

MSG No. 150.28 P_c321 [Type IV, trigonal]

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

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

Table 2: Wyckoff site: 2b, site symmetry: 32'.

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

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

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

Table 5: Wyckoff site: 6e, site symmetry: .2.

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

Table 6: Wyckoff site: **6f**, site symmetry: $.2^1$.

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

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	$[x - y, -y, -z]$	[4]
5	$[y, x, -z]$	[5]
6	$[-x, -x + y, -z]$	[6]
7	$[x, y, z + \frac{1}{2}]$	[7]
8	$[-y, x - y, z + \frac{1}{2}]$	[8]
9	$[-x + y, -x, z + \frac{1}{2}]$	[9]
10	$[x - y, -y, \frac{1}{2} - z]$	[10]
11	$[y, x, \frac{1}{2} - z]$	[11]
12	$[-x, -x + y, \frac{1}{2} - z]$	[12]