SACADA Database Code: 24

Topology: etb

# of independent nodes (IN): 1
Transitivity: [1221]
Space Group: R-3m
Pearson: hR18
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
etb (SACADA #24)		2.277		1.085	243.8	57.6	9.2	SACADA[1]
								link
Structure VI								doi: 10.1007/bf00750899
								doi: 10.1070/RC1984v053n07ABEH003084
								doi: 10.1007/bf00749588
cR6		2.26	2.79		276			doi: 10.1103/PhysRevB.57.R661
6(3)2-22b		2.31						doi: 10.1016/S0009-2614(01)00126-9
cR6			2.93		262			doi: 10.1038/srep03077
cR6								doi: 10.1038/srep04339
cR6			2.95		268			doi: 10.1103/PhysRevLett.116.195501

Elasticity tensor (kBar)[1]

2622.6702	1972.8230	2101.2535	25.1254	-718.5814	-0.3315
1972.8230	2619.0848	2110.0115	-14.1216	704.5670	4.6369
2101.2535	2110.0115	5686.6318	-3.1862	8.0419	-2.5572
25.1254	-14.1216	-3.1862	317.6783	-15.4451	-701.9103
-718.5814	704.5670	8.0419	-15.4451	1750.1113	6.9908
-0.3315	4.6369	-2.5572	-701.9103	6.9908	1742.6620

[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].