

SG No. 85  $C_{4h}^3$   $P4/n$  [ tetragonal ]

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

Table 1: Wyckoff site: 2a, site symmetry:  $-4..$

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

Table 2: Wyckoff site: 2b, site symmetry:  $-4..$

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

Table 3: Wyckoff site: 2c, site symmetry:  $4..$

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

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

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

Table 5: Wyckoff site: 4e, 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	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[3, 7]$
4	$[0, \frac{1}{2}, \frac{1}{2}]$	$[4, 8]$

Table 6: Wyckoff site: **4f**, site symmetry: **2**.

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

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	$[\frac{1}{2} - y, x, z]$	[3]
4	$[y, \frac{1}{2} - x, z]$	[4]
5	$[-x, -y, -z]$	[5]
6	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[6]
7	$[y + \frac{1}{2}, -x, -z]$	[7]
8	$[-y, x + \frac{1}{2}, -z]$	[8]