SG No. 58 D_{2h}^{12} $Pnnm$ [orthorhombic]

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

Table 1: Wyckoff site: `2a`, site symmetry: `..2/m`

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

Table 2: Wyckoff site: `2b`, site symmetry: `..2/m`

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

Table 3: Wyckoff site: `2c`, site symmetry: `..2/m`

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

Table 4: Wyckoff site: `2d`, site symmetry: `..2/m`

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

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

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

Table 6: Wyckoff site: `4f`, site symmetry: `..2`

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

Table 7: Wyckoff site: `4g`, site symmetry: `..m`

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,6]`
2	$[-x,\ -y,\ 0]$	`[2,5]`
3	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[3,8]`
4	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[4,7]`

Table 8: Wyckoff site: `8h`, site symmetry: `1`

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