

SG No. 54 D_{2h}^8 $Pcc\bar{a}$ [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	[0, 0, \frac{1}{2}]	[3, 7]
4	[\frac{1}{2}, 0, \frac{1}{2}]	[4, 8]

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: ..2

No.	position	mapping
1	[\frac{1}{4}, \frac{1}{2}, z]	[1, 2]

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 1

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