

SG No. 110 C_{4v}^{12} $I4_1cd$ [tetragonal]

* plus set: $+ [0, 0, 0]$, $+ [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

Table 1: Wyckoff site: 8a, site symmetry: 2..

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

Table 2: Wyckoff site: 16b, site symmetry: 1

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