

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]