

Table 1: Wyckoff site: 2a, site symmetry: 2.22

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

Table 2: Wyckoff site: 2b, site symmetry: 2.22

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

Table 3: Wyckoff site: 2c, site symmetry: 4..

No.	position	mapping
1	$[0, \frac{1}{2}, z]$	$[1, 2, 3, 6]$
2	$[\frac{1}{2}, 0, -z]$	$[4, 5, 7, 8]$

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 6]$
2	$[\frac{1}{2}, \frac{1}{2}, z]$	$[2, 3]$
3	$[\frac{1}{2}, \frac{1}{2}, -z]$	$[4, 5]$
4	$[0, 0, -z]$	$[7, 8]$

Table 5: Wyckoff site: 4e, site symmetry: ..2

No.	position	mapping
1	$[x, x, 0]$	$[1, 7]$
2	$[\frac{1}{2} - x, x + \frac{1}{2}, 0]$	$[2, 5]$
3	$[x + \frac{1}{2}, \frac{1}{2} - x, 0]$	$[3, 4]$
4	$[-x, -x, 0]$	$[6, 8]$

Table 6: Wyckoff site: $4f$, site symmetry: $\dots 2$

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

Table 7: Wyckoff site: $8g$, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[2]
3	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[3]
4	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[4]
5	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[5]
6	$[-x, -y, z]$	[6]
7	$[y, x, -z]$	[7]
8	$[-y, -x, -z]$	[8]