

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: . . 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]