Abbreviations and symbols

B3LYP - Becke's three exchange functional and the gradient corrected functional of Lee, Yang and Parr

BF<sub>i</sub> - Percentage of bond formation of the i<sup>th</sup> bond of a given species on the reaction path

BC<sub>j</sub> - Percentage of bond cleavage of the j<sup>th</sup> bond

BF<sub>Ave</sub> - Average percentage of bond formation

BC<sub>Ave</sub> - Average percentage of bond cleavage

BF<sub>CAVE</sub> - Average percentage of bond formation and cleavage

CCSD - Coupled-Cluster Single and Double

DFT - Density Functional Theory

E<sub>a</sub> - Activation barrier

ESP - Charges derived by fitting the Electrostatic Potential

HF - Hartree-Fock

FOE - Frontier Orbital Energy

HOMO - Highest Occupied Molecular Orbital

HLEG - (HOMO - LUMO) energy gaps

ΔH - Reaction enthalpy

IRC - Intrinsic Reaction Coordinate

LUMO - Lowest Unoccupied Molecular Orbital

MP - MØller-Plesset perturbation theory

NBO - Natural Bond Orbital

NHO - Natural Hybrid Orbital

NLMO - Natural Localized Molecular Orbital

NPA - Natural Population Analysis

PES - Potential Energy Surface

QCISD - Quadratic Configuration Interaction Single and Double

q<sub>ct</sub> - Quantum of charge transfer

SOSP - Second-Order Saddle Point

TS - Transition State