

SG No. 98  $D_4^{10}$   $I4_122$  [ 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	$[0, 0, 0]$	$[1, 2, 7, 8]$
2	$[0, \frac{1}{2}, \frac{1}{4}]$	$[3, 4, 5, 6]$

Table 2: Wyckoff site: 4b, site symmetry: 2.22

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

Table 3: Wyckoff site: 8c, site symmetry: 2..

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

Table 4: Wyckoff site: 8d, site symmetry: ..2

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

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

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

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

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

Table 7: Wyckoff site: 16g, site symmetry: 1

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