

MSG No. 53.321 $Pmna$ [Type I, orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: **4g**, site symmetry: $.2.$

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

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

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

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

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