SACADA Database Code: 201

Topology: 3^2,4T207

# of independent nodes (IN): 3
Transitivity: -
Space Group: R-3m
Pearson: hR54
Coordination Number (CN): 3, 4 (2:1)

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
3^2,4T207 (SACADA #201)		2.394		0.900	268.2	185.1	21.5	SACADA[1]
Tri-C54	0-20	2.442	1.55		270.1	195.1	26.6	doi: 10.1016/j.carbon.2015.05.027

Elasticity tensor (kBar)[1]

4360.9649	2080.5956	622.3589	-0.0000	106.8656	0.0000
2080.5956	4360.9649	622.3589	0.0000	-106.8656	-0.0000
622.3589	622.3589	9307.0482	0.0000	0.0000	0.0000
-0.0000	0.0000	-0.0000	1140.1846	-0.0000	106.8656
106.8656	-106.8656	-0.0000	0.0000	2076.3346	0.0000
-0.0000	-0.0000	0.0000	106.8656	-0.0000	2076.3346

[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].