

MSG No. 18.24 $P_I2_12_12$ [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: **2c**, site symmetry: $2'2'2$

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

Table 4: Wyckoff site: **2d**, site symmetry: $2'2'2$

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

Table 5: Wyckoff site: **4e**, site symmetry: $2' \dots$

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

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

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

Table 7: Wyckoff site: **4g**, site symmetry: $.2'.$

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

Table 8: Wyckoff site: **4h**, site symmetry: $.2'.$

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

Table 9: Wyckoff site: **4i**, site symmetry: $..2$

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

Table 10: Wyckoff site: **4j**, site symmetry: $..2$

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

Table 11: Wyckoff site: $8k$, site symmetry: 1

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