

SG No. 17 D_2^2 $P222_1$ [orthorhombic]

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

* Wyckoff site: **2a**, site symmetry: $2..$

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

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

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

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

Table 3: Wyckoff bond: **4c@2a**

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

* Wyckoff site: **2b**, site symmetry: $2..$

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

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

Table 5: Wyckoff bond: **2b@2b**

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

Table 6: Wyckoff bond: **4c@2b**

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

* Wyckoff site: **2c**, site symmetry: $.2$.

Table 7: Wyckoff bond: **2a@2c**

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

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

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

Table 9: Wyckoff bond: **4c@2c**

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

* Wyckoff site: **2d**, site symmetry: $.2$.

Table 10: Wyckoff bond: **2a@2d**

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

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

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

Table 12: Wyckoff bond: **4c@2d**

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

* Wyckoff site: **4e**, site symmetry: 1

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

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