SACADA Database Code: 219

Topology: $3,4^3T71$

# of independent nodes (IN): 4
Transitivity: [4753]
Space Group: C2/m
Pearson: mS16
Coordination Number (CN): 3, 4 (1:3)

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3,4^3T71$ (SACADA #219)		2.910		0.224	348.2	268.6	35.7	SACADA[1]
m-C_8	60		Semimetal					doi: 10.1038/am.2017.26

Elasticity tensor (kBar)[1]

7717.2709	407.6869	621.8808	-0.0000	-0.0000	209.2992
407.6869	10849.5398	1007.4672	-0.0000	-0.0000	75.3599
621.8808	1007.4672	9057.7926	0.0000	0.0000	911.0604
-0.0000	-0.0000	0.0000	3108.5698	516.5111	-0.0000
-0.0000	-0.0000	0.0000	516.5111	3551.6194	-0.0000
209.2992	75.3599	911.0604	-0.0000	-0.0000	818.1318

[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].