

# SG No. 97 $D_4^9$ $I422$ [ tetragonal ]

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

Table 1: Wyckoff site: 2a, site symmetry: 422

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

Table 2: Wyckoff site: 2b, site symmetry: 422

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: 2.22

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: 2. .

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

*continued ...*

Table 6

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

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

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

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

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

Table 9: Wyckoff site: 8i, 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 10: Wyckoff site: 8j, site symmetry:  $.2$ 

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

Table 11: Wyckoff site:  $16k$ , 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]