

SG No. 136 D_{4h}^{14} $P4_2/mnm$ [tetragonal]

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

Table 1: Wyckoff site: 2a, site symmetry: m.m̄m̄

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

Table 2: Wyckoff site: 2b, site symmetry: m.m̄m̄

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

Table 3: Wyckoff site: 4c, site symmetry: 2/m..

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

Table 4: Wyckoff site: 4d, site symmetry: -4..

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

Table 5: Wyckoff site: 4e, site symmetry: 2.m̄m̄

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

Table 6: Wyckoff site: 4f, site symmetry: m.2m

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

Table 7: Wyckoff site: 4g, site symmetry: m.2m

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: m..

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

Table 10: Wyckoff site: 8j, site symmetry: . . m

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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