

SACADA Database Code: 271

Topology: $3^4,4^2T38$

of independent nodes (IN): 6

Transitivity: -

Space Group: Cmc₂m

Pearson: oS72

Coordination Number (CN): 3, 4 (2:1)

Year: 2015

Data

Name	Pressure, GPa	Density, g/cm ³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^4,4^2T38$ (SACADA #271)		2.218		0.733	255.2	196.3	26.0	SACADA ¹
Orth-C72	0-20	2.262	1.74		257.9	202.0	29.9	doi: 10.1016/j.carbon.2015.05.027 

Elasticity tensor (kBar)¹

4320.3126	1713.2991	622.6558	-0.0000	0.0000	-0.0000
1713.2991	4112.6082	894.9530	0.0000	-0.0000	0.0000
622.6558	894.9530	8681.8325	0.0000	0.0000	-0.0000
-0.0000	0.0000	0.0000	1358.2513	0.0000	-0.0000
0.0000	0.0000	-0.0000	0.0000	2183.5954	-0.0000
-0.0000	0.0000	-0.0000	0.0000	-0.0000	2329.3432

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].