Title: Focal Point Analysis of the Low Temperature Combustion of Dimethyl ether

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In order to provide a chemically accuracte surface, we have applied focal point analysis (FPA) to the decomposition of the adduct of dimethyl ether radical + O2. The ideal procedure for focal point analysis, and other high accuracy composite methods would utilize quadruple-zeta or, at least, triple-zeta quality basis sets for the optimization of all stationary points at the CCSD(T) level of theory; however, this becomes intractable for moderately sized molecules ($>$ 6 heavy atoms). Therefore, we test a modification to the standard FPA approach for combustion processes: utilizing a composite gradient method to achieve CCSD(T)/cc-pVQZ quality geometries at significantly reduced cost compared to the CCSD(T)/cc-pVTZ level of theory. For the surface, the CCSDT(Q)/CBS energy is targeted through basis set extrapolations up to CCSD(T)/cc-pV5Z and correlation treatment up through CCSDT(Q)/cc-pVDZ. Exact two-component scalar-relativistic, diagonal Born–Oppenheimer, frozen-core, and zero-point vibrational energy corrections are also applied.