

MSG No. 103.201 P_C4cc [Type IV, tetragonal]

Table 1: Wyckoff site: **4a**, site symmetry: 4..

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

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

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

Table 3: Wyckoff site: **8c**, site symmetry: 2'..

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

Table 4: Wyckoff site: **16d**, site symmetry: 1

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

continued ...

Table 4

No.	position	mapping
10	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[10]
11	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[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	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[15]
16	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[16]