MSG No. 133.460 $P4_2/nbc1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 222.1'

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

Table 2: Wyckoff site: 4b, site symmetry: 222.1'

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

Table 3: Wyckoff site: 4c, site symmetry: 2.221'

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

Table 4: Wyckoff site: 4d, site symmetry: -4..1'

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

Table 5: Wyckoff site: 8e, site symmetry: -11'

No.	position	mapping
1	[0, 0, 0]	[1,9,17,25]
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[2,10,18,26]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 2..1'

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

Table 7: Wyckoff site: 8g, site symmetry: 2..1'

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

Table 8: Wyckoff site: 8h, site symmetry: .2.1'

No.	position	mapping
1	$\left[x, \frac{1}{4}, 0\right]$	[1,4,17,20]
2	$\left[\frac{1}{4}, x, \frac{1}{2}\right]$	[2,7,18,23]
3	$\left[\frac{1}{4}, \frac{1}{2}-x, \frac{1}{2}\right]$	[3,8,19,24]
4	$\left[\frac{1}{2}-x, \frac{1}{4}, 0\right]$	[5,6,21,22]
5	$\left[-x, \frac{3}{4}, 0\right]$	[9,12,25,28]

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{3}{4}, -x, \frac{1}{2}\right]$	`[10,15,26,31]`
7	$\left[\frac{3}{4}, x+\frac{1}{2}, \frac{1}{2}\right]$	`[11,16,27,32]`
8	$\left[x+\frac{1}{2}, \frac{3}{4}, 0\right]$	`[13,14,29,30]`

Table 9: Wyckoff site: `8i`, site symmetry: `.2.1'`

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

Table 10: Wyckoff site: `8j`, site symmetry: `..21'`

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

Table 11: Wyckoff site: `16k`, site symmetry: `11'`

No.	position	mapping
1	$[x, y, z]$	`[1,17]`
2	$\left[\frac{1}{2}-y, x, z+\frac{1}{2}\right]$	`[2,18]`
3	$\left[y, \frac{1}{2}-x, z+\frac{1}{2}\right]$	`[3,19]`
4	$\left[x, \frac{1}{2}-y, -z\right]$	`[4,20]`
5	$\left[\frac{1}{2}-x, y, -z\right]$	`[5,21]`
6	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z\right]$	`[6,22]`
7	$\left[y, x, \frac{1}{2}-z\right]$	`[7,23]`
8	$\left[\frac{1}{2}-y, \frac{1}{2}-x, \frac{1}{2}-z\right]$	`[8,24]`

continued ...

Table 11

No.	position	mapping
9	$[-x,\, -y,\, -z]$	[9,25]
10	$\left[y+\frac{1}{2},\, -x,\, \frac{1}{2}-z\right]$	[10,26]
11	$\left[-y,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[11,27]
12	$\left[-x,\, y+\frac{1}{2},\, z\right]$	[12,28]
13	$\left[x+\frac{1}{2},\, -y,\, z\right]$	[13,29]
14	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[14,30]
15	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[15,31]
16	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[16,32]