

MSG No. 114.277 $P\bar{4}'2'_1c$ [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}, \frac{1}{2}]	[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}, 0]	[3, 4, 5, 6]

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

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: 1

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

continued ...

Table 5

No.	position	mapping
7	$[y, -x, -z]$	[7]
8	$[-y, x, -z]$	[8]