**SACADA Database Code: 332**

Topology: ajk10

# of independent nodes (IN): 13
Transitivity: [(13)(20)(14)5]
Space Group: P63/mmc
Pearson: hP136
Coordination Number (CN): 4

Year: 2011

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| ajk10 (SACADA #332) | | 3.063 | | 0.671 | 371.1 | 416.3 | 78.0 | SACADA[1] |
| clathrates II-4H | | 3.05 | | | 404 | | | doi: 10.1021/jp205676p |
| clathrates II-4H | | 3.05 | 6.0 | | | | | doi: 10.1021/ic102178d |
| clathrates II-4H | | | | | | | | doi: 10.1002/cphc.201300133 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 9249.4135 | 949.9215 | 920.2092 | 1.0935 | 0.0062 | -0.7026 |
| 949.9215 | 9249.1778 | 919.3599 | 1.9622 | 1.1314 | -0.6669 |
| 920.2092 | 919.3599 | 9324.1293 | 3.0983 | 0.1448 | 2.4009 |
| 1.0935 | 1.9622 | 3.0983 | 4155.9077 | 1.3041 | 0.2906 |
| 0.0062 | 1.1314 | 0.1448 | 1.3041 | 4157.9703 | 0.7296 |
| -0.7026 | -0.6669 | 2.4009 | 0.2906 | 0.7296 | 4159.1253 |

[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 $2\pi \times 0.025$ Å$^{-1}$ 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 Å$^{-1}$ 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].