

MSG No. 82.42 $I_c\bar{4}$ [Type IV, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: -4..

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

Table 2: Wyckoff site: 4b, site symmetry: -4'..

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

Table 3: Wyckoff site: 4c, site symmetry: -4'..

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: 2..

No.	position	mapping
1	[0, 0, z]	[1,2]
2	[0, 0, -z]	[3,4]

continued ...

Table 5

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

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

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

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

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

Table 8: Wyckoff site: 16h, 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	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]

continued ...

Table 8

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