SACADA Database Code: 74

Topology: can

# of independent nodes (IN): 1
Transitivity: [1342]
Space Group: P63/mmc
Pearson: hP12
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
12-hexa(3,3)can (SACADA #74)		2.924		0.435	343.3	319.0	54.4	SACADA[1]
tubulane								doi: 10.1016/0009-2614(93)80059-X
TA2								doi: 10.1134/s1063776111060173
TA2	35							link
3D (3,3)-II					345.6	324.3	85.5	doi: 10.1038/srep01331
α-C		1.50	2.28		330		73.1	doi: 10.1016/j.physleta.2015.06.037

Elasticity tensor (kBar)[1]

7626.9522	1840.1969	671.7928	0.0025	0.0000	-0.0000
1840.1969	7626.9579	671.7930	0.0025	-0.0000	0.0000
671.7928	671.7930	9287.7638	0.0002	-0.0000	0.0000
0.0025	0.0025	0.0002	2893.3791	0.0000	-0.0000
0.0000	-0.0000	-0.0000	0.0000	3051.3465	0.0010
-0.0000	0.0000	0.0000	-0.0000	0.0010	3051.3454

[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].