

SG No. 59  $D_{2h}^{13}$   $Pmmn$  [ orthorhombic ]

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

Table 1: Wyckoff site: 2a, site symmetry:  $mm2$

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

Table 2: Wyckoff site: 2b, site symmetry:  $mm2$

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

Table 3: Wyckoff site: 4c, site symmetry:  $-1$

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

Table 4: Wyckoff site: 4d, site symmetry:  $-1$

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

Table 5: Wyckoff site: 4e, site symmetry:  $m..$

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

Table 6: Wyckoff site:  $4f$ , site symmetry:  $\bar{4}2m$ .

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

Table 7: Wyckoff site:  $8g$ , site symmetry:  $1$ 

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