

SG No. 66 D_{2h}^{20} $Cccm$ [orthorhombic]

* plus set: $+ [0, 0, 0]$, $+ [\frac{1}{2}, \frac{1}{2}, 0]$

Table 1: Wyckoff site: 4a, site symmetry: 222

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

Table 2: Wyckoff site: 4b, site symmetry: 222

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

Table 3: Wyckoff site: 4c, site symmetry: $\dots 2/m$

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

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

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

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

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

Table 6: Wyckoff site: $4\mathbf{f}$, site symmetry: $\dots 2/m$

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

Table 7: Wyckoff site: $8\mathbf{g}$, site symmetry: $2\dots$

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

Table 8: Wyckoff site: $8\mathbf{h}$, site symmetry: $\dots 2$

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

Table 9: Wyckoff site: $8\mathbf{i}$, site symmetry: $\dots 2$

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

Table 10: Wyckoff site: $8\mathbf{j}$, site symmetry: $\dots 2$

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

Table 11: Wyckoff site: $8k$, site symmetry: $\dots 2$

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

Table 12: Wyckoff site: $8l$, site symmetry: $\dots m$

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

Table 13: Wyckoff site: $16m$, site symmetry: 1

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