

MSG No. 126.375 $P4/nnc$ [Type I, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 422

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

Table 2: Wyckoff site: 2b, site symmetry: 422

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

Table 3: Wyckoff site: 4c, site symmetry: 222.

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

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

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

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

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

Table 6: Wyckoff site: 8f, site symmetry: -1

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

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

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: .2.

No.	position	mapping
1	[x, $\frac{1}{4}$, $\frac{1}{4}$]	[1, 4]
2	[$\frac{1}{4}$, x, $\frac{1}{4}$]	[2, 7]
3	[$\frac{1}{4}$, $\frac{1}{2}$ - x, $\frac{1}{4}$]	[3, 8]

continued ...

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: .2.

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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