SACADA Database Code: 206

Topology: $3^2,4^2$T201

# of independent nodes (IN): 4
Transitivity: [4454]
Space Group: P-6m2
Pearson: hP10
Coordination Number (CN): 3, 4 (2:3)

Year: 2010

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
$3^2,4^2$T201 (SACADA #206)		3.120		1.234	368.0	296.2	42.1	SACADA[1]
trigohexagonite		3.178	Metal					doi: 10.1007/s10910-010-9713-3

Elasticity tensor (kBar)[1]

9274.4599	1732.7111	962.5893	12.4508	-1.0490	0.8813
1732.7111	9284.7551	960.6647	11.4866	2.8978	0.4794
962.5893	960.6647	7531.9864	-2.0263	1.3077	-0.6259
12.4508	11.4866	-2.0263	3764.5582	0.2173	2.1223
-1.0490	2.8978	1.3077	0.2173	2096.6366	-2.8514
0.8813	0.4794	-0.6259	2.1223	-2.8514	2088.0566

[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].