SACADA Database Code: 279

Topology: 4^7T4

# of independent nodes (IN): 7
Transitivity: [7(12)(10)3]
Space Group: Immm
Pearson: oI56
Coordination Number (CN): 4

Year: 2010

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^7T4 (SACADA #279)		2.973		0.829	354.8	368.9	67.5	SACADA[1]
bco-C28			3.3		341			link
bco-C28								doi: 10.1007/978-94-007-6371-5_4

Elasticity tensor (kBar)[1]

9717.8684	714.8634	788.8970	-0.0000	-0.0000	0.0000
714.8634	8628.2609	1116.3685	0.0000	0.0000	0.0000
788.8970	1116.3685	8369.9108	-0.0000	0.0000	0.0000
0.0000	0.0000	0.0000	3652.1452	-0.0000	-0.0000
-0.0000	0.0000	0.0000	-0.0000	3135.3150	0.0000
-0.0000	-0.0000	0.0000	-0.0000	0.0000	3724.2594

[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].