SACADA Database Code: 10

Topology: sod

# of independent nodes (IN): 1
Transitivity: [1121]
Space Group: Im-3m
Pearson: cI12
Coordination Number (CN): 4

Year: 1968

Data

Name	Pressure, GPa	Density, g/cm³	Gap, eV	Relative energy, eV/atom	Bulk, GPa	Shear, GPa	Vickers, GPa	Refs
sod (SACADA #10)		2.880		0.993	345.8	324.8	55.9	SACADA[1]
truncated octahedrel								link
truncated octahedrel								doi: 10.1080/153638X9508545737
truncated octahedrel								doi: 10.1080/10641229608001571
C6					352		84.5	doi: 10.1103/PhysRevB.74.172101
C6								doi: 10.3103/s1063457610030056
CA6								doi: 10.1134/s1063776111060173
clathrate VII								doi: 10.1021/ic102178d
clathrate VII		2.87						doi: 10.1021/jp205676p
CA6					363			link
sodalite								doi: 10.1002/pssb.201248185
KI		2.84	3.07		328.6		77.4	doi: 10.1063/1.4802002
bcc-C_6			2.5					doi: 10.1039/C5CP00803D

Elasticity tensor (kBar)[1]

8224.8676	1073.8732	1073.8732	-0.0000	0.0000	-0.0000
1073.8732	8224.8676	1073.8732	0.0000	-0.0000	-0.0000
1073.8732	1073.8732	8224.8676	0.0000	-0.0000	0.0000
-0.0000	-0.0000	0.0000	3047.4240	-0.0000	0.0000
0.0000	-0.0000	-0.0000	0.0000	3047.4240	0.0000
-0.0000	-0.0000	0.0000	0.0000	0.0000	3047.4240

[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].