

MSG No. 136.496 $P4_2/mnm1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: m.mmm1'

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

Table 2: Wyckoff site: 2b, site symmetry: m.mmm1'

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

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	[0, \frac{1}{2}, \frac{1}{2}]	[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	[\frac{1}{2}, 0, 0]	[7, 8, 15, 16, 23, 24, 31, 32]

Table 4: Wyckoff site: 4d, site symmetry: -4..1'

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

Table 5: Wyckoff site: 4e, site symmetry: 2.mmm1'

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

Table 6: Wyckoff site: **4f**, site symmetry: **m.2m1'**

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

Table 7: Wyckoff site: **4g**, site symmetry: **m.m21'**

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

Table 8: Wyckoff site: **8h**, site symmetry: **2..1'**

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

Table 9: Wyckoff site: **8i**, site symmetry: **m..1'**

No.	position	mapping
1	$[x, y, 0]$	[1, 14, 17, 30]
2	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2}]$	[2, 11, 18, 27]
3	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[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	$[y, x, 0]$	[7, 16, 23, 32]
8	$[-y, -x, 0]$	[8, 15, 24, 31]

Table 10: Wyckoff site: 8j, site symmetry: ..m1'

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

Table 11: Wyckoff site: 16k, site symmetry: 11'

No.	position	mapping
1	[x, y, z]	[1,17]
2	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[2,18]
3	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[3,19]
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, x, -z]	[7,23]
8	[-y, -x, -z]	[8,24]
9	[-x, -y, -z]	[9,25]
10	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[10,26]
11	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[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	[-y, -x, z]	[15,31]
16	[y, x, z]	[16,32]