SACADA Database Code: 274

Topology: 4^7T3

# of independent nodes (IN): 7
Transitivity: [7(10)(10)7]
Space Group: P2221
Pearson: oP18
Coordination Number (CN): 4

Year: 2013

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
4^7T3 (SACADA #274)		3.424		0.697	429.0	470.5	87.7	SACADA[1]
P2221	0-100	3.375			409	469	85.9	doi: 10.1063/1.4794424
P-carbon								doi: 10.1088/0253-6102/64/2/237
P2221								doi: 10.1007/s10853-015-9266-8

Elasticity tensor (kBar)[1]

9673.8299	1333.0188	1631.3671	0.0000	0.0000	-0.0000
1333.0188	10925.8465	1235.5813	-0.0000	-0.0000	0.0000
1631.3671	1235.5813	9639.7805	0.0000	-0.0000	-0.0000
0.0000	0.0000	0.0000	4369.6976	-0.0000	-0.0000
0.0000	-0.0000	-0.0000	-0.0000	5332.3828	-0.0000
-0.0000	0.0000	0.0000	-0.0000	0.0000	5291.0808

[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].