

SACADA Database Code: 23

Topology: [eta](#) 

of independent nodes (IN): 1
Transitivity: [1221]
Space Group: P6222
Pearson: hP6
Coordination Number (CN): 3

Year: 1981

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
eta (SACADA #23)		2.384		1.285	253.9	49.5	8.0	SACADA ¹
								link 
Structure IV-V								doi: 10.1007/bf00750899 
C1(32)-C1(32)								doi: 10.1070/RC1984v053n07ABEH003084 
C1(32)-C1(32)								doi: 10.1007/bf00749588 
C1(31)								doi: 10.1007/bf00752165 
6(3)6-11		2.42						doi: 10.1016/S0009-2614(01)00126-9 
cH6					272			doi: 10.1038/srep03077 

Elasticity tensor (kBar)¹

8489.4531	1447.5431	1451.4449	0.6195	0.4250	4.9307
1447.5431	2626.6699	2420.9906	6.9538	-1.9645	0.7303
1451.4449	2420.9906	2589.1160	-2.4886	3.6372	2.2809
0.6195	6.9538	-2.4886	542.1153	3.0364	6.1319
0.4250	-1.9645	3.6372	3.0364	94.2820	2.5519
4.9307	0.7303	2.2809	6.1319	2.5519	534.2902

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 $2\pi \times 0.025 \text{ \AA}^{-1}$ 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 $\text{\AA}^{-1}$ 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].