

SG No. 74 D_{2h}^{28} *Imma* [orthorhombic]

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

* Wyckoff site: **4a**, site symmetry: $2/m..$

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

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

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

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

Table 3: Wyckoff bond: **8c@4a**

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

* Wyckoff site: **4b**, site symmetry: $2/m..$

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

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

Table 5: Wyckoff bond: **4b@4b**

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

Table 6: Wyckoff bond: 8c@4b

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

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

Table 7: Wyckoff bond: 4a@4c

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

Table 8: Wyckoff bond: 4b@4c

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

Table 9: Wyckoff bond: 8c@4c

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

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

Table 10: Wyckoff bond: 4a@4d

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

Table 11: Wyckoff bond: **4b@4d**

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

Table 12: Wyckoff bond: **8c@4d**

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

* Wyckoff site: **4e**, site symmetry: **mm2**

Table 13: Wyckoff bond: **4a@4e**

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

Table 14: Wyckoff bond: **4b@4e**

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

Table 15: Wyckoff bond: **4c@4e**

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

Table 16: Wyckoff bond: **8d@4e**

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

Table 17: Wyckoff bond: **8e@4e**

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

Table 18: Wyckoff bond: **8f@4e**

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

Table 19: Wyckoff bond: **16g@4e**

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

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

Table 20: Wyckoff bond: **8a@8f**

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

Table 21: Wyckoff bond: **8b@8f**

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

Table 22: Wyckoff bond: **16c@8f**

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

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

Table 23: Wyckoff bond: **8a@8g**

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

Table 24: Wyckoff bond: **8b@8g**

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

Table 25: Wyckoff bond: **16c@8g**

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

* Wyckoff site: **8h**, site symmetry: **m** . .

Table 26: Wyckoff bond: **8a@8h**

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

Table 27: Wyckoff bond: **8b@8h**

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

Table 28: Wyckoff bond: **16c@8h**

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

* Wyckoff site: **8i**, site symmetry: **.m**.

Table 29: Wyckoff bond: **8a@8i**

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

Table 30: Wyckoff bond: **8b@8i**

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

Table 31: Wyckoff bond: **16c@8i**

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

* Wyckoff site: 16j, site symmetry: 1

Table 32: Wyckoff bond: 16a@16j

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