

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]