

SG No. 114 D_{2d}^4 $P\bar{4}2_1c$ [tetragonal]

* plus set: + [0, 0, 0]

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

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

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

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

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

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

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

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

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

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

continued ...

Table 5

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