Abstract

Hydrogen bonding has been an active field of research for a long time. On the contrary, there is a lack of knowledge about the weak intermolecular interactions involving C–H···F hydrogen bonds. Intermolecular interactions involving organic fluorine are important in medicinal chemistry, drug-protein interaction study and crystal packing. Hence, a vivid investigation of this weak interaction is attempted in our current study. A group of dimers involving ethylene, benzene, fluorinated ethylene and fluorinated benzene have been studied to reveal the structure, stability and energetics of the dimers of these molecules formed by C–H···F hydrogen bonds. The molecules have been studied at MP2 level of theory using different basis sets such as 6- 31++g*, aug-cc-pVDZ and aug-cc-pVTZ. Frequency calculations were performed to ensure that the geometries correspond to real minima in potential energy surface. Later the energy values of the optimized geometries were extrapolated to CBS limit to calculate their energetics with highest accuracy. The contribution of energy of the formed hydrogen bond in the total stabilization energy is also determined by substitution methods. All the structural and energetic details explain the formation of intermolecular C–H···F hydrogen bonds. Further, AIM calculations and Energy Decomposition analysis (EDA) were done to explore the nature of interactions existing among the studied molecules. Our results emphasize on the impact of these weak interactions in overall stability of the dimers.