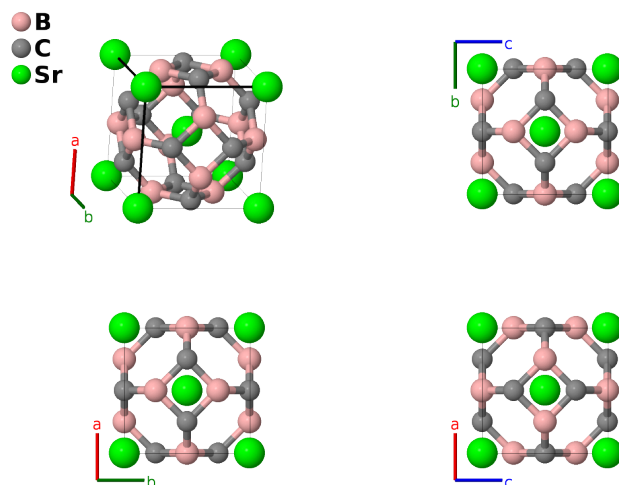


# SrB<sub>3</sub>C<sub>3</sub> Clathrate Structure: A3B3C\_cP14\_223\_c\_d\_a-001

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<https://aflow.org/p/FACW>

[https://aflow.org/p/A3B3C\\_cP14\\_223\\_c\\_d\\_a-001](https://aflow.org/p/A3B3C_cP14_223_c_d_a-001)



Prototype	B <sub>3</sub> C <sub>3</sub> Sr
AFLOW prototype label	A3B3C_cP14_223_c_d_a-001
CCDC	1949948
Pearson symbol	cP14
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	<code>aflow --proto=A3B3C_cP14_223_c_d_a-001 --params=a</code>

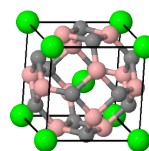
## Simple Cubic primitive vectors

$$\mathbf{a}_1 = a \hat{x}$$

$$\mathbf{a}_2 = a \hat{y}$$

$$\mathbf{a}_3 = a \hat{z}$$

a<sub>1</sub>  
a<sub>2</sub>  
a<sub>3</sub>



## Basis vectors

	Lattice coordinates	=	Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) Sr I
$\mathbf{B}_2$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(2a) Sr I
$\mathbf{B}_3$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$	(6c) B I
$\mathbf{B}_4$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{z}}$	(6c) B I
$\mathbf{B}_5$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_2$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{y}}$	(6c) B I
$\mathbf{B}_6$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_2$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{y}}$	(6c) B I
$\mathbf{B}_7$	=	$\frac{1}{2}\mathbf{a}_2 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{1}{4}a\hat{\mathbf{z}}$	(6c) B I
$\mathbf{B}_8$	=	$\frac{1}{2}\mathbf{a}_2 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{y}} + \frac{3}{4}a\hat{\mathbf{z}}$	(6c) B I
$\mathbf{B}_9$	=	$\frac{1}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	=	$\frac{1}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}}$	(6d) C I
$\mathbf{B}_{10}$	=	$\frac{3}{4}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2$	=	$\frac{3}{4}a\hat{\mathbf{x}} + \frac{1}{2}a\hat{\mathbf{y}}$	(6d) C I
$\mathbf{B}_{11}$	=	$\frac{1}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{1}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(6d) C I
$\mathbf{B}_{12}$	=	$\frac{3}{4}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	=	$\frac{3}{4}a\hat{\mathbf{y}} + \frac{1}{2}a\hat{\mathbf{z}}$	(6d) C I
$\mathbf{B}_{13}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{1}{4}a\hat{\mathbf{z}}$	(6d) C I
$\mathbf{B}_{14}$	=	$\frac{1}{2}\mathbf{a}_1 + \frac{3}{4}\mathbf{a}_3$	=	$\frac{1}{2}a\hat{\mathbf{x}} + \frac{3}{4}a\hat{\mathbf{z}}$	(6d) C I

## References

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