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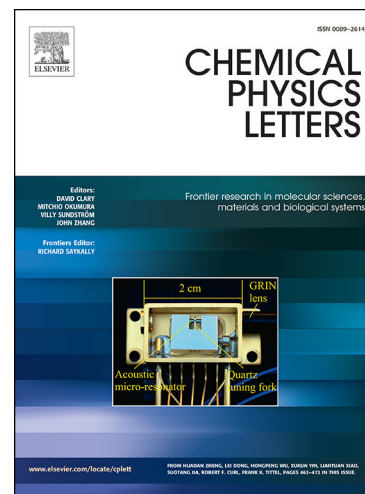
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Halogen Bonding in the framework of classical force fields: the case of chlorine

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ABSTRACT

Halogen bonding is nowadays a consolidated tool in chemistry. Only recently, the importance of halogen bonding has been demonstrated also in biological systems, owing to the presence of halogens in drugs. This interaction is due to the anisotropy of the electron density around the halogen that leads to the formation of the ‘ σ -hole’, which is responsible for the interaction with a nucleophile site. Unfortunately, classical force fields used in the study of ligand-receptor systems

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