

MSG No. 115.284 $P\bar{4}m21'$ [Type II, tetragonal]

Table 1: Wyckoff site: 1a, site symmetry: -4m21'

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

Table 2: Wyckoff site: 1b, site symmetry: -4m21'

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

Table 3: Wyckoff site: 1c, site symmetry: -4m21'

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

Table 4: Wyckoff site: 1d, site symmetry: -4m21'

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

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

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

Table 6: Wyckoff site: 2f, site symmetry: 2mm.1'

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

Table 7: Wyckoff site: 2g, site symmetry: 2mm.1'

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

Table 8: Wyckoff site: 4h, site symmetry: ..21'

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

Table 9: Wyckoff site: 4i, site symmetry: ..21'

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

Table 10: Wyckoff site: 4j, site symmetry: .m.1'

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

Table 11: Wyckoff site: 4k, site symmetry: .m.1'

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

Table 12: Wyckoff site: 81, site symmetry: 11'

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