

MSG No. 121.331 $I\bar{4}2'm'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, x, z]$	$[1, 8]$
2	$[-x, -x, z]$	$[2, 7]$
3	$[x, -x, -z]$	$[3, 5]$

continued ...

Table 9

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

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

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