

MSG No. 117.302 $P\bar{4}'b2'$ [Type III, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: 2.2'2'

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

Table 4: Wyckoff site: 2d, site symmetry: 2.2'2'

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

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

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

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

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

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

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

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

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

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

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