

MSG No. 114.276 $P\bar{4}2_1c1'$ [Type II, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: 2..1'

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

Table 4: Wyckoff site: 4d, site symmetry: 2..1'

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

Table 5: Wyckoff site: 8e, site symmetry: 11'

No.	position	mapping
1	[x, y, z]	[1,9]
2	[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]	[2,10]
3	[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]	[3,11]
4	[-x, -y, z]	[4,12]
5	[y, -x, -z]	[5,13]
6	[-y, x, -z]	[6,14]

continued ...

Table 5

No.	position	mapping
7	$\left[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}\right]$	[7, 15]
8	$\left[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}\right]$	[8, 16]