SACADA Database Code: 12

Topology: lcv

# of independent nodes (IN): 1
Transitivity: [1121]
Space Group: I4132
Pearson: cI12
Coordination Number (CN): 4

Year: 2014

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
lcv (SACADA #12)		2.102		2.025	217.1	50.0	8.0	SACADA[1]
K6 carbon		2.169	Metal		228	52		doi: 10.1063/1.4864109
Tri-carbon			Metal					doi: 10.1088/0953-8984/26/23/235402
K6 carbon		2.101			226	61		doi: 10.1021/acs.cgd.5b01490

Elasticity tensor (kBar)[1]

3294.0286	1609.7379	1609.7379	0.0000	-0.0000	0.0000
1609.7379	3294.0286	1609.7379	0.0000	-0.0000	-0.0000
1609.7379	1609.7379	3294.0286	-0.0000	0.0000	0.0000
0.0000	0.0000	-0.0000	346.5165	0.0000	-0.0000
-0.0000	-0.0000	0.0000	0.0000	346.5165	-0.0000
-0.0000	-0.0000	0.0000	-0.0000	-0.0000	346.5165

[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].