

MSG No. 23.50 $I2221'$ [Type II, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: $2221'$

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

Table 2: Wyckoff site: 2b, site symmetry: $2221'$

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

Table 3: Wyckoff site: 2c, site symmetry: $2221'$

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

Table 4: Wyckoff site: 2d, site symmetry: $2221'$

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

Table 5: Wyckoff site: 4e, site symmetry: $2..1'$

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

Table 6: Wyckoff site: $4\mathbf{f}$, site symmetry: $2..1'$

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

Table 7: Wyckoff site: $4\mathbf{g}$, site symmetry: $.2.1'$

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

Table 8: Wyckoff site: $4\mathbf{h}$, site symmetry: $.2.1'$

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

Table 9: Wyckoff site: $4\mathbf{i}$, site symmetry: $..21'$

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

Table 10: Wyckoff site: $4\mathbf{j}$, site symmetry: $..21'$

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

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

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