

MPG No. 8.5.28 $m'm'm'$ [Type III, orthorhombic]

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: $\mathbf{m'm'm'}$

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

Table 2: Wyckoff site: $2\mathbf{a}$, site symmetry: $2\mathbf{m'm'}$

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2, 7, 8]$
2	$[-x, 0, 0]$	$[3, 4, 5, 6]$

Table 3: Wyckoff site: $2\mathbf{b}$, site symmetry: $\mathbf{m'2m'}$

No.	position	mapping
1	$[0, y, 0]$	$[1, 3, 6, 8]$
2	$[0, -y, 0]$	$[2, 4, 5, 7]$

Table 4: Wyckoff site: $2\mathbf{c}$, site symmetry: $\mathbf{m'm'2}$

No.	position	mapping
1	$[0, 0, z]$	$[1, 4, 6, 7]$
2	$[0, 0, -z]$	$[2, 3, 5, 8]$

Table 5: Wyckoff site: $4\mathbf{d}$, site symmetry: $\mathbf{m'..}$

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

Table 6: Wyckoff site: $4\mathbf{e}$, site symmetry: $\mathbf{.m'..}$

No.	position	mapping
1	$[x, 0, z]$	$[1, 7]$

continued ...

Table 6

No.	position	mapping
2	$[-x, 0, z]$	[4,6]
3	$[-x, 0, -z]$	[3,5]
4	$[x, 0, -z]$	[2,8]

Table 7: Wyckoff site: $4f$, site symmetry: $\bar{3}m'$

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

Table 8: Wyckoff site: $8g$, site symmetry: 1

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