SG No. 72 D_{2h}^{26} *Ibam* [orthorhombic]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$
* Wyckoff site: `4a`, site symmetry: `222`

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

No.	vector	center	mapping
1	$[0,\ 0,\ Z]$	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[1,2,-3,-4]`
2	$[0,\ 0,\ -Z]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[5,6,-7,-8]`

Table 2: Wyckoff bond: `4b@4a`

No.	vector	center	mapping
1	$[0,\ Y,\ 0]$	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[1,-2,3,-4]`
2	$[0,\ -Y,\ 0]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[5,-6,7,-8]`

Table 3: Wyckoff bond: `4c@4a`

No.	vector	center	mapping
1	$[X,\ 0,\ 0]$	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[1,-2,-3,4]`
2	$[-X,\ 0,\ 0]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[5,-6,-7,8]`

Table 4: Wyckoff bond: `8d@4a`

No.	vector	center	mapping
1	$[X,\ Y,\ 0]$	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[1,-2]`
2	$[-X,\ Y,\ 0]$	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[3,-4]`
3	$[-X,\ -Y,\ 0]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[5,-6]`
4	$[X,\ -Y,\ 0]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[7,-8]`

Table 5: Wyckoff bond: `8e@4a`

No.	vector	center	mapping
1	$[X,\ 0,\ Z]$	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[1,-3]`
2	$[-X,\ 0,\ Z]$	$\left[0,\ 0,\ \frac{1}{4}\right]$	`[2,-4]`
3	$[-X,\ 0,\ -Z]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[5,-7]`
4	$[X,\ 0,\ -Z]$	$\left[0,\ 0,\ \frac{3}{4}\right]$	`[6,-8]`

Table 6: Wyckoff bond: `8f@4a`

No.	vector	center	mapping
1	$[0, Y, Z]$	$\left[0, 0, \frac{1}{4}\right]$	`[1,-4]`
2	$[0, -Y, Z]$	$\left[0, 0, \frac{1}{4}\right]$	`[2,-3]`
3	$[0, -Y, -Z]$	$\left[0, 0, \frac{3}{4}\right]$	`[5,-8]`
4	$[0, Y, -Z]$	$\left[0, 0, \frac{3}{4}\right]$	`[6,-7]`

Table 7: Wyckoff bond: `16g@4a`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[0, 0, \frac{1}{4}\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[0, 0, \frac{1}{4}\right]$	`[2]`
3	$[-X, Y, -Z]$	$\left[0, 0, \frac{1}{4}\right]$	`[3]`
4	$[X, -Y, -Z]$	$\left[0, 0, \frac{1}{4}\right]$	`[4]`
5	$[-X, -Y, -Z]$	$\left[0, 0, \frac{3}{4}\right]$	`[5]`
6	$[X, Y, -Z]$	$\left[0, 0, \frac{3}{4}\right]$	`[6]`
7	$[X, -Y, Z]$	$\left[0, 0, \frac{3}{4}\right]$	`[7]`
8	$[-X, Y, Z]$	$\left[0, 0, \frac{3}{4}\right]$	`[8]`

* Wyckoff site: `4b`, site symmetry: `222`

Table 8: Wyckoff bond: `4a@4b`

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[1,2,-3,-4]`
2	$[0, 0, -Z]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[5,6,-7,-8]`

Table 9: Wyckoff bond: `4b@4b`

No.	vector	center	mapping
1	$[0, Y, 0]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[1,-2,3,-4]`
2	$[0, -Y, 0]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[5,-6,7,-8]`

Table 10: Wyckoff bond: `4c@4b`

No.	vector	center	mapping
1	$[X, 0, 0]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[1,-2,-3,4]`
2	$[-X, 0, 0]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[5,-6,-7,8]`

Table 11: Wyckoff bond: `8d@4b`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[1,-2]`
2	$[-X, Y, 0]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[3,-4]`
3	$[-X, -Y, 0]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[5,-6]`
4	$[X, -Y, 0]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[7,-8]`

Table 12: Wyckoff bond: `8e@4b`

No.	vector	center	mapping
1	$[X, 0, Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[1,-3]`
2	$[-X, 0, Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[2,-4]`
3	$[-X, 0, -Z]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[5,-7]`
4	$[X, 0, -Z]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[6,-8]`

Table 13: Wyckoff bond: `8f@4b`

No.	vector	center	mapping
1	$[0, Y, Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[1,-4]`
2	$[0, -Y, Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[2,-3]`
3	$[0, -Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[5,-8]`
4	$[0, Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[6,-7]`

Table 14: Wyckoff bond: `16g@4b`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[2]`
3	$[-X, Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[3]`
4	$[X, -Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[4]`
5	$[-X, -Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[5]`
6	$[X, Y, -Z]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[6]`
7	$[X, -Y, Z]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[7]`
8	$[-X, Y, Z]$	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[8]`

* Wyckoff site: `4c`, site symmetry: `..2/m`

Table 15: Wyckoff bond: `4a@4c`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, 0]$	`[1,-2,-5,6]`
2	$[-X, Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[3,-4,-7,8]`

Table 16: Wyckoff bond: `4b@4c`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, 0]$	`[1,2,-5,-6]`
2	$[0, 0, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[3,4,-7,-8]`

Table 17: Wyckoff bond: `8c@4c`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	`[1,-5]`
2	$[-X, -Y, Z]$	$[0, 0, 0]$	`[2,-6]`
3	$[-X, Y, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[3,-7]`
4	$[X, -Y, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[4,-8]`

* Wyckoff site: `4d`, site symmetry: `..2/m`

Table 18: Wyckoff bond: `4a@4d`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[\frac{1}{2}, 0, 0\right]$	`[1,-2,-5,6]`
2	$[-X, Y, 0]$	$\left[0, \frac{1}{2}, 0\right]$	`[3,-4,-7,8]`

Table 19: Wyckoff bond: `4b@4d`

No.	vector	center	mapping
1	$[0, 0, Z]$	$\left[\frac{1}{2}, 0, 0\right]$	`[1,2,-5,-6]`
2	$[0, 0, -Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[3,4,-7,-8]`

Table 20: Wyckoff bond: `8c@4d`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{2}, 0, 0\right]$	`[1,-5]`
2	$[-X, -Y, Z]$	$\left[\frac{1}{2}, 0, 0\right]$	`[2,-6]`
3	$[-X, Y, -Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[3,-7]`
4	$[X, -Y, -Z]$	$\left[0, \frac{1}{2}, 0\right]$	`[4,-8]`

* Wyckoff site: `8e`, site symmetry: `-1`

Table 21: Wyckoff bond: `8a@8e`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,-5]`
2	$[-X, -Y, Z]$	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[2,-6]`
3	$[-X, Y, -Z]$	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[3,-7]`
4	$[X, -Y, -Z]$	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[4,-8]`

* Wyckoff site: `8f`, site symmetry: `2..`

Table 22: Wyckoff bond: `8a@8f`

No.	vector	center	mapping
1	$[0, Y, Z]$	$\left[x, 0, \frac{1}{4}\right]$	`[1,-4]`
2	$[0, -Y, Z]$	$\left[-x, 0, \frac{1}{4}\right]$	`[2,-3]`
3	$[0, -Y, -Z]$	$\left[-x, 0, \frac{3}{4}\right]$	`[5,-8]`
4	$[0, Y, -Z]$	$\left[x, 0, \frac{3}{4}\right]$	`[6,-7]`

Table 23: Wyckoff bond: `8b@8f`

No.	vector	center	mapping
1	$[X, 0, 0]$	$\left[x, 0, \frac{1}{4}\right]$	`[1,4]`
2	$[-X, 0, 0]$	$\left[-x, 0, \frac{1}{4}\right]$	`[2,3]`
3	$[-X, 0, 0]$	$\left[-x, 0, \frac{3}{4}\right]$	`[5,8]`
4	$[X, 0, 0]$	$\left[x, 0, \frac{3}{4}\right]$	`[6,7]`

Table 24: Wyckoff bond: `16c@8f`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[x, 0, \frac{1}{4}\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[-x, 0, \frac{1}{4}\right]$	`[2]`

continued ...

Table 24

No.	vector	center	mapping
3	$[-X, Y, -Z]$	$\left[-x, 0, \frac{1}{4}\right]$	`[3]`
4	$[X, -Y, -Z]$	$\left[x, 0, \frac{1}{4}\right]$	`[4]`
5	$[-X, -Y, -Z]$	$\left[-x, 0, \frac{3}{4}\right]$	`[5]`
6	$[X, Y, -Z]$	$\left[x, 0, \frac{3}{4}\right]$	`[6]`
7	$[X, -Y, Z]$	$\left[x, 0, \frac{3}{4}\right]$	`[7]`
8	$[-X, Y, Z]$	$\left[-x, 0, \frac{3}{4}\right]$	`[8]`

* Wyckoff site: `8g`, site symmetry: `.2.`

Table 25: Wyckoff bond: `8a@8g`

No.	vector	center	mapping
1	$[X, 0, Z]$	$\left[0, y, \frac{1}{4}\right]$	`[1,-3]`
2	$[-X, 0, Z]$	$\left[0, -y, \frac{1}{4}\right]$	`[2,-4]`
3	$[-X, 0, -Z]$	$\left[0, -y, \frac{3}{4}\right]$	`[5,-7]`
4	$[X, 0, -Z]$	$\left[0, y, \frac{3}{4}\right]$	`[6,-8]`

Table 26: Wyckoff bond: `8b@8g`

No.	vector	center	mapping
1	$[0, Y, 0]$	$\left[0, y, \frac{1}{4}\right]$	`[1,3]`
2	$[0, -Y, 0]$	$\left[0, -y, \frac{1}{4}\right]$	`[2,4]`
3	$[0, -Y, 0]$	$\left[0, -y, \frac{3}{4}\right]$	`[5,7]`
4	$[0, Y, 0]$	$\left[0, y, \frac{3}{4}\right]$	`[6,8]`

Table 27: Wyckoff bond: `16c@8g`

No.	vector	center	mapping
1	$[X, Y, Z]$	$\left[0, y, \frac{1}{4}\right]$	`[1]`
2	$[-X, -Y, Z]$	$\left[0, -y, \frac{1}{4}\right]$	`[2]`
3	$[-X, Y, -Z]$	$\left[0, y, \frac{1}{4}\right]$	`[3]`
4	$[X, -Y, -Z]$	$\left[0, -y, \frac{1}{4}\right]$	`[4]`
5	$[-X, -Y, -Z]$	$\left[0, -y, \frac{3}{4}\right]$	`[5]`
6	$[X, Y, -Z]$	$\left[0, y, \frac{3}{4}\right]$	`[6]`
7	$[X, -Y, Z]$	$\left[0, -y, \frac{3}{4}\right]$	`[7]`
8	$[-X, Y, Z]$	$\left[0, y, \frac{3}{4}\right]$	`[8]`

* Wyckoff site: `8h`, site symmetry: `..2`

Table 28: Wyckoff bond: `8a@8h`

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	`[1,-2]`
2	$[-X, Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[3,-4]`
3	$[-X, -Y, 0]$	$[0, 0, -z]$	`[5,-6]`
4	$[X, -Y, 0]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[7,-8]`

Table 29: Wyckoff bond: `8b@8h`

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	`[1,2]`
2	$[0, 0, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[3,4]`
3	$[0, 0, -Z]$	$[0, 0, -z]$	`[5,6]`
4	$[0, 0, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[7,8]`

Table 30: Wyckoff bond: `16c@8h`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, z]$	`[1]`
2	$[-X, -Y, Z]$	$[0, 0, z]$	`[2]`
3	$[-X, Y, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[3]`
4	$[X, -Y, -Z]$	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	`[4]`
5	$[-X, -Y, -Z]$	$[0, 0, -z]$	`[5]`
6	$[X, Y, -Z]$	$[0, 0, -z]$	`[6]`
7	$[X, -Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[7]`
8	$[-X, Y, Z]$	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	`[8]`

* Wyckoff site: `8i`, site symmetry: `..2`

Table 31: Wyckoff bond: `8a@8i`

No.	vector	center	mapping
1	$[X, Y, 0]$	$\left[0, \frac{1}{2}, z\right]$	`[1,-2]`
2	$[-X, Y, 0]$	$\left[\frac{1}{2}, 0, -z\right]$	`[3,-4]`
3	$[-X, -Y, 0]$	$\left[0, \frac{1}{2}, -z\right]$	`[5,-6]`
4	$[X, -Y, 0]$	$\left[\frac{1}{2}, 0, z\right]$	`[7,-8]`

Table 32: Wyckoff bond: `8b@8i`

No.	vector	center	mapping
1	$[0,\ 0,\ Z]$	$\left[0,\ \frac{1}{2},\ z\right]$	`[1,2]`
2	$[0,\ 0,\ -Z]$	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[3,4]`
3	$[0,\ 0,\ -Z]$	$\left[0,\ \frac{1}{2},\ -z\right]$	`[5,6]`
4	$[0,\ 0,\ Z]$	$\left[\frac{1}{2},\ 0,\ z\right]$	`[7,8]`

Table 33: Wyckoff bond: `16c@8i`

No.	vector	center	mapping
1	$[X,\ Y,\ Z]$	$\left[0,\ \frac{1}{2},\ z\right]$	`[1]`
2	$[-X,\ -Y,\ Z]$	$\left[0,\ \frac{1}{2},\ z\right]$	`[2]`
3	$[-X,\ Y,\ -Z]$	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[3]`
4	$[X,\ -Y,\ -Z]$	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[4]`
5	$[-X,\ -Y,\ -Z]$	$\left[0,\ \frac{1}{2},\ -z\right]$	`[5]`
6	$[X,\ Y,\ -Z]$	$\left[0,\ \frac{1}{2},\ -z\right]$	`[6]`
7	$[X,\ -Y,\ Z]$	$\left[\frac{1}{2},\ 0,\ z\right]$	`[7]`
8	$[-X,\ Y,\ Z]$	$\left[\frac{1}{2},\ 0,\ z\right]$	`[8]`

* Wyckoff site: `8j`, site symmetry: `..m`

Table 34: Wyckoff bond: `8a@8j`

No.	vector	center	mapping
1	$[X,\ Y,\ 0]$	$[x,\ y,\ 0]$	`[1,6]`
2	$[-X,\ -Y,\ 0]$	$[-x,\ -y,\ 0]$	`[2,5]`
3	$[-X,\ Y,\ 0]$	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0\right]$	`[3,8]`
4	$[X,\ -Y,\ 0]$	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	`[4,7]`

Table 35: Wyckoff bond: `8b@8j`

No.	vector	center	mapping
1	$[0,\ 0,\ Z]$	$[x,\ y,\ 0]$	`[1,-6]`
2	$[0,\ 0,\ Z]$	$[-x,\ -y,\ 0]$	`[2,-5]`
3	$[0,\ 0,\ -Z]$	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0\right]$	`[3,-8]`
4	$[0,\ 0,\ -Z]$	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	`[4,-7]`

Table 36: Wyckoff bond: `16c@8j`

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, 0]$	`[1]`
2	$[-X, -Y, Z]$	$[-x, -y, 0]$	`[2]`
3	$[-X, Y, -Z]$	$\left[\frac{1}{2} - x, y + \frac{1}{2}, 0\right]$	`[3]`
4	$[X, -Y, -Z]$	$\left[x + \frac{1}{2}, \frac{1}{2} - y, 0\right]$	`[4]`
5	$[-X, -Y, -Z]$	$[-x, -y, 0]$	`[5]`
6	$[X, Y, -Z]$	$[x, y, 0]$	`[6]`
7	$[X, -Y, Z]$	$\left[x + \frac{1}{2}, \frac{1}{2} - y, 0\right]$	`[7]`
8	$[-X, Y, Z]$	$\left[\frac{1}{2} - x, y + \frac{1}{2}, 0\right]$	`[8]`

* Wyckoff site: `16k`, site symmetry: `1`

Table 37: Wyckoff bond: `16a@16k`

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