Supplementary Information

Mayer's Chemical Energy Component Analysis as a tool to identify the factors determining the shapes of potential surfaces of chemical reactions

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Calculational protocol

The following protocol can be used to reproduce the results reported in this paper:
1. Download the Program NEWENPART from http://occam.ttk.hu/programs/ unzip it. A directory called newenpart/ will be generated.
2. With Gaussian, get the geometry of the saddle point on the potential energy surface of reaction R1 using the command line
UHF/6-31G** Opt(TS,Nolinear,Noeigentest,CalcFC)
3. to locate the minimum energy path, transfer the optimized saddle point geometry from the output and start a calculation using the command lines
UHF/6-31G** IRC(Maxpoints=35,CalcFC)
(Modify Maxpoints to match your needs.
4. Extract the geometries for the points along the minimum energy path and at each point run a calculation with the command line
UHF/6-31G** SCF=Tight Formcheck
5. For each point along the MEP, copy the formatted checkpoint file to Test.FChk in the newenpart directory and run the script "fut" as
...path../newenpart/fut [any_desired_outputfilename]
The mehhircfwd_border01.apost etc. files zipped in the Supplementary Information were generated according to this protocol.

Figures

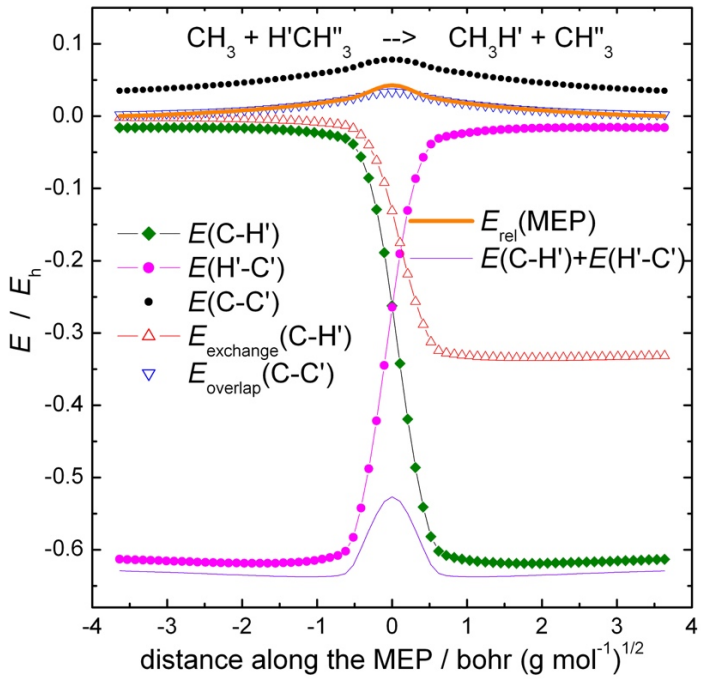


Fig. S1 Diatomic energy contributions of atom pairs involved in reaction R2 as a function of the position along the minimum energy path, obtained with the CECA method from the UHF/6-31G** wave function. The exchange contribution for the forming C–H' bond and the overlap contribution for the C–C' end/atom pair is also shown.

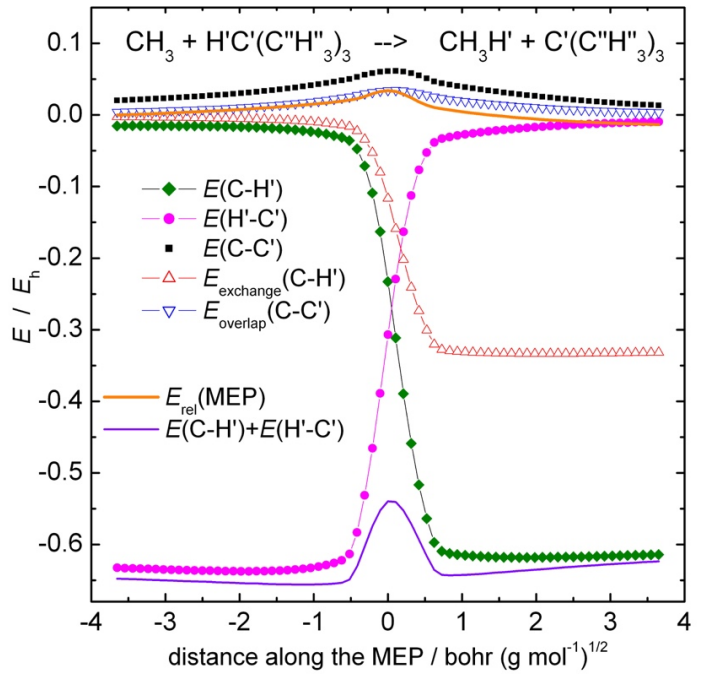


Fig. S2 Same as Fig. S1 but for reaction R3

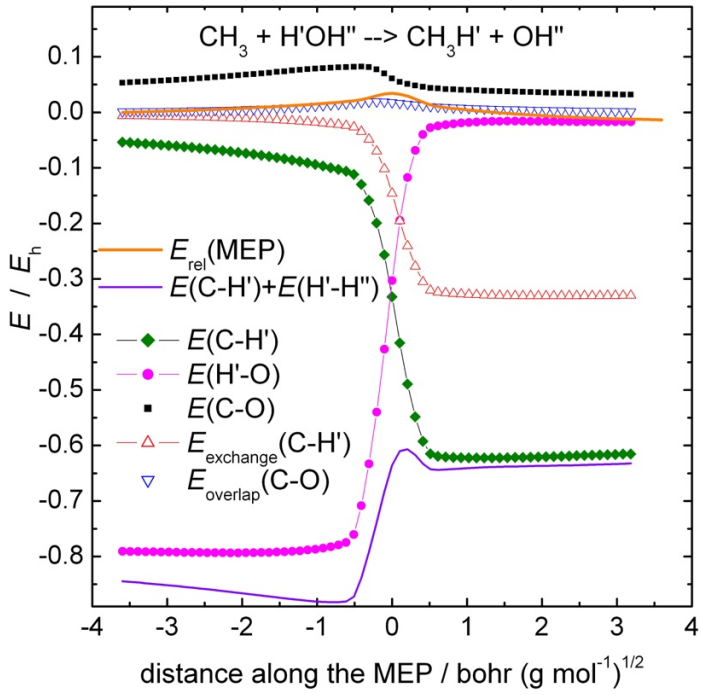


Fig. S3 Same as Fig. S1 but for reaction R4

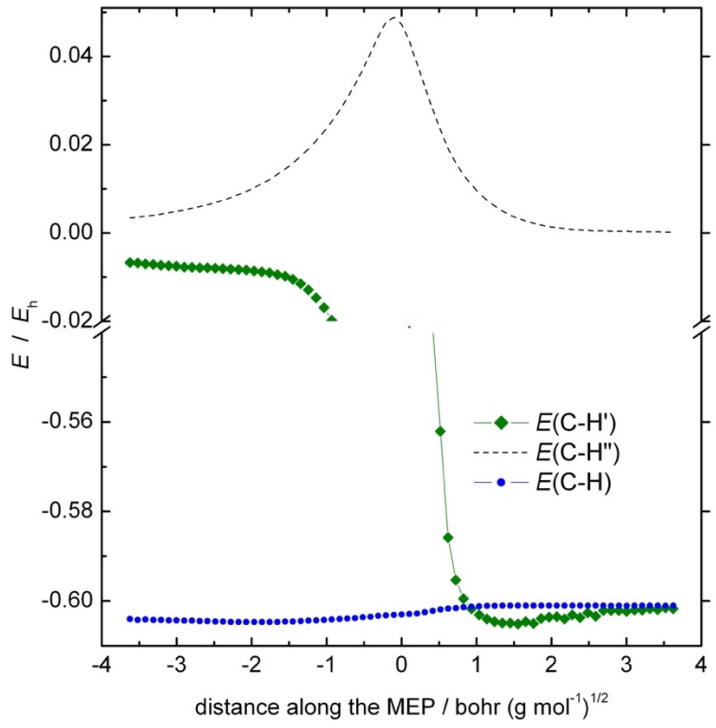


Fig. S4 The diatomic CECA energy components corresponding to the carbon–hydrogen atom pairs along the MEP of reaction R1 obtained at the UHF/6-31G** level.

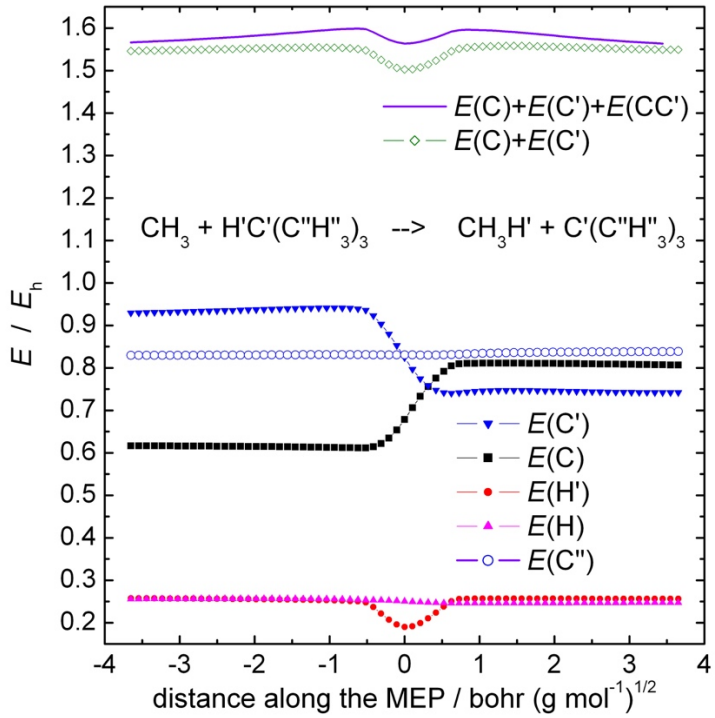
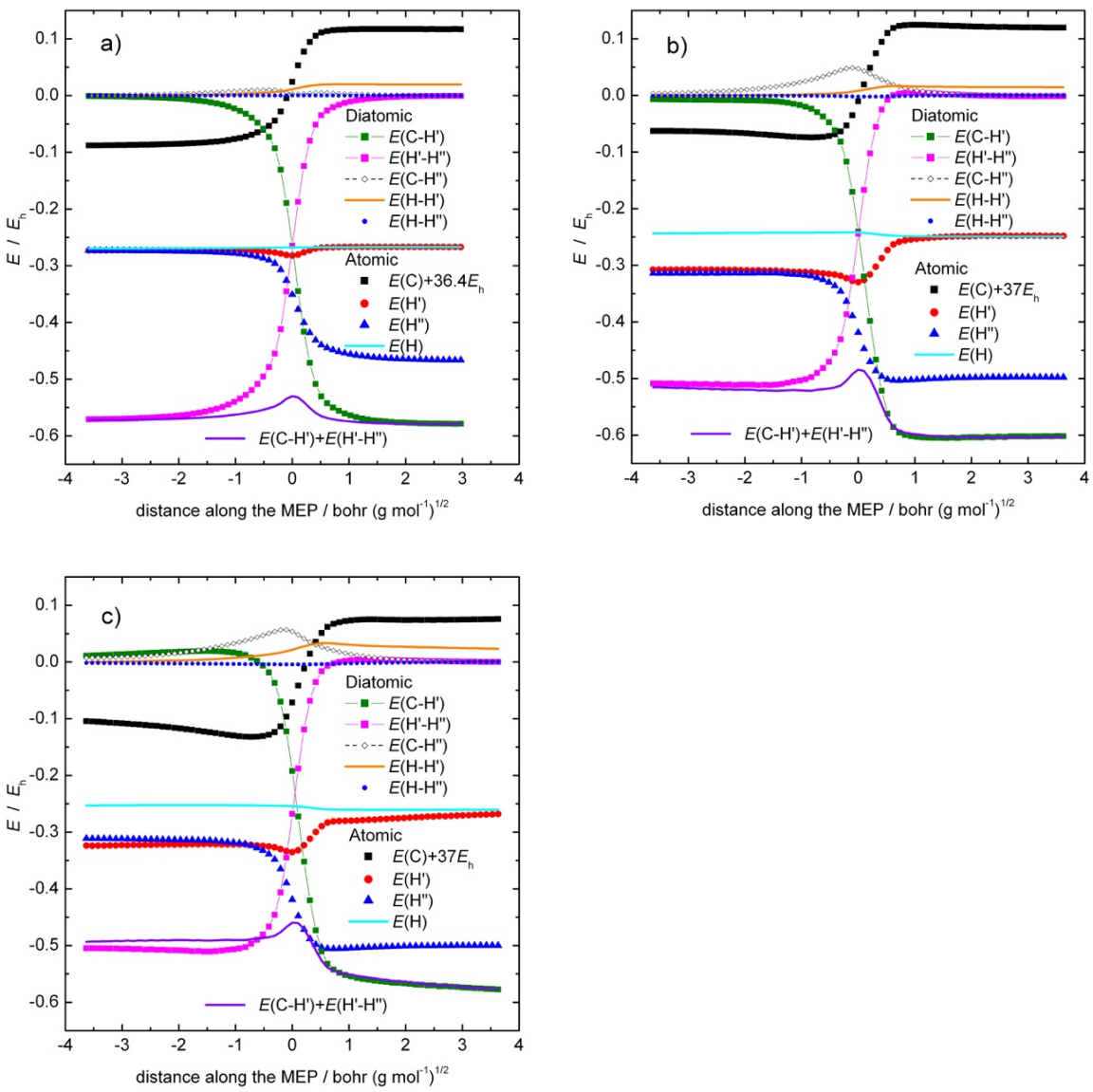


Fig. S5 Same as Fig. 6 in the main text but for reaction R3



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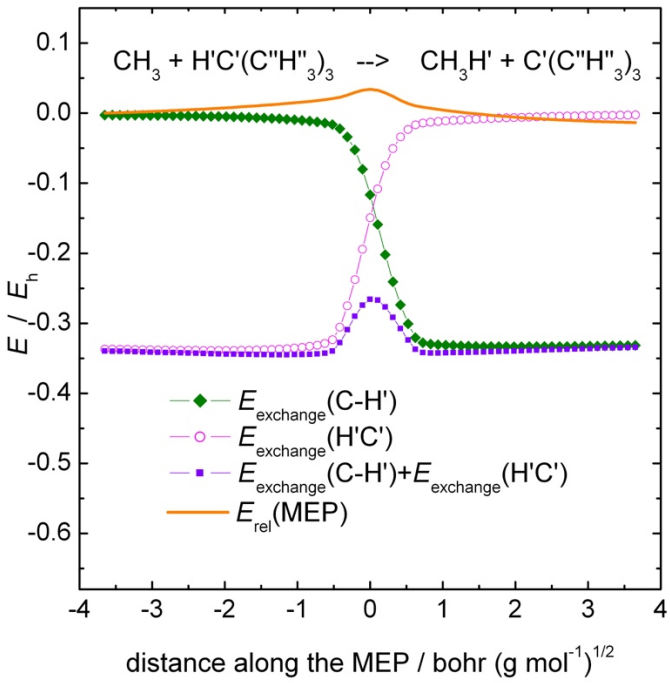

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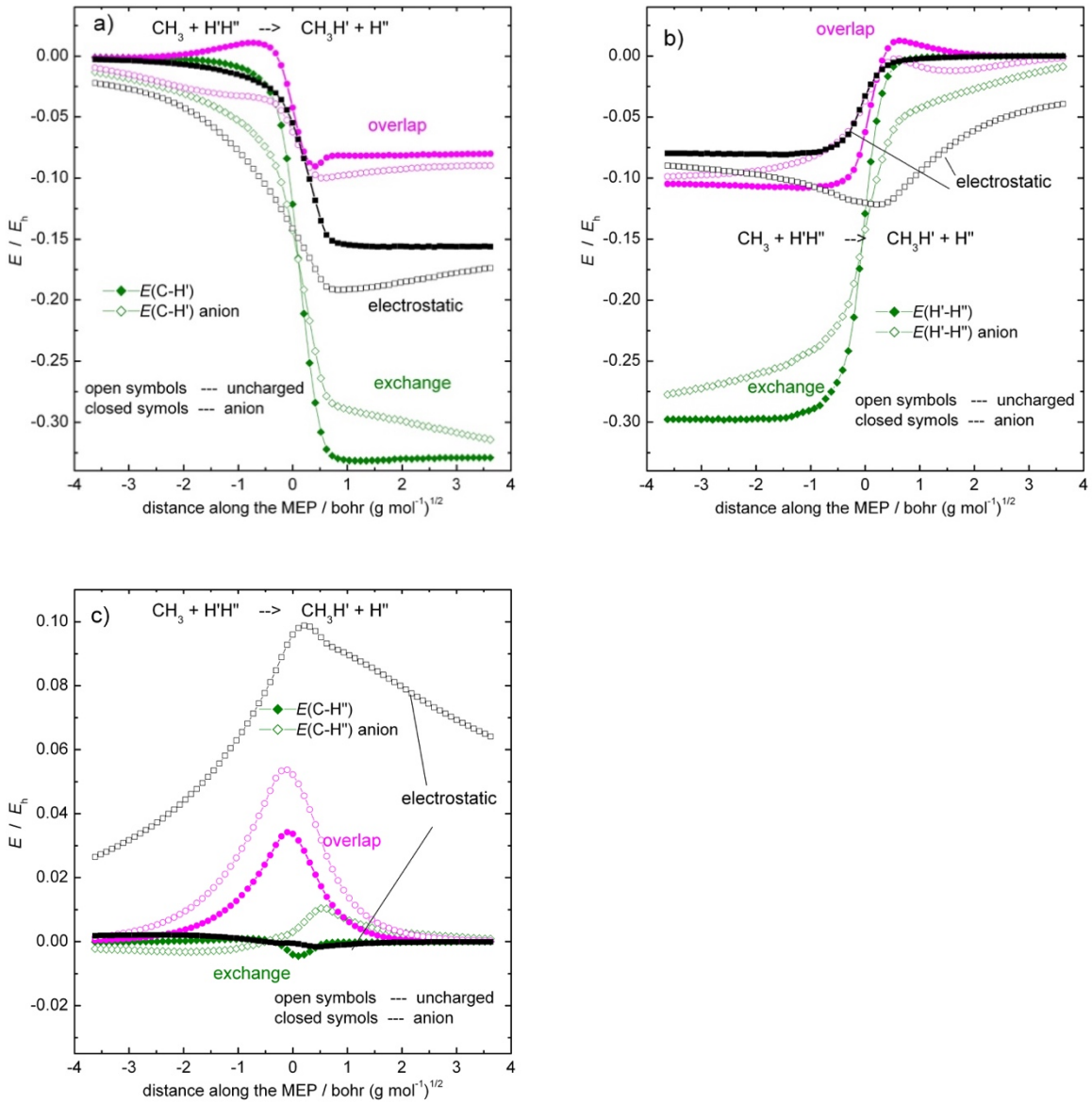

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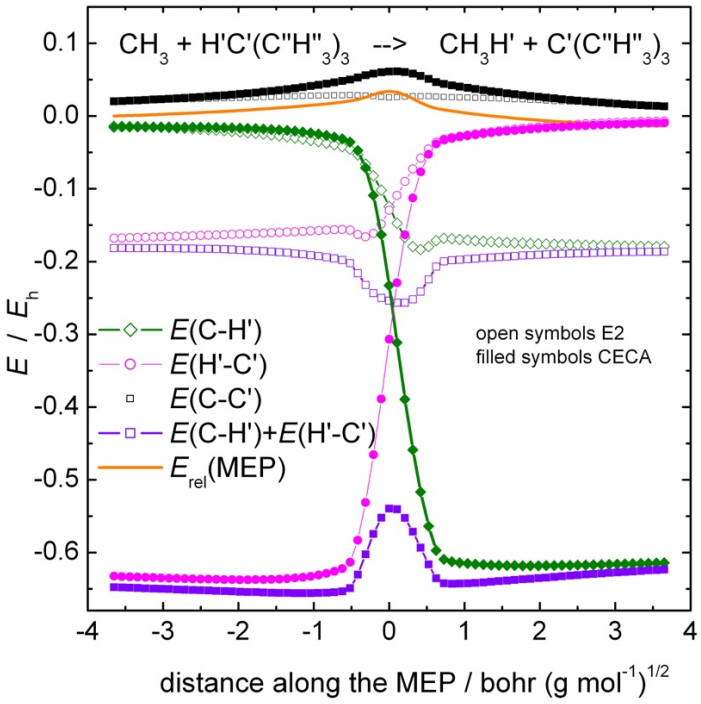

Fig. S9a The diatomic energy components along the MEP of reaction R3 derived according to the CECA (closed symbols) and E2 (open symbols) schemes from the UHF/6-31G** wave functions

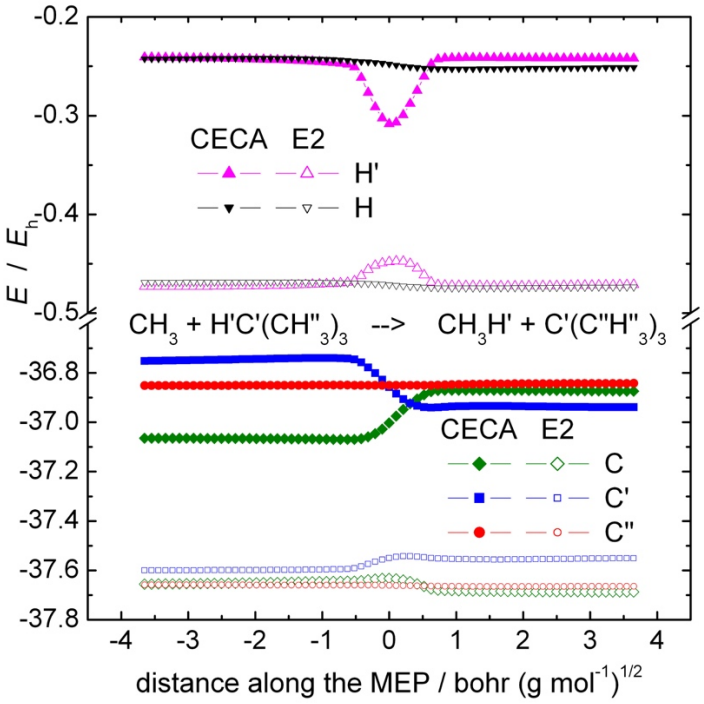

Fig. S9b The monoatomic energy components along the MEP of reaction R3 derived according to the CECA (closed symbols) and E2 (open symbols) schemes from the UHF/6-31G** wave functions