

MSG No. 205.33  $Pa\bar{3}$  [ Type I, cubic ]

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

No.	position	mapping
1	[0, 0, 0]	[1,5,6,13,17,18]
2	[\frac{1}{2}, \frac{1}{2}, 0]	[2,10,11,14,22,23]
3	[0, \frac{1}{2}, \frac{1}{2}]	[3,7,12,15,19,24]
4	[\frac{1}{2}, 0, \frac{1}{2}]	[4,8,9,16,20,21]

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

No.	position	mapping
1	[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]	[1,5,6,13,17,18]
2	[0, 0, \frac{1}{2}]	[2,10,11,14,22,23]
3	[\frac{1}{2}, 0, 0]	[3,7,12,15,19,24]
4	[0, \frac{1}{2}, 0]	[4,8,9,16,20,21]

Table 3: Wyckoff site: 8c, site symmetry: .3.

No.	position	mapping
1	[x, x, x]	[1,5,6]
2	[x + \frac{1}{2}, \frac{1}{2} - x, -x]	[2,10,11]
3	[-x, x + \frac{1}{2}, \frac{1}{2} - x]	[3,7,12]
4	[\frac{1}{2} - x, -x, x + \frac{1}{2}]	[4,8,9]
5	[-x, -x, -x]	[13,17,18]
6	[\frac{1}{2} - x, x + \frac{1}{2}, x]	[14,22,23]
7	[x, \frac{1}{2} - x, x + \frac{1}{2}]	[15,19,24]
8	[x + \frac{1}{2}, x, \frac{1}{2} - x]	[16,20,21]

Table 4: Wyckoff site: 24d, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1]
2	[x + \frac{1}{2}, \frac{1}{2} - y, -z]	[2]
3	[-x, y + \frac{1}{2}, \frac{1}{2} - z]	[3]
4	[\frac{1}{2} - x, -y, z + \frac{1}{2}]	[4]
5	[z, x, y]	[5]
6	[y, z, x]	[6]
7	[-y, z + \frac{1}{2}, \frac{1}{2} - x]	[7]
8	[\frac{1}{2} - z, -x, y + \frac{1}{2}]	[8]
9	[\frac{1}{2} - y, -z, x + \frac{1}{2}]	[9]

*continued ...*

Table 4

No.	position	mapping
10	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[10]
11	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[11]
12	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[12]
13	$[-x, -y, -z]$	[13]
14	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[14]
15	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[15]
16	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[16]
17	$[-z, -x, -y]$	[17]
18	$[-y, -z, -x]$	[18]
19	$[y, \frac{1}{2} - z, x + \frac{1}{2}]$	[19]
20	$[z + \frac{1}{2}, x, \frac{1}{2} - y]$	[20]
21	$[y + \frac{1}{2}, z, \frac{1}{2} - x]$	[21]
22	$[\frac{1}{2} - z, x + \frac{1}{2}, y]$	[22]
23	$[\frac{1}{2} - y, z + \frac{1}{2}, x]$	[23]
24	$[z, \frac{1}{2} - x, y + \frac{1}{2}]$	[24]