

SG No. 24 D_2^9 $I2_12_12_1$ [orthorhombic]

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff bond: **8c@4b**

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

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

Table 7: Wyckoff bond: **4a@4c**

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

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

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

Table 9: Wyckoff bond: **8c@4c**

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	$[-X, Y, -Z]$	$[0, \frac{3}{4}, \frac{1}{2} - z]$	[3]
4	$[X, -Y, -Z]$	$[0, \frac{3}{4}, \frac{1}{2} - z]$	[4]

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

Table 10: Wyckoff bond: **8a@8d**

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