

## SACADA Database Code: 447

Topology: [cfe](#)

# of independent nodes (IN): 3

Transitivity: [3443]

Space Group: R-3m

Pearson: hR18

Coordination Number (CN): 4

Year: 2017

## Data

Name	Pressure, GPa	Density, g/cm <sup>3</sup>	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
cfe (SACADA #447)		3.545		0.579	450.1	531.8	100.7	SACADA <sup>1</sup>
G153								doi: <a href="https://doi.org/10.1002/cphc.201700151">10.1002/cphc.201700151</a>

### Elasticity tensor (kBar)<sup>1</sup>

12045.6867	1067.8323	321.4576	0.2052	179.0637	2.0258
1067.8323	12047.2056	319.4254	1.2509	-180.0046	-0.6167
321.4576	319.4254	13002.1429	-1.7947	0.7022	0.3707
0.2052	1.2509	-1.7947	5484.9784	-1.0117	180.2015
179.0637	-180.0046	0.7022	-1.0117	4735.6309	2.6707
2.0258	-0.6167	0.3707	180.2015	2.6707	4739.8523

<sup>1</sup> 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  $\Gamma$ -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  $\nu$  — 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].