MSG No. 138.526 $P4'_2/n'cm'$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `2.22`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[1,2,3,4]
2	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[5,6,7,8]
3	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[9,10,11,12]
4	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[13,14,15,16]

Table 2: Wyckoff site: `4b`, site symmetry: `-4..`

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

Table 3: Wyckoff site: `4c`, site symmetry: `..2/m'`

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	[1,4,13,16]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[2,3,14,15]
3	$\left[\frac{1}{2}, 0, 0\right]$	[5,7,9,11]
4	$\left[0, \frac{1}{2}, 0\right]$	[6,8,10,12]

Table 4: Wyckoff site: `4d`, site symmetry: `..2/m'`

No.	position	mapping
1	$[0, 0, 0]$	[1,4,13,16]
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[2,3,14,15]
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[5,7,9,11]
4	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[6,8,10,12]

Table 5: Wyckoff site: `4e`, site symmetry: `2.m'm'`

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, z\right]$	[1,2,15,16]
2	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	[3,4,13,14]

continued ...

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Table 5

No.	position	mapping
3	$\left[\frac{3}{4},\, \frac{3}{4},\, \frac{1}{2} - z\right]$	[5,6,11,12]
4	$\left[\frac{1}{4},\, \frac{1}{4},\, z + \frac{1}{2}\right]$	[7,8,9,10]

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

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

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

No.	position	mapping
1	$\left[x,\, -x,\, \frac{1}{2}\right]$	[1,4]
2	$\left[\frac{1}{2} - x,\, x + \frac{1}{2},\, \frac{1}{2}\right]$	[2,3]
3	$\left[\frac{1}{2} - x,\, -x,\, 0\right]$	[5,7]
4	$\left[x,\, x + \frac{1}{2},\, 0\right]$	[6,8]
5	$\left[x + \frac{1}{2},\, x,\, 0\right]$	[9,11]
6	$\left[-x,\, \frac{1}{2} - x,\, 0\right]$	[10,12]
7	$\left[-x,\, x,\, \frac{1}{2}\right]$	[13,16]
8	$\left[x + \frac{1}{2},\, \frac{1}{2} - x,\, \frac{1}{2}\right]$	[14,15]

Table 8: Wyckoff site: 8h, site symmetry: ..2

No.	position	mapping
1	$\left[x,\, -x,\, 0\right]$	[1,4]
2	$\left[\frac{1}{2} - x,\, x + \frac{1}{2},\, 0\right]$	[2,3]
3	$\left[\frac{1}{2} - x,\, -x,\, \frac{1}{2}\right]$	[5,7]
4	$\left[x,\, x + \frac{1}{2},\, \frac{1}{2}\right]$	[6,8]
5	$\left[x + \frac{1}{2},\, x,\, \frac{1}{2}\right]$	[9,11]
6	$\left[-x,\, \frac{1}{2} - x,\, \frac{1}{2}\right]$	[10,12]
7	$\left[-x,\, x,\, 0\right]$	[13,16]
8	$\left[x + \frac{1}{2},\, \frac{1}{2} - x,\, 0\right]$	[14,15]

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

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

Table 10: Wyckoff site: `16j`, site symmetry: `1`

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