

SG No. 121 D_{2d}^{11} $I\bar{4}2m$ [tetragonal]

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

Table 1: Wyckoff site: 2a, site symmetry: $-42m$

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

Table 2: Wyckoff site: 2b, site symmetry: $-42m$

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

Table 3: Wyckoff site: 4c, site symmetry: $222.$

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	$[0, \frac{1}{2}, \frac{1}{4}]$	$[1, 2, 3, 4]$
2	$[0, \frac{1}{2}, \frac{3}{4}]$	$[5, 6, 7, 8]$

Table 5: Wyckoff site: 4e, site symmetry: $2.mm$

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

Table 6: Wyckoff site: 8f, site symmetry: $.2.$

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

continued ...

Table 6

No.	position	mapping
4	$[0, x, 0]$	$[4, 8]$

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

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

Table 8: Wyckoff site: $8h$, 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 9: Wyckoff site: $8i$, site symmetry: $..m$

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

Table 10: Wyckoff site: $16j$, 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	$[y, x, z]$	$[8]$