

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

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

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]