

MSG No. 85.62 $P4/n'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: $-4'$. .

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

Table 2: Wyckoff site: 2b, site symmetry: $-4'$. .

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

Table 3: Wyckoff site: 2c, site symmetry: 4 . .

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

Table 4: Wyckoff site: 4d, site symmetry: $-1'$

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

Table 5: Wyckoff site: 4e, site symmetry: $-1'$

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

Table 6: Wyckoff site: $4f$, site symmetry: $2..$

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

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

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