

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: $\dots m$

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: $\dots m'$.

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]