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PREDICTION OF THE THERMOPHYSICAL PROPERTIES AND PHASE BEHAVIOR OF ALTERNATIVE REFRIGERANTS VIA COMPUTATIONAL CHEMISTRY. *Maurizio Fermeglia, and Sabrina Pricl, Department of Chemical Engineering, University of Trieste, Piazzale Europa 1, Trieste 34127, Italy, Fax: 0039-040-569823, mauf@dicamp.units.it, sabrinap@dicamp.units.it*

In recent years, numerous investigations have identified chemicals, which are alternatives to the CFCs and HCFCs, for the purpose of protecting the stratospheric ozone hole. In particular, hydrocarbons (HC), fluorocarbons (HFCs), fluoroethers (FE), fluorothioethers (FTE) and their mixtures have received notable attentions as promising candidates for retaining the good environmental properties and minimizing the relevant shortcomings. In this paper we present the results of the application of an intensive computational chemistry approach to the determination of the thermophysical properties and phase behavior of a series of alternative refrigerants and their mixtures. We employed a hybrid approach to derive a new force field (FF) for these classes of substances, based on the CFF91 force field. This FF was then applied to calculate, via Molecular Dynamics (MD), the PVT properties of all pure components considered, and to derive the Perturbed Hard Sphere Chain Therory Equation of State (PHSCT EOS) parameters, by which the phase behavior of the corresponding mixtures was predicted. All virtual results were compared with the relevant experimental data, showing a good agreement in all cases.