A Car-Parrinello and path integral molecular dynamics study of the intramolecular lithium bond in the lithium 2-pyridyl-*N*-oxide acetate.

Autorzy

Piotr Durlak

Zdzisław Latajka

Sławomir Berski

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Streszczenie

Lithium bonding in lithium 2-pyridyl-N-oxide acetate has been investigated using classic Car–Parrinello molecular dynamics (CPMD) and the path integral approach [path integrals molecular dynamics (PIMD)]. The simulations have been performed in 300 K. Structures, energies, and lithium trajectories have been determined. The CPMD results show that the lithium atom is generally equidistant between heavy atoms in the (O⋯Li⋯O) bridge. Applying quantum effects through the PIMD leads to similar conclusion. The theoretical lithium 2-pyridyl-N-oxide acetate infrared spectrum has also been determined using the CPMD calculations. This shows very good agreement with available experimental results and reproduces well the broad low-frequency band observed experimentally. In order to gain deeper understanding of the nature of the lithium bonding topological analysis of the electron localization function has been applied.

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