

MSG No. 99.166 $P4'mm'$ [Type III, tetragonal]

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

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

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

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: $2mm.$

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

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

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

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

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

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

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

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

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