

SACADA Database Code: 91

Topology: [baa](#) 

of independent nodes (IN): 2
Transitivity: [2221]
Space Group: I-42d
Pearson: tI12
Coordination Number (CN): 4

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
baa (SACADA #91)		3.438		1.075	399.6	396.2	70.8	SACADA ¹
iceXII-carbon		3.38	2.01		373.5		85.5	doi: 10.1021/jp5080048 

Elasticity tensor (kBar)¹

10523.6687	1553.8655	1280.6302	-0.0000	-0.0000	0.0000
1553.8655	10523.6687	1280.6302	0.0000	0.0000	-0.0000
1280.6302	1280.6302	7264.6839	-0.0000	-0.0000	0.0000
-0.0000	0.0000	-0.0000	4574.8334	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	3676.6861	0.0000
0.0000	-0.0000	0.0000	-0.0000	-0.0000	3676.6858

¹ We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) to calculate the total energy and properties of carbon allotropes.

DFT calculations

We apply the density functional theory (DFT) approach by using the Vienna Ab Initio Simulation Package (VASP) package [6] to calculate the total energy of carbon allotropes. The Generalized Gradient Approximation [7] (GGA) for exchange-correlational functional is used everywhere. The energy cutoff set to 600 eV. Fully automatic Γ -centered k-points mesh with a reciprocal-space resolution of $2\pi \times 0.025 \text{ \AA}^{-1}$ is applied. We used tetrahedron method with Blöchl corrections to perform the k-point integration. The convergence thresholds are set at 10^{-6} eV for energy and 10^{-5} eV $\text{\AA}^{-1}$ for ionic forces. Polycrystalline elastic moduli — the bulk modulus, the shear modulus, Young’s modulus, and the Poisson’s ratio ν — have been calculated within the Voigt-Reuss-Hill [8] approximation. The Vicker’s hardness H_v has been estimated according to Oganov’s model [9].