

MSG No. 104.208 P_c4nc [Type IV, tetragonal]

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

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

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

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

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

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

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	[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]	[5]
6	[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]	[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, y, z + \frac{1}{2}]	[9]

continued ...

Table 4

No.	position	mapping
10	$[-y, x, z + \frac{1}{2}]$	[10]
11	$[y, -x, z + \frac{1}{2}]$	[11]
12	$[-x, -y, z + \frac{1}{2}]$	[12]
13	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[13]
14	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[14]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[15]
16	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[16]