

SG No. 55  $D_{2h}^9$   $Pbam$  [ orthorhombic ]

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

Table 1: Wyckoff site: 2a, site symmetry:  $\dots 2/m$

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site: **4f**, site symmetry:  $\bar{3}2$ 

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

Table 7: Wyckoff site: **4g**, site symmetry:  $\bar{3}m$ 

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

Table 8: Wyckoff site: **4h**, site symmetry:  $\bar{3}m$ 

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

Table 9: Wyckoff site: **8i**, site symmetry:  $\bar{1}$ 

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