

SG No. 99 C_{4v}^1 $P4mm$ [tetragonal]

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

Table 1: Wyckoff site: **1a**, site symmetry: **4mm**

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 4, 5, 6, 7, 8]$

Table 2: Wyckoff site: **1b**, site symmetry: **4mm**

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

Table 3: Wyckoff site: **2c**, site symmetry: **2mm**.

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

Table 4: Wyckoff site: **4d**, site symmetry: **. . m**

No.	position	mapping
1	$[x, x, z]$	$[1, 8]$
2	$[-x, -x, z]$	$[2, 7]$
3	$[-x, x, z]$	$[3, 6]$
4	$[x, -x, z]$	$[4, 5]$

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

No.	position	mapping
1	$[x, 0, z]$	$[1, 5]$
2	$[-x, 0, z]$	$[2, 6]$
3	$[0, x, z]$	$[3, 8]$
4	$[0, -x, z]$	$[4, 7]$

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

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

Table 7: Wyckoff site: $8\mathbf{g}$, 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	$[x, -y, z]$	$[5]$
6	$[-x, y, z]$	$[6]$
7	$[-y, -x, z]$	$[7]$
8	$[y, x, z]$	$[8]$