SACADA Database Code: 106

Topology: tna

# of independent nodes (IN): 2
Transitivity: [2332]
Space Group: R32
Pearson: hR18
Coordination Number (CN): 3

Year: 2001

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
tna (SACADA #106)		1.729		1.800	-	-	-	SACADA[1]
6(3)2-27a		1.77						doi: 10.1016/S0009-2614(01)00126-9

Elasticity tensor (kBar)[1]

1192.1066	3266.4883	1091.9051	8.2403	-64.3665	-3.0605
3266.4883	1212.1128	1080.4862	5.5345	49.0606	-1.7452
1091.9051	1080.4862	3127.4080	12.1471	-5.3937	-0.5940
8.2403	5.5345	12.1471	-1029.5995	-11.6837	-43.1467
-64.3665	49.0606	-5.3937	-11.6837	-76.5615	-0.4450
-3.0605	-1.7452	-0.5940	-43.1467	-0.4450	-73.2767

[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].