

MSG No. 135.486 $P4'_2/m'b'c$ [Type III, tetragonal]

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: 2.22

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

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

No.	position	mapping
1	[0, 0, z]	[1,2]
2	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[3,4]

continued ...

Table 5

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

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

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

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

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

continued ...

Table 8

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

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

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