

SACADA Database Code: 204

Topology: ajk3

of independent nodes (IN): 4
Transitivity: [4432]
Space Group: I-43m
Pearson: cI46
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ajk3 (SACADA #204)		3.206		0.798	399.5	424.2	78.2	SACADA ¹
clathrates VIII		3.20			421			doi: 10.1021/jp205676p ☞
clathrates VIII		3.20	7.3					doi: 10.1021/ic102178d ☞

Elasticity tensor (kBar)¹

10031.9549	975.7748	975.7748	0.0000	-0.0000	0.0000
975.7748	10031.9549	975.7748	-0.0000	0.0000	-0.0000
975.7748	975.7748	10031.9549	-0.0000	0.0000	-0.0000
0.0000	-0.0000	-0.0000	4062.2083	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	4062.2083	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	-0.0000	4062.2083

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].

