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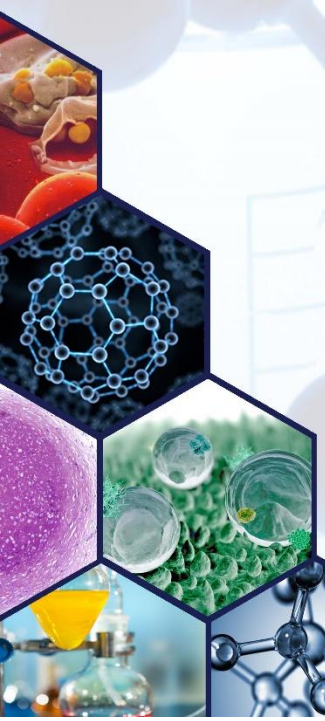

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Study of phenol and toluene stacking interactions, including interactions at large horizontal displacements, in crystal structures and calculated potential energy surfaces

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Importance of aromatic interactions has been widely documented. The arrangements of molecules in solids, liquid crystals and solution are influenced by aromatic stacking interactions. In biological systems, the role of aromatic residues has been identified as very important in protein-protein, protein-folding, protein function, protein-ligand, protein-lipid, protein-nucleic acids interactions and protein structure stability.

Here, we searched the Cambridge Structural Database to find interactions of stacking benzene, *p*-phenol and toluene dimers. Beside this, we calculated interaction energies of phenol and toluene dimers and compared with benzene dimers previously calculated. The results have shown that stacking p-phenol/p-phenol dimer tends to be orientated in parallel and antiparallel fashion while stacking toluene/toluene dimers have almost exclusively antiparallel orientation of two rings. As for benzene molecules, number of interactions for stacking p-phenol/p-phenol and toluene/toluene dimers is increasing at the large offsets (4.0 - 6.0 Å). Additionally, interactions of p-phenol/p-phenol and toluene/toluene dimers show peak at offset 1.5 Å.

The potential surfaces of stacking interactions of phenol-phenol and toluene-toluene were investigated, including interactions at large offsets. Three different geometries of parallel and antiparallel phenol-phenol and toluene-toluene dimers were considered. The DFT calculations have shown that the interaction energies for phenol/phenol and toluene/toluene dimers have similar trends. For parallel orientations at negative and positive offsets for toluene/toluene, the strongest interaction energy is –3.98 kcal/mol. For antiparallel orientations, at negative offsets, the strongest interaction energy is –5.39 kcal/mol, while at positive offset the strongest interaction has energy of –2.83 kcal/mol. Both systems phenol/phenol and toluene/toluene, in crystal structures show preference for large offsets (4.0 - 6.0 Å) and have significant calculated interaction energy similar to benzene dimer.