SACADA Database Code: 18

Topology: ths (Allotrope with "sp" atoms)

# of independent nodes (IN): 1
Transitivity: [1211]
Space Group: C2/c
Pearson: mS16
Coordination Number (CN): 2, 3 (1:1)

Year: 1993

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ths (SACADA #18)		1.865		1.338	107.2	54.9	7.0	SACADA[1]
Trans hinged polydiacetylene		1.789						doi: 10.1038/365735a0

Elasticity tensor (kBar)[1]

6912.1253	1189.8488	1663.4342	0.0000	0.0000	879.6429
1189.8488	341.1437	461.3599	0.0000	0.0000	69.0629
1663.4342	461.3599	3688.8908	-0.0000	0.0000	-159.9657
0.0000	0.0000	-0.0000	987.9858	88.5887	0.0000
-0.0000	0.0000	0.0000	88.5887	184.5458	0.0000
879.6429	69.0629	-159.9657	0.0000	0.0000	624.4978

[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].