

SG No. 85 C_{4h}^3 $P4/n$ [tetragonal]

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

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

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

Table 2: Wyckoff site: 2b, site symmetry: $-4..$

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: -1

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

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

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

Table 7: Wyckoff site: $8g$, site symmetry: 1

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