

MSG No. 58.396  $Pnnm'$  [ Type III, orthorhombic ]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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