

MSG No. 58.399 $Pn'n'm'$ [Type III, orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[3]
4	$[-x, -y, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[7]
8	$[x, y, -z]$	[8]