

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

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

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	$[-y, -x, \frac{1}{2} - z]$	$[8]$