

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]