

SG No. 87 C_{4h}^5 $I4/m$ [tetragonal]

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

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

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

Table 2: Wyckoff site: 2b, site symmetry: $4/m..$

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: $-4..$

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

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4]$
2	$[0, 0, -z]$	$[5, 6, 7, 8]$

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

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

continued ...

Table 6

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

Table 7: Wyckoff site: 8g, site symmetry: 2. .

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

Table 8: Wyckoff site: 8h, site symmetry: m. .

No.	position	mapping
1	$[x, y, 0]$	[1,6]
2	$[-x, -y, 0]$	[2,5]
3	$[-y, x, 0]$	[3,8]
4	$[y, -x, 0]$	[4,7]

Table 9: Wyckoff site: 16i, site symmetry: 1

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