

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

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

* Wyckoff site: **8a**, site symmetry: $.3$.

Table 1: Wyckoff bond: **8a@8a**

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

Table 2: Wyckoff bond: **24b@8a**

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

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

Table 3: Wyckoff bond: **12a@12b**

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

Table 4: Wyckoff bond: 12b@12b

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

Table 5: Wyckoff bond: 24c@12b

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

* Wyckoff site: 24c, site symmetry: 1

Table 6: Wyckoff bond: 24a@24c

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