

Table 1: Wyckoff site: 2a, site symmetry:  $. . 2' / m$

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

Table 2: Wyckoff site: 2b, site symmetry:  $. . 2' / m$

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

Table 3: Wyckoff site: 2c, site symmetry:  $. . 2' / m$

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

Table 4: Wyckoff site: 2d, site symmetry:  $. . 2' / m$

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

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

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

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

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

Table 7: Wyckoff site: 4g, site symmetry:  $\dots m$ 

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

Table 8: Wyckoff site: 4h, site symmetry:  $\dots m$ 

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

Table 9: Wyckoff site: 8i, site symmetry: 1

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