

MSG No. 118.307 $P\bar{4}n2$ [Type I, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: -4..

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

Table 2: Wyckoff site: 2b, site symmetry: -4..

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

Table 3: Wyckoff site: 2c, site symmetry: 2.22

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

Table 4: Wyckoff site: 2d, site symmetry: 2.22

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

Table 5: Wyckoff site: 4e, site symmetry: 2..

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

Table 6: Wyckoff site: 4f, site symmetry: ...2

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

Table 7: Wyckoff site: 4g, site symmetry: ...2

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

Table 8: Wyckoff site: 4h, site symmetry: 2..

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

Table 9: Wyckoff site: 8i, site symmetry: 1

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