

MSG No. 58.397  $Pn'n'm$  [ Type III, orthorhombic ]

Table 1: Wyckoff site: 2a, site symmetry:  $\dots 2/m$

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

Table 2: Wyckoff site: 2b, site symmetry:  $\dots 2/m$

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

Table 3: Wyckoff site: 2c, site symmetry:  $\dots 2/m$

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

Table 4: Wyckoff site: 2d, site symmetry:  $\dots 2/m$

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

Table 5: Wyckoff site: 4e, site symmetry:  $\dots 2$

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

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

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

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

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

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

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