Kinetics of the OH reaction with 2-Methyl-2-Propen-1-ol and the Analogue Alkene

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**MPO221 BHandHLYP/cc-pVDZ**

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**Frequencies**

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$\sigma$-PC$_{pr\text{i}}$ BHandHLYP/cc-pVDZ

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σ-PC_ter  BHandHLYP/cc-pVDZ

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**E(BHandHLYP)**

-308.0215015

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**TS_{pri} BHandHLYP/cc-pVDZ**

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Frequencies

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1494.02  1504.41  1515.91  1529.83  1643.18
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\(E(\text{BHandHLYP})\) ...........................................-308.0183809
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C     -1.648760   -0.310634   -0.600310
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Frequencies

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E(BHandHLYP).............................-308.0582132
B: Cartesian coordinates (angstroms), vibrational frequencies (cm-1) and electronic energies (hartrees) for the stationary points on the MPO221 + OH Potential Energy Surface calculated at BHandHLYP/aug-cc-pVDZ

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$\sigma$-PC$_{pri}$ BHandHLYP/ aug-cc-pVDZ

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H   -0.056750  -1.366780  -1.279730
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1100.71 1168.47 1266.81 1318.96 1435.83 1449.08
1478.13 1481.35 1507.78 1520.16 1530.47 1746.60
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σ-PC_{ter} BHandHLYP/ aug-cc-pVDZ

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| 735.63 | 873.10 | 974.53 | 993.61 | 998.02 | 1050.07 |
| 1098.01| 1163.88| 1266.96| 1322.37| 1438.23| 1447.54 |
| 1474.86| 1479.57| 1509.75| 1519.98| 1530.31| 1744.68 |
| 3094.38| 3112.09| 3147.68| 3170.79| 3213.01| 3240.71 |
| 3342.60| 3901.95| 3926.96|        |        |        |

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\[ \pi-\text{PC BHandHLYP/ aug-cc-pVDZ} \]

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IM_{pri} BHandHLYP/ aug-cc-pVDZ

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M2 BHandHLYP/ cc-pVDZ

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**BHandHLYP/ cc-pVDZ**

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D: Cartesian coordinates (angstroms), vibrational frequencies (cm-1) and electronic energies (hartrees) for the stationary points on the M2 + OH Potential Energy Surface calculated at BHandHLYP/aug-cc-pVDZ

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-232.8540993
π-PC BHandHLYP/ aug-cc-pVDZ

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**TS\textsubscript{ter} BHandHLYP/ aug-cc-pVDZ**

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E(BHandHLYP).............................-232.8520136
**IM$_{pri}$ BHandHLYP/ aug-cc-pVDZ**

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**IM**

**BHandHLYP/ aug-cc-pVDZ**

**Cartesian Coordinates**

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**E(BHandHLYP).............................-232.8933573**
Figure: Reaction Profile showing the contribution of both $\pi$-PC (denoted as 1$\pi$-PC in this Figure) and 2$\pi$-PC paths. A: Comparison of the optimized geometries, located at the BHandHLYP/aug-cc-pVDZ level, for the $\pi$-PC. A: 1$\pi$-PC, as reported at the manuscript, representing an upward OH attack to MPO221. B: 1$\pi$-PC, from another view. C: 2$\pi$-PC, representing an upward OH attack to the mirror image of MPO221 and resembling Zhang’s PC. C: 2$\pi$-PC, from another view.
Figure: Reaction Profile showing the contribution of both $\pi$-PC (denoted as 1$\pi$-PC in this Figure) and 2$\pi$-PC paths. B: Reaction profile showing the contribution of both upward and downward attack to MPO221, resulting from two conformers (mirror images) of the reactant. The blue lines represent the upward attacks; the red lines represent the downward attack; the yellow lines represent the connection between the $\pi$-PC and TSpri along the $\pi$-PC $\rightarrow$ IMpri reaction path; the green lines represent the connection between the $\pi$-PC and TSter along the $\pi$-PC $\rightarrow$ IMter reaction path.
Table: Electronic energies (hartree) calculated for the stationary points along the MPO221 + OH reaction path at different theoretical levels with the cc-pVDZ basis set.

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