

MSG No. 90.98 $P42_1'2'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 2.2'2'

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

Table 2: Wyckoff site: 2b, site symmetry: 2.2'2'

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

Table 3: Wyckoff site: 2c, site symmetry: 4..

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

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

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

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

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

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

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

Table 7: Wyckoff site: 8g, site symmetry: 1

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