

SG No. 56  $D_{2h}^{10}$   $Pccn$  [ orthorhombic ]

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

\* Wyckoff site: **4a**, site symmetry:  $-1$

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

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, 0]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, \frac{1}{2}]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[4, -8]$

\* Wyckoff site: **4b**, site symmetry:  $-1$

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

No.	vector	center	mapping
1	$[X, Y, Z]$	$[0, 0, \frac{1}{2}]$	$[1, -5]$
2	$[-X, -Y, Z]$	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[2, -6]$
3	$[-X, Y, -Z]$	$[0, \frac{1}{2}, 0]$	$[3, -7]$
4	$[X, -Y, -Z]$	$[\frac{1}{2}, 0, 0]$	$[4, -8]$

\* Wyckoff site: **4c**, site symmetry:  $. . 2$

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

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{4}, \frac{1}{4}, z]$	$[1, -2]$
2	$[-X, Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	$[3, -4]$
3	$[-X, -Y, 0]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	$[5, -6]$
4	$[X, -Y, 0]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	$[7, -8]$

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

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{4}, \frac{1}{4}, z]$	$[1, 2]$
2	$[0, 0, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	$[3, 4]$
3	$[0, 0, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	$[5, 6]$
4	$[0, 0, Z]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	$[7, 8]$

Table 5: Wyckoff bond: **8c@4c**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, z]$	[2]
3	$[-X, Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[3]
4	$[X, -Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[4]
5	$[-X, -Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[5]
6	$[X, Y, -Z]$	$[\frac{3}{4}, \frac{3}{4}, -z]$	[6]
7	$[X, -Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[7]
8	$[-X, Y, Z]$	$[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[8]

\* Wyckoff site: **4d**, site symmetry:  $\dots 2$

Table 6: Wyckoff bond: **4a@4d**

No.	vector	center	mapping
1	$[X, Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, z]$	[1,-2]
2	$[-X, Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[3,-4]
3	$[-X, -Y, 0]$	$[\frac{3}{4}, \frac{1}{4}, -z]$	[5,-6]
4	$[X, -Y, 0]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[7,-8]

Table 7: Wyckoff bond: **4b@4d**

No.	vector	center	mapping
1	$[0, 0, Z]$	$[\frac{1}{4}, \frac{3}{4}, z]$	[1,2]
2	$[0, 0, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[3,4]
3	$[0, 0, -Z]$	$[\frac{3}{4}, \frac{1}{4}, -z]$	[5,6]
4	$[0, 0, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[7,8]

Table 8: Wyckoff bond: **8c@4d**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[\frac{1}{4}, \frac{3}{4}, z]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{4}, \frac{3}{4}, z]$	[2]
3	$[-X, Y, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[3]
4	$[X, -Y, -Z]$	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[4]
5	$[-X, -Y, -Z]$	$[\frac{3}{4}, \frac{1}{4}, -z]$	[5]
6	$[X, Y, -Z]$	$[\frac{3}{4}, \frac{1}{4}, -z]$	[6]
7	$[X, -Y, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[7]
8	$[-X, Y, Z]$	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[8]

\* Wyckoff site: **8e**, site symmetry: **1**

Table 9: Wyckoff bond: **8a@8e**

No.	vector	center	mapping
1	$[X, Y, Z]$	$[x, y, z]$	[1]
2	$[-X, -Y, Z]$	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[2]
3	$[-X, Y, -Z]$	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[3]
4	$[X, -Y, -Z]$	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[4]
5	$[-X, -Y, -Z]$	$[-x, -y, -z]$	[5]
6	$[X, Y, -Z]$	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[6]
7	$[X, -Y, Z]$	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[7]
8	$[-X, Y, Z]$	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[8]