

SG No. 205 T_h^6 $Pa\bar{3}$ [cubic]

* plus set: $+ [0, 0, 0]$

* Wyckoff site: **4a**, site symmetry: $.-\bar{3}$.

Table 1: Wyckoff bond: **4a@4a**

No.	vector	center	mapping
1	$[X, X, X]$	$[0, 0, 0]$	$[1, 5, 9, -13, -17, -21]$
2	$[-X, -X, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, 7, 12, -14, -19, -24]$
3	$[-X, X, -X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, 8, 10, -15, -20, -22]$
4	$[X, -X, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[4, 6, 11, -16, -18, -23]$

Table 2: Wyckoff bond: **12b@4a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1, -13]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[2, -14]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -15]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[4, -16]$
5	$[Z, X, Y]$	$[0, 0, 0]$	$[5, -17]$
6	$[Z, -X, -Y]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[6, -18]$
7	$[-Z, -X, Y]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[7, -19]$
8	$[-Z, X, -Y]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[8, -20]$
9	$[Y, Z, X]$	$[0, 0, 0]$	$[9, -21]$
10	$[-Y, Z, -X]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[10, -22]$
11	$[Y, -Z, -X]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[11, -23]$
12	$[-Y, -Z, X]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[12, -24]$

* Wyckoff site: **4b**, site symmetry: $.-\bar{3}$.

Table 3: Wyckoff bond: **4a@4b**

No.	vector	center	mapping
1	$[X, X, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, 5, 9, -13, -17, -21]$
2	$[-X, -X, X]$	$[0, \frac{1}{2}, 0]$	$[2, 7, 12, -14, -19, -24]$
3	$[-X, X, -X]$	$[\frac{1}{2}, 0, 0]$	$[3, 8, 10, -15, -20, -22]$
4	$[X, -X, -X]$	$[0, 0, \frac{1}{2}]$	$[4, 6, 11, -16, -18, -23]$

Table 4: Wyckoff bond: **12b@4b**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, -13]$

continued ...

Table 4

No.	vector	center	mapping
2	$[-X, -Y, Z]$	$[0, \frac{1}{2}, 0]$	[2,-14]
3	$[-X, Y, -Z]$	$[\frac{1}{2}, 0, 0]$	[3,-15]
4	$[X, -Y, -Z]$	$[0, 0, \frac{1}{2}]$	[4,-16]
5	$[Z, X, Y]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[5,-17]
6	$[Z, -X, -Y]$	$[0, 0, \frac{1}{2}]$	[6,-18]
7	$[-Z, -X, Y]$	$[0, \frac{1}{2}, 0]$	[7,-19]
8	$[-Z, X, -Y]$	$[\frac{1}{2}, 0, 0]$	[8,-20]
9	$[Y, Z, X]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[9,-21]
10	$[-Y, Z, -X]$	$[\frac{1}{2}, 0, 0]$	[10,-22]
11	$[Y, -Z, -X]$	$[0, 0, \frac{1}{2}]$	[11,-23]
12	$[-Y, -Z, X]$	$[0, \frac{1}{2}, 0]$	[12,-24]

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

Table 5: Wyckoff bond: 8a@8c

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]
5	$[-X, -X, -X]$	$[-x, -x, -x]$	[13,17,21]
6	$[X, X, -X]$	$[x + \frac{1}{2}, x, \frac{1}{2} - x]$	[14,19,24]
7	$[X, -X, X]$	$[x, \frac{1}{2} - x, x + \frac{1}{2}]$	[15,20,22]
8	$[-X, X, X]$	$[\frac{1}{2} - x, x + \frac{1}{2}, x]$	[16,18,23]

Table 6: Wyckoff bond: 24b@8c

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]
13	$[-X, -Y, -Z]$	$[-x, -x, -x]$	[13]

continued ...

Table 6

No.	vector	center	mapping
14	$[X, Y, -Z]$	$[x + \frac{1}{2}, x, \frac{1}{2} - x]$	[14]
15	$[X, -Y, Z]$	$[x, \frac{1}{2} - x, x + \frac{1}{2}]$	[15]
16	$[-X, Y, Z]$	$[\frac{1}{2} - x, x + \frac{1}{2}, x]$	[16]
17	$[-Z, -X, -Y]$	$[-x, -x, -x]$	[17]
18	$[-Z, X, Y]$	$[\frac{1}{2} - x, x + \frac{1}{2}, x]$	[18]
19	$[Z, X, -Y]$	$[x + \frac{1}{2}, x, \frac{1}{2} - x]$	[19]
20	$[Z, -X, Y]$	$[x, \frac{1}{2} - x, x + \frac{1}{2}]$	[20]
21	$[-Y, -Z, -X]$	$[-x, -x, -x]$	[21]
22	$[Y, -Z, X]$	$[x, \frac{1}{2} - x, x + \frac{1}{2}]$	[22]
23	$[-Y, Z, X]$	$[\frac{1}{2} - x, x + \frac{1}{2}, x]$	[23]
24	$[Y, Z, -X]$	$[x + \frac{1}{2}, x, \frac{1}{2} - x]$	[24]

* Wyckoff site: 24d, site symmetry: 1

Table 7: Wyckoff bond: 24a@24d

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]
13	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[13]
14	$[X, Y, -Z]$	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[14]
15	$[X, -Y, Z]$	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[15]
16	$[-X, Y, Z]$	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[16]
17	$[-Z, -X, -Y]$	$[-z, -x, -y]$	[17]
18	$[-Z, X, Y]$	$[\frac{1}{2} - z, x + \frac{1}{2}, y]$	[18]
19	$[Z, X, -Y]$	$[z + \frac{1}{2}, x, \frac{1}{2} - y]$	[19]
20	$[Z, -X, Y]$	$[z, \frac{1}{2} - x, y + \frac{1}{2}]$	[20]
21	$[-Y, -Z, -X]$	$[-y, -z, -x]$	[21]
22	$[Y, -Z, X]$	$[y, \frac{1}{2} - z, x + \frac{1}{2}]$	[22]
23	$[-Y, Z, X]$	$[\frac{1}{2} - y, z + \frac{1}{2}, x]$	[23]
24	$[Y, Z, -X]$	$[y + \frac{1}{2}, z, \frac{1}{2} - x]$	[24]