MSG No. 126.376 $P4/nnc1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4221'

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

Table 2: Wyckoff site: 2b, site symmetry: 4221'

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

Table 3: Wyckoff site: 4c, site symmetry: 222.1'

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: 4..1'

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

Table 6: Wyckoff site: `8f`, site symmetry: `-11'`

No.	position	mapping
1	$[0, 0, 0]$	`[1,9,17,25]`
2	$\left[\frac{1}{2}, 0, 0\right]$	`[2,10,18,26]`
3	$\left[0, \frac{1}{2}, 0\right]$	`[3,11,19,27]`
4	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[4,12,20,28]`
5	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[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 7: Wyckoff site: `8g`, site symmetry: `2..1'`

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

Table 8: Wyckoff site: `8h`, site symmetry: `..21'`

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

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

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

continued ...

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: .2.1'

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

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

No.	position	mapping
1	$[x,\ y,\ z]$	[1,17]
2	$\left[\frac{1}{2}-y,\ x,\ z\right]$	[2,18]
3	$\left[y,\ \frac{1}{2}-x,\ z\right]$	[3,19]
4	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[4,20]
5	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	[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]
9	$[-x,\ -y,\ -z]$	[9,25]
10	$\left[y+\frac{1}{2},\ -x,\ -z\right]$	[10,26]
11	$\left[-y,\ x+\frac{1}{2},\ -z\right]$	[11,27]
12	$\left[-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[12,28]
13	$\left[x+\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[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]