

SG No. 109  $C_{4v}^{11}$   $I4_1md$  [ tetragonal ]

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

Table 1: Wyckoff site: 4a, site symmetry:  $2mm$ .

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

Table 2: Wyckoff site: 8b, site symmetry:  $.m$ .

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

Table 3: Wyckoff site: 16c, 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	$[x, -y, z]$	$[5]$
6	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	$[6]$
7	$[-y, \frac{1}{2} - x, z + \frac{1}{4}]$	$[7]$
8	$[y + \frac{1}{2}, x, z + \frac{3}{4}]$	$[8]$