

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

Table 1: Wyckoff site: 2a, site symmetry: 32.

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: -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: -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]