

MSG No. 59.406 $Pmmn1'$ [Type II, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: $mm21'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, z]$	$[1, 4, 6, 7, 9, 12, 14, 15]$
2	$[\frac{3}{4}, \frac{3}{4}, -z]$	$[2, 3, 5, 8, 10, 11, 13, 16]$

Table 2: Wyckoff site: 2b, site symmetry: $mm21'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{3}{4}, z]$	$[1, 4, 6, 7, 9, 12, 14, 15]$
2	$[\frac{3}{4}, \frac{1}{4}, -z]$	$[2, 3, 5, 8, 10, 11, 13, 16]$

Table 3: Wyckoff site: 4c, site symmetry: $-11'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 5, 9, 13]$
2	$[\frac{1}{2}, 0, 0]$	$[2, 6, 10, 14]$
3	$[0, \frac{1}{2}, 0]$	$[3, 7, 11, 15]$
4	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[4, 8, 12, 16]$

Table 4: Wyckoff site: 4d, site symmetry: $-11'$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 5, 9, 13]$
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, 6, 10, 14]$
3	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, 7, 11, 15]$
4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[4, 8, 12, 16]$

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

No.	position	mapping
1	$[\frac{1}{4}, y, z]$	$[1, 6, 9, 14]$
2	$[\frac{3}{4}, -y, -z]$	$[2, 5, 10, 13]$
3	$[\frac{3}{4}, y + \frac{1}{2}, -z]$	$[3, 8, 11, 16]$
4	$[\frac{1}{4}, \frac{1}{2} - y, z]$	$[4, 7, 12, 15]$

Table 6: Wyckoff site: **4f**, site symmetry: $\bar{4}2m$

No.	position	mapping
1	$[x, \frac{1}{4}, z]$	$[1, 7, 9, 15]$
2	$[x + \frac{1}{2}, \frac{3}{4}, -z]$	$[2, 8, 10, 16]$
3	$[-x, \frac{3}{4}, -z]$	$[3, 5, 11, 13]$
4	$[\frac{1}{2} - x, \frac{1}{4}, z]$	$[4, 6, 12, 14]$

Table 7: Wyckoff site: **8g**, site symmetry: $\bar{4}2m$

No.	position	mapping
1	$[x, y, z]$	$[1, 9]$
2	$[x + \frac{1}{2}, -y, -z]$	$[2, 10]$
3	$[-x, y + \frac{1}{2}, -z]$	$[3, 11]$
4	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	$[4, 12]$
5	$[-x, -y, -z]$	$[5, 13]$
6	$[\frac{1}{2} - x, y, z]$	$[6, 14]$
7	$[x, \frac{1}{2} - y, z]$	$[7, 15]$
8	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	$[8, 16]$