Cyanogen [$(CN)_2$] Structure: AB_oP16_61_c_c-002

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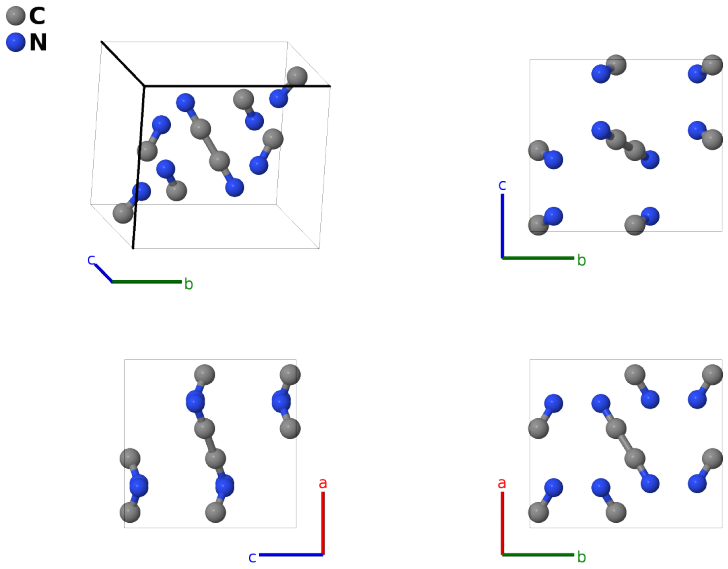
https://aflow.org/p/NEGW

https://aflow.org/p/AB_oP16_61_c_c-002

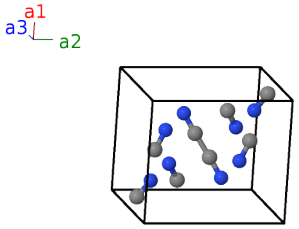


Prototype	CN
AFLOW prototype label	AB_oP16_61_c_c-002
Mineral name	cyanogen
ICSD	15870
Pearson symbol	oP16
Space group number	61
Space group symbol	*Pbca*
AFLOW prototype command	`aflow --proto=AB_oP16_61_c_c-002 --params=`$a, b/a, c/a, x_1, y_1, z_1, x_2, y_2, z_2$

- We use the data for solid cyanogen at −95°C from (Parkes, 1963).
- (Parkes, 1963) give the structure in the *Pcab* setting of space group #61. We rotated this 90° about the y-axis to transform this to the standard *Pbca* setting.
- This structure has the same AFLOW label as B_e, CdSb. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_5}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_6}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_7}$	=	$x_1\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_8}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8c)	C I
$\mathbf{B_9}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_{10}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_{11}}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_{12}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_{13}}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_{14}}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_{15}}$	=	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8c)	N I
$\mathbf{B_{16}}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(8c)	N I

References

[1] A. S. Parkes and R. E. Hughes, *The Crystal Structure of Cyanogen*, Acta Cryst. **16**, 734–736 (1963), doi:10.1107/S0365110X63001924.

Found in

[1] *Crystal structure of Cyanogen*, Wikipedia.