

MSG No. 135.485 $P4_2/m'bc$ [Type III, tetragonal]

Table 1: Wyckoff site: **4a**, site symmetry: $2/m' \dots$

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

Table 2: Wyckoff site: **4b**, site symmetry: $-4' \dots$

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

Table 3: Wyckoff site: **4c**, site symmetry: $2/m' \dots$

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

Table 4: Wyckoff site: **4d**, site symmetry: $2.2'2'$

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

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

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

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[x, y, 0]$	[1,16]
2	$[-y, x, \frac{1}{2}]$	[2,15]
3	$[y, -x, \frac{1}{2}]$	[3,14]
4	$[-x, -y, 0]$	[4,13]
5	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	[5,10]

continued ...

Table 8

No.	position	mapping
6	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	[6,9]
7	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2}]$	[7,12]
8	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[8,11]

Table 9: Wyckoff site: 16i, 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	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[5]
6	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[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	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[9]
10	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[10]
11	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[12]
13	$[-x, -y, -z]$	[13]
14	$[y, -x, \frac{1}{2} - z]$	[14]
15	$[-y, x, \frac{1}{2} - z]$	[15]
16	$[x, y, -z]$	[16]