

Table 1: Wyckoff site: 1a, site symmetry: $-6'..$

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6]$

Table 2: Wyckoff site: 1b, site symmetry: $-6'..$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6]$

Table 3: Wyckoff site: 1c, site symmetry: $-6'..$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 2, 3, 4, 5, 6]$

Table 4: Wyckoff site: 1d, site symmetry: $-6'..$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6]$

Table 5: Wyckoff site: 1e, site symmetry: $-6'..$

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[1, 2, 3, 4, 5, 6]$

Table 6: Wyckoff site: 1f, site symmetry: $-6'..$

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6]$

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3]$
2	$[0, 0, -z]$	$[4, 5, 6]$

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

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 2, 3]$
2	$[\frac{1}{3}, \frac{2}{3}, -z]$	$[4, 5, 6]$

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

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, z]$	$[1, 2, 3]$
2	$[\frac{2}{3}, \frac{1}{3}, -z]$	$[4, 5, 6]$

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

No.	position	mapping
1	$[x, y, 0]$	$[1, 5]$
2	$[-y, x - y, 0]$	$[2, 6]$
3	$[-x + y, -x, 0]$	$[3, 4]$

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

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	$[1, 5]$
2	$[-y, x - y, \frac{1}{2}]$	$[2, 6]$
3	$[-x + y, -x, \frac{1}{2}]$	$[3, 4]$

Table 12: Wyckoff site: $6l$, site symmetry: 1

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

continued ...

Table 12

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