SACADA Database Code: 67

Topology: sra

# of independent nodes (IN): 1
Transitivity: [1331]
Space Group: Imma
Pearson: oI8
Coordination Number (CN): 4

Year: 1993

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
sra (SACADA #67)		3.056		0.393	364.2	293.1	41.7	SACADA[1]
8-tetra(3,3)tubulane		3.179			312			doi: 10.1016/0009-2614(93)80059-X
E		3.031	2.8		324.7			doi: 10.1103/PhysRevB.70.045101
LA6								doi: 10.1134/s1063776111060173
LA6								link
Imma C	13.4	3.13	2.68		367	301	76.2	doi: 10.1016/j.diamond.2014.01.012

Elasticity tensor (kBar)[1]

7810.5548	3469.0675	341.9670	0.0000	-0.0000	-0.0000
3469.0675	5295.6299	1357.4805	-0.0000	0.0000	0.0000
341.9670	1357.4805	9559.6395	0.0000	-0.0000	0.0000
0.0000	-0.0000	0.0000	3662.3545	0.0000	0.0000
-0.0000	0.0000	-0.0000	0.0000	2776.2249	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	3619.7889

[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].