MSG No. 65.489 C_ammm [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `mmm`

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

Table 2: Wyckoff site: `4b`, site symmetry: `m'mm`

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

Table 3: Wyckoff site: `4c`, site symmetry: `mmm`

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

Table 4: Wyckoff site: `4d`, site symmetry: `m'mm`

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

Table 5: Wyckoff site: `4e`, site symmetry: `mm'm`

No.	position	mapping
1	$\left[0, \frac{1}{4}, 0\right]$	`[1,3,6,8,26,28,29,31]`
2	$\left[0, \frac{3}{4}, 0\right]$	`[2,4,5,7,25,27,30,32]`

continued ...

Table 5

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

Table 6: Wyckoff site: `4f`, site symmetry: `m'm'm`

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

Table 7: Wyckoff site: `4g`, site symmetry: `mm'm`

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

Table 8: Wyckoff site: `4h`, site symmetry: `m'm'm`

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

Table 9: Wyckoff site: `8i`, site symmetry: `2mm`

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

continued ...

Table 9

No.	position	mapping
8	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[27,28,29,30]`

Table 10: Wyckoff site: `8j`, site symmetry: `2mm`

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

Table 11: Wyckoff site: `8k`, site symmetry: `2'm'm`

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

Table 12: Wyckoff site: `8l`, site symmetry: `2'm'm`

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

Table 13: Wyckoff site: `8m`, site symmetry: `m2m`

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

Table 14: Wyckoff site: `8n`, site symmetry: `m2m`

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

Table 15: Wyckoff site: `8o`, site symmetry: `m'2'm`

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

Table 16: Wyckoff site: `8p`, site symmetry: `m'2'm`

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ \frac{1}{2}\right]$	`[1,8,19,22]`
2	$\left[\frac{1}{4},\ -y,\ \frac{1}{2}\right]$	`[2,7,20,21]`
3	$\left[\frac{3}{4},\ y,\ \frac{1}{2}\right]$	`[3,6,17,24]`

continued ...

Table 16

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

Table 17: Wyckoff site: 8q, site symmetry: mm2

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

Table 18: Wyckoff site: 8r, site symmetry: mm'2'

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

Table 19: Wyckoff site: 8s, site symmetry: m'm2'

No.	position	mapping
1	$\left[\frac{1}{4}, 0, z\right]$	[1,7,20,22]
2	$\left[\frac{1}{4}, 0, -z\right]$	[2,8,19,21]
3	$\left[\frac{3}{4}, 0, -z\right]$	[3,5,18,24]
4	$\left[\frac{3}{4}, 0, z\right]$	[4,6,17,23]
5	$\left[\frac{3}{4}, \frac{1}{2}, z\right]$	[9,15,28,30]
6	$\left[\frac{3}{4}, \frac{1}{2}, -z\right]$	[10,16,27,29]

continued ...

Table 19

No.	position	mapping
7	$\left[\frac{1}{4}, \frac{1}{2}, -z\right]$	`[11,13,26,32]`
8	$\left[\frac{1}{4}, \frac{1}{2}, z\right]$	`[12,14,25,31]`

Table 20: Wyckoff site: `8t`, site symmetry: `m'm'2`

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

Table 21: Wyckoff site: `16u`, site symmetry: `m..`

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

Table 22: Wyckoff site: `16v`, site symmetry: `m'..`

No.	position	mapping
1	$\left[\frac{1}{4}, y, z\right]$	`[1,22]`

continued ...

Table 22

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

Table 23: Wyckoff site: 16w, site symmetry: .m.

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

Table 24: Wyckoff site: 16x, site symmetry: .m'.

No.	position	mapping
1	$\left[x, \frac{1}{4}, z\right]$	[1,31]
2	$\left[x, \frac{3}{4}, -z\right]$	[2,32]
3	$\left[-x, \frac{1}{4}, -z\right]$	[3,29]

continued ...

Table 24

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

Table 25: Wyckoff site: 16y, site symmetry: ..m

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

Table 26: Wyckoff site: 16z, site symmetry: ..m

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{2}\right]$	[1,8]
2	$\left[x,\ -y,\ \frac{1}{2}\right]$	[2,7]
3	$\left[-x,\ y,\ \frac{1}{2}\right]$	[3,6]
4	$\left[-x,\ -y,\ \frac{1}{2}\right]$	[4,5]
5	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[9,16]

continued ...

Table 26

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

Table 27: Wyckoff site: 32A, 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	$[-x,\ -y,\ -z]$	[5]
6	$[-x,\ y,\ z]$	[6]
7	$[x,\ -y,\ z]$	[7]
8	$[x,\ y,\ -z]$	[8]
9	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[9]
10	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[10]
11	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$	[11]
12	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[12]
13	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ -z\right]$	[13]
14	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[14]
15	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	[15]
16	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[16]
17	$\left[x+\frac{1}{2},\ y,\ z\right]$	[17]
18	$\left[x+\frac{1}{2},\ -y,\ -z\right]$	[18]
19	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	[19]
20	$\left[\frac{1}{2}-x,\ -y,\ z\right]$	[20]
21	$\left[\frac{1}{2}-x,\ -y,\ -z\right]$	[21]
22	$\left[\frac{1}{2}-x,\ y,\ z\right]$	[22]
23	$\left[x+\frac{1}{2},\ -y,\ z\right]$	[23]
24	$\left[x+\frac{1}{2},\ y,\ -z\right]$	[24]
25	$\left[x,\ y+\frac{1}{2},\ z\right]$	[25]
26	$\left[x,\ \frac{1}{2}-y,\ -z\right]$	[26]
27	$\left[-x,\ y+\frac{1}{2},\ -z\right]$	[27]
28	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	[28]
29	$\left[-x,\ \frac{1}{2}-y,\ -z\right]$	[29]

continued ...

Table 27

No.	position	mapping
30	$\left[-x,\, y+\frac{1}{2},\, z\right]$	[30]
31	$\left[x,\, \frac{1}{2}-y,\, z\right]$	[31]
32	$\left[x,\, y+\frac{1}{2},\, -z\right]$	[32]