

MSG No. 121.328 $I\bar{4}2m1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: -42m1'

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

Table 2: Wyckoff site: 2b, site symmetry: -42m1'

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

Table 3: Wyckoff site: 4c, site symmetry: 222.1'

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

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

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

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

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

Table 6: Wyckoff site: 8f, site symmetry: .2.1'

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

Table 7: Wyckoff site: 8g, site symmetry: .2.1'

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: ..m1'

No.	position	mapping
1	[x, x, z]	[1,8,17,24]
2	[$x, -x, -z$]	[2,5,18,21]
3	[$-x, x, -z$]	[3,6,19,22]

continued ...

Table 9

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

Table 10: Wyckoff site: 16j, site symmetry: 11'

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