

SG No. 11  $C_{2h}^2$   $P2_1/m$  (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	$[-X, Y, -Z]$	$[0, \frac{1}{2}, 0]$	$[2, -4]$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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