

SG No. 55 D_{2h}^9 $Pbam$ [orthorhombic]

* plus set: $+ [0, 0, 0]$

Table 1: Wyckoff site: 2a, site symmetry: $\dots 2/m$

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

Table 2: Wyckoff site: 2b, site symmetry: $\dots 2/m$

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

Table 3: Wyckoff site: 2c, site symmetry: $\dots 2/m$

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

Table 4: Wyckoff site: 2d, site symmetry: $\dots 2/m$

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

Table 5: Wyckoff site: 4e, site symmetry: $\dots 2$

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

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

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

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

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

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

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

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

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