

SG No. 88 C_{4h}^6 $I4_1/a$ [tetragonal]

* plus set: $+ [0, 0, 0], + [\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: -1

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

Table 4: Wyckoff site: 8d, site symmetry: -1

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

Table 5: Wyckoff site: 8e, site symmetry: $2..$

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

Table 6: Wyckoff site: 16f, site symmetry: 1

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