

MSG No. 149.22 $P3121'$ [Type II, trigonal]

Table 1: Wyckoff site: 1a, site symmetry: $3.21'$

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

Table 2: Wyckoff site: 1b, site symmetry: $3.21'$

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

Table 3: Wyckoff site: 1c, site symmetry: $3.21'$

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

Table 4: Wyckoff site: 1d, site symmetry: $3.21'$

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

Table 5: Wyckoff site: 1e, site symmetry: $3.21'$

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

Table 6: Wyckoff site: 1f, site symmetry: $3.21'$

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

Table 7: Wyckoff site: 2g, site symmetry: $3..1'$

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

Table 8: Wyckoff site: 2h, site symmetry: $3..1'$

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

Table 9: Wyckoff site: 2i, site symmetry: $3..1'$

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

Table 10: Wyckoff site: 3j, site symmetry: $..21'$

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

Table 11: Wyckoff site: 3k, site symmetry: $..21'$

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

Table 12: Wyckoff site: 6l, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 7]$
2	$[-y, x - y, z]$	$[2, 8]$

continued ...

Table 12

No.	position	mapping
3	$[-x + y, -x, z]$	[3,9]
4	$[x, x - y, -z]$	[4,10]
5	$[-x + y, y, -z]$	[5,11]
6	$[-y, -x, -z]$	[6,12]