**SACADA Database Code: 37**

Topology: lon

# of independent nodes (IN): 1
Transitivity: [1222]
Space Group: P63/mmc
Pearson: hP4
Coordination Number (CN): 4

Year: 1967

## Data

| Name | Pressure, GPa | Density, g/cm³ | Gap, eV | Relative energy, eV/atom | Bulk, GPa | Shear, GPa | Vickers, GPa | Refs |
|---|---|---|---|---|---|---|---|---|
| Hexagonallon (SACADA #37) | | 3.540 | | 0.023 | 452.6 | 532.7 | 100.8 | SACADA[1] |
| Lonsdaleite | | | | | | | | doi: 10.1038/214587a0 |
| L2 | | 3.521 | 3.7 | | 405.3 | | | doi: 10.1016/S0379-6779(97)81165-4 |
| Lonsdaleite | | 3.511 | 3.05 | | | | | doi: 10.1006/jssc.1999.8448 |
| Lonsdaleite | | | | | | | | doi: 10.1103/PhysRevB.70.045101 |
| Lonsdaleite | | | | | | | | doi: 10.1063/1.3479478 |
| Lonsdaleite | | | | | | | | doi: 10.1063/1.3452220 |
| Lonsdaleite | | 3.623 | | | 437.1 | | 152.0 | doi: 10.1016/j.scriptamat.2011.04.013 |
| 3D-(3,0) | | 3.623 | | | 454.5 | 551.2 | 96.9 | doi: 10.1021/nn202053t |
| LA2 | | 3.51 | | | 454.5 | | | doi: 10.1134/s1063776111060173 |
| Lonsdaleite | | | | | | | | doi: 10.1021/ja304380p |
| diamond | | | | | | | | doi: 10.1103/PhysRevB.85.155428 |
| L2 | | | | | | | | link |
| Lonsdaleite | | | | | | | | doi: 10.1524/zkri.2013.1620 |
| 2H-diamond | | | | | 455.3 | 551.6 | 97.3 | doi: 10.1016/j.diamond.2014.04.005 |
| hd | | | | | | | | doi: 10.1103/PhysRevB.91.214104 |

## Elasticity tensor (kBar)[1]

| | | | | | |
|---|---|---|---|---|---|
| 12170.7043 | 1079.3223 | 213.7101 | 7.6285 | -0.4187 | -0.1684 |
| 1079.3223 | 12174.3249 | 213.2098 | 8.6004 | -0.5226 | -0.0804 |
| 213.7101 | 213.2098 | 13384.5801 | -3.9833 | 0.0280 | -0.3246 |
| 7.6285 | 8.6004 | -3.9833 | 5530.8357 | -2.4841 | 0.4457 |
| -0.4187 | -0.5226 | 0.0280 | -2.4841 | 4624.6072 | 0.2178 |
| -0.1684 | -0.0804 | -0.3246 | 0.4457 | 0.2178 | 4625.7615 |

[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].