

SG No. 52 D_{2h}^6 $Pnna$ [orthorhombic]

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

Table 1: Wyckoff site: 4a, site symmetry: -1

No.	position	mapping
1	[0, 0, 0]	[1, 5]
2	[\frac{1}{2}, 0, 0]	[2, 6]
3	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[3, 7]
4	[0, \frac{1}{2}, \frac{1}{2}]	[4, 8]

Table 2: Wyckoff site: 4b, site symmetry: -1

No.	position	mapping
1	[0, 0, \frac{1}{2}]	[1, 5]
2	[\frac{1}{2}, 0, \frac{1}{2}]	[2, 6]
3	[\frac{1}{2}, \frac{1}{2}, 0]	[3, 7]
4	[0, \frac{1}{2}, 0]	[4, 8]

Table 3: Wyckoff site: 4c, site symmetry: ...2

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

Table 4: Wyckoff site: 4d, site symmetry: 2...

No.	position	mapping
1	[x, \frac{1}{4}, \frac{1}{4}]	[1, 4]
2	[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]	[2, 3]
3	[-x, \frac{3}{4}, \frac{3}{4}]	[5, 8]
4	[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]	[6, 7]

Table 5: Wyckoff site: 8e, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1]

continued ...

Table 5

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