

MSG No. 80.31 $I4'_1$ [Type III, tetragonal]

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

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

Table 2: Wyckoff site: **8b**, site symmetry: 1

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