

SG No. 45 C_{2v}^{21} $Iba2$ [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	$[X, Y, 0]$	$[0, 0, z]$	$[1, -2]$
2	$[X, -Y, 0]$	$[\frac{1}{2}, \frac{1}{2}, z]$	$[3, -4]$

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff bond: **8a@8c**

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