AB INITIO REACTION PATHWAYS FOR $\beta-$ HYDROGEN ELIMINATION FROM SMALL RADICALS

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Reaction pathways have been calculated for the elimination of a $\beta-$ hydrogen from several small radicals. Structural and thermodynamic information is predicted by the calculations. Calculated structural changes are consistent with very simple models of chemical bonding involving a change in the orbital hybridization of the large fragment atom involved in the bond that is dissociated. Calculations at the MP2/6-311g* level give thermodynamic values which are in modest agreement with experiment.