

Supplementary Material

Theoretical Study on the H-atom Abstraction Reactions of Pentanol + HO₂, Part I : Five Branched Pentanol Isomers

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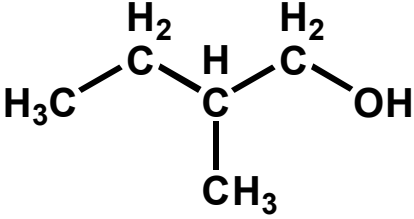
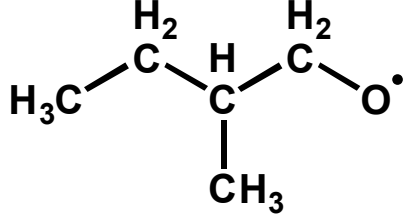
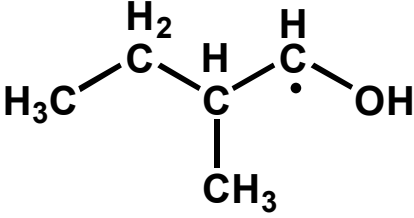
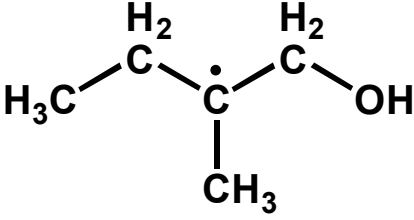
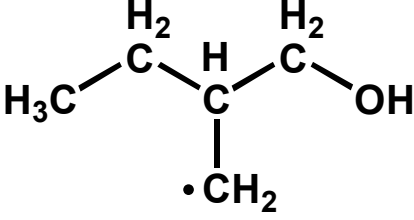
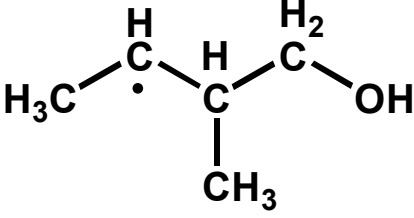
Section 2: Species and structures of some reactants and products identified calculated in this work.

Table S1**T1 diagnostic values for reactants, transition states, and products calculated in this work.**

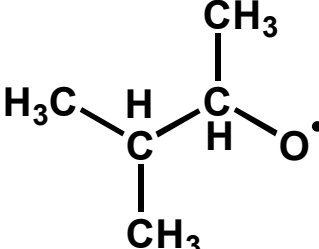
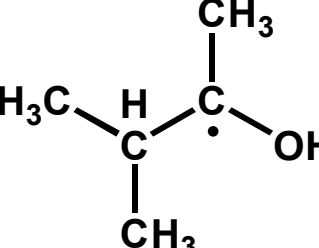
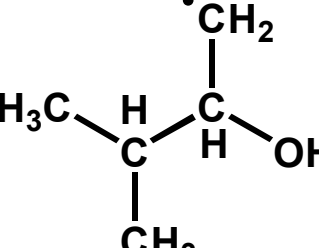
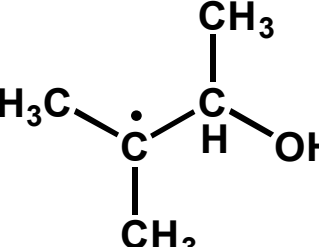
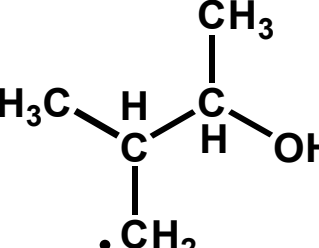
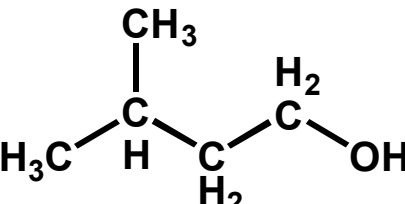
| Species | T1 | Species | T1 |
|--|-------|---|-------|
| $\text{H}\dot{\text{O}}_2$ | 0.038 | H_2O_2 | 0.010 |
| 2-Methyl-1-butanol+ $\text{H}\dot{\text{O}}_2$ radical | | 1,2-Dimethyl-1-propanol+ $\text{H}\dot{\text{O}}_2$ radical | |
| $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{OH}$ | 0.009 | $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{OH}$ | 0.009 |
| TS- δ_p | 0.022 | TS- γ_p | 0.022 |
| $\dot{\text{C}}\text{H}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{OH}$ | 0.010 | $\dot{\text{C}}\text{H}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{OH}$ | 0.010 |
| TS- γ_s | 0.019 | TS- β_t | 0.017 |
| $\text{CH}_3\dot{\text{C}}\text{HCH}(\text{CH}_3)\text{CH}_2\text{OH}$ | 0.011 | $\text{CH}_3\dot{\text{C}}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{OH}$ | 0.011 |
| TS- β_t | 0.017 | TS- α_t | 0.019 |
| $\text{CH}_3\text{CH}_2\dot{\text{C}}(\text{CH}_3)\text{CH}_2\text{OH}$ | 0.012 | $\text{CH}_3\text{CH}(\text{CH}_3)\dot{\text{C}}(\text{CH}_3)\text{OH}$ | 0.014 |
| TS- γ_p | 0.022 | TS- β_p | 0.022 |
| $\text{CH}_3\text{CH}_2\text{CH}(\dot{\text{C}}\text{H}_2)\text{CH}_2\text{OH}$ | 0.010 | $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}(\dot{\text{C}}\text{H}_2)\text{OH}$ | 0.011 |
| TS- α_s | 0.017 | TS-OH | 0.072 |
| $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\dot{\text{C}}\text{HOH}$ | 0.014 | $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\dot{\text{O}}$ | 0.017 |
| TS-OH | 0.073 | 3-Methyl-1-butanol + $\text{H}\dot{\text{O}}_2$ radical | |
| $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\dot{\text{O}}$ | 0.016 | $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{OH}$ | 0.009 |
| 1,1-Dimethyl-1-propanol+ $\text{H}\dot{\text{O}}_2$ radical | | TS- δ_p | 0.022 |
| $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_2)(\text{CH}_3)\text{OH}$ | 0.009 | $\text{CH}_3\text{CH}(\dot{\text{C}}\text{H}_2)\text{CH}_2\text{CH}_2\text{OH}$ | 0.010 |
| TS- γ_p | 0.022 | TS- γ_t | 0.015 |
| $\dot{\text{C}}\text{H}_2\text{CH}_2\text{C}(\text{CH}_3)_2\text{OH}$ | 0.010 | $\text{CH}_3\dot{\text{C}}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{OH}$ | 0.012 |
| TS- β_s | 0.020 | TS- β_s | 0.020 |
| $\text{CH}_3\dot{\text{C}}\text{HC}(\text{CH}_3)_2\text{OH}$ | 0.011 | $\text{CH}_3\text{CH}(\text{CH}_3)\dot{\text{C}}\text{HCH}_2\text{OH}$ | 0.011 |
| TS- β_p | 0.021 | TS- α_s | 0.018 |
| $\text{CH}_3\text{CH}_2\text{C}(\dot{\text{C}}\text{H}_2)(\text{CH}_3)\text{OH}$ | 0.011 | $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\dot{\text{C}}\text{HOH}$ | 0.014 |
| TS-OH | 0.076 | TS-OH | 0.145 |
| $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\dot{\text{O}}$ | 0.016 | $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2\dot{\text{O}}$ | 0.016 |
| 2,2-Dimethyl-1-propanol+ $\text{H}\dot{\text{O}}_2$ radical | | | |
| $\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{OH}$ | 0.009 | | |
| TS- γ_p | 0.022 | | |
| $\dot{\text{C}}\text{H}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{OH}$ | 0.011 | | |
| TS- α_s | 0.017 | | |
| $\text{CH}_3\text{C}(\text{CH}_3)_2\dot{\text{C}}\text{HOH}$ | 0.014 | | |
| TS-OH | 0.064 | | |
| $\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\dot{\text{O}}$ | 0.016 | | |

Table S2

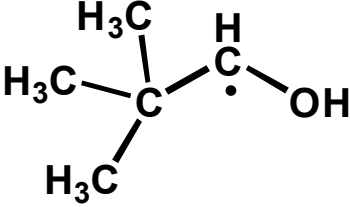
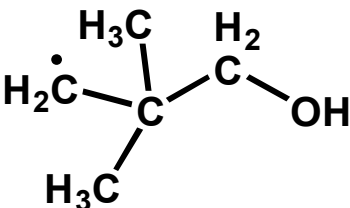
Species and structures of some reactants and products identified calculated in this work.

| Species | Molecular structure |
|---|--|
| $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{OH}$ |  |
| $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\dot{\text{O}}$ |  |
| $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\dot{\text{C}}\text{HOH}$ |  |
| $\text{CH}_3\text{CH}_2\dot{\text{C}}(\text{CH}_3)\text{CH}_2\text{OH}$ |  |
| $\text{CH}_3\text{CH}_2\text{CH}(\dot{\text{C}}\text{H}_2)\text{CH}_2\text{OH}$ |  |
| $\text{CH}_3\dot{\text{C}}\text{HCH}(\text{CH}_3)\text{CH}_2\text{OH}$ |  |

| | |
|--|--|
| $\dot{\text{C}}\text{H}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{OH}$ | |
| $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{OH}$ | |
| $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\dot{\text{O}}$ | |
| $\text{CH}_3\text{CH}_2\text{C}(\dot{\text{C}}\text{H}_2)(\text{CH}_3)\text{OH}$ | |
| $\text{CH}_3\dot{\text{C}}\text{H}\text{C}(\text{CH}_3)_2\text{OH}$ | |
| $\dot{\text{C}}\text{H}_2\text{CH}_2\text{C}(\text{CH}_3)_2\text{OH}$ | |
| $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{OH}$ | |

| | |
|---|---|
| $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\dot{\text{O}}$ |  <p>Structural formula showing a central carbon atom bonded to three methyl groups (CH₃) and a hydrogen atom (H). This central carbon is bonded to another carbon atom, which is bonded to two methyl groups (CH₃) and a hydrogen atom (H). The second carbon atom is bonded to an oxygen atom (O) with a radical dot (·).</p> |
| $\text{CH}_3\text{CH}(\text{CH}_3)\dot{\text{C}}(\text{CH}_3)\text{OH}$ |  <p>Structural formula showing a central carbon atom bonded to three methyl groups (CH₃) and a hydrogen atom (H). This central carbon is bonded to another carbon atom, which is bonded to one methyl group (CH₃) and a hydroxyl group (OH). The second carbon atom has a radical dot (·) on its central carbon.</p> |
| $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}(\dot{\text{C}}\text{H}_2)\text{OH}$ |  <p>Structural formula showing a central carbon atom bonded to three methyl groups (CH₃) and a hydrogen atom (H). This central carbon is bonded to another carbon atom, which is bonded to one methyl group (CH₃) and a hydroxyl group (OH). The second carbon atom has a radical dot (·) on its CH₂ group.</p> |
| $\text{CH}_3\dot{\text{C}}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{OH}$ |  <p>Structural formula showing a central carbon atom bonded to three methyl groups (CH₃) and a hydrogen atom (H). This central carbon has a radical dot (·) on its central carbon. It is bonded to another carbon atom, which is bonded to one methyl group (CH₃) and a hydroxyl group (OH).</p> |
| $\dot{\text{C}}\text{H}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{OH}$ |  <p>Structural formula showing a central carbon atom bonded to three methyl groups (CH₃) and a hydrogen atom (H). This central carbon is bonded to another carbon atom, which is bonded to one methyl group (CH₃) and a hydroxyl group (OH). The second carbon atom has a radical dot (·) on its CH₂ group.</p> |
| $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{OH}$ |  <p>Structural formula showing a four-carbon chain. The first carbon is bonded to three methyl groups (CH₃) and a hydrogen atom (H). The second carbon is bonded to one methyl group (CH₃) and a hydrogen atom (H). The third carbon is bonded to two hydrogen atoms (H₂). The fourth carbon is bonded to one hydrogen atom (H) and one hydroxyl group (OH).</p> |

| | |
|---|--|
| $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2\dot{\text{O}}$ | |
| $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\dot{\text{C}}\text{HOH}$ | |
| $\text{CH}_3\text{CH}(\text{CH}_3)\dot{\text{C}}\text{HCH}_2\text{OH}$ | |
| $\text{CH}_3\dot{\text{C}}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{OH}$ | |
| $\text{CH}_3\text{CH}(\dot{\text{C}}\text{H}_2)\text{CH}_2\text{CH}_2\text{OH}$ | |
| $\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{OH}$ | |
| $\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\dot{\text{O}}$ | |

| | |
|---|--|
| $\text{CH}_3\text{C}(\text{CH}_3)_2\dot{\text{C}}\text{HOH}$ |  <p>The diagram shows a central carbon atom bonded to three methyl groups (H₃C) and a CH₂OH group. The radical dot is located on the carbon atom of the CH₂OH group.</p> |
| $\dot{\text{C}}\text{H}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{OH}$ |  <p>The diagram shows a central carbon atom bonded to two methyl groups (H₃C) and two CH₂ groups. One of the CH₂ groups is bonded to an OH group. The radical dot is located on the carbon atom of the CH₂ group that is not bonded to the OH group.</p> |