

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]