45.7	6	0	2	85.3	79.3	6	0	6x	29.9	29.9
-14	0	8x	.0	32.7	-8	0	9	152.9	161.0	-6	0	12x	34.1	32.2
-14	0	6x	44.3	36.6	8	0	1	169.8	165.7	-8	0	13x	48.9	53.4
0	0	2	38.6	38.0	10	0	0	66.5	63.1	8	0	5x	47.5	50.2
-2	0	3	267.9	271.7	-10	0	10	64.3	62.2	-10	0	4x	18.4	21.4
2	0	1	260.5	267.6	-12	0	11	55.3	69.5	-10	0	14x	13.5	23.3
4	0	0	39.1	40.6	-12	0	1	80.9	74.6	0	0	10	77.7	76.2
-4	0	4	37.6	39.6	0	0	6	51.9	56.9	2	0	9x	27.1	22.2
-6	0	5	189.5	189.1	-2	0	7	47.5	33.6	-2	0	11x	29.5	20.5
-6	0	1	173.3	178.9	2	0	5	43.9	37.1	-4	0	12	66.3	68.5
-8	0	6x	42.3	34.3	-4	0	8	61.9	60.1	4	0	8	72.4	71.8
-8	0	2x	44.4	36.3	4	0	4	59.7	56.6	6	0	7x	36.1	22.6
-10	0	3	96.7	99.7	-6	0	9	59.4	62.8	-6	0	13x	32.4	21.3
-10	0	7	112.7	110.0	6	0	3	59.6	67.3	-8	0	14x	31.8	54.1
-12	0	4x	29.7	22.7	8	0	2	49.9	48.1	8	0	6x	53.9	59.4
-12	0	8x	30.1	20.8	-8	0	10	55.6	51.5	10	0	5x	32.8	25.0
-14	0	5	57.9	52.7	10	0	1x	47.8	58.0	-10	0	15x	30.9	25.7
-14	0	9	58.1	59.0	-10	0	11x	44.5	54.1	0	0	11	29.3	28.5
0	0	3x	8.1	3.3	12	0	0x	23.3	32.4	-2	0	12	46.6	23.3
2	0	2	58.2	63.4	-12	0	12x	23.3	34.1	2	0	10	44.0	26.0
-2	0	4	55.7	57.0	0	0	7	99.2	100.1	-4	0	13x	17.9	37.7
-4	0	5x	14.8	13.6	2	0	6	249.7	247.7	4	0	9x	32.8	42.1
4	0	1x	15.7	14.6	-2	0	8	249.7	248.9	6	0	8	40.4	33.9
-6	0	6	80.6	85.8	-4	0	9	89.0	88.7	-6	0	14	43.5	32.0
6	0	0	92.1	95.6	4	0	5	98.0	95.3	8	0	7x	27.2	47.5
-8	0	1x	.0	8.3	-6	0	10	162.8	167.5	-8	0	15x	20.5	42.4
-8	0	7x	15.7	7.4	6	0	4	163.4	164.0	0	0	12	89.6	86.7
-10	0	2	92.4	85.7	-8	0	11	57.4	63.0	-2	0	13	122.2	119.0
-10	0	8	78.3	77.7	8	0	3	71.7	69.7	2	0	11	122.6	117.8
-12	0	3x	20.0	5.4	10	0	2	74.9	78.0	-4	0	14	70.7	74.7
-12	0	9x	17.4	5.9	-10	0	12	77.3	82.7	4	0	10	77.7	80.9

h	k	l	/Fo/	/Fc/	h	k	l	/Fo/	/Fc/	h	k	l	/Fo/	/Fc/
-6	0	15	72.5	80.4	-7	1	6	114.4	111.8	3	1	5	63.8	57.1
6	0	9	79.9	78.0	-7	1	1	115.6	111.1	-3	1	8	65.4	58.5
8	0	8	52.5	55.9	-9	1	7	175.9	173.0	-5	1	9	35.3	36.7
-8	0	16	32.7	50.0	-9	1	2	184.4	176.0	5	1	4	32.9	33.6
0	0	13	42.6	33.0	-11	1	8	34.1	27.4	7	1	3	58.8	59.9
-2	0	14	61.5	64.4	-11	1	3	36.4	29.2	-7	1	10	64.4	63.7
2	0	12	62.3	62.2	-13	1	4	83.3	80.4	-9	1	11*	28.2	35.1
4	0	11*	.0	22.6	-13	1	9	70.2	78.5	9	1	2*	21.2	32.3
-4	0	15*	32.3	24.0	1	1	3*	16.5	36.5	11	1	1	39.1	40.2
-6	0	16	46.6	54.5	-1	1	4*	24.4	40.8	-11	1	12	39.0	43.7
6	0	10	51.0	50.4	3	1	2	68.0	61.0	-1	1	8	144.7	137.5
0	0	14*	.0	50.8	-3	1	5	71.4	62.1	1	1	7	147.3	145.5
-2	0	15	35.1	36.3	-5	1	6	49.5	57.0	-3	1	9	100.2	104.7
2	0	13	41.6	36.3	5	1	1	47.9	58.0	3	1	6	98.2	99.9
-4	0	16*	.0	44.0	7	1	0	71.1	66.6	5	1	5	140.5	134.8
4	0	12*	34.9	45.3	-7	1	7	77.9	69.0	-5	1	10	131.2	128.0
1	1	0	115.1	119.8	-9	1	8	55.0	52.9	-7	1	11	35.9	47.7
-1	1	1	114.9	116.5	-9	1	1	62.2	56.0	7	1	4	39.8	48.8
-3	1	1	101.0	104.2	-11	1	2	48.8	49.6	9	1	3	94.4	93.3
-3	1	2	96.1	99.8	-11	1	9	50.9	50.6	-9	1	12	81.9	88.6
-5	1	2	110.7	113.5	-13	1	10*	34.7	32.2	11	1	2*	22.2	25.3
-5	1	3	97.7	103.5	-13	1	3*	47.2	34.6	-11	1	13*	21.5	22.8
-7	1	4	71.8	75.6	1	1	4	194.4	194.3	-1	1	9	36.9	26.0
-7	1	3	83.4	82.6	-1	1	5	202.5	206.0	1	1	8	39.0	24.0
-9	1	5	75.4	75.4	3	1	3	196.2	195.4	-3	1	10	61.5	55.4
9	1	4	86.8	84.5	-3	1	6	192.5	187.0	3	1	7	56.7	58.9
-11	1	6	54.0	51.8	5	1	2	137.7	136.6	-5	1	11*	19.4	1.9
-11	1	5	60.0	57.9	-5	1	7	151.1	149.0	5	1	6*	22.0	1.8
-13	1	7	51.7	46.2	7	1	1	128.5	127.3	7	1	5	57.9	69.6
-13	1	6	53.7	50.9	-7	1	8	124.1	123.6	-7	1	12	60.1	65.8
-1	1	2	47.2	51.3	-9	1	9	90.8	85.7	9	1	4*	9.8	4.1
1	1	1	47.0	50.1	9	1	0	80.2	76.6	-9	1	13*	13.7	4.6
3	1	0*	3.2	9.4	-11	1	10	54.1	61.7	-11	1	14	35.7	50.0
-3	1	3*	18.6	10.4	-11	1	1	58.7	61.1	11	1	3	38.7	52.7
-5	1	4	86.9	88.1	-13	1	2*	38.7	39.8	-1	1	10	147.7	146.9
-5	1	1	85.0	85.8	-13	1	11*	48.1	44.0	1	1	9	141.2	133.2
-7	1	5*	22.1	25.1	-1	1	6	28.2	35.2	3	1	8	152.4	152.7
-7	1	2*	16.6	23.4	1	1	5	26.8	31.4	-3	1	11	142.7	140.6
-9	1	6	83.3	80.1	-3	1	7	40.4	36.4	5	1	7	83.3	86.3
-9	1	3	75.1	76.5	3	1	4	36.9	32.5	-5	1	12	92.5	96.6
-11	1	4*	17.9	16.5	-5	1	8	42.0	50.1	-7	1	13	87.8	99.3
-11	1	7*	16.4	16.8	5	1	3	39.1	48.8	7	1	6	104.7	106.5
-13	1	8	51.7	51.5	7	1	2	48.9	44.9	-9	1	14*	39.7	48.1
-13	1	5	48.6	47.9	-7	1	9	48.7	46.5	9	1	5*	35.4	43.5
-1	1	3	367.3	360.9	-9	1	10*	36.3	46.0	-1	1	11	69.4	69.1
1	1	2	365.7	368.4	9	1	1*	30.9	46.9	1	1	10	63.5	62.8
-3	1	4	264.3	260.8	-11	1	11	46.3	42.3	3	1	9	47.5	52.0
3	1	1	259.7	255.2	11	1	0	45.4	44.4	-3	1	12	44.8	51.0
-5	1	5	301.6	294.3	-1	1	7	44.9	38.9	-5	1	13	61.0	62.3
5	1	0	306.4	299.6	1	1	6	44.2	35.6	5	1	8	57.1	55.7

h	k	l	/Fo/	/Fc/	h	k	l	/Fo/	/Fc/	h	k	l	/Fo/	/Fc/
7	1	7*	30.8	33.4	2	2	1	194.8	195.5	0	2	6	49.9	51.5
-7	1	14*	33.9	37.0	4	2	0	33.2	30.8	2	2	5*	34.0	31.3
9	1	6	34.8	34.6	-4	2	4	35.4	30.3	-2	2	7*	36.8	28.0
-9	1	15	38.6	38.6	-6	2	5	147.0	148.4	4	2	4	53.3	49.7
-1	1	12*	38.9	39.4	-6	2	1	141.3	140.2	-4	2	8	52.7	52.4
1	1	11*	38.3	43.1	-8	2	2	38.8	28.3	6	2	3	48.0	55.7
-3	1	13*	48.9	49.5	-8	2	6	35.1	27.1	-6	2	9	48.3	51.5
3	1	10*	44.6	46.0	-10	2	7	93.9	90.9	8	2	2	44.3	42.3
5	1	9*	31.5	34.1	-10	2	3	85.5	82.3	-8	2	10	49.7	44.9
-5	1	14*	26.2	30.5	-12	2	8*	7.8	16.7	-10	2	1*	44.9	49.0
7	1	8	44.2	41.7	-12	2	4*	28.5	18.0	-10	2	11*	40.4	45.5
-7	1	15	38.1	45.3	0	2	3*	17.3	.5	0	2	7	84.7	80.7
1	1	12*	12.9	5.4	-2	2	4	44.2	43.6	2	2	6	199.7	198.2
-1	1	13*	6.0	6.0	2	2	2	47.0	48.5	-2	2	8	201.5	199.2
3	1	11*	16.7	15.9	-4	2	5*	2.6	10.3	4	2	5	82.7	77.5
-3	1	14*	13.1	14.8	4	2	1*	11.5	10.9	-4	2	9	75.7	72.4
5	1	15*	13.1	12.7	-6	2	6	68.6	67.2	-6	2	10	133.3	137.4
5	1	10*	14.5	14.0	6	2	0	72.9	74.6	6	2	4	134.2	134.5
7	1	9*	10.2	24.4	-8	2	1*	15.6	7.8	-8	2	11	50.6	52.4
-7	1	16*	23.0	23.0	-8	2	7*	4.1	7.2	8	2	3	61.5	57.8
-1	1	14*	29.5	14.0	-10	2	2	72.4	71.0	-10	2	12	59.5	70.0
1	1	13*	32.9	12.5	-10	2	8	65.0	64.6	-10	2	2	64.8	66.0
-3	1	15*	19.3	32.1	-12	2	9*	8.1	3.4	0	2	8*	23.1	25.7
3	1	12*	17.3	35.6	-12	2	3*	8.8	3.1	2	2	7	68.2	68.9
5	1	11*	10.2	15.1	0	2	4	38.2	28.7	-2	2	9	72.0	73.5
-5	1	16*	34.0	14.2	-2	2	5*	39.7	34.5	4	2	6*	3.4	18.0
-1	1	15	64.3	63.9	2	2	3*	37.4	37.1	-4	2	10*	13.1	17.2
1	1	14	63.4	57.1	4	2	2	54.3	49.7	-6	2	11	59.4	65.3
0	2	0	400.3	437.3	-4	2	6	57.0	55.4	6	2	5	54.9	58.3
-2	2	1*	40.7	38.8	-6	2	7	41.1	35.3	-8	2	12*	12.8	1.9
-4	2	2	353.0	348.7	6	2	1	41.1	39.2	8	2	4*	6.5	1.8
-6	2	3	79.1	78.7	8	2	0	57.9	57.0	-10	2	13	39.8	46.2
-8	2	4	195.8	191.3	-8	2	8	63.6	63.0	-10	2	3	37.0	43.1
-10	2	5	68.1	67.9	-10	2	1*	23.7	26.8	0	2	9	54.6	50.7
-12	2	6	74.9	76.6	-10	2	9*	26.9	24.5	-2	2	10*	16.5	15.1
0	2	1*	21.8	29.1	-12	2	2*	30.4	41.2	2	2	8*	10.7	13.8
2	2	0*	29.7	42.4	-12	2	10*	44.7	45.6	-4	2	11	50.8	50.4
-2	2	2*	25.7	39.8	0	2	5	279.9	278.8	4	2	7	49.0	48.9
-4	2	1	61.5	55.4	2	2	4	55.1	57.2	6	2	6*	29.6	25.9
-4	2	3	63.0	60.4	-2	2	6	52.4	52.0	-6	2	12*	29.1	27.6
-6	2	2	46.6	51.3	4	2	3	237.0	230.7	-8	2	13	32.7	44.7
-6	2	4	41.3	46.3	-4	2	7	231.1	228.6	8	2	5	39.7	42.1
-8	2	5	68.6	62.5	-6	2	8	61.5	58.6	0	2	10	68.1	61.9
-8	2	3	64.6	59.5	6	2	2	65.8	63.7	2	2	9*	26.4	19.1
-10	2	4	44.8	46.6	-8	2	9	127.2	132.5	-2	2	11*	19.7	17.7
-10	2	6	39.3	41.7	8	2	1	137.1	136.5	4	2	8	60.9	59.1
-12	2	7*	41.8	39.8	10	2	0	53.4	52.0	-4	2	12	53.9	56.3
-12	2	5*	43.7	38.4	-10	2	10	51.1	51.1	6	2	7*	30.9	18.9
0	2	2	31.2	28.9	-12	2	1	68.9	63.8	-6	2	13*	21.9	17.7
-2	2	3	197.4	198.8	-12	2	11	53.5	59.3	8	2	6	43.7	50.3

h	k	l	/Fo/	/Fc/	h	k	l	/Fo/	/Fc/	h	k	l	/Fo/	/Fc/
-8	2	14	30.5	45.8	-7	3	6	75.6	76.2	3	3	6	66.9	67.3
0	2	11	30.8	25.7	-7	3	1	77.8	75.7	-3	3	9	65.8	70.8
2	2	10*	38.4	22.6	-9	3	2	122.6	120.9	-5	3	10	85.5	87.1
-2	2	12*	42.8	20.3	-9	3	7	118.2	118.6	5	3	5	95.8	92.1
4	2	9*	9.8	37.2	-11	3	3*	23.5	22.6	7	3	4*	30.7	34.5
-4	2	13*	23.9	33.3	-11	3	8*	27.9	21.3	-7	3	11*	.0	33.8
6	2	8	35.8	28.8	-1	3	4*	12.3	36.2	9	3	3	65.8	66.7
-6	2	14	36.4	27.0	1	3	3*	23.6	32.3	-9	3	12	49.6	62.9
0	2	12	78.0	74.0	3	3	2	42.7	45.3	1	3	8*	31.9	20.2
-2	2	13	102.1	100.6	-3	3	5	47.7	44.6	-1	3	9*	25.0	22.1
2	2	11	105.3	99.7	-5	3	6*	33.9	41.6	3	3	7*	42.5	44.8
-4	2	14	56.4	64.0	5	3	1*	35.0	40.7	-3	3	10*	45.9	41.8
4	2	10	69.6	69.2	7	3	0	48.2	48.1	-5	3	11*	27.4	4.4
-6	2	15	59.4	68.7	-7	3	7	55.0	48.8	5	3	6*	14.1	3.9
6	2	9	64.6	66.7	-9	3	1*	44.4	39.8	7	3	5*	44.9	52.6
0	2	13*	25.2	27.6	-9	3	8*	36.4	38.5	-7	3	12*	43.7	49.4
-2	2	14	53.6	56.6	-11	3	9*	36.4	37.2	1	3	9	100.7	93.3
2	2	12	59.1	54.7	-11	3	2*	40.4	37.0	-1	3	10	107.4	102.9
-4	2	15*	5.8	20.0	-1	3	5	127.2	128.5	-3	3	11	100.3	98.7
4	2	11*	25.3	18.9	1	3	4	123.0	121.4	3	3	8	109.7	107.4
1	3	0	66.5	68.7	-3	3	6	116.4	117.4	-5	3	12	65.8	69.5
-1	3	1	66.9	66.9	3	3	3	124.5	122.9	5	3	7	60.4	62.1
-3	3	1	60.1	61.0	5	3	2	94.0	90.5	7	3	6*	75.7	76.8
-3	3	2	58.3	57.9	-5	3	7	97.7	98.6	-7	3	13*	52.5	71.4
-5	3	2	67.9	70.7	7	3	1	84.6	84.1	-1	3	11	52.8	51.1
5	3	3	65.9	64.5	-7	3	8	79.9	81.6	1	3	10	53.6	46.7
-7	3	3	50.6	51.0	9	3	0	58.4	54.9	3	3	9	39.2	40.0
-7	3	4	47.1	46.2	-9	3	9	59.7	61.3	-3	3	12	36.1	39.5
-9	3	5	55.7	52.2	1	3	5*	18.8	23.2	5	3	8	45.2	41.1
-9	3	4	60.1	58.5	-1	3	6*	19.0	25.6	-5	3	13	42.6	45.9
-11	3	5	43.0	40.2	-3	3	7	31.0	30.3	-1	3	12*	24.5	28.0
-11	3	6	32.4	35.9	3	3	4	32.6	27.3	1	3	11*	9.7	30.7
-1	3	2	32.2	34.8	5	3	3*	28.2	31.6	-3	3	13*	20.4	36.0
1	3	1	33.5	35.8	-5	3	8*	25.0	33.0	3	3	10*	29.1	33.5
-3	3	3*	6.9	2.6	-7	3	9*	35.5	35.9	0	4	0	223.9	227.9
3	3	0*	9.5	2.6	7	3	2*	35.1	33.7	-2	4	1*	25.1	19.5
-5	3	4	59.8	59.1	9	3	1	28.0	32.2	-4	4	2	193.8	190.5
-5	3	1	58.2	59.3	-9	3	10	25.0	31.6	-6	4	3	45.2	42.5
-7	3	2*	5.3	11.6	-1	3	7*	26.1	23.9	-8	4	4	112.0	113.0
-7	3	5*	17.0	12.3	1	3	6*	25.0	21.5	0	4	1*	31.3	26.6
-9	3	6	57.6	56.8	-3	3	8	38.3	36.8	-2	4	2*	3.3	29.4
-9	3	3	57.7	55.2	3	3	5	44.5	36.6	2	4	0*	20.2	30.5
-11	3	4*	11.9	9.7	5	3	4*	23.8	23.6	-4	4	3*	42.0	38.0
-11	3	7*	9.7	9.9	-5	3	9*	20.5	25.1	-4	4	1*	39.3	34.0
1	3	2	213.6	215.4	7	3	3*	44.2	41.8	-6	4	4*	25.5	31.2
-1	3	3	211.6	210.9	-7	3	10*	39.8	44.0	-6	4	2*	29.2	33.9
-3	3	4	160.7	160.6	9	3	2*	20.0	23.6	-8	4	3	42.2	35.7
3	3	1	159.9	157.3	-9	3	11*	23.1	25.2	-8	4	5	42.4	38.5
-5	3	5	193.0	188.1	-1	3	8	92.7	91.3	0	4	2*	17.1	13.5
5	3	0	195.2	191.7	1	3	7	100.8	96.9	2	4	1	101.5	100.5

h	k	l	/Fo/	/Fc/	h	k	l	/Fo/	/Fc/	h	k	l	/Fo/	/Fc/
-2	4	3	101.9	102.3	-8	4	8*	22.7	36.0	0	4	8*	3.0	12.4
4	4	0*	14.3	14.7	8	4	0*	35.0	32.8	2	4	7*	49.7	47.0
-4	4	4*	24.2	15.0	0	4	5	151.2	153.9	-2	4	9*	50.4	49.8
-6	4	1	79.9	77.4	-2	4	6	26.9	30.8	-4	4	10*	.0	7.9
-6	4	5	79.9	82.1	2	4	4	32.7	33.6	4	4	6*	20.7	8.5
-8	4	6*	4.6	14.6	-4	4	7	127.0	129.8	0	4	9	34.8	29.3
-8	4	2*	22.9	14.5	4	4	3	130.9	131.1	-2	4	10*	.0	9.0
0	4	3*	21.7	3.5	-6	4	8*	24.3	33.5	2	4	8*	6.0	8.5
-2	4	4*	17.2	18.2	6	4	2*	40.6	36.7	1	5	0*	30.5	29.9
2	4	2*	21.4	20.4	0	4	6*	26.9	37.1	-1	5	1*	28.5	29.6
4	4	1*	2.6	8.6	-2	4	7*	22.8	19.4	-3	5	1*	25.8	27.0
-4	4	5*	17.2	9.1	2	4	5*	22.1	21.7	-3	5	2*	33.2	25.0
-6	4	6	39.4	37.1	-4	4	8	31.6	37.0	-1	5	2*	6.9	23.0
6	4	0	38.2	40.6	4	4	4	34.4	35.6	1	5	1*	1.1	24.7
-8	4	1*	15.8	7.0	-6	4	9*	21.2	31.4	3	5	0*	8.4	7.3
-8	4	7*	4.3	7.2	6	4	3*	29.3	34.5	-3	5	3*	16.6	8.0
0	4	4*	9.6	8.5	0	4	7	54.3	47.3	1	5	2	107.4	105.8
-2	4	5*	28.0	25.4	2	4	6	119.6	114.9	-1	5	3	105.8	103.3
2	4	3*	25.0	27.2	-2	4	8	113.3	115.4	-3	5	4	81.3	81.1
4	4	2*	31.1	25.2	-4	4	9	43.5	43.1	3	5	1	81.0	79.3
-4	4	6*	32.5	27.6	4	4	5	48.2	45.9	-1	5	4*	26.4	26.3
-6	4	7	25.1	26.1	-6	4	10	73.3	83.0	1	5	3*	26.4	23.5
6	4	1	34.0	29.0	6	4	4	81.2	81.3	0	0	0	.0	.0

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 $I < 2\sigma(I)$.