SACADA Database Code: 11

Topology: qtz

# of independent nodes (IN): 1
Transitivity: [1121]
Space Group: P6222
Pearson: hP3
Coordination Number (CN): 4

Year: 2011

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
qtz (SACADA #11)		3.690		1.647	447.0	556.6	106.1	SACADA[1]
hP3			2.0		432.7		87.6	doi: 10.1103/PhysRevB.83.193410
hP3								link
hP3								doi: 10.3103/s1063457613010012
qtz								doi: 10.1524/zkri.2013.1620
cintet					428			doi: 10.1103/PhysRevB.91.214104

Elasticity tensor (kBar)[1]

12008.7124	857.1308	705.3271	0.0000	-0.0000	-0.0000
857.1308	12008.7124	705.3271	0.0000	0.0000	0.0000
705.3271	705.3271	11688.6951	0.0000	-0.0000	-0.0000
0.0000	0.0000	0.0000	5575.7908	0.0000	0.0000
-0.0000	0.0000	-0.0000	0.0000	5553.7364	0.0000
-0.0000	0.0000	-0.0000	0.0000	0.0000	5553.7364

[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].