

SG No. 160  $C_{3v}^5$   $R3m$  [ trigonal ]

\* plus set:  $+ [0, 0, 0]$ ,  $+ [\frac{2}{3}, \frac{1}{3}, \frac{1}{3}]$ ,  $+ [\frac{1}{3}, \frac{2}{3}, \frac{2}{3}]$

\* Wyckoff site: **3a**, site symmetry:  $3m$

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[0, 0, z]$	$[1, 2, 3, 4, 5, 6]$

Table 2: Wyckoff bond: **9b@3a**

No.	vector	center	mapping
1	$[X, -X, Z]$	$[0, 0, z]$	$[1, 4]$
2	$[X, 2X, Z]$	$[0, 0, z]$	$[2, 6]$
3	$[-2X, -X, Z]$	$[0, 0, z]$	$[3, 5]$

Table 3: Wyckoff bond: **9c@3a**

No.	vector	center	mapping
1	$[X, 0, 0]$	$[0, 0, z]$	$[1, -5]$
2	$[0, X, 0]$	$[0, 0, z]$	$[2, -4]$
3	$[-X, -X, 0]$	$[0, 0, z]$	$[3, -6]$

Table 4: Wyckoff bond: **18d@3a**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, z]$	$[1]$
2	$[-Y, X - Y, Z]$	$[0, 0, z]$	$[2]$
3	$[-X + Y, -X, Z]$	$[0, 0, z]$	$[3]$
4	$[-Y, -X, Z]$	$[0, 0, z]$	$[4]$
5	$[-X + Y, Y, Z]$	$[0, 0, z]$	$[5]$
6	$[X, X - Y, Z]$	$[0, 0, z]$	$[6]$

\* Wyckoff site: **9b**, site symmetry:  $.m$

Table 5: Wyckoff bond: **9a@9b**

No.	vector	center	mapping
1	$[X, -X, Z]$	$[x, -x, z]$	$[1, 4]$
2	$[X, 2X, Z]$	$[x, 2x, z]$	$[2, 6]$

*continued ...*

Table 5

No.	vector	center	mapping
3	$[-2X, -X, Z]$	$[-2x, -x, z]$	[3, 5]

Table 6: Wyckoff bond: 9b@9b

No.	vector	center	mapping
1	$[X, X, 0]$	$[x, -x, z]$	[1, -4]
2	$[-X, 0, 0]$	$[x, 2x, z]$	[2, -6]
3	$[0, -X, 0]$	$[-2x, -x, z]$	[3, -5]

Table 7: Wyckoff bond: 18c@9b

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, -x, z]$	[1]
2	$[-Y, X - Y, Z]$	$[x, 2x, z]$	[2]
3	$[-X + Y, -X, Z]$	$[-2x, -x, z]$	[3]
4	$[-Y, -X, Z]$	$[x, -x, z]$	[4]
5	$[-X + Y, Y, Z]$	$[-2x, -x, z]$	[5]
6	$[X, X - Y, Z]$	$[x, 2x, z]$	[6]

\* Wyckoff site: 18c, site symmetry: 1

Table 8: Wyckoff bond: 18a@18c

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-Y, X - Y, Z]$	$[-y, x - y, z]$	[2]
3	$[-X + Y, -X, Z]$	$[-x + y, -x, z]$	[3]
4	$[-Y, -X, Z]$	$[-y, -x, z]$	[4]
5	$[-X + Y, Y, Z]$	$[-x + y, y, z]$	[5]
6	$[X, X - Y, Z]$	$[x, x - y, z]$	[6]