

MSG No. 55.354 *Pbam1'* [Type II, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: . . 2/m1'

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

Table 2: Wyckoff site: 2b, site symmetry: . . 2/m1'

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

Table 3: Wyckoff site: 2c, site symmetry: . . 2/m1'

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

Table 4: Wyckoff site: 2d, site symmetry: . . 2/m1'

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

Table 5: Wyckoff site: 4e, site symmetry: . . 21'

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

Table 6: Wyckoff site: 4f, site symmetry: . . 21'

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

Table 7: Wyckoff site: 4g, site symmetry: . . m1'

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

Table 8: Wyckoff site: 4h, site symmetry: . . m1'

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	[1, 8, 9, 16]
2	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[2, 7, 10, 15]
3	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$	[3, 6, 11, 14]
4	$[-x, -y, \frac{1}{2}]$	[4, 5, 12, 13]

Table 9: Wyckoff site: 8i, site symmetry: 11'

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