SACADA Database Code: 95

Topology: tfi

# of independent nodes (IN): 2
Transitivity: [2232]
Space Group: P42/mmc
Pearson: tP6
Coordination Number (CN): 3, 4 (2:1)

Year: 1994

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
tfi (SACADA #95)		3.004		0.500	341.5	152.9	21.0	SACADA[1]
glitter		3.12			440.0			doi: 10.1021/ja00104a027
glitter								doi: 10.1016/S0008-6223(96)00119-4
glitter								doi: 10.1007/978-94-010-1013-9_1
glitter								link
glitter								doi: 10.1023/B:JOMC.0000044525.92511.ab
glitter								doi: 10.1007/s10910-005-4528-3
glitter								doi: 10.1142/S0219633606002209
glitter								nonelink
glitter								doi: 10.1016/j.diamond.2009.11.004
glitter								doi: 10.1007/978-1-4020-9718-8_3
glitter								doi: 10.1007/s10910-011-9954-9
glitter								doi: 10.1016/j.diamond.2013.01.010
T6		2.952			337.4			doi: 10.1073/pnas.1311028110
tP6-carbon			Metal		341.1	175.9	16.8	doi: 10.3103/s1063457614040042
T6					337	197		doi: 10.1038/srep21879
T6		3.057			357	157		doi: 10.1021/acs.cgd.5b01490

Elasticity tensor (kBar)[1]

7277.3729	558.3129	1057.4160	-0.0000	0.0000	-0.0000
558.3129	7277.3729	1057.4160	0.0000	-0.0000	0.0000
1057.4160	1057.4160	11752.0247	0.0000	0.0000	0.0000

-0.0000	0.0000	0.0000	665.7333	0.0000	0.0000
0.0000	-0.0000	0.0000	0.0000	737.5073	-0.0000
-0.0000	0.0000	0.0000	0.0000	-0.0000	737.5054

[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].