

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

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

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:  $2/m..$

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:  $.2/m.$

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:  $..2/m$

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:  $\dots 2$ 

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:  $\dots 2.$ 

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: 16l, 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]