

MSG No. 58.395 $Pn'nm$ [Type III, orthorhombic]

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

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site: 4f, site symmetry: $\dots 2'$

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

Table 7: Wyckoff site: 4g, site symmetry: $\dots m$

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

Table 8: Wyckoff site: 8h, site symmetry: 1

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