

MSG No. 87.75 $I4/m$ [Type I, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4/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: 4/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: 2/m..

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

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

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

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

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

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

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

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

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

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

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

Table 9: Wyckoff site: 16i, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-y, x, z]$	[2]
3	$[y, -x, z]$	[3]

continued ...

Table 9

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