

SG No. 120 D_{2d}^{10} $I\bar{4}c2$ [tetragonal]

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

Table 1: Wyckoff site: 4a, site symmetry: 2.22

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

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

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

Table 3: Wyckoff site: 4c, 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 4: Wyckoff site: 4d, site symmetry: 2.22

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

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

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

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

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

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

Table 8: Wyckoff site: **8h**, site symmetry: $..2$

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

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	$[x, -y, z + \frac{1}{2}]$	[5]
6	$[-x, y, z + \frac{1}{2}]$	[6]
7	$[y, x, \frac{1}{2} - z]$	[7]
8	$[-y, -x, \frac{1}{2} - z]$	[8]