

MSG No. 55.353 *Pbam* [Type I, orthorhombic]

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

No.	position	mapping
1	[0, 0, 0]	[1, 4, 5, 8]
2	[\frac{1}{2}, \frac{1}{2}, 0]	[2, 3, 6, 7]

Table 2: Wyckoff site: 2b, site symmetry: . . 2/m

No.	position	mapping
1	[0, 0, \frac{1}{2}]	[1, 4, 5, 8]
2	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[2, 3, 6, 7]

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

No.	position	mapping
1	[0, \frac{1}{2}, 0]	[1, 4, 5, 8]
2	[\frac{1}{2}, 0, 0]	[2, 3, 6, 7]

Table 4: Wyckoff site: 2d, site symmetry: . . 2/m

No.	position	mapping
1	[0, \frac{1}{2}, \frac{1}{2}]	[1, 4, 5, 8]
2	[\frac{1}{2}, 0, \frac{1}{2}]	[2, 3, 6, 7]

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

No.	position	mapping
1	[0, 0, z]	[1, 4]
2	[\frac{1}{2}, \frac{1}{2}, -z]	[2, 3]
3	[0, 0, -z]	[5, 8]
4	[\frac{1}{2}, \frac{1}{2}, z]	[6, 7]

Table 6: Wyckoff site: 4f, site symmetry: ...2

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	[1,4]
2	$[\frac{1}{2}, 0, -z]$	[2,3]
3	$[0, \frac{1}{2}, -z]$	[5,8]
4	$[\frac{1}{2}, 0, z]$	[6,7]

Table 7: Wyckoff site: 4g, site symmetry: ...m

No.	position	mapping
1	$[x, y, 0]$	[1,8]
2	$[x + \frac{1}{2}, \frac{1}{2} - y, 0]$	[2,7]
3	$[\frac{1}{2} - x, y + \frac{1}{2}, 0]$	[3,6]
4	$[-x, -y, 0]$	[4,5]

Table 8: Wyckoff site: 4h, site symmetry: ...m

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	[1,8]
2	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[2,7]
3	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	[3,6]
4	$[-x, -y, \frac{1}{2}]$	[4,5]

Table 9: Wyckoff site: 8i, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[2]
3	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[3]
4	$[-x, -y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[6]
7	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[7]
8	$[x, y, -z]$	[8]