

SG No. 23 D_2^8 $I222$ [orthorhombic]

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

* Wyckoff site: **2a**, site symmetry: 222

Table 1: Wyckoff bond: **2a@2a**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, 0]$	$[1, 2, -3, -4]$

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

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, 0, 0]$	$[1, -2, 3, -4]$

Table 3: Wyckoff bond: **2c@2a**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, 0]$	$[1, -2, -3, 4]$

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

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, 0]$	$[1, -2]$
2	$[-X, Y, 0]$	$[0, 0, 0]$	$[3, -4]$

Table 5: Wyckoff bond: **4e@2a**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, 0, 0]$	$[1, -3]$
2	$[-X, 0, Z]$	$[0, 0, 0]$	$[2, -4]$

Table 6: Wyckoff bond: **4f@2a**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[0, 0, 0]$	$[1, -4]$
2	$[0, -Y, Z]$	$[0, 0, 0]$	$[2, -3]$

Table 7: Wyckoff bond: **8g@2a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[0, 0, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[0, 0, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[0, 0, 0]$	$[4]$

* Wyckoff site: **2b**, site symmetry: **222**

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

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

Table 9: Wyckoff bond: **2b@2b**

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

Table 10: Wyckoff bond: **2c@2b**

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

Table 11: Wyckoff bond: **4d@2b**

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

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

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

Table 13: Wyckoff bond: **4f@2b**

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

Table 14: Wyckoff bond: **8g@2b**

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

* Wyckoff site: **2c**, site symmetry: **222**

Table 15: Wyckoff bond: **2a@2c**

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

Table 16: Wyckoff bond: **2b@2c**

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

Table 17: Wyckoff bond: **2c@2c**

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

Table 18: Wyckoff bond: **4d@2c**

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

Table 19: Wyckoff bond: **4e@2c**

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

Table 20: Wyckoff bond: **4f@2c**

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

Table 21: Wyckoff bond: **8g@2c**

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

* Wyckoff site: **2d**, site symmetry: **222**

Table 22: Wyckoff bond: **2a@2d**

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

Table 23: Wyckoff bond: **2b@2d**

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

Table 24: Wyckoff bond: **2c@2d**

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

Table 25: Wyckoff bond: **4d@2d**

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

Table 26: Wyckoff bond: **4e@2d**

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

Table 27: Wyckoff bond: **4f@2d**

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

Table 28: Wyckoff bond: **8g@2d**

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

* Wyckoff site: **4e**, site symmetry: $2..$

Table 29: Wyckoff bond: **4a@4e**

No.	vector	center	mapping
1	$[0, Y, Z]$	$[x, 0, 0]$	$[1, -4]$
2	$[0, -Y, Z]$	$[-x, 0, 0]$	$[2, -3]$

Table 30: Wyckoff bond: **4b@4e**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[x, 0, 0]$	$[1, 4]$
2	$[-X, 0, 0]$	$[-x, 0, 0]$	$[2, 3]$

Table 31: Wyckoff bond: **8c@4e**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, 0, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, 0, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[-x, 0, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[x, 0, 0]$	$[4]$

* Wyckoff site: **4f**, site symmetry: $2..$

Table 32: Wyckoff bond: **4a@4f**

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

Table 33: Wyckoff bond: **4b@4f**

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

Table 34: Wyckoff bond: **8c@4f**

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

* Wyckoff site: **4g**, site symmetry: $.2.$

Table 35: Wyckoff bond: **4a@4g**

No.	vector	center	mapping
1	$[X, 0, Z]$	$[0, y, 0]$	$[1, -3]$
2	$[-X, 0, Z]$	$[0, -y, 0]$	$[2, -4]$

Table 36: Wyckoff bond: **4b@4g**

No.	vector	center	mapping
1	$[0, Y, 0]$	$[0, y, 0]$	$[1, 3]$
2	$[0, -Y, 0]$	$[0, -y, 0]$	$[2, 4]$

Table 37: Wyckoff bond: **8c@4g**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, y, 0]$	$[1]$
2	$[-X, -Y, Z]$	$[0, -y, 0]$	$[2]$
3	$[-X, Y, -Z]$	$[0, y, 0]$	$[3]$
4	$[X, -Y, -Z]$	$[0, -y, 0]$	$[4]$

* Wyckoff site: **4h**, site symmetry: $.2$.

Table 38: Wyckoff bond: **4a@4h**

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

Table 39: Wyckoff bond: **4b@4h**

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

Table 40: Wyckoff bond: **8c@4h**

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

* Wyckoff site: **4i**, site symmetry: $\dots 2$

Table 41: Wyckoff bond: **4a@4i**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[0, 0, z]$	[1, -2]
2	$[-X, Y, 0]$	$[0, 0, -z]$	[3, -4]

Table 42: Wyckoff bond: **4b@4i**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	[1, 2]
2	$[0, 0, -Z]$	$[0, 0, -z]$	[3, 4]

Table 43: Wyckoff bond: **8c@4i**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, z]$	[1]
2	$[-X, -Y, Z]$	$[0, 0, z]$	[2]
3	$[-X, Y, -Z]$	$[0, 0, -z]$	[3]
4	$[X, -Y, -Z]$	$[0, 0, -z]$	[4]

* Wyckoff site: **4j**, site symmetry: $\dots 2$

Table 44: Wyckoff bond: **4a@4j**

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

Table 45: Wyckoff bond: **4b@4j**

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

Table 46: Wyckoff bond: **8c@4j**

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

* Wyckoff site: **8k**, site symmetry: **1**

Table 47: Wyckoff bond: **8a@8k**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	$[1]$
2	$[-X, -Y, Z]$	$[-x, -y, z]$	$[2]$
3	$[-X, Y, -Z]$	$[-x, y, -z]$	$[3]$
4	$[X, -Y, -Z]$	$[x, -y, -z]$	$[4]$