

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: 4f, 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: 4g, 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: 4h, 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: 4i, 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: 4j, 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]