

SACADA Database Code: 352

Topology: ajk7

of independent nodes (IN): 25

Transitivity: [(25)(38)(26)9]

Space Group: P63/mmc

Pearson: hP272

Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ajk7 (SACADA #352)		3.063		0.673	370.5	415.1	77.8	SACADA ¹
Clathrate II-8H								doi: 10.1002/cphc.201300133 

Elasticity tensor (kBar)¹

9231.4654	954.6410	909.5716	-0.0000	0.0000	-0.0000
954.6410	9231.4654	909.5716	-0.0000	0.0000	0.0000
909.5716	909.5716	9332.1875	-0.0000	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	4138.4122	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	4137.6189	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	0.0000	4137.6189

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].