

MSG No. 165.92  $P\bar{3}c11'$  [ Type II, trigonal ]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 6e, site symmetry:  $-11'$

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

Table 6: Wyckoff site:  $6\mathbf{f}$ , site symmetry:  $.2.1'$ 

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

Table 7: Wyckoff site:  $12\mathbf{g}$ , site symmetry:  $11'$ 

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