

MSG No. 53.326 $Pm'n'a$ [Type III, orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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