

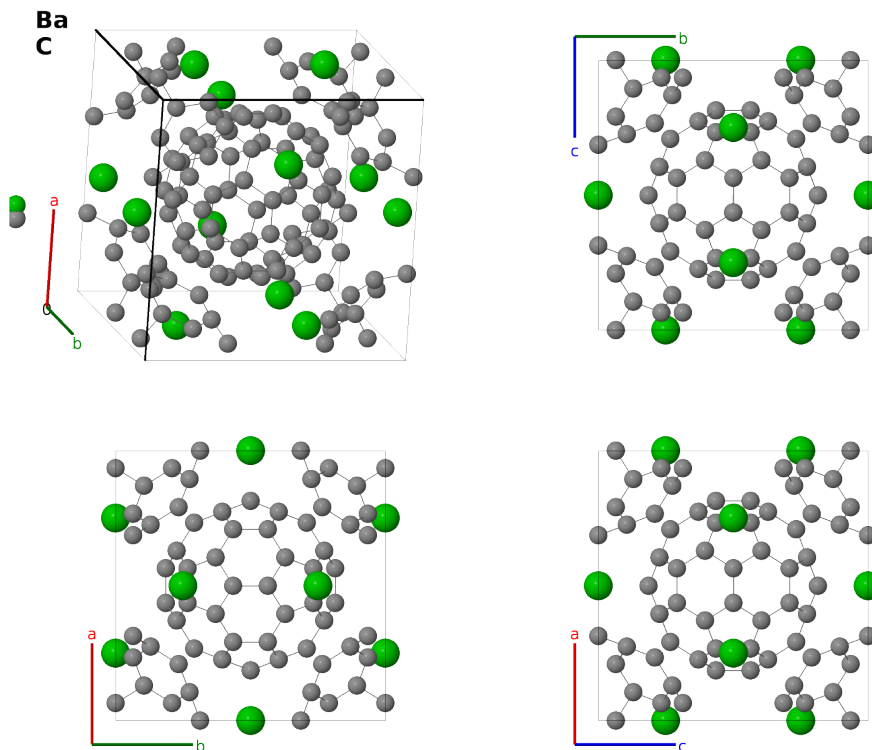
“A15” Fullerene (Ba_3C_{60}) Structure: AB20_cP126_223_c_k2l-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettl, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/HV0S>

https://aflow.org/prototype-encyclopedia/AB20_cP126_223_c_k2l-001



Prototype	Ba_3C_{60}
AFLOW prototype label	AB20_cP126_223_c_k2l-001
ICSD	70063
CCDC	1631887
Pearson symbol	cP126
Space group number	223
Space group symbol	$Pm\bar{3}n$
AFLOW prototype command	<pre>aflow --proto=AB20_cP126_223_c_k2l-001 --params=a, y2, z2, x3, y3, z3, x4, y4, z4</pre>

Other compounds with this structure
 Sr_3C_{60}

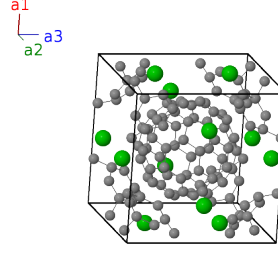
- The barium atoms are on the chromium sites in the $A15$ (Cr_3Si) structure, while the fullerene molecules are centered on the silicon site.

Simple Cubic primitive vectors

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

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

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{4}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$	(6c)	Ba I
$\mathbf{B}_2$	$= \frac{3}{4} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{3}{4}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{z}}$	(6c)	Ba I
$\mathbf{B}_3$	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{4}a \hat{\mathbf{y}}$	(6c)	Ba I
$\mathbf{B}_4$	$= \frac{1}{2} \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{3}{4}a \hat{\mathbf{y}}$	(6c)	Ba I
$\mathbf{B}_5$	$= \frac{1}{2} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{4}a \hat{\mathbf{z}}$	(6c)	Ba I
$\mathbf{B}_6$	$= \frac{1}{2} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{y}} + \frac{3}{4}a \hat{\mathbf{z}}$	(6c)	Ba I
$\mathbf{B}_7$	$= y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_8$	$= -y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{y}} + az_2 \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_9$	$= y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{10}$	$= -y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ay_2 \hat{\mathbf{y}} - az_2 \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{11}$	$= z_2 \mathbf{a}_1 + y_2 \mathbf{a}_3$	$=$	$az_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{12}$	$= z_2 \mathbf{a}_1 - y_2 \mathbf{a}_3$	$=$	$az_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{13}$	$= -z_2 \mathbf{a}_1 + y_2 \mathbf{a}_3$	$=$	$-az_2 \hat{\mathbf{x}} + ay_2 \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{14}$	$= -z_2 \mathbf{a}_1 - y_2 \mathbf{a}_3$	$=$	$-az_2 \hat{\mathbf{x}} - ay_2 \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{15}$	$= y_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$=$	$ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}}$	(24k)	C I
$\mathbf{B}_{16}$	$= -y_2 \mathbf{a}_1 + z_2 \mathbf{a}_2$	$=$	$-ay_2 \hat{\mathbf{x}} + az_2 \hat{\mathbf{y}}$	(24k)	C I
$\mathbf{B}_{17}$	$= y_2 \mathbf{a}_1 - z_2 \mathbf{a}_2$	$=$	$ay_2 \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}}$	(24k)	C I
$\mathbf{B}_{18}$	$= -y_2 \mathbf{a}_1 - z_2 \mathbf{a}_2$	$=$	$-ay_2 \hat{\mathbf{x}} - az_2 \hat{\mathbf{y}}$	(24k)	C I
$\mathbf{B}_{19}$	$= (y_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - a(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{20}$	$= -(y_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - a(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{21}$	$= (y_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$a(y_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{22}$	$= -(y_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(y_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{23}$	$= \frac{1}{2} \mathbf{a}_1 + (z_2 + \frac{1}{2}) \mathbf{a}_2 - (y_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{y}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{24}$	$= \frac{1}{2} \mathbf{a}_1 + (z_2 + \frac{1}{2}) \mathbf{a}_2 + (y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + a(z_2 + \frac{1}{2}) \hat{\mathbf{y}} + a(y_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	C I
$\mathbf{B}_{25}$	$= \frac{1}{2} \mathbf{a}_1 - (z_2 - \frac{1}{2}) \mathbf{a}_2 - (y_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - a(z_2 - \frac{1}{2}) \hat{\mathbf{y}} - a(y_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	C I

[illegible]

[illegible]

[illegible]

$$\begin{aligned}
\mathbf{B}_{118} &= \begin{pmatrix} (y_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2 - \\ (z_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \begin{pmatrix} (y_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{y}} - a (z_4 - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (48l) & \text{C III} \\
\mathbf{B}_{119} &= \begin{pmatrix} -(x_4 - \frac{1}{2}) \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2 + \\ (y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} - a (z_4 - \frac{1}{2}) \hat{\mathbf{y}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (48l) & \text{C III} \\
\mathbf{B}_{120} &= \begin{pmatrix} (x_4 + \frac{1}{2}) \mathbf{a}_1 - (z_4 - \frac{1}{2}) \mathbf{a}_2 - \\ (y_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \begin{pmatrix} (x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (z_4 - \frac{1}{2}) \hat{\mathbf{y}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (48l) & \text{C III} \\
\mathbf{B}_{121} &= \begin{pmatrix} (x_4 + \frac{1}{2}) \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (y_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \begin{pmatrix} (x_4 + \frac{1}{2}) \hat{\mathbf{x}} + a (z_4 + \frac{1}{2}) \hat{\mathbf{y}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (48l) & \text{C III} \\
\mathbf{B}_{122} &= \begin{pmatrix} -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (z_4 + \frac{1}{2}) \mathbf{a}_2 - \\ (y_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -a (x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (z_4 + \frac{1}{2}) \hat{\mathbf{y}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (48l) & \text{C III} \\
\mathbf{B}_{123} &= \begin{pmatrix} -(z_4 - \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -a (z_4 - \frac{1}{2}) \hat{\mathbf{x}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{y}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (48l) & \text{C III} \\
\mathbf{B}_{124} &= \begin{pmatrix} -(z_4 - \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - \\ (x_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = \begin{pmatrix} -a (z_4 - \frac{1}{2}) \hat{\mathbf{x}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{y}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (48l) & \text{C III} \\
\mathbf{B}_{125} &= \begin{pmatrix} (z_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - \\ (x_4 - \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \begin{pmatrix} (z_4 + \frac{1}{2}) \hat{\mathbf{x}} - a (y_4 - \frac{1}{2}) \hat{\mathbf{y}} - a (x_4 - \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (48l) & \text{C III} \\
\mathbf{B}_{126} &= \begin{pmatrix} (z_4 + \frac{1}{2}) \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 + \\ (x_4 + \frac{1}{2}) \mathbf{a}_3 \end{pmatrix} = a \begin{pmatrix} (z_4 + \frac{1}{2}) \hat{\mathbf{x}} + a (y_4 + \frac{1}{2}) \hat{\mathbf{y}} + a (x_4 + \frac{1}{2}) \hat{\mathbf{z}} \end{pmatrix} & (48l) & \text{C III}
\end{aligned}$$

References

- [1] A. R. Kortan, N. Kopylov, R. M. Fleming, O. Zhou, F. A. Thiel, R. C. Haddon, and K. M. Rabe, *Novel A15 phase in barium-doped fullerite*, Phys. Rev. B **47**, 13070–13074 (R) (1993), doi:10.1103/PhysRevB.47.13070.

Found in

- [1] M. C. Böhm, T. Schedel-Niedrig, H. Werner, R. Schlögl, and J. Schulte, *Solid state electronic structure of Ba_3C_{60} – A model approach*, Solid State Commun. **98**, 463–468 (1996), doi:10.1016/0038-1098(95)00752-0.

First cited in

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.