

MSG No. 99.167 $P4m'm'$ [Type III, tetragonal]

Table 1: Wyckoff site: $1a$, site symmetry: $4m'm'$

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

Table 2: Wyckoff site: $1b$, site symmetry: $4m'm'$

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: $8g$, site symmetry: 1

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