SACADA Database Code: 75

Topology: atn

# of independent nodes (IN): 1
Transitivity: [1342]
Space Group: I4/mmm
Pearson: tI16
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
16-tetra(2,2)atn (SACADA #75)		2.968		0.502	349.3	279.6	39.4	SACADA[1]
tubulane								doi: 10.1016/0009-2614(93)80059-X
3D (2,2)-I								doi: 10.1088/0953-8984/16/49/023
TA1								doi: 10.1134/s1063776111060173
TA1								link
3D (2,2)-I					371.1	289.2	88.1	doi: 10.1038/srep01331
bct C_8	16-35		1.66					doi: 10.1016/j.carbon.2017.05.011

Elasticity tensor (kBar)[1]

8037.8444	2228.4807	261.6970	1.2724	2.0448	0.0671
2228.4807	7976.0988	296.4572	6.0528	0.7435	-0.5986
261.6970	296.4572	9851.4848	7.5183	-0.0917	-0.4004
1.2724	6.0528	7.5183	1181.8920	2.6362	0.3708
2.0448	0.7435	-0.0917	2.6362	3311.1094	-0.6729
0.0671	-0.5986	-0.4004	0.3708	-0.6729	3304.3701

[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].