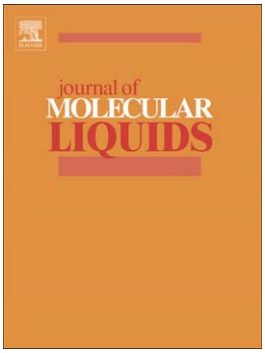

Li^+ binding to fluorinated carbonate solvents studied by ab initio quantum chemical calculations

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Li^+ binding to fluorinated carbonate solvents studied by ab initio quantum chemical calculations

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Ab initio quantum-chemical calculations have been performed for fluorinated ethylene carbonate and fluorinated diethylcarbonate and their complexes with Li^+ ion. Structures of complexes, binding energies and harmonic vibrational frequencies have been obtained in vacuum and in the PCM solvent. Calculated parameters suggest that fluorination of carbonates generally reduces strength of solvent-Li^+ interactions. Frequencies of vibrational modes computed in the solvent agree well with available experimental IR data.

Keywords: quantum-chemical calculations; fluorinated carbonates; lithium ion binding; vibrational spectra

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