

MSG No. 86.67 $P4_2/n$ [Type I, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: -1

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $2..$

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

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

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

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

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