

SG No. 70  $D_{2h}^{24}$   $Fddd$  [ orthorhombic ]

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

Table 1: Wyckoff site: 8a, site symmetry: 222

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

Table 2: Wyckoff site: 8b, site symmetry: 222

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

Table 3: Wyckoff site: 16c, site symmetry: -1

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

Table 4: Wyckoff site: 16d, site symmetry: -1

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

Table 5: Wyckoff site: 16e, site symmetry: 2..

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

Table 6: Wyckoff site: 16f, site symmetry: .2.

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

Table 7: Wyckoff site: 16g, site symmetry: . .2

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

Table 8: Wyckoff site: 32h, site symmetry: 1

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