

MSG No. 134.471 $P4_2/nnm$ [Type I, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: $-42m$

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

Table 2: Wyckoff site: 2b, site symmetry: $-42m$

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: 2.22

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

Table 5: Wyckoff site: 4e, site symmetry: $.2/m$

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

Table 6: Wyckoff site: **4f**, site symmetry: $\dots 2/m$

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

Table 7: Wyckoff site: **4g**, site symmetry: $2.mm$

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

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

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

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

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

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

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

Table 11: Wyckoff site: $8k$, site symmetry: $.2$

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

Table 12: Wyckoff site: $8l$, site symmetry: $.2$

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

Table 13: Wyckoff site: $8m$, site symmetry: $.m$

No.	position	mapping
1	$[x, -x, z]$	$[1, 15]$
2	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	$[2, 13]$
3	$[-x, \frac{1}{2} - x, z + \frac{1}{2}]$	$[3, 12]$

continued ...

Table 13

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

Table 14: Wyckoff site: 16n, site symmetry: 1

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