

MSG No. 128.404  $P4'/m'n'c$  [ Type III, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $4'/\text{m}'..$

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

Table 2: Wyckoff site: 2b, site symmetry:  $4'/\text{m}'..$

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

Table 3: Wyckoff site: 4c, site symmetry:  $2/\text{m}'..$

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{1}{4}]	[2,3,9,10]
3	[\frac{1}{2}, 0, \frac{3}{4}]	[5,6,14,15]
4	[0, \frac{1}{2}, \frac{3}{4}]	[7,8,13,16]

Table 5: Wyckoff site: 4e, site symmetry:  $4'..$

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

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

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

*continued ...*

Table 9

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