

MSG No. 99.165  $P4'm'm$  [ Type III, tetragonal ]

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

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

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

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	$[\frac{1}{2}, 0, z]$	$[1, 2, 7, 8]$
2	$[0, \frac{1}{2}, z]$	$[3, 4, 5, 6]$

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

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

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

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

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

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

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

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