

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

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: $3..$

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

Table 4: Wyckoff site: 2d, site symmetry: $3..$

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

Table 5: Wyckoff site: 3e, site symmetry: $.2'$.

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

Table 6: Wyckoff site: 3f, site symmetry: $.2'$.

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

Table 7: Wyckoff site: $6g$, 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]