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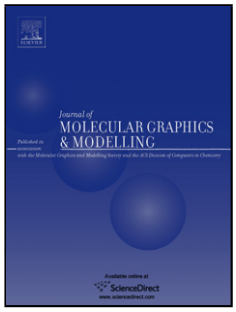

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Theoretical investigation of the π^+-π^+ stacking interactions in substituted pyridinium ion

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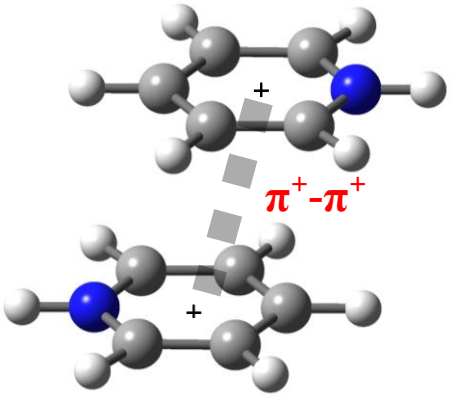
Graphical abstract



Aromatic cations have the ability to form π^+-π^+ stacked complexes, which can have a significant influence over many key chemical and biological processes. the propensity of pyridinium rings to form stable π^+-π^+ stacked dimer structures have been studied in several solvents in the absence of counterions using the ab initio calculations.

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