

MSG No. 26.73 $Pcm2_1$ [Type IV, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: $mm'2'$

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

Table 2: Wyckoff site: 2b, site symmetry: $mm'2'$

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

Table 3: Wyckoff site: 2c, site symmetry: $mm'2'$

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

Table 4: Wyckoff site: 2d, site symmetry: $mm'2'$

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

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

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

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

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

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

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

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

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

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

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