

MSG No. 218.82  $P\bar{4}3n1'$  [ Type II, cubic ]

Table 1: Wyckoff site: 2a, site symmetry:  $23..1'$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36]$
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]$

Table 2: Wyckoff site: 6b, site symmetry:  $222..1'$

No.	position	mapping
1	$[0, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, 3, 4, 25, 26, 27, 28]$
2	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[5, 8, 10, 12, 29, 32, 34, 36]$
3	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[6, 7, 9, 11, 30, 31, 33, 35]$
4	$[\frac{1}{2}, 0, 0]$	$[13, 14, 21, 22, 37, 38, 45, 46]$
5	$[0, 0, \frac{1}{2}]$	$[15, 16, 23, 24, 39, 40, 47, 48]$
6	$[0, \frac{1}{2}, 0]$	$[17, 18, 19, 20, 41, 42, 43, 44]$

Table 3: Wyckoff site: 6c, site symmetry:  $-4..1'$

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[1, 2, 13, 14, 25, 26, 37, 38]$
2	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[3, 4, 21, 22, 27, 28, 45, 46]$
3	$[0, \frac{1}{4}, \frac{1}{2}]$	$[5, 12, 17, 19, 29, 36, 41, 43]$
4	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[6, 9, 16, 23, 30, 33, 40, 47]$
5	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[7, 11, 15, 24, 31, 35, 39, 48]$
6	$[0, \frac{3}{4}, \frac{1}{2}]$	$[8, 10, 18, 20, 32, 34, 42, 44]$

Table 4: Wyckoff site: 6d, site symmetry:  $-4..1'$

No.	position	mapping
1	$[\frac{1}{4}, 0, \frac{1}{2}]$	$[1, 2, 13, 14, 25, 26, 37, 38]$
2	$[\frac{3}{4}, 0, \frac{1}{2}]$	$[3, 4, 21, 22, 27, 28, 45, 46]$
3	$[\frac{1}{2}, \frac{1}{4}, 0]$	$[5, 12, 17, 19, 29, 36, 41, 43]$
4	$[0, \frac{1}{2}, \frac{1}{4}]$	$[6, 9, 16, 23, 30, 33, 40, 47]$
5	$[0, \frac{1}{2}, \frac{3}{4}]$	$[7, 11, 15, 24, 31, 35, 39, 48]$
6	$[\frac{1}{2}, \frac{3}{4}, 0]$	$[8, 10, 18, 20, 32, 34, 42, 44]$

Table 5: Wyckoff site:  $8e$ , site symmetry:  $.3.1'$ 

No.	position	mapping
1	$[x, x, x]$	$[1, 5, 6, 25, 29, 30]$
2	$[x, -x, -x]$	$[2, 10, 11, 26, 34, 35]$
3	$[-x, x, -x]$	$[3, 7, 12, 27, 31, 36]$
4	$[-x, -x, x]$	$[4, 8, 9, 28, 32, 33]$
5	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	$[13, 18, 23, 37, 42, 47]$
6	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	$[14, 15, 19, 38, 39, 43]$
7	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	$[16, 17, 21, 40, 41, 45]$
8	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	$[20, 22, 24, 44, 46, 48]$

Table 6: Wyckoff site:  $12f$ , site symmetry:  $2..1'$ 

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2, 25, 26]$
2	$[-x, 0, 0]$	$[3, 4, 27, 28]$
3	$[0, x, 0]$	$[5, 12, 29, 36]$
4	$[0, 0, x]$	$[6, 9, 30, 33]$
5	$[0, 0, -x]$	$[7, 11, 31, 35]$
6	$[0, -x, 0]$	$[8, 10, 32, 34]$
7	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	$[13, 14, 37, 38]$
8	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	$[15, 24, 39, 48]$
9	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	$[16, 23, 40, 47]$
10	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	$[17, 19, 41, 43]$
11	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	$[18, 20, 42, 44]$
12	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[21, 22, 45, 46]$

Table 7: Wyckoff site:  $12g$ , site symmetry:  $2..1'$ 

No.	position	mapping
1	$[x, \frac{1}{2}, 0]$	$[1, 2, 25, 26]$
2	$[-x, \frac{1}{2}, 0]$	$[3, 4, 27, 28]$
3	$[0, x, \frac{1}{2}]$	$[5, 12, 29, 36]$
4	$[\frac{1}{2}, 0, x]$	$[6, 9, 30, 33]$
5	$[\frac{1}{2}, 0, -x]$	$[7, 11, 31, 35]$
6	$[0, -x, \frac{1}{2}]$	$[8, 10, 32, 34]$
7	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	$[13, 14, 37, 38]$
8	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	$[15, 24, 39, 48]$
9	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	$[16, 23, 40, 47]$
10	$[0, \frac{1}{2} - x, \frac{1}{2}]$	$[17, 19, 41, 43]$
11	$[0, x + \frac{1}{2}, \frac{1}{2}]$	$[18, 20, 42, 44]$
12	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	$[21, 22, 45, 46]$

Table 8: Wyckoff site: 12h, site symmetry:  $2..1'$ 

No.	position	mapping
1	$[x, 0, \frac{1}{2}]$	[1, 2, 25, 26]
2	$[-x, 0, \frac{1}{2}]$	[3, 4, 27, 28]
3	$[\frac{1}{2}, x, 0]$	[5, 12, 29, 36]
4	$[0, \frac{1}{2}, x]$	[6, 9, 30, 33]
5	$[0, \frac{1}{2}, -x]$	[7, 11, 31, 35]
6	$[\frac{1}{2}, -x, 0]$	[8, 10, 32, 34]
7	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[13, 14, 37, 38]
8	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[15, 24, 39, 48]
9	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[16, 23, 40, 47]
10	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[17, 19, 41, 43]
11	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	[18, 20, 42, 44]
12	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[21, 22, 45, 46]

Table 9: Wyckoff site: 24i, site symmetry:  $11'$ 

No.	position	mapping
1	$[x, y, z]$	[1, 25]
2	$[x, -y, -z]$	[2, 26]
3	$[-x, y, -z]$	[3, 27]
4	$[-x, -y, z]$	[4, 28]
5	$[z, x, y]$	[5, 29]
6	$[y, z, x]$	[6, 30]
7	$[-y, z, -x]$	[7, 31]
8	$[-z, -x, y]$	[8, 32]
9	$[-y, -z, x]$	[9, 33]
10	$[z, -x, -y]$	[10, 34]
11	$[y, -z, -x]$	[11, 35]
12	$[-z, x, -y]$	[12, 36]
13	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y]$	[13, 37]
14	$[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}]$	[14, 38]
15	$[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}]$	[15, 39]
16	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x]$	[16, 40]
17	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[17, 41]
18	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[18, 42]
19	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[19, 43]
20	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[20, 44]
21	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[21, 45]
22	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[22, 46]
23	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x]$	[23, 47]
24	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[24, 48]