

SG No. 13  $C_{2h}^4$   $P2/c$  (b-axis setting) [ monoclinic ]

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

\* Wyckoff site: **2a**, site symmetry:  $-1$

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

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

\* Wyckoff site: **2b**, site symmetry:  $-1$

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

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

\* Wyckoff site: **2c**, site symmetry:  $-1$

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

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

\* Wyckoff site: **2d**, site symmetry:  $-1$

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

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

\* Wyckoff site: **2e**, site symmetry:  $2$

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

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

Table 6: Wyckoff bond: **2b@2e**

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

Table 7: Wyckoff bond: **4c@2e**

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

\* Wyckoff site: **2f**, site symmetry: 2

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

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

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

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

Table 10: Wyckoff bond: **4c@2f**

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

\* Wyckoff site: **4g**, site symmetry: 1

Table 11: Wyckoff bond: **4a@4g**

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