

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: $\dots m'$

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]