SACADA Database Code: 212

Topology: ton

# of independent nodes (IN): 4
Transitivity: [4653]
Space Group: Cmcm
Pearson: oS24
Coordination Number (CN): 4

Year: 1993

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
ton (SACADA #212)		3.086		0.879	359.8	369.1	67.1	SACADA[1]
C-TON			3.28					doi: 10.1002/anie.199307011

Elasticity tensor (kBar)[1]

7631.8406	2227.5880	478.2344	-0.0000	0.0000	0.0000
2227.5880	7711.3783	833.9195	0.0000	-0.0000	0.0000
478.2344	833.9195	9985.2566	0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	3598.5512	0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	4318.3330	-0.0000
0.0000	0.0000	0.0000	0.0000	-0.0000	3581.6937

[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].