

MSG No. 22.48 F_S222 [Type IV, orthorhombic]

Table 1: Wyckoff site: **8a**, site symmetry: 222

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4]
2	[0, $\frac{1}{2}$, $\frac{1}{2}$]	[5,6,7,8]
3	[$\frac{1}{2}$, 0, $\frac{1}{2}$]	[9,10,11,12]
4	[$\frac{1}{2}$, $\frac{1}{2}$, 0]	[13,14,15,16]
5	[0, 0, $\frac{1}{2}$]	[17,18,19,20]
6	[0, $\frac{1}{2}$, 0]	[21,22,23,24]
7	[$\frac{1}{2}$, 0, 0]	[25,26,27,28]
8	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[29,30,31,32]

Table 2: Wyckoff site: **8b**, site symmetry: 22'2'

No.	position	mapping
1	[$\frac{1}{4}$, 0, 0]	[1,2,27,28]
2	[$\frac{3}{4}$, 0, 0]	[3,4,25,26]
3	[$\frac{1}{4}$, $\frac{1}{2}$, $\frac{1}{2}$]	[5,6,31,32]
4	[$\frac{3}{4}$, $\frac{1}{2}$, $\frac{1}{2}$]	[7,8,29,30]
5	[$\frac{3}{4}$, 0, $\frac{1}{2}$]	[9,10,19,20]
6	[$\frac{1}{4}$, 0, $\frac{1}{2}$]	[11,12,17,18]
7	[$\frac{3}{4}$, $\frac{1}{2}$, 0]	[13,14,23,24]
8	[$\frac{1}{4}$, $\frac{1}{2}$, 0]	[15,16,21,22]

Table 3: Wyckoff site: **8c**, site symmetry: 2'22'

No.	position	mapping
1	[0, $\frac{1}{4}$, 0]	[1,3,22,24]
2	[0, $\frac{3}{4}$, 0]	[2,4,21,23]
3	[0, $\frac{3}{4}$, $\frac{1}{2}$]	[5,7,18,20]
4	[0, $\frac{1}{4}$, $\frac{1}{2}$]	[6,8,17,19]
5	[$\frac{1}{2}$, $\frac{1}{4}$, $\frac{1}{2}$]	[9,11,30,32]
6	[$\frac{1}{2}$, $\frac{3}{4}$, $\frac{1}{2}$]	[10,12,29,31]
7	[$\frac{1}{2}$, $\frac{3}{4}$, 0]	[13,15,26,28]
8	[$\frac{1}{2}$, $\frac{1}{4}$, 0]	[14,16,25,27]

Table 4: Wyckoff site: 8d, site symmetry: 2'2'2

No.	position	mapping
1	$[0, 0, \frac{1}{4}]$	$[1, 4, 18, 19]$
2	$[0, 0, \frac{3}{4}]$	$[2, 3, 17, 20]$
3	$[0, \frac{1}{2}, \frac{3}{4}]$	$[5, 8, 22, 23]$
4	$[0, \frac{1}{2}, \frac{1}{4}]$	$[6, 7, 21, 24]$
5	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[9, 12, 26, 27]$
6	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[10, 11, 25, 28]$
7	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	$[13, 16, 30, 31]$
8	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	$[14, 15, 29, 32]$

Table 5: Wyckoff site: 8e, site symmetry: 2'2'2

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[1, 16, 22, 27]$
2	$[\frac{1}{4}, \frac{3}{4}, 0]$	$[2, 15, 21, 28]$
3	$[\frac{3}{4}, \frac{1}{4}, 0]$	$[3, 14, 24, 25]$
4	$[\frac{3}{4}, \frac{3}{4}, 0]$	$[4, 13, 23, 26]$
5	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	$[5, 12, 18, 31]$
6	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	$[6, 11, 17, 32]$
7	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	$[7, 10, 20, 29]$
8	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	$[8, 9, 19, 30]$

Table 6: Wyckoff site: 8f, site symmetry: 2'22'

No.	position	mapping
1	$[\frac{1}{4}, 0, \frac{1}{4}]$	$[1, 11, 18, 28]$
2	$[\frac{1}{4}, 0, \frac{3}{4}]$	$[2, 12, 17, 27]$
3	$[\frac{3}{4}, 0, \frac{3}{4}]$	$[3, 9, 20, 26]$
4	$[\frac{3}{4}, 0, \frac{1}{4}]$	$[4, 10, 19, 25]$
5	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	$[5, 15, 22, 32]$
6	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	$[6, 16, 21, 31]$
7	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	$[7, 13, 24, 30]$
8	$[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}]$	$[8, 14, 23, 29]$

Table 7: Wyckoff site: 8g, site symmetry: 22'2'

No.	position	mapping
1	$[0, \frac{1}{4}, \frac{1}{4}]$	$[1, 6, 19, 24]$
2	$[0, \frac{3}{4}, \frac{3}{4}]$	$[2, 5, 20, 23]$
3	$[0, \frac{1}{4}, \frac{3}{4}]$	$[3, 8, 17, 22]$

continued ...

Table 7

No.	position	mapping
4	$[0, \frac{3}{4}, \frac{1}{4}]$	[4, 7, 18, 21]
5	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[9, 14, 27, 32]
6	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[10, 13, 28, 31]
7	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[11, 16, 25, 30]
8	$[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[12, 15, 26, 29]

Table 8: Wyckoff site: 8h, site symmetry: 222

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[1, 6, 11, 16]
2	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[2, 5, 12, 15]
3	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[3, 8, 9, 14]
4	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[4, 7, 10, 13]
5	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[17, 22, 27, 32]
6	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[18, 21, 28, 31]
7	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[19, 24, 25, 30]
8	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[20, 23, 26, 29]

Table 9: Wyckoff site: 16i, site symmetry: 2..

No.	position	mapping
1	$[x, 0, 0]$	[1, 2]
2	$[-x, 0, 0]$	[3, 4]
3	$[x, \frac{1}{2}, \frac{1}{2}]$	[5, 6]
4	$[-x, \frac{1}{2}, \frac{1}{2}]$	[7, 8]
5	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[9, 10]
6	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[11, 12]
7	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[13, 14]
8	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[15, 16]
9	$[x, 0, \frac{1}{2}]$	[17, 18]
10	$[-x, 0, \frac{1}{2}]$	[19, 20]
11	$[x, \frac{1}{2}, 0]$	[21, 22]
12	$[-x, \frac{1}{2}, 0]$	[23, 24]
13	$[x + \frac{1}{2}, 0, 0]$	[25, 26]
14	$[\frac{1}{2} - x, 0, 0]$	[27, 28]
15	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[29, 30]
16	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[31, 32]

Table 10: Wyckoff site: 16j, site symmetry: $2^1\ldots$

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1,18]
2	$[x, 0, \frac{3}{4}]$	[2,17]
3	$[-x, 0, \frac{3}{4}]$	[3,20]
4	$[-x, 0, \frac{1}{4}]$	[4,19]
5	$[x, \frac{1}{2}, \frac{3}{4}]$	[5,22]
6	$[x, \frac{1}{2}, \frac{1}{4}]$	[6,21]
7	$[-x, \frac{1}{2}, \frac{1}{4}]$	[7,24]
8	$[-x, \frac{1}{2}, \frac{3}{4}]$	[8,23]
9	$[x + \frac{1}{2}, 0, \frac{3}{4}]$	[9,26]
10	$[x + \frac{1}{2}, 0, \frac{1}{4}]$	[10,25]
11	$[\frac{1}{2} - x, 0, \frac{1}{4}]$	[11,28]
12	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[12,27]
13	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[13,30]
14	$[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[14,29]
15	$[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$	[15,32]
16	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{4}]$	[16,31]

Table 11: Wyckoff site: 16k, site symmetry: $2^1\ldots$

No.	position	mapping
1	$[x, \frac{1}{4}, 0]$	[1,22]
2	$[x, \frac{3}{4}, 0]$	[2,21]
3	$[-x, \frac{1}{4}, 0]$	[3,24]
4	$[-x, \frac{3}{4}, 0]$	[4,23]
5	$[x, \frac{3}{4}, \frac{1}{2}]$	[5,18]
6	$[x, \frac{1}{4}, \frac{1}{2}]$	[6,17]
7	$[-x, \frac{3}{4}, \frac{1}{2}]$	[7,20]
8	$[-x, \frac{1}{4}, \frac{1}{2}]$	[8,19]
9	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[9,30]
10	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}]$	[10,29]
11	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{2}]$	[11,32]
12	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{2}]$	[12,31]
13	$[x + \frac{1}{2}, \frac{3}{4}, 0]$	[13,26]
14	$[x + \frac{1}{2}, \frac{1}{4}, 0]$	[14,25]
15	$[\frac{1}{2} - x, \frac{3}{4}, 0]$	[15,28]
16	$[\frac{1}{2} - x, \frac{1}{4}, 0]$	[16,27]

Table 12: Wyckoff site: 16l, site symmetry: $2\ldots$

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1,6]

continued ...

Table 12

No.	position	mapping
2	$[x, \frac{3}{4}, \frac{3}{4}]$	[2,5]
3	$[-x, \frac{1}{4}, \frac{3}{4}]$	[3,8]
4	$[-x, \frac{3}{4}, \frac{1}{4}]$	[4,7]
5	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[9,14]
6	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[10,13]
7	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[11,16]
8	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[12,15]
9	$[x, \frac{1}{4}, \frac{3}{4}]$	[17,22]
10	$[x, \frac{3}{4}, \frac{1}{4}]$	[18,21]
11	$[-x, \frac{1}{4}, \frac{1}{4}]$	[19,24]
12	$[-x, \frac{3}{4}, \frac{3}{4}]$	[20,23]
13	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[25,30]
14	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[26,29]
15	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[27,32]
16	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[28,31]

Table 13: Wyckoff site: 16m, site symmetry: .2.

No.	position	mapping
1	$[0, y, 0]$	[1,3]
2	$[0, -y, 0]$	[2,4]
3	$[0, y + \frac{1}{2}, \frac{1}{2}]$	[5,7]
4	$[0, \frac{1}{2} - y, \frac{1}{2}]$	[6,8]
5	$[\frac{1}{2}, y, \frac{1}{2}]$	[9,11]
6	$[\frac{1}{2}, -y, \frac{1}{2}]$	[10,12]
7	$[\frac{1}{2}, y + \frac{1}{2}, 0]$	[13,15]
8	$[\frac{1}{2}, \frac{1}{2} - y, 0]$	[14,16]
9	$[0, y, \frac{1}{2}]$	[17,19]
10	$[0, -y, \frac{1}{2}]$	[18,20]
11	$[0, y + \frac{1}{2}, 0]$	[21,23]
12	$[0, \frac{1}{2} - y, 0]$	[22,24]
13	$[\frac{1}{2}, y, 0]$	[25,27]
14	$[\frac{1}{2}, -y, 0]$	[26,28]
15	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[29,31]
16	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[30,32]

Table 14: Wyckoff site: 16n, site symmetry: .2'.

No.	position	mapping
1	$[0, y, \frac{1}{4}]$	[1,19]
2	$[0, -y, \frac{3}{4}]$	[2,20]
3	$[0, y, \frac{3}{4}]$	[3,17]

continued ...

Table 14

No.	position	mapping
4	$[0, -y, \frac{1}{4}]$	[4,18]
5	$[0, y + \frac{1}{2}, \frac{3}{4}]$	[5,23]
6	$[0, \frac{1}{2} - y, \frac{1}{4}]$	[6,24]
7	$[0, y + \frac{1}{2}, \frac{1}{4}]$	[7,21]
8	$[0, \frac{1}{2} - y, \frac{3}{4}]$	[8,22]
9	$[\frac{1}{2}, y, \frac{3}{4}]$	[9,27]
10	$[\frac{1}{2}, -y, \frac{1}{4}]$	[10,28]
11	$[\frac{1}{2}, y, \frac{1}{4}]$	[11,25]
12	$[\frac{1}{2}, -y, \frac{3}{4}]$	[12,26]
13	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$	[13,31]
14	$[\frac{1}{2}, \frac{1}{2} - y, \frac{3}{4}]$	[14,32]
15	$[\frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[15,29]
16	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$	[16,30]

Table 15: Wyckoff site: 16o, site symmetry: .2'.

No.	position	mapping
1	$[\frac{1}{4}, y, 0]$	[1,27]
2	$[\frac{1}{4}, -y, 0]$	[2,28]
3	$[\frac{3}{4}, y, 0]$	[3,25]
4	$[\frac{3}{4}, -y, 0]$	[4,26]
5	$[\frac{1}{4}, y + \frac{1}{2}, \frac{1}{2}]$	[5,31]
6	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2}]$	[6,32]
7	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2}]$	[7,29]
8	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{2}]$	[8,30]
9	$[\frac{3}{4}, y, \frac{1}{2}]$	[9,19]
10	$[\frac{3}{4}, -y, \frac{1}{2}]$	[10,20]
11	$[\frac{1}{4}, y, \frac{1}{2}]$	[11,17]
12	$[\frac{1}{4}, -y, \frac{1}{2}]$	[12,18]
13	$[\frac{3}{4}, y + \frac{1}{2}, 0]$	[13,23]
14	$[\frac{3}{4}, \frac{1}{2} - y, 0]$	[14,24]
15	$[\frac{1}{4}, y + \frac{1}{2}, 0]$	[15,21]
16	$[\frac{1}{4}, \frac{1}{2} - y, 0]$	[16,22]

Table 16: Wyckoff site: 16p, site symmetry: .2.

No.	position	mapping
1	$[\frac{1}{4}, y, \frac{1}{4}]$	[1,11]
2	$[\frac{1}{4}, -y, \frac{3}{4}]$	[2,12]
3	$[\frac{3}{4}, y, \frac{3}{4}]$	[3,9]
4	$[\frac{3}{4}, -y, \frac{1}{4}]$	[4,10]
5	$[\frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}]$	[5,15]

continued ...

Table 16

No.	position	mapping
6	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{4}]$	[6,16]
7	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{4}]$	[7,13]
8	$[\frac{3}{4}, \frac{1}{2} - y, \frac{3}{4}]$	[8,14]
9	$[\frac{1}{4}, y, \frac{3}{4}]$	[17,27]
10	$[\frac{1}{4}, -y, \frac{1}{4}]$	[18,28]
11	$[\frac{3}{4}, y, \frac{1}{4}]$	[19,25]
12	$[\frac{3}{4}, -y, \frac{3}{4}]$	[20,26]
13	$[\frac{1}{4}, y + \frac{1}{2}, \frac{1}{4}]$	[21,31]
14	$[\frac{1}{4}, \frac{1}{2} - y, \frac{3}{4}]$	[22,32]
15	$[\frac{3}{4}, y + \frac{1}{2}, \frac{3}{4}]$	[23,29]
16	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{4}]$	[24,30]

Table 17: Wyckoff site: 16q, site symmetry: ...2

No.	position	mapping
1	$[0, 0, z]$	[1,4]
2	$[0, 0, -z]$	[2,3]
3	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[5,8]
4	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[6,7]
5	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[9,12]
6	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[10,11]
7	$[\frac{1}{2}, \frac{1}{2}, z]$	[13,16]
8	$[\frac{1}{2}, \frac{1}{2}, -z]$	[14,15]
9	$[0, 0, z + \frac{1}{2}]$	[17,20]
10	$[0, 0, \frac{1}{2} - z]$	[18,19]
11	$[0, \frac{1}{2}, z]$	[21,24]
12	$[0, \frac{1}{2}, -z]$	[22,23]
13	$[\frac{1}{2}, 0, z]$	[25,28]
14	$[\frac{1}{2}, 0, -z]$	[26,27]
15	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[29,32]
16	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[30,31]

Table 18: Wyckoff site: 16r, site symmetry: ...2'

No.	position	mapping
1	$[\frac{1}{4}, 0, z]$	[1,28]
2	$[\frac{1}{4}, 0, -z]$	[2,27]
3	$[\frac{3}{4}, 0, -z]$	[3,26]
4	$[\frac{3}{4}, 0, z]$	[4,25]
5	$[\frac{1}{4}, \frac{1}{2}, z + \frac{1}{2}]$	[5,32]
6	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{2} - z]$	[6,31]
7	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{2} - z]$	[7,30]

continued ...

Table 18

No.	position	mapping
8	$[\frac{3}{4}, \frac{1}{2}, z + \frac{1}{2}]$	[8,29]
9	$[\frac{3}{4}, 0, z + \frac{1}{2}]$	[9,20]
10	$[\frac{3}{4}, 0, \frac{1}{2} - z]$	[10,19]
11	$[\frac{1}{4}, 0, \frac{1}{2} - z]$	[11,18]
12	$[\frac{1}{4}, 0, z + \frac{1}{2}]$	[12,17]
13	$[\frac{3}{4}, \frac{1}{2}, z]$	[13,24]
14	$[\frac{3}{4}, \frac{1}{2}, -z]$	[14,23]
15	$[\frac{1}{4}, \frac{1}{2}, -z]$	[15,22]
16	$[\frac{1}{4}, \frac{1}{2}, z]$	[16,21]

Table 19: Wyckoff site: 16s, site symmetry: ...2'

No.	position	mapping
1	$[0, \frac{1}{4}, z]$	[1,24]
2	$[0, \frac{3}{4}, -z]$	[2,23]
3	$[0, \frac{1}{4}, -z]$	[3,22]
4	$[0, \frac{3}{4}, z]$	[4,21]
5	$[0, \frac{3}{4}, z + \frac{1}{2}]$	[5,20]
6	$[0, \frac{1}{4}, \frac{1}{2} - z]$	[6,19]
7	$[0, \frac{3}{4}, \frac{1}{2} - z]$	[7,18]
8	$[0, \frac{1}{4}, z + \frac{1}{2}]$	[8,17]
9	$[\frac{1}{2}, \frac{1}{4}, z + \frac{1}{2}]$	[9,32]
10	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z]$	[10,31]
11	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - z]$	[11,30]
12	$[\frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$	[12,29]
13	$[\frac{1}{2}, \frac{3}{4}, z]$	[13,28]
14	$[\frac{1}{2}, \frac{1}{4}, -z]$	[14,27]
15	$[\frac{1}{2}, \frac{3}{4}, -z]$	[15,26]
16	$[\frac{1}{2}, \frac{1}{4}, z]$	[16,25]

Table 20: Wyckoff site: 16t, site symmetry: ...2

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	[1,16]
2	$[\frac{1}{4}, \frac{3}{4}, -z]$	[2,15]
3	$[\frac{3}{4}, \frac{1}{4}, -z]$	[3,14]
4	$[\frac{3}{4}, \frac{3}{4}, z]$	[4,13]
5	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[5,12]
6	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[6,11]
7	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[7,10]
8	$[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[8,9]
9	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[17,32]

continued ...

Table 20

No.	position	mapping
10	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[18,31]
11	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[19,30]
12	$[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[20,29]
13	$[\frac{1}{4}, \frac{3}{4}, z]$	[21,28]
14	$[\frac{1}{4}, \frac{1}{4}, -z]$	[22,27]
15	$[\frac{3}{4}, \frac{3}{4}, -z]$	[23,26]
16	$[\frac{3}{4}, \frac{1}{4}, z]$	[24,25]

Table 21: Wyckoff site: 32u, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -y, -z]$	[2]
3	$[-x, y, -z]$	[3]
4	$[-x, -y, z]$	[4]
5	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[6]
7	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[7]
8	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[8]
9	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[9]
10	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[10]
11	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[12]
13	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[13]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[14]
15	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[15]
16	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[16]
17	$[x, y, z + \frac{1}{2}]$	[17]
18	$[x, -y, \frac{1}{2} - z]$	[18]
19	$[-x, y, \frac{1}{2} - z]$	[19]
20	$[-x, -y, z + \frac{1}{2}]$	[20]
21	$[x, y + \frac{1}{2}, z]$	[21]
22	$[x, \frac{1}{2} - y, -z]$	[22]
23	$[-x, y + \frac{1}{2}, -z]$	[23]
24	$[-x, \frac{1}{2} - y, z]$	[24]
25	$[x + \frac{1}{2}, y, z]$	[25]
26	$[x + \frac{1}{2}, -y, -z]$	[26]
27	$[\frac{1}{2} - x, y, -z]$	[27]
28	$[\frac{1}{2} - x, -y, z]$	[28]
29	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[29]
30	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[30]
31	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[31]
32	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[32]