

MSG No. 128.400  $P4/mnc1'$  [ Type II, tetragonal ]

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

No.	position	mapping
1	[0, 0, 0]	[1, 2, 3, 6, 9, 10, 11, 14, 17, 18, 19, 22, 25, 26, 27, 30]
2	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[4, 5, 7, 8, 12, 13, 15, 16, 20, 21, 23, 24, 28, 29, 31, 32]

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

No.	position	mapping
1	[0, 0, \frac{1}{2}]	[1, 2, 3, 6, 9, 10, 11, 14, 17, 18, 19, 22, 25, 26, 27, 30]
2	[\frac{1}{2}, \frac{1}{2}, 0]	[4, 5, 7, 8, 12, 13, 15, 16, 20, 21, 23, 24, 28, 29, 31, 32]

Table 3: Wyckoff site: 4c, site symmetry: 2/m..1'

No.	position	mapping
1	[0, \frac{1}{2}, 0]	[1, 6, 9, 14, 17, 22, 25, 30]
2	[\frac{1}{2}, 0, 0]	[2, 3, 10, 11, 18, 19, 26, 27]
3	[\frac{1}{2}, 0, \frac{1}{2}]	[4, 5, 12, 13, 20, 21, 28, 29]
4	[0, \frac{1}{2}, \frac{1}{2}]	[7, 8, 15, 16, 23, 24, 31, 32]

Table 4: Wyckoff site: 4d, site symmetry: 2..221'

No.	position	mapping
1	[0, \frac{1}{2}, \frac{1}{4}]	[1, 6, 7, 8, 17, 22, 23, 24]
2	[\frac{1}{2}, 0, \frac{1}{4}]	[2, 3, 4, 5, 18, 19, 20, 21]
3	[0, \frac{1}{2}, \frac{3}{4}]	[9, 14, 15, 16, 25, 30, 31, 32]
4	[\frac{1}{2}, 0, \frac{3}{4}]	[10, 11, 12, 13, 26, 27, 28, 29]

Table 5: Wyckoff site: 4e, site symmetry: 4..1'

No.	position	mapping
1	[0, 0, z]	[1, 2, 3, 6, 17, 18, 19, 22]
2	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]	[4, 5, 7, 8, 20, 21, 23, 24]
3	[0, 0, -z]	[9, 10, 11, 14, 25, 26, 27, 30]
4	[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]	[12, 13, 15, 16, 28, 29, 31, 32]

Table 6: Wyckoff site: 8f, site symmetry: 2..1'

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	[1,6,17,22]
2	$[\frac{1}{2}, 0, z]$	[2,3,18,19]
3	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[4,5,20,21]
4	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[7,8,23,24]
5	$[0, \frac{1}{2}, -z]$	[9,14,25,30]
6	$[\frac{1}{2}, 0, -z]$	[10,11,26,27]
7	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[12,13,28,29]
8	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[15,16,31,32]

Table 7: Wyckoff site: 8g, site symmetry: ..21'

No.	position	mapping
1	$[x, x + \frac{1}{2}, \frac{1}{4}]$	[1,7,17,23]
2	$[\frac{1}{2} - x, x, \frac{1}{4}]$	[2,5,18,21]
3	$[x + \frac{1}{2}, -x, \frac{1}{4}]$	[3,4,19,20]
4	$[-x, \frac{1}{2} - x, \frac{1}{4}]$	[6,8,22,24]
5	$[-x, \frac{1}{2} - x, \frac{3}{4}]$	[9,15,25,31]
6	$[x + \frac{1}{2}, -x, \frac{3}{4}]$	[10,13,26,29]
7	$[\frac{1}{2} - x, x, \frac{3}{4}]$	[11,12,27,28]
8	$[x, x + \frac{1}{2}, \frac{3}{4}]$	[14,16,30,32]

Table 8: Wyckoff site: 8h, site symmetry: m..1'

No.	position	mapping
1	$[x, y, 0]$	[1,14,17,30]
2	$[-y, x, 0]$	[2,11,18,27]
3	$[y, -x, 0]$	[3,10,19,26]
4	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[4,13,20,29]
5	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	[5,12,21,28]
6	$[-x, -y, 0]$	[6,9,22,25]
7	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[7,16,23,32]
8	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2}]$	[8,15,24,31]

Table 9: Wyckoff site: 16i, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,17]
2	$[-y, x, z]$	[2,18]
3	$[y, -x, z]$	[3,19]

*continued ...*

Table 9

No.	position	mapping
4	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[4,20]
5	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[5,21]
6	$[-x, -y, z]$	[6,22]
7	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[7,23]
8	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[8,24]
9	$[-x, -y, -z]$	[9,25]
10	$[y, -x, -z]$	[10,26]
11	$[-y, x, -z]$	[11,27]
12	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[12,28]
13	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[13,29]
14	$[x, y, -z]$	[14,30]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[15,31]
16	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[16,32]