

MPG No. 15.2.54 4/mmm1' [Type II, tetragonal]

Table 1: Wyckoff site: 1o, site symmetry: 4/mmm1'

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

Table 2: Wyckoff site: 2a, site symmetry: 4mm

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

Table 3: Wyckoff site: 4b, site symmetry: m.m2

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

Table 4: Wyckoff site: 4c, site symmetry: m2m.

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

Table 5: Wyckoff site: 8d, site symmetry: m..

No.	position	mapping
1	[x, y, 0]	[1,12,17,28]
2	[-x, -y, 0]	[4,9,20,25]
3	[-y, x, 0]	[6,15,22,31]
4	[y, -x, 0]	[7,14,23,30]
5	[-x, y, 0]	[3,10,19,26]
6	[x, -y, 0]	[2,11,18,27]

continued ...

Table 5

No.	position	mapping
7	[$y, x, 0$]	[8,13,24,29]
8	[$-y, -x, 0$]	[5,16,21,32]

Table 6: Wyckoff site: 8e, site symmetry: ...m

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

Table 7: Wyckoff site: 8f, site symmetry: .m.

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

Table 8: Wyckoff site: 16g, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1,17]
2	[$-x, -y, z$]	[4,20]
3	[$-y, x, z$]	[6,22]
4	[$y, -x, z$]	[7,23]
5	[$-x, y, -z$]	[3,19]
6	[$x, -y, -z$]	[2,18]
7	[$y, x, -z$]	[8,24]
8	[$-y, -x, -z$]	[5,21]
9	[$-x, -y, -z$]	[9,25]

continued ...

Table 8

No.	position	mapping
10	$[x, y, -z]$	[12, 28]
11	$[y, -x, -z]$	[14, 30]
12	$[-y, x, -z]$	[15, 31]
13	$[x, -y, z]$	[11, 27]
14	$[-x, y, z]$	[10, 26]
15	$[-y, -x, z]$	[16, 32]
16	$[y, x, z]$	[13, 29]