

SACADA Database Code: 502

Topology: 4⁷T31

of independent nodes (IN): 7
Transitivity: [7(15)(15)6]
Space Group: P-1
Pearson: aP14
Coordination Number (CN): 4

Year: 2017

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4 ⁷ T31 (SACADA #502)		3.366		1.075	382.5	414.0	76.8	SACADA ¹
G215								doi: 10.1002/cphc.201700151 ✉

Elasticity tensor (kBar)¹

9560.6690	1032.2805	1198.5912	-161.2701	-71.1383	-116.1910
1032.2805	8456.0114	1500.8260	-488.8963	369.9736	-101.6549
1198.5912	1500.8260	8997.1992	303.0342	194.9372	-104.3690
-161.2701	-488.8963	303.0342	4257.4260	-261.2042	196.3184
-71.1383	369.9736	194.9372	-261.2042	4449.4187	-106.4184
-116.1910	-101.6549	-104.3690	196.3184	-106.4184	4314.5452

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 $2\pi \times 0.025 \text{ \AA}^{-1}$ 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 $\text{\AA}^{-1}$ 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].