

MSG No. 138.519  $P4_2/ncm$  [ Type I, tetragonal ]

Table 1: Wyckoff site: 4a, site symmetry: 2.22

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: ..2/m

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

Table 4: Wyckoff site: 4d, site symmetry: ..2/m

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

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

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	[1,6,15,16]
2	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[2,3,12,13]

*continued ...*

Table 5

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

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

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

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

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

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

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

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

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

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

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