

MSG No. 129.411  $P4/nmm$  [ Type I, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $-4m2$

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

Table 2: Wyckoff site: 2b, site symmetry:  $-4m2$

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

Table 3: Wyckoff site: 2c, site symmetry:  $4mm$

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

Table 4: Wyckoff site: 4d, site symmetry:  $\dots 2/m$

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

Table 5: Wyckoff site: 4e, site symmetry:  $\dots 2/m$

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

Table 6: Wyckoff site: 4f, site symmetry:  $2mm$ .

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

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

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

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

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

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

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

*continued ...*

Table 9

No.	position	mapping
8	$[-y, \frac{3}{4}, -z]$	[8,11]

Table 10: Wyckoff site: 8j, site symmetry:  $\bar{3}m$ 

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

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

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