

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]