

SG No. 130 D_{4h}^8 $P4/ncc$ [tetragonal]

* plus set: + [0, 0, 0]

Table 1: Wyckoff site: 4a, site symmetry: 2..22

No.	position	mapping
1	[$\frac{3}{4}$, $\frac{1}{4}$, $\frac{1}{4}$]	[1,2,7,8]
2	[$\frac{1}{4}$, $\frac{3}{4}$, $\frac{1}{4}$]	[3,4,5,6]
3	[$\frac{1}{4}$, $\frac{3}{4}$, $\frac{3}{4}$]	[9,10,15,16]
4	[$\frac{3}{4}$, $\frac{1}{4}$, $\frac{3}{4}$]	[11,12,13,14]

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

No.	position	mapping
1	[$\frac{3}{4}$, $\frac{1}{4}$, 0]	[1,2,11,12]
2	[$\frac{1}{4}$, $\frac{3}{4}$, 0]	[3,4,9,10]
3	[$\frac{1}{4}$, $\frac{3}{4}$, $\frac{1}{2}$]	[5,6,15,16]
4	[$\frac{3}{4}$, $\frac{1}{4}$, $\frac{1}{2}$]	[7,8,13,14]

Table 3: Wyckoff site: 4c, site symmetry: 4..

No.	position	mapping
1	[$\frac{1}{4}$, $\frac{1}{4}$, z]	[1,2,3,4]
2	[$\frac{3}{4}$, $\frac{3}{4}$, $\frac{1}{2} - z$]	[5,6,7,8]
3	[$\frac{3}{4}$, $\frac{3}{4}$, $-z$]	[9,10,11,12]
4	[$\frac{1}{4}$, $\frac{1}{4}$, $z + \frac{1}{2}$]	[13,14,15,16]

Table 4: Wyckoff site: 8d, site symmetry: -1

No.	position	mapping
1	[0, 0, 0]	[1,9]
2	[$\frac{1}{2}$, $\frac{1}{2}$, 0]	[2,10]
3	[$\frac{1}{2}$, 0, 0]	[3,11]
4	[0, $\frac{1}{2}$, 0]	[4,12]
5	[0, $\frac{1}{2}$, $\frac{1}{2}$]	[5,13]
6	[$\frac{1}{2}$, 0, $\frac{1}{2}$]	[6,14]
7	[$\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$]	[7,15]
8	[0, 0, $\frac{1}{2}$]	[8,16]

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

No.	position	mapping
1	$[\frac{3}{4}, \frac{1}{4}, z]$	[1,2]
2	$[\frac{1}{4}, \frac{3}{4}, z]$	[3,4]
3	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$	[5,6]
4	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$	[7,8]
5	$[\frac{1}{4}, \frac{3}{4}, -z]$	[9,10]
6	$[\frac{3}{4}, \frac{1}{4}, -z]$	[11,12]
7	$[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$	[13,14]
8	$[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$	[15,16]

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

No.	position	mapping
1	$[x, -x, \frac{1}{4}]$	[1,8]
2	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}]$	[2,7]
3	$[x + \frac{1}{2}, x, \frac{1}{4}]$	[3,6]
4	$[-x, \frac{1}{2} - x, \frac{1}{4}]$	[4,5]
5	$[-x, x, \frac{3}{4}]$	[9,16]
6	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[10,15]
7	$[\frac{1}{2} - x, -x, \frac{3}{4}]$	[11,14]
8	$[x, x + \frac{1}{2}, \frac{3}{4}]$	[12,13]

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[2]
3	$[\frac{1}{2} - y, x, z]$	[3]
4	$[y, \frac{1}{2} - x, z]$	[4]
5	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[5]
6	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[6]
7	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[7]
8	$[-y, -x, \frac{1}{2} - z]$	[8]
9	$[-x, -y, -z]$	[9]
10	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[10]
11	$[y + \frac{1}{2}, -x, -z]$	[11]
12	$[-y, x + \frac{1}{2}, -z]$	[12]
13	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[13]
14	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[14]
15	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[15]
16	$[y, x, z + \frac{1}{2}]$	[16]