MPG No. 15.1.53 $4/mmm$ [Type I, tetragonal]

Table 1: Wyckoff site: 1o, site symmetry: 4/mmm

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

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

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

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

No.	position	mapping
1	$[x, x, 0]$	[1,8,12,13]
2	$[-x, -x, 0]$	[4,5,9,16]
3	$[-x, x, 0]$	[3,6,10,15]
4	$[x, -x, 0]$	[2,7,11,14]

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

No.	position	mapping
1	$[x, 0, 0]$	[1,2,11,12]
2	$[-x, 0, 0]$	[3,4,9,10]
3	$[0, x, 0]$	[6,8,13,15]
4	$[0, -x, 0]$	[5,7,14,16]

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

No.	position	mapping
1	$[x, y, 0]$	[1,12]
2	$[-x, -y, 0]$	[4,9]
3	$[-y, x, 0]$	[6,15]
4	$[y, -x, 0]$	[7,14]
5	$[-x, y, 0]$	[3,10]
6	$[x, -y, 0]$	[2,11]
7	$[y, x, 0]$	[8,13]

continued …

Table 5

No.	position	mapping
8	$[-y, -x, 0]$	[5,16]

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

No.	position	mapping
1	$[x, x, z]$	[1,13]
2	$[-x, -x, z]$	[4,16]
3	$[-x, x, z]$	[6,10]
4	$[x, -x, z]$	[7,11]
5	$[-x, x, -z]$	[3,15]
6	$[x, -x, -z]$	[2,14]
7	$[x, x, -z]$	[8,12]
8	$[-x, -x, -z]$	[5,9]

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

No.	position	mapping
1	$[x, 0, z]$	[1,11]
2	$[-x, 0, z]$	[4,10]
3	$[0, x, z]$	[6,13]
4	$[0, -x, z]$	[7,16]
5	$[-x, 0, -z]$	[3,9]
6	$[x, 0, -z]$	[2,12]
7	$[0, x, -z]$	[8,15]
8	$[0, -x, -z]$	[5,14]

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[4]
3	$[-y, x, z]$	[6]
4	$[y, -x, z]$	[7]
5	$[-x, y, -z]$	[3]
6	$[x, -y, -z]$	[2]
7	$[y, x, -z]$	[8]
8	$[-y, -x, -z]$	[5]
9	$[-x, -y, -z]$	[9]
10	$[x, y, -z]$	[12]

continued …

Table 8

No.	position	mapping
11	$[y, -x, -z]$	[14]
12	$[-y, x, -z]$	[15]
13	$[x, -y, z]$	[11]
14	$[-x, y, z]$	[10]
15	$[-y, -x, z]$	[16]
16	$[y, x, z]$	[13]

11	$[y, -x, -z]$	[14]
12	$[-y, x, -z]$	[15]
13	$[x, -y, z]$	[11]
14	$[-x, y, z]$	