

SG No. 51 D_{2h}^5 $Pmma$ [orthorhombic]

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

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: **2e**, site symmetry: $mm2$

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

Table 6: Wyckoff site: **2f**, site symmetry: **mm2**

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

Table 7: Wyckoff site: **4g**, site symmetry: **.2.**

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

Table 8: Wyckoff site: **4h**, site symmetry: **.2.**

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

Table 9: Wyckoff site: **4i**, site symmetry: **.m.**

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

Table 10: Wyckoff site: **4j**, site symmetry: **.m.**

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

Table 11: Wyckoff site: $4\mathbf{k}$, site symmetry: $\mathbf{m} . .$

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

Table 12: Wyckoff site: $8\mathbf{l}$, site symmetry: $\mathbf{1}$

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