

MSG No. 136.495 $P4_2/mnm$ [Type I, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: m.m̄m̄

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

Table 2: Wyckoff site: 2b, site symmetry: m.m̄m̄

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

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

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

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

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

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

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

Table 6: Wyckoff site: 4f, site symmetry: m.2m

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

Table 7: Wyckoff site: 4g, site symmetry: m.m2

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

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

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

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

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

Table 10: Wyckoff site: 8j, site symmetry: . . m

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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