

SG No. 122  $D_{2d}^{12}$   $I\bar{4}2d$  [ tetragonal ]

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

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

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

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

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

Table 3: Wyckoff site: **8c**, site symmetry:  $2..$

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

Table 4: Wyckoff site: **8d**, site symmetry:  $.2.$

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

Table 5: Wyckoff site: **16e**, site symmetry:  $1$

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

*continued ...*

Table 5

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