

SG No. 69 D_{2h}^{23} $Fmmm$ [orthorhombic]

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

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

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

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

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

Table 3: Wyckoff site: 8c, site symmetry: $2/\text{m..}$

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

Table 4: Wyckoff site: 8d, site symmetry: $.2/\text{m.}$

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

Table 5: Wyckoff site: 8e, site symmetry: $..\text{2}/\text{m}$

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

Table 6: Wyckoff site: 8f, site symmetry: 222

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

Table 7: Wyckoff site: 8g, site symmetry: 2mm

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

Table 8: Wyckoff site: 8h, site symmetry: m2m

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

Table 9: Wyckoff site: 8i, site symmetry: mm2

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

Table 10: Wyckoff site: 16j, site symmetry: ..2

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

Table 11: Wyckoff site: 16k, site symmetry: .2.

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

Table 12: Wyckoff site: 161, site symmetry: 2..

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

Table 13: Wyckoff site: 16m, site symmetry: m..

No.	position	mapping
1	$[0, y, z]$	[1,8]
2	$[0, -y, z]$	[2,7]
3	$[0, y, -z]$	[3,6]
4	$[0, -y, -z]$	[4,5]

Table 14: Wyckoff site: 16n, site symmetry: .m.

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

Table 15: Wyckoff site: 16o, site symmetry: ..m

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

Table 16: Wyckoff site: 32p, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[2]
3	$[-x, y, -z]$	[3]
4	$[x, -y, -z]$	[4]

continued ...

Table 16

No.	position	mapping
5	$[-x, -y, -z]$	[5]
6	$[x, y, -z]$	[6]
7	$[x, -y, z]$	[7]
8	$[-x, y, z]$	[8]