

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:  $2'..$ 

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:  $2'..$ 

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:  $2..$ 

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:  $\dots 2$ 

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:  $\dots 2'$ 

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:  $\dots 2'$ 

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:  $\dots 2$ 

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]