

MSG No. 113.274 $P\bar{4}2_1m$ [Type IV, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: $-4'2'm$

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

Table 2: Wyckoff site: 2b, site symmetry: $-4'2'm$

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

Table 3: Wyckoff site: 4c, site symmetry: $22'2'$

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, x + \frac{1}{2}, z]$	$[1, 8]$
2	$[x + \frac{1}{2}, -x, -z]$	$[2, 5]$
3	$[\frac{1}{2} - x, x, -z]$	$[3, 6]$

continued ...

Table 9

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

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

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