



FOUNDATIONS
ADVANCES

1

2 **Volume 76 (2020)**

3 **Supporting information for article:**

4 **Domain formation and phase transitions in the wurtzite-based**
5 **heterovalent ternaries: a Landau theory analysis**

6 **Paul C. Quayle**

7

8

Setting Transformation

Initial structure

Initial Setting: $Pna2_1$ (33)

```

33
5.8500000000 6.7600000000 5.5800000000 90.0000000000 90.0000000000 90.0000000000
4
Zn      1      4a      0.083500      0.125000      0.000000
N       1      4a      0.083500      0.125000      0.375000
Sn      1      4a     -0.083500      0.375000     -0.500000
N       2      4a     -0.083500      0.375000     -0.125000

```

Final structure

Final Setting: $Pbn2_1$ (33)

```

33 #Pbn21
6.7600 5.8500 5.5800 90.00 90.00 90.00
4
Zn      1      -      0.125000      0.083500      0.000000
N       1      -      0.125000      0.083500     -0.375000
Sn      1      -      0.375000     -0.083500      0.500000
N       2      -      0.375000     -0.083500      0.125000

```

Transformation matrix (P, p): **b,a,-c; 0,0,0**

Matrix form:

$$(\mathbf{P}, \mathbf{p}) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Atoms Data:

AT.	WP	SS	Initial setting Atomic Orbit	Final setting Atomic orbit
Zn1	4a x,y,z	1	(0.083500,0.125000,0.000000) (0.916500,0.875000,0.500000) (0.583500,0.375000,0.000000) (0.416500,0.625000,0.500000)	(0.125000,0.083500,0.000000) (0.875000,0.916500,-0.500000) (0.375000,0.583500,0.000000) (0.625000,0.416500,-0.500000)

N1	4a x,y,z	1	(0.083500,0.125000,0.375000) (0.916500,0.875000,0.875000) (0.583500,0.375000,0.375000) (0.416500,0.625000,0.875000)	(0.125000,0.083500,-0.375000) (0.875000,0.916500,-0.875000) (0.375000,0.583500,-0.375000) (0.625000,0.416500,-0.875000)
Sn1	4a x,y,z	1	(0.916500,0.375000,0.500000) (0.083500,0.625000,0.000000) (0.416500,0.125000,0.500000) (0.583500,0.875000,0.000000)	(0.375000,0.916500,-0.500000) (0.625000,0.083500,0.000000) (0.125000,0.416500,-0.500000) (0.875000,0.583500,0.000000)
N2	4a x,y,z	1	(0.916500,0.375000,0.875000) (0.083500,0.625000,0.375000) (0.416500,0.125000,0.875000) (0.583500,0.875000,0.375000)	(0.375000,0.916500,-0.875000) (0.625000,0.083500,-0.375000) (0.125000,0.416500,-0.875000) (0.875000,0.583500,-0.375000)

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For comments, please mail to
administrador.bcs@ehu.eus

Setting Transformation

Initial structure

Initial Setting: $Pca2_1$ (29)

```

29
5.8500000000 6.7600000000 5.5800000000 90.0000000000 90.0000000000 90.0000000000
4
Zn      1      4a      0.083500      0.875000      0.000000
N       1      4a      0.083500      0.875000      0.375000
Sn      1      4a     -0.083500      0.625000     -0.500000
N       2      4a     -0.083500      0.625000     -0.125000

```

Final structure

Final Setting: $Pbc2_1$ (29)

```

29 #Pbc21
6.7600 5.8500 5.5800 90.00 90.00 90.00
4
Zn      1      -      0.875000      0.083500      0.000000
N       1      -      0.875000      0.083500     -0.375000
Sn      1      -      0.625000     -0.083500      0.500000
N       2      -      0.625000     -0.083500      0.125000

```

Transformation matrix (P, p): **b,a,-c; 0,0,0**

Matrix form:

$$(\mathbf{P}, \mathbf{p}) = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Atoms Data:

AT.	WP	SS	Initial setting Atomic Orbit	Final setting Atomic orbit
Zn1	4a x,y,z	1	(0.083500,0.875000,0.000000) (0.916500,0.125000,0.500000) (0.583500,0.125000,0.000000) (0.416500,0.875000,0.500000)	(0.875000,0.083500,0.000000) (0.125000,0.916500,-0.500000) (0.125000,0.583500,0.000000) (0.875000,0.416500,-0.500000)

N1	4a x,y,z	1	(0.083500,0.875000,0.375000) (0.916500,0.125000,0.875000) (0.583500,0.125000,0.375000) (0.416500,0.875000,0.875000)	(0.875000,0.083500,-0.375000) (0.125000,0.916500,-0.875000) (0.125000,0.583500,-0.375000) (0.875000,0.416500,-0.875000)
Sn1	4a x,y,z	1	(0.916500,0.625000,0.500000) (0.083500,0.375000,0.000000) (0.416500,0.375000,0.500000) (0.583500,0.625000,0.000000)	(0.625000,0.916500,-0.500000) (0.375000,0.083500,0.000000) (0.375000,0.416500,-0.500000) (0.625000,0.583500,0.000000)
N2	4a x,y,z	1	(0.916500,0.625000,0.875000) (0.083500,0.375000,0.375000) (0.416500,0.375000,0.875000) (0.583500,0.625000,0.375000)	(0.625000,0.916500,-0.875000) (0.375000,0.083500,-0.375000) (0.375000,0.416500,-0.875000) (0.625000,0.583500,-0.375000)

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