

MSG No. 205.34 $Pa\bar{3}1'$ [Type II, cubic]

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

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

Table 2: Wyckoff site: 4b, site symmetry: $.-3'.1'$

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

Table 3: Wyckoff site: 8c, site symmetry: $.3.1'$

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

Table 4: Wyckoff site: 24d, site symmetry: $11'$

No.	position	mapping
1	[x, y, z]	[1,25]
2	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[2,26]
3	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[3,27]
4	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[4,28]
5	[z, x, y]	[5,29]
6	[y, z, x]	[6,30]
7	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[7,31]
8	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[8,32]
9	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[9,33]

continued ...

Table 4

No.	position	mapping
10	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[10,34]
11	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[11,35]
12	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[12,36]
13	$[-x, -y, -z]$	[13,37]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[14,38]
15	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[15,39]
16	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[16,40]
17	$[-z, -x, -y]$	[17,41]
18	$[-y, -z, -x]$	[18,42]
19	$[y, \frac{1}{2} - z, x + \frac{1}{2}]$	[19,43]
20	$[z + \frac{1}{2}, x, \frac{1}{2} - y]$	[20,44]
21	$[y + \frac{1}{2}, z, \frac{1}{2} - x]$	[21,45]
22	$[\frac{1}{2} - z, x + \frac{1}{2}, y]$	[22,46]
23	$[\frac{1}{2} - y, z + \frac{1}{2}, x]$	[23,47]
24	$[z, \frac{1}{2} - x, y + \frac{1}{2}]$	[24,48]