

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

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

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: **4f**, 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: **8g**, 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: **8h**, 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: **8i**, 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: **8j**, 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:  $8\mathbf{k}$ , 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:  $8\mathbf{l}$ , 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:  $16\mathbf{m}$ , 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	$[-x, y, z + \frac{1}{2}]$	$[8]$