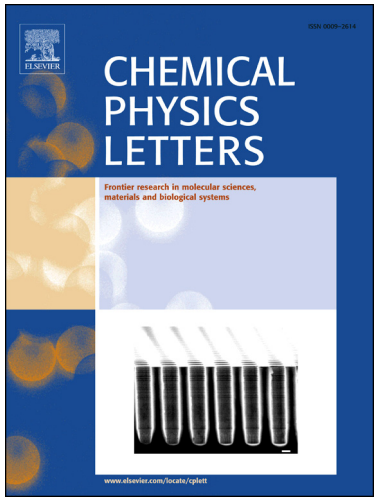

Ground-state dipole moment of the spatially confined carbon monoxide and boron fluoride molecules

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Ground-state dipole moment of the spatially confined carbon monoxide and boron fluoride molecules

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Abstract

In this contribution the influence of spatial confinement on the dipole moment of carbon monoxide and boron fluoride was investigated. The spatial confinement was modeled by applying the two-dimensional harmonic oscillator potential. The dipole moment calculations were performed for both molecules using their experimental geometries and also including the effect of geometry relaxation in the presence of confining potential. Our results demonstrate that the dipole moment is noticeably affected by the confinement. Moreover, it was found that the changes in the dipole moment, caused by the presence of harmonic oscillator potential, are substantially different for each of the studied molecules.

Keywords: spatial confinement, dipole moment, carbon monoxide, boron fluoride, Hirshfeld analysis

1. Introduction

In the course of the last few decades a considerable amount of scientific work has been devoted to the studies of molecular systems under spatial confinement [1–28]. The classic examples of this phenomenon are the inclusion compounds (chemical objects trapped inside molecular cages of different topology) - the key structures in supramolecular chemistry, artificial atoms (quantum dots) and matter under high pressure. It is well established that the physical and chemical properties of spatially limited atoms and molecules can be substantially different from those observed in the free space [1–4, 6–13]. For this reason, such systems attract much attention from researchers working in various areas of science, including spectroscopy, photonics, nanotechnology, crystallography, astrophysics, etc [1, 2, 4, 8, 10, 12].