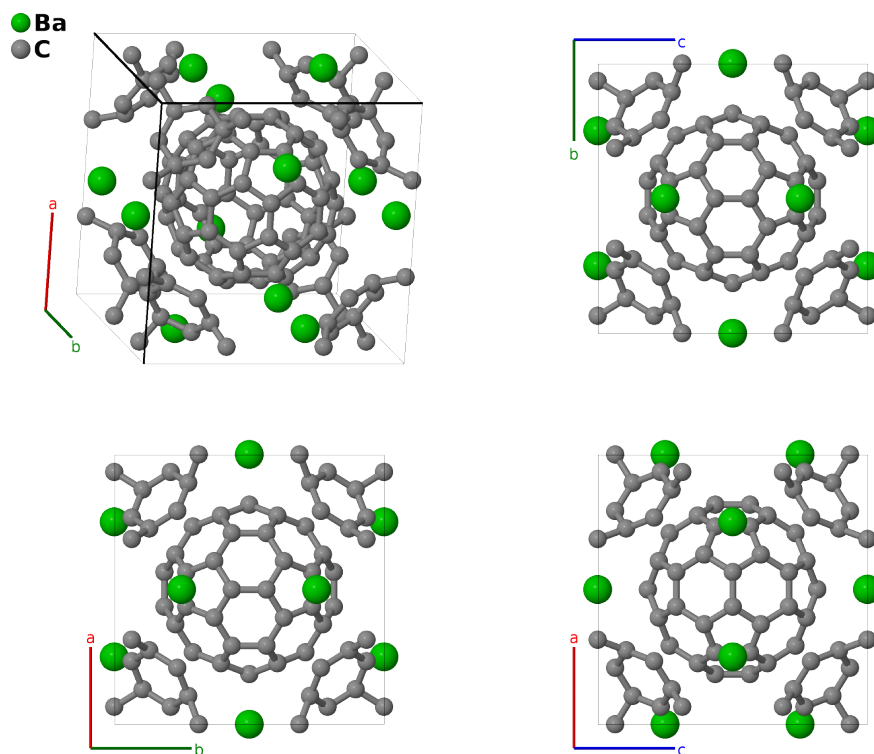


“A15” Fullerene (Ba_3C_{60}) Structure: AB20_cP126_223_c_k2l-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

<https://aflow.org/p/HV0S>

https://aflow.org/p/AB20_cP126_223_c_k2l-001



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

Other compounds with this structure

Sr_3C_{60}

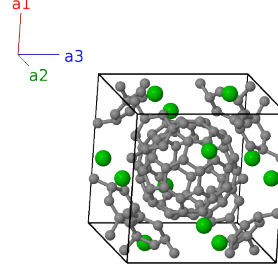
- The barium atoms are on the chromium sites in the A15 (Cr_3Si) structure, while the fullerene molecules are centered on the silicon site.

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
\mathbf{B}_{26}	$= \frac{1}{2} \mathbf{a}_1 - (z_2 - \frac{1}{2}) \mathbf{a}_2 + (y_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - a (z_2 - \frac{1}{2}) \hat{\mathbf{y}} + a (y_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(24k)	C I
\mathbf{B}_{27}	$= (z_2 + \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a (z_2 + \frac{1}{2}) \hat{\mathbf{x}} + a (y_2 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	(24k)	C I

$$\begin{aligned}
\mathbf{B}_{119} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(481) & \text{C III} \\
\mathbf{B}_{120} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(z_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(481) & \text{C III} \\
\mathbf{B}_{121} &= \left(x_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_2 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(481) & \text{C III} \\
\mathbf{B}_{122} &= -\left(x_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(z_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(481) & \text{C III} \\
\mathbf{B}_{123} &= -\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(481) & \text{C III} \\
\mathbf{B}_{124} &= -\left(z_4 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3 &= -a\left(z_4 - \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(481) & \text{C III} \\
\mathbf{B}_{125} &= \left(z_4 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right) \mathbf{a}_2 - \left(x_4 - \frac{1}{2}\right) \mathbf{a}_3 &= a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{x}} - a\left(y_4 - \frac{1}{2}\right) \hat{\mathbf{y}} - a\left(x_4 - \frac{1}{2}\right) \hat{\mathbf{z}} &(481) & \text{C III} \\
\mathbf{B}_{126} &= \left(z_4 + \frac{1}{2}\right) \mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right) \mathbf{a}_2 + \left(x_4 + \frac{1}{2}\right) \mathbf{a}_3 &= a\left(z_4 + \frac{1}{2}\right) \hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right) \hat{\mathbf{y}} + a\left(x_4 + \frac{1}{2}\right) \hat{\mathbf{z}} &(481) & \text{C III}
\end{aligned}$$

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