

MSG No. 126.377  $P4/n'nc$  [ Type III, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry: 42'2'

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

Table 2: Wyckoff site: 2b, site symmetry: 42'2'

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

Table 3: Wyckoff site: 4c, site symmetry: 22'2'.

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

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

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

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

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

Table 6: Wyckoff site: 8f, site symmetry: -1'

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

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

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: .2'.

No.	position	mapping
1	[x, $\frac{1}{4}$ , $\frac{1}{4}$ ]	[1, 9]
2	[ $\frac{1}{4}$ , x, $\frac{1}{4}$ ]	[2, 11]
3	[ $\frac{1}{4}$ , $\frac{1}{2} - x$ , $\frac{1}{4}$ ]	[3, 12]

*continued ...*

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: .2'.

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

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	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[4]
5	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[5]
6	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[6]
7	$[-y, -x, z + \frac{1}{2}]$	[7]
8	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[8]
9	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[9]
10	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[10]
11	$[y, x, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[12]
13	$[-x, -y, -z]$	[13]
14	$[y + \frac{1}{2}, -x, -z]$	[14]
15	$[-y, x + \frac{1}{2}, -z]$	[15]
16	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[16]