

MSG No. 101.185 P_{C42cm} [Type IV, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 2.m̄m̄

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: 2.m̄m̄

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

Table 4: Wyckoff site: 8d, site symmetry: . .m̄

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

Table 5: Wyckoff site: **8e**, site symmetry: $\dots \cdot m'$

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

Table 6: Wyckoff site: **16f**, site symmetry: 1

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