

SG No. 199  $T^5$   $I2_13$  [ cubic ]

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

Table 1: Wyckoff site: 8a, site symmetry:  $.3$ .

No.	position	mapping
1	$[x, x, x]$	[1,5,9]
2	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	[2,7,12]
3	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	[3,8,10]
4	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	[4,6,11]

Table 2: Wyckoff site: 12b, site symmetry:  $2..$

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1,4]
2	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[2,3]
3	$[\frac{1}{4}, x, 0]$	[5,8]
4	$[\frac{3}{4}, \frac{1}{2} - x, 0]$	[6,7]
5	$[0, \frac{1}{4}, x]$	[9,12]
6	$[0, \frac{3}{4}, \frac{1}{2} - x]$	[10,11]

Table 3: Wyckoff site: 24c, site symmetry:  $1$

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[2]
3	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[3]
4	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[4]
5	$[z, x, y]$	[5]
6	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[6]
7	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[7]
8	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[8]
9	$[y, z, x]$	[9]
10	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[10]
11	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[11]
12	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[12]