

SG No. 197 T^3 $I23$ [cubic]

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

Table 1: Wyckoff site: 2a, site symmetry: 23.

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$

Table 2: Wyckoff site: 6b, site symmetry: 222..

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

Table 3: Wyckoff site: 8c, site symmetry: .3.

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

Table 4: Wyckoff site: 12d, site symmetry: 2..

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

Table 5: Wyckoff site: 12e, site symmetry: 2..

No.	position	mapping
1	$[x, \frac{1}{2}, 0]$	$[1, 4]$
2	$[-x, \frac{1}{2}, 0]$	$[2, 3]$
3	$[0, x, \frac{1}{2}]$	$[5, 8]$

continued ...

Table 5

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

Table 6: Wyckoff site: 24f, site symmetry: 1

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