Cope Elimination: Elucidation of Solvent Effects from QM/MM Simulations

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Supporting Material

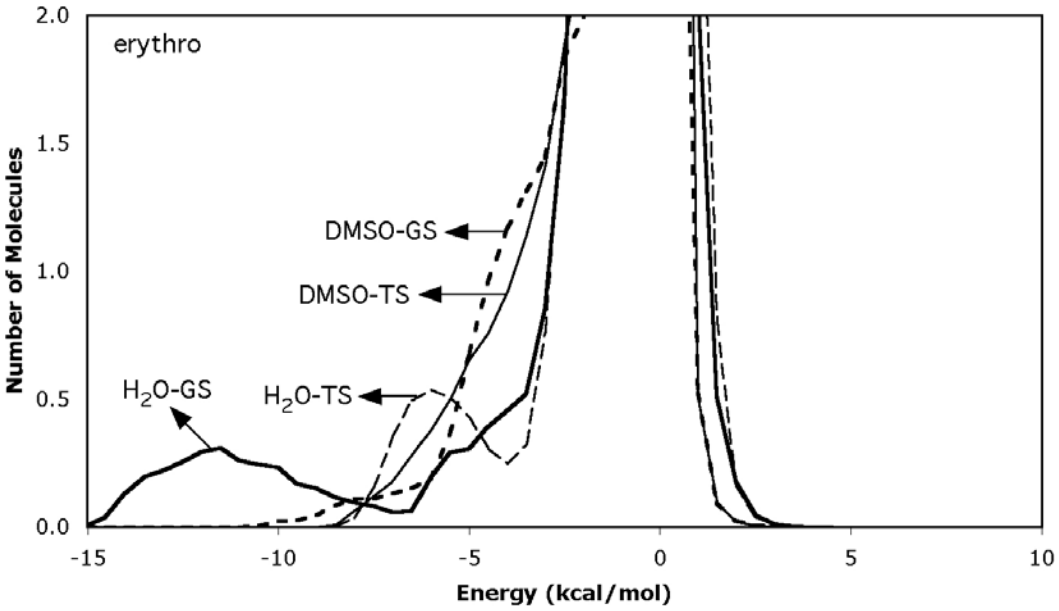

Figure S1. Solute-solvent energy pair distributions for the Cope elimination of *erythro* amine oxide in water and DMSO for the reactant (GS) and transition structure (TS). The ordinate records the number of solvent molecules that interact with the solutes with their interaction energy on the abscissa. Units for the ordinate are number of molecules per kcal/mol.

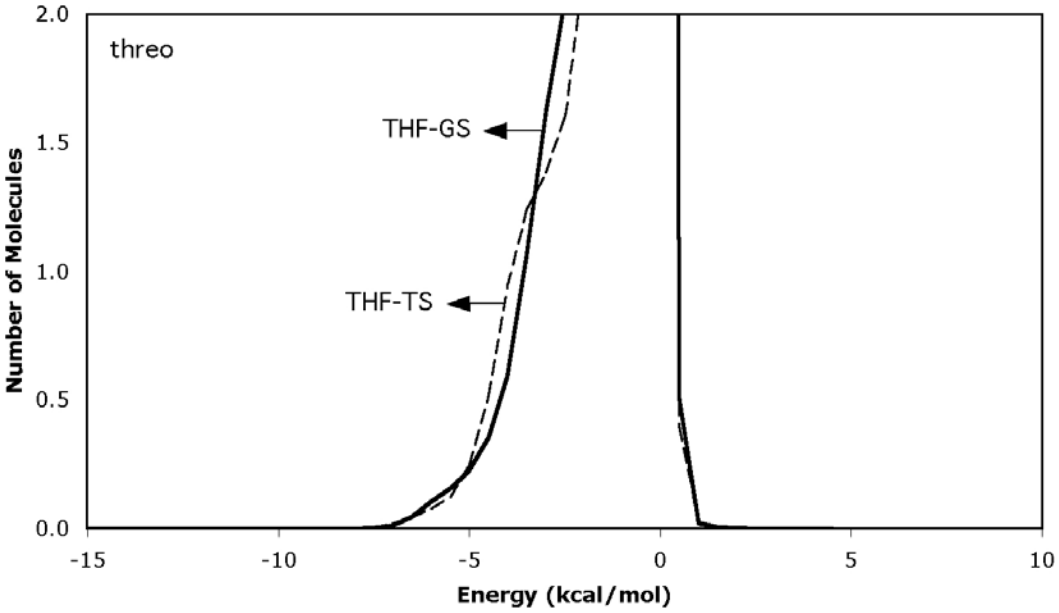

Figure S2. Solute-solvent energy pair distributions for the Cope elimination of *threo* amine oxide in THF for the reactant (GS) and transition structure (TS). The ordinate records the number of solvent molecules that interact with the solutes with their interaction energy on the abscissa. Units for the ordinate are number of molecules per kcal/mol.

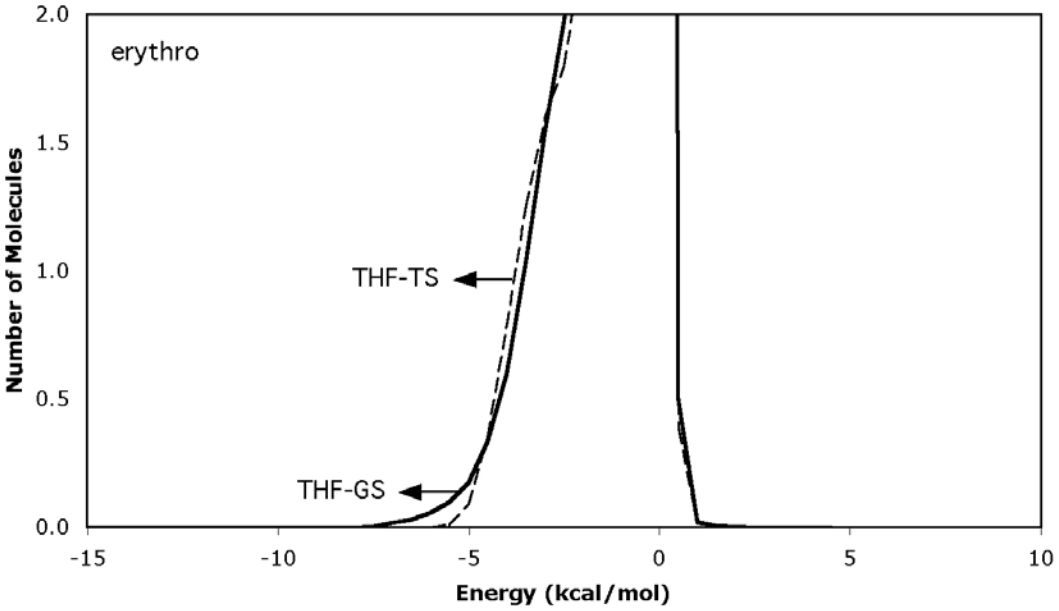

Figure S3. Solute-solvent energy pair distributions for the Cope elimination of *erythro* amine oxide in THF for the reactant (GS) and transition structure (TS). The ordinate records the number of solvent molecules that interact with the solutes with their interaction energy on the abscissa. Units for the ordinate are number of molecules per kcal/mol.

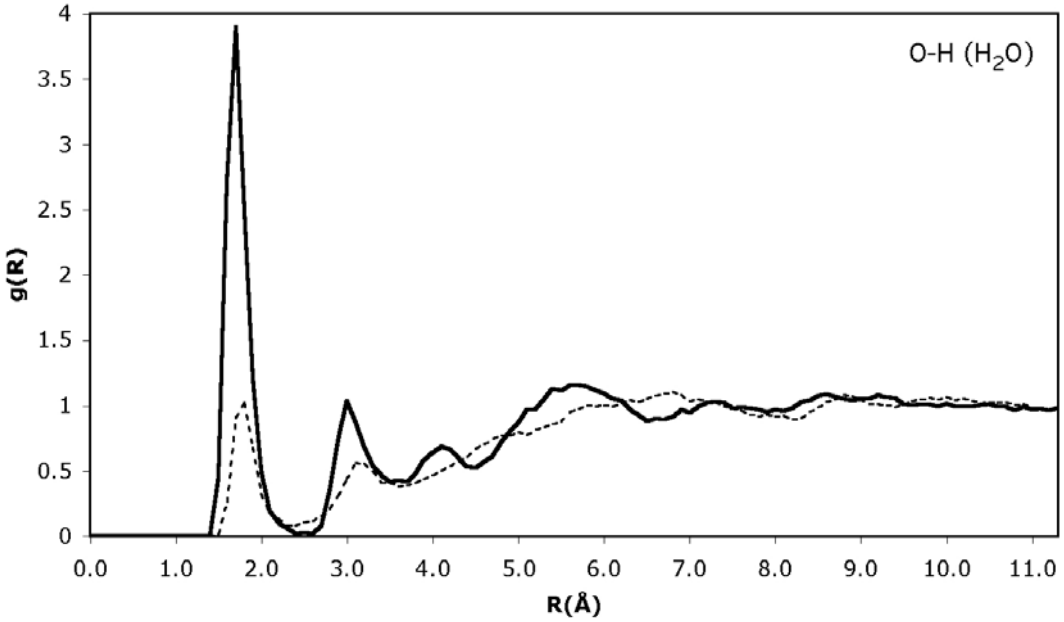

Figure S4. Computed (Cope)-O···H-(H_2O) radial distribution functions for the reactant (solid curve) and transition state (dashed curve) for the reaction of *erythro*-N,N-dimethyl-3-phenyl-2-butylamine oxide.

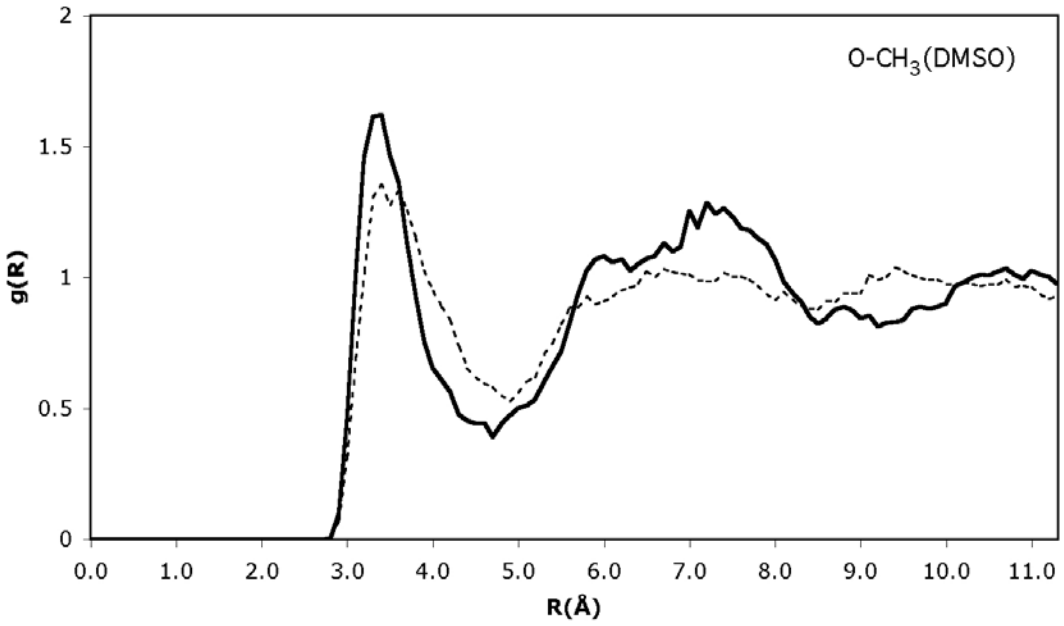

Figure S5. Computed (Cope)-O···CH_3-(DMSO) radial distribution functions for the reactant (solid curve) and transition state (dashed curve) for the reaction of *erythro*-N,N-dimethyl-3-phenyl-2-butylamine oxide.

Gaussian 03 Reference

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