Table 1: Wyckoff site: 2a, site symmetry: -4..1'

No.	position	mapping
1	$[0, 0, 0]$	[1,2,3,4,9,10,11,12]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[5,6,7,8,13,14,15,16]

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

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	[1,2,3,4,9,10,11,12]
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[5,6,7,8,13,14,15,16]

Table 3: Wyckoff site: 2c, site symmetry: -4..1'

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[1,2,7,8,9,10,15,16]
2	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[3,4,5,6,11,12,13,14]

Table 4: Wyckoff site: 2d, site symmetry: -4..1'

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[1,2,7,8,9,10,15,16]
2	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[3,4,5,6,11,12,13,14]

Table 5: Wyckoff site: 4e, site symmetry: 2..1'

No.	position	mapping
1	$[0, 0, z]$	[1,2,9,10]
2	$[0, 0, -z]$	[3,4,11,12]
3	$\left[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}\right]$	[5,6,13,14]
4	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z\right]$	[7,8,15,16]

Table 6: Wyckoff site: `4f`, site symmetry: `2..1'`

No.	position	mapping
1	$\left[0, \frac{1}{2}, z\right]$	[1,2,9,10]
2	$\left[\frac{1}{2}, 0, -z\right]$	[3,4,11,12]
3	$\left[\frac{1}{2}, 0, z + \frac{1}{2}\right]$	[5,6,13,14]
4	$\left[0, \frac{1}{2}, \frac{1}{2} - z\right]$	[7,8,15,16]

Table 7: Wyckoff site: `8g`, site symmetry: `11'`

No.	position	mapping
1	$[x, y, z]$	[1,9]
2	$[-x, -y, z]$	[2,10]
3	$[y, -x, -z]$	[3,11]
4	$[-y, x, -z]$	[4,12]
5	$\left[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[5,13]
6	$\left[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[6,14]
7	$\left[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z\right]$	[7,15]
8	$\left[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z\right]$	[8,16]