

SG No. 22 D_2^7 $F222$ [orthorhombic]

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

* Wyckoff site: **4a**, site symmetry: 222

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

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

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

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

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

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

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

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: **8e@4a**

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: **8f@4a**

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: **16g@4a**

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

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

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

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

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

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

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

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

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 12: Wyckoff bond: **8e@4b**

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 13: Wyckoff bond: **8f@4b**

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 14: Wyckoff bond: **16g@4b**

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: **4c**, site symmetry: **222**

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

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

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

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

Table 17: Wyckoff bond: **4c@4c**

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

Table 18: Wyckoff bond: **8d@4c**

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

Table 19: Wyckoff bond: **8e@4c**

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

Table 20: Wyckoff bond: **8f@4c**

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

Table 21: Wyckoff bond: **16g@4c**

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

* Wyckoff site: **4d**, site symmetry: **222**

Table 22: Wyckoff bond: **4a@4d**

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

Table 23: Wyckoff bond: **4b@4d**

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

Table 24: Wyckoff bond: **4c@4d**

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

Table 25: Wyckoff bond: **8d@4d**

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

Table 26: Wyckoff bond: **8e@4d**

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

Table 27: Wyckoff bond: **8f@4d**

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

Table 28: Wyckoff bond: **16g@4d**

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

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

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

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: **8b@8e**

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: **16c@8e**

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

Table 32: Wyckoff bond: **8a@8f**

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

Table 33: Wyckoff bond: **8b@8f**

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

Table 34: Wyckoff bond: **16c@8f**

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

Table 35: Wyckoff bond: **8a@8g**

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

Table 36: Wyckoff bond: **8b@8g**

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

Table 37: Wyckoff bond: **16c@8g**

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: **8h**, site symmetry: $\dots 2$

Table 38: Wyckoff bond: **8a@8h**

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

Table 39: Wyckoff bond: **8b@8h**

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

Table 40: Wyckoff bond: **16c@8h**

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

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

Table 41: Wyckoff bond: **8a@8i**

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

Table 42: Wyckoff bond: **8b@8i**

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

Table 43: Wyckoff bond: **16c@8i**

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

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

Table 44: Wyckoff bond: **8a@8j**

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

Table 45: Wyckoff bond: **8b@8j**

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

Table 46: Wyckoff bond: **16c@8j**

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

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

Table 47: 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	$[-X, Y, -Z]$	$[-x, y, -z]$	$[3]$
4	$[X, -Y, -Z]$	$[x, -y, -z]$	$[4]$