SACADA Database Code: 242

Topology: zra-d

# of independent nodes (IN): 5
Transitivity: [5873]
Space Group: P6/mmm
Pearson: hP40
Coordination Number (CN): 4

Year: 1995

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
zra-d (SACADA #242)		3.058		0.723	373.5	421.1	79.0	SACADA[1]
hex-C40								doi: 10.1016/0009-2614(95)00946-2
hex-C40								doi: 10.1007/BF02451606
hex-C40								nonelink
Clathrate IV								link
hex-C40								doi: 10.1103/PhysRevB.61.12689
hex-C40								doi: 10.1016/j.crci.2009.05.004
hex-C40								doi: 10.1063/1.3359682
Clathrate IV								doi: 10.1021/ic102178d
Clathrate IV		3.05			394			doi: 10.1021/jp205676p
KV		3.03	3.70		357.8		81.7	doi: 10.1063/1.4802002
hex-C40								doi: 10.1007/978-94-007-6371-5_4

Elasticity tensor (kBar)[1]

9361.8358	1021.3579	961.6814	0.0000	-0.0000	0.0000
1021.3579	9361.8358	961.6814	0.0000	0.0000	0.0000
961.6814	961.6814	9001.8485	0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	4170.2390	-0.0000	-0.0000
-0.0000	0.0000	-0.0000	-0.0000	4316.0559	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	4316.0559

[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].