

MSG No. 165.91 $P\bar{3}c1$ [Type I, trigonal]

Table 1: Wyckoff site: 2a, site symmetry: $\bar{3}2$.

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

Table 2: Wyckoff site: 2b, site symmetry: $\bar{3}..$

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

Table 3: Wyckoff site: 4c, site symmetry: $3..$

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

Table 4: Wyckoff site: 4d, site symmetry: $3..$

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

Table 5: Wyckoff site: 6e, site symmetry: $\bar{1}$

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

Table 6: Wyckoff site: **6f**, site symmetry: $.2$.

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

Table 7: Wyckoff site: **12g**, site symmetry: 1

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