**Supporting Information**

# $^{13}C$ and $^{2}H$ Kinetic Isotope Effects and the Mechanism of Bromination of 1-Pentene under Synthetic Conditions

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## Structure 1

SCF Done: E(RB+HF-LYP) = -5265.64314558

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 35 | 0 | -0.109828 | -0.235482 | -0.019589 |
| 2 | 35 | 0 | 2.248611 | 0.172958 | 0.012316 |
| 3 | 6 | 0 | -3.056538 | -0.026401 | -0.444657 |
| 4 | 6 | 0 | -2.809792 | -1.160099 | 0.239744 |
| 5 | 6 | 0 | -3.432021 | 1.289036 | 0.168106 |
| 6 | 1 | 0 | -2.735046 | 2.077771 | -0.139734 |
| 7 | 1 | 0 | -3.438876 | 1.239863 | 1.261283 |
| 8 | 1 | 0 | -4.430204 | 1.596581 | -0.171510 |
| 9 | 1 | 0 | -3.006619 | -0.054409 | -1.533231 |
| 10 | 1 | 0 | -2.867841 | -1.191843 | 1.325184 |
| 11 | 1 | 0 | -2.588713 | -2.094821 | -0.266601 |

Zero-point correction= 0.081970 (Hartree/Particle)
Thermal correction to Energy= 0.090216
Thermal correction to Enthalpy= 0.091160
Thermal correction to Gibbs Free Energy= 0.046077
Sum of electronic and zero-point Energies= -5265.561175
Sum of electronic and thermal Energies= -5265.552930
Sum of electronic and thermal Enthalpies= -5265.551986
Sum of electronic and thermal Free Energies= -5265.597069

| | E (Thermal) KCAL/MOL | CV CAL/MOL-KELVIN | S CAL/MOL-KELVIN |
|---|---|---|---|
| TOTAL | 56.611 | 24.326 | 94.886 |

## Structure 2

SCF Done: E(RB+HF-LYP) = -2691.48291242

Standard orientation:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 35 | 0 | 0.905503 | -0.210584 | -0.013481 |
| 2 | 6 | 0 | -1.163644 | 0.252811 | 0.487817 |
| 3 | 6 | 0 | -0.415396 | 1.313661 | -0.175942 |
| 4 | 6 | 0 | -2.171426 | -0.595903 | -0.190350 |
| 5 | 1 | 0 | -1.146800 | 0.254902 | 1.577055 |
| 6 | 1 | 0 | -0.599162 | 1.503857 | -1.231168 |
| 7 | 1 | 0 | -0.041301 | 2.149698 | 0.410355 |
| 8 | 1 | 0 | -3.144413 | -0.116013 | 0.018118 |
| 9 | 1 | 0 | -2.219497 | -1.599107 | 0.241851 |
| 10 | 1 | 0 | -2.038635 | -0.646305 | -1.273520 |

Zero-point correction= 0.082796 (Hartree/Particle)
Thermal correction to Energy= 0.087895
Thermal correction to Enthalpy= 0.088839
Thermal correction to Gibbs Free Energy= 0.053861
Sum of electronic and zero-point Energies= -2691.400117
Sum of electronic and thermal Energies= -2691.395018
Sum of electronic and thermal Enthalpies= -2691.394074
Sum of electronic and thermal Free Energies= -2691.429051

| | E (Thermal) KCAL/MOL | CV CAL/MOL-KELVIN | S CAL/MOL-KELVIN |
|---|---|---|---|
| TOTAL | 55.155 | 17.107 | 73.617 |

## Structure 3

SCF Done: E(RB+HF-LYP) = -2809.41126840

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.209881 | -0.057891 | -2.363706 |
| 2 | 6 | 0 | 0.171760 | -0.065071 | -2.413378 |
| 3 | 6 | 0 | -2.075338 | -1.261901 | -2.442103 |
| 4 | 1 | 0 | -1.709812 | 0.909607 | -2.320814 |
| 5 | 1 | 0 | 0.715598 | -0.995616 | -2.552881 |
| 6 | 1 | 0 | 0.726615 | 0.859331 | -2.540419 |
| 7 | 1 | 0 | -2.593451 | -1.241447 | -3.413796 |
| 8 | 1 | 0 | -2.863398 | -1.238165 | -1.681054 |
| 9 | 1 | 0 | -1.512434 | -2.195506 | -2.369178 |
| 10 | 35 | 0 | 0.000000 | 0.000000 | 0.000000 |
| 11 | 6 | 0 | 1.209881 | 0.057891 | 2.363706 |
| 12 | 6 | 0 | -0.171760 | 0.065071 | 2.413378 |
| 13 | 6 | 0 | 2.075338 | 1.261901 | 2.442103 |
| 14 | 1 | 0 | 1.709812 | -0.909607 | 2.320814 |
| 15 | 1 | 0 | -0.715598 | 0.995616 | 2.552881 |

| | | | | | |
|---|---|---|---|---|---|
| 16 | 1 | 0 | -0.726615 | -0.859331 | 2.540419 |
| 17 | 1 | 0 | 2.593451 | 1.241447 | 3.413796 |
| 18 | 1 | 0 | 2.863398 | 1.238165 | 1.681054 |
| 19 | 1 | 0 | 1.512434 | 2.195506 | 2.369178 |

| | |
|---|---|
| Zero-point correction= | 0.163491 (Hartree/Particle) |
| Thermal correction to Energy= | 0.173845 |
| Thermal correction to Enthalpy= | 0.174789 |
| Thermal correction to Gibbs Free Energy= | 0.126643 |
| Sum of electronic and zero-point Energies= | -2809.247777 |
| Sum of electronic and thermal Energies= | -2809.237423 |
| Sum of electronic and thermal Enthalpies= | -2809.236479 |
| Sum of electronic and thermal Free Energies= | -2809.284625 |

| | E (Thermal) KCAL/MOL | CV CAL/MOL-KELVIN | S CAL/MOL-KELVIN |
|---|---|---|---|
| TOTAL | 109.089 | 34.400 | 101.332 |