SACADA Database Code: 100

Topology: kea

# of independent nodes (IN): 2
Transitivity: [2321]
Space Group: P43212
Pearson: tP12
Coordination Number (CN): 4

Year: 1987

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
kea (SACADA #100)		3.594		1.429	417.2	501.9	95.3	SACADA[1]
st12			5.4		396		88.3	doi: 10.1103/PhysRevB.35.9559
tP12-carbon								doi: 10.1103/PhysRevB.83.193410
tP12-carbon		3.53	4.96		393.4		87.7	link
tP12-carbon								doi: 10.3103/s1063457613010012
iceIII-carbon								doi: 10.1021/jp5080048
st12					395			doi: 10.1103/PhysRevB.91.214104
st12		3.536			379			doi: 10.1103/PhysRevB.94.174102

Elasticity tensor (kBar)[1]

12077.0740	493.8352	897.5580	-0.0000	0.0000	-0.0000
493.8352	12077.0740	897.5580	0.0000	-0.0000	0.0000
897.5580	897.5580	9070.0606	-0.0000	-0.0000	0.0000
0.0000	0.0000	0.0000	5144.5416	0.0000	-0.0000
0.0000	0.0000	-0.0000	0.0000	4878.8926	-0.0000
-0.0000	0.0000	0.0000	-0.0000	-0.0000	4878.8923

[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].