

SG No. 3 C_2^1 $P2$ (b-axis setting) [monoclinic]

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

* Wyckoff site: **1a**, site symmetry: 2

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

No.	vector	center	mapping
1	[$X, 0, Z$]	[$0, y, 0$]	[$1, -2$]

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

No.	vector	center	mapping
1	[$0, Y, 0$]	[$0, y, 0$]	[$1, 2$]

Table 3: Wyckoff bond: **2c@1a**

No.	vector	center	mapping
1	[X, Y, Z]	[$0, y, 0$]	[1]
2	[$-X, Y, -Z$]	[$0, y, 0$]	[2]

* Wyckoff site: **1b**, site symmetry: 2

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

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

Table 5: Wyckoff bond: **1b@1b**

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

Table 6: Wyckoff bond: **2c@1b**

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

* Wyckoff site: **1c**, site symmetry: 2

Table 7: Wyckoff bond: **1a@1c**

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

Table 8: Wyckoff bond: **1b@1c**

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

Table 9: Wyckoff bond: **2c@1c**

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

* Wyckoff site: **1d**, site symmetry: 2

Table 10: Wyckoff bond: **1a@1d**

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

Table 11: Wyckoff bond: **1b@1d**

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

Table 12: Wyckoff bond: **2c@1d**

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

* Wyckoff site: **2e**, site symmetry: 1

Table 13: Wyckoff bond: **2a@2e**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-X, Y, -Z]$	$[-x, y, -z]$	[2]