

MSG No. 52.315  $P_b n n a$  [ Type IV, orthorhombic ]

Table 1: Wyckoff site: 4a, site symmetry:  $22'2'$

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

Table 2: Wyckoff site: 4b, site symmetry:  $22'2'$

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

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

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

Table 4: Wyckoff site: 4d, site symmetry:  $2'2'2$

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

Table 5: Wyckoff site: 8e, site symmetry:  $-1'$

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[1,13]
2	$[\frac{1}{2}, \frac{1}{4}, 0]$	[2,14]

*continued ...*

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$[x, 0, \frac{3}{4}]$	[1, 10]
2	$[x, \frac{1}{2}, \frac{3}{4}]$	[2, 9]
3	$[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$	[3, 12]
4	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[4, 11]
5	$[-x, 0, \frac{1}{4}]$	[5, 14]

*continued ...*

Table 8

No.	position	mapping
6	$[-x, \frac{1}{2}, \frac{1}{4}]$	[6,13]
7	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[7,16]
8	$[x + \frac{1}{2}, 0, \frac{1}{4}]$	[8,15]

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

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

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

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

Table 11: Wyckoff site: 8k, site symmetry:  $. 2'$ .

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

Table 12: Wyckoff site:  $81$ , site symmetry:  $.2'$ .

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

Table 13: Wyckoff site:  $16m$ , site symmetry:  $1$ 

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