

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

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

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	$[y + \frac{1}{2}, x, z + \frac{1}{4}]$	$[8]$