The Atmospheric Oxidation of CH$_3$OOH by OH radical.

The effect of water vapor

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(Supplementary information)
Figure S1: Selected geometrical parameters (distances in Å, and angles in °) for the optimized structures of the reactants. Plain values obtained at BH&HLYP/6-311+G(2df,2p). Values in parenthesis optimized at QCISD/6-311+G(2df,2p).

Table S1: Calculated equilibrium constant ($K_{eq}$ in cm$^3$ molec$^{-1}$) computed at different Temperatures (T in Kelvin) for the formation of the CH$_3$OOH···H$_2$O, H$_2$O···OH (M1), and H$_2$O···OH (M2). The rate constants for the decomposition of the complexes into the reactants (in s$^{-1}$) are also given in each case.$^a$

<table>
<thead>
<tr>
<th></th>
<th>CH$_3$OOH···H$_2$O</th>
<th>H$_2$O···OH (M1)</th>
<th>H$_2$O···OH (M2)</th>
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<tbody>
<tr>
<td>T</td>
<td>$K_{eqa}$</td>
<td>$k_a$</td>
<td>$K_{eqb}$</td>
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$^a$
Table S2: Calculated, at different temperatures (T, in Kelvin) of the equilibrium constant ($K_{eq}$ in cm$^3$ molec$^{-1}$) for the pre-reactive complexes, tunneling factor ($\Gamma$), rate constant ($k_{uni}$ in s$^{-1}$) of the unimolecular decomposition of the reactive complexes into the products, and the bimolecular rate constant ($k_t=K_{eq} \cdot \Gamma \cdot k_{uni}$, in cm$^3$ molec$^{-1}$·s$^{-1}$) for the four elementary reactions in the oxidation of CH$_3$OOH by OH.

<table>
<thead>
<tr>
<th>T</th>
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a) Calculated according to the conventional transition state theory.
Table S3: Calculated and fitted overall rate constants ($k_{tot} = k_{5a} + k_{5b}$, in cm$^3$ molec$^{-1}$·s$^{-1}$) and branching ratios, at different temperatures (T in K) for reactions 5a and 5b ($\Gamma_{5a}$ and $\Gamma_{5b}$, in %) obtained from the calculated and fitted rate constants.

<table>
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<th>T</th>
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<th>fitted $k_{tot}$</th>
<th>Calc. $\Gamma_{5a}$</th>
<th>Calc $\Gamma_{5b}$</th>
<th>Fitted $\Gamma_{5a}$</th>
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Table S4: Kinetic equations S1 – S11 according to Scheme 2 of the main text. [M1] stands for the concentration of the M1 complex of the H$_2$O···OH

\[
d[\text{CH}_3\text{OOH}] / dt = - k_a[\text{CH}_3\text{OOH}][\text{H}_2\text{O}] + k_a[\text{CH}_3\text{OOH} \cdot \text{H}_2\text{O}] \quad \text{(S1)}
\]

\[
d[\text{H}_2\text{O}] / dt = - k_a[\text{CH}_3\text{OOH}][\text{H}_2\text{O}] + k_a[\text{CH}_3\text{OOH} \cdot \text{H}_2\text{O}] - k_b[\text{OH}][\text{H}_2\text{O}] + k_b[\text{M1}] \quad \text{(S2)}
\]

\[
d[\text{OH}] / dt = - k[\text{CH}_3\text{OOH} \cdot \text{H}_2\text{O}][\text{OH}] + k_1[\text{BCR1}] - k_b[\text{OH}][\text{H}_2\text{O}] + k_b[\text{M1}] \quad \text{(S3)}
\]

\[
d[\text{CH}_3\text{OOH} \cdot \text{H}_2\text{O}] / dt = - k[\text{CH}_3\text{OOH} \cdot \text{H}_2\text{O}][\text{OH}] + k_1[\text{BCR1}] + k_a[\text{CH}_3\text{OOH}][\text{H}_2\text{O}] - k_a[\text{CH}_3\text{OOH} \cdot \text{H}_2\text{O}] \quad \text{(S4)}
\]

\[
d[\text{H}_2\text{O} \cdot \cdot \cdot \text{OH} (\text{M1})] / dt = - k_b[\text{M1}] + k_b[\text{OH}][\text{H}_2\text{O}] + k_4[\text{BCR1}] - k_4[\text{CH}_3\text{OOH}] [\text{M1}] + k_5[\text{BCR2}] - k_5[\text{CH}_3\text{OOH}] [\text{M1}] + k_6[\text{BCR3}] - k_6[\text{CH}_3\text{OOH}] [\text{M1}] \quad \text{(S5)}
\]

\[
d[\text{BCR1}] / dt = k[\text{CH}_3\text{OOH} \cdot \text{H}_2\text{O}][\text{OH}] - k_1[\text{BCR1}] - k_2[\text{BCR2}] - k_4[\text{BCR1}] + k_4[\text{CH}_3\text{OOH}] [\text{M1}] \quad \text{(S6)}
\]

\[
d[\text{BCR2}] / dt = k_4[\text{BCR1}] - k_2[\text{BCR2}] - k_3[\text{BCR2}] + k_3[\text{BCR3}] - k_5[\text{BCR2}] + k_5*[\text{CH}_3\text{OOH}] [\text{M1}] - k_7[\text{BCR2}] - k_8*[\text{BCR2}] \quad \text{(S7)}
\]
\[ \frac{d[BCR3]}{dt} = k_3[BCR2] - k_3[BCR3] - k_6[BCR3] + k_6[CH_3OOH][M1] - k_9[BCR3] \] (S8)

\[ \frac{d[P1]}{dt} = + k_7[BCR2] \] (S9)
\[ \frac{d[P2]}{dt} = + k_8[BCR2] \] (S10)
\[ \frac{d[P3]}{dt} = + k_9[BCR3] \] (S11)

**Table S5:** Kinetic equations S12 – S25 according to Scheme 3 of the main text. [M2] stands for the concentration of the M2 complex of the H_2O···OH

\[ \frac{d[CH_3OOH]}{dt} = -ka[CH_3OOH][H_2O] + k_a[CH_3OOH··H_2O] \] (S12)
\[ \frac{d[H_2O]}{dt} = -ka[CH_3OOH][H_2O] + k_a[CH_3OOH··H_2O] - kc[H_2O][OH] + k_c[M2] \] (S13)
\[ \frac{d[OH]}{dt} = -k_1[CH_3OOH··H_2O][OH] + k_1*[BCR4] - kc[H_2O][OH] + k_c[M2] \] (S14)
\[ \frac{d[CH_3OOH··H_2O]}{dt} = -k_1[CH_3OOH··H_2O][OH] + k_1*[BCR4] + ka[CH_3OOH][H_2O] - k_a[CH_3OOH··H_2O] \] (S15)
\[ \frac{d[BCR4]}{dt} = k_1[CH_3OOH··H_2O][OH] - k_1*[BCR4] - k_2[BCR4] + k_2[BCR5] \] (S17)
\[ \frac{d[BCR7]}{dt} = k_4[BCR5] - k_4[BCR7] - k_5[BCR7] + k_5[BCR8] - k_7[BCR7] + k_7[CH_3OOH][M2] - k_12[BCR7] \] (S20)
\[ \frac{d[BCR8]}{dt} = k_5[BCR7] - k_5[BCR8] - k_8[BCR8] + k_8[CH_3OOH][M2] - k_13[BCR7] \] (S21)
\[ \frac{d[P1]}{dt} = k_10[BCR6] \] (S22)
\[ \frac{d[P2]}{dt} = k_11[BCR6] \] (S23)
\[ \frac{d[P3]}{dt} = k_12[BCR7] \] (S24)
Figure S2: Concentration of the BCR4 – BCR8 pre-reactive complexes as a function of time in the steady state regime. For the numerical integration we have used [OH]=2 x 10^6 molecule·cm⁻³, [CH₃OOH] = 6.45 x 10^10 molecule·cm⁻³, Temperatures ranging from 275 to 325 K and the water concentrations corresponding to RH of 20%, 40%, 60%, 80%, and 100% for each temperature.
Table S6: Calculated equilibrium constant ($K_{eq}$ in cm$^3$ molec$^{-1}$) computed at different Temperatures (T in Kelvin) for the formation of the complexes from scheme 2 of the main text. The rate constants for the decomposition of the complexes into the reactants (in s$^{-1}$) are also given in each case.a,b

<table>
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<tr>
<th>T</th>
<th>$K_{eq1}$</th>
<th>$K_{-1}$</th>
<th>$k_{eq4}$</th>
<th>$k_{4}$</th>
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a) Calculated according to the conventional transition state theory.
b) The corresponding values for the CH$_3$OOH + H$_2$O $\leftrightarrow$ CH$_3$OOH···H$_2$O and H$_2$O···OH $\leftrightarrow$ H$_2$O···OH (M1) are listed in Table S1.

Table S7: Calculated rate constants (in s$^{-1}$) computed at different Temperatures (T in Kelvin) for the unimolecular reactions described in Scheme 2.

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**Table S8:** Calculated equilibrium constant ($K_{eq}$ in cm$^3$ molec$^{-1}$) computed at different Temperatures (T in Kelvin) for the formation of the complexes from scheme 3 of the main text. The rate constants for the decomposition of the complexes into the reactants (in s$^{-1}$) are also given in each case.$^{\text{a,b}}$

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<th>$k_{-6}$</th>
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<td>2.77e+13</td>
<td>1.63e-20</td>
<td>9.54e+13</td>
<td>6.27e-20</td>
<td>2.48e+13</td>
<td>5.41e-20</td>
<td>2.87e+13</td>
<td>5.25e-21</td>
<td>2.95e+14</td>
</tr>
<tr>
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<td>1.65e+14</td>
<td>3.63e-20</td>
<td>4.57e+13</td>
<td>3.07e-20</td>
<td>5.39e+13</td>
<td>3.46e-21</td>
<td>4.78e+14</td>
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<tr>
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<td>3.35e-20</td>
<td>5.41e+13</td>
<td>5.17e-21</td>
<td>3.52e+14</td>
<td>1.71e-20</td>
<td>1.07e+14</td>
<td>1.40e-20</td>
<td>1.30e+14</td>
<td>1.95e-21</td>
<td>9.35e+14</td>
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</tbody>
</table>

**Table S9:** Calculated rate constants (in s$^{-1}$) computed at different Temperatures (T in Kelvin) for the unimolecular reactions described in Scheme 3.

<table>
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<tr>
<th>#</th>
<th>T</th>
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<th>$k_5$</th>
<th>$k_6$</th>
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<th>$k_8$</th>
<th>$k_9$</th>
<th>$k_{10}$</th>
<th>$k_{11}$</th>
<th>$k_{12}$</th>
<th>$k_{13}$</th>
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</thead>
<tbody>
<tr>
<td>275</td>
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<td>1.19e+11</td>
<td>4.61e+11</td>
<td>3.46e+12</td>
<td>7.83e+11</td>
<td>3.09e+12</td>
<td>3.23e+12</td>
<td>2.72e+09</td>
<td>4.12e+09</td>
<td>9.42e+07</td>
<td>8.34e+07</td>
<td></td>
</tr>
<tr>
<td>280</td>
<td>4.51e+11</td>
<td>1.06e+12</td>
<td>1.24e+11</td>
<td>4.62e+11</td>
<td>3.43e+12</td>
<td>8.06e+11</td>
<td>3.08e+12</td>
<td>3.27e+12</td>
<td>2.94e+09</td>
<td>4.33e+09</td>
<td>1.09e+08</td>
<td>9.80e+07</td>
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<tr>
<td>290</td>
<td>4.53e+11</td>
<td>1.19e+12</td>
<td>1.34e+11</td>
<td>4.63e+11</td>
<td>3.38e+12</td>
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<td>3.07e+12</td>
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<td>3.78e+09</td>
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<td>9.01e+11</td>
<td>3.07e+12</td>
<td>3.41e+12</td>
<td>3.88e+09</td>
<td>4.33e+09</td>
<td>1.57e+08</td>
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<td>9.47e+11</td>
<td>3.06e+12</td>
<td>3.48e+12</td>
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<td>4.70e+09</td>
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<tr>
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<td>4.68e+11</td>
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<td>3.57e+12</td>
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<td>5.27e+09</td>
<td>2.82e+08</td>
<td>3.35e+08</td>
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</tr>
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</table>
Table S10: Computed rate constants (in cm$^3$·molecule$^{-1}$·s$^{-1}$) for the oxidation of CH$_3$OOH by OH without water vapor and including the effect of water vapor at different relative humidity (% RH), and different temperatures (T in Kelvin)

<table>
<thead>
<tr>
<th>T (K)</th>
<th>No water</th>
<th>20%RH</th>
<th>40%RH</th>
<th>60%RH</th>
<th>80%RH</th>
<th>100%RH</th>
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<tbody>
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<td>275</td>
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<td>4.96 x 10^{-12}</td>
<td>5.07 x 10^{-12}</td>
<td>5.19 x 10^{-12}</td>
<td>5.30 x 10^{-12}</td>
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<tr>
<td>280</td>
<td>4.43 x 10^{-12}</td>
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<td>4.66 x 10^{-12}</td>
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<td>4.88 x 10^{-12}</td>
<td>5.00 x 10^{-12}</td>
</tr>
<tr>
<td>290</td>
<td>3.92 x 10^{-12}</td>
<td>4.03 x 10^{-12}</td>
<td>4.14 x 10^{-12}</td>
<td>4.25 x 10^{-12}</td>
<td>4.36 x 10^{-12}</td>
<td>4.47 x 10^{-12}</td>
</tr>
<tr>
<td>298</td>
<td>3.59 x 10^{-12}</td>
<td>3.70 x 10^{-12}</td>
<td>3.80 x 10^{-12}</td>
<td>3.91 x 10^{-12}</td>
<td>4.02 x 10^{-12}</td>
<td>4.13 x 10^{-12}</td>
</tr>
<tr>
<td>300</td>
<td>3.50 x 10^{-12}</td>
<td>3.61 x 10^{-12}</td>
<td>3.72 x 10^{-12}</td>
<td>3.83 x 10^{-12}</td>
<td>3.94 x 10^{-12}</td>
<td>4.05 x 10^{-12}</td>
</tr>
<tr>
<td>310</td>
<td>3.17 x 10^{-12}</td>
<td>3.28 x 10^{-12}</td>
<td>3.39 x 10^{-12}</td>
<td>3.49 x 10^{-12}</td>
<td>3.60 x 10^{-12}</td>
<td>3.71 x 10^{-12}</td>
</tr>
<tr>
<td>325</td>
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<td>2.97 x 10^{-12}</td>
<td>3.07 x 10^{-12}</td>
<td>3.18 x 10^{-12}</td>
<td>3.28 x 10^{-12}</td>
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</tbody>
</table>

Reaction 5a+w: CH$_3$OOH + OH (+H$_2$O) $\rightarrow$ CH$_3$O$_2$ + H$_2$O (+ H$_2$O)

<table>
<thead>
<tr>
<th>T (K)</th>
<th>No water</th>
<th>20%RH</th>
<th>40%RH</th>
<th>60%RH</th>
<th>80%RH</th>
<th>100%RH</th>
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<td>280</td>
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<td>290</td>
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<td>1.87 x 10^{-12}</td>
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<td>1.89 x 10^{-12}</td>
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<tr>
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<td>1.69 x 10^{-12}</td>
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<td>1.69 x 10^{-12}</td>
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<tr>
<td>310</td>
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<td>1.51 x 10^{-12}</td>
<td>1.52 x 10^{-12}</td>
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<td>1.25 x 10^{-12}</td>
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<td>1.30 x 10^{-12}</td>
<td>1.31 x 10^{-12}</td>
<td>1.32 x 10^{-12}</td>
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</table>

Reaction 5b+w: CH$_3$OOH + OH (+H$_2$O) $\rightarrow$ CH$_2$OOH + H$_2$O (+ H$_2$O)

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<th>T (K)</th>
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<th>20%RH</th>
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<td>6.26 x 10^{-12}</td>
<td>6.38 x 10^{-12}</td>
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<tr>
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<td>5.62 x 10^{-12}</td>
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Table S11. Increase (in percent) of the rate constant of Reaction 5a at different temperatures (T in Kelvin), and relative humidity (%RH).
Table S12. Increase (in percent) of the rate constant of Reaction 2 at different temperatures (T in Kelvin), and relative humidity (%RH).

<table>
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<th>100%RH</th>
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<td>0.99</td>
<td>1.32</td>
<td>1.65</td>
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<tr>
<td>280.00</td>
<td>0.39</td>
<td>0.78</td>
<td>1.17</td>
<td>1.56</td>
<td>1.95</td>
</tr>
<tr>
<td>290.00</td>
<td>0.52</td>
<td>1.03</td>
<td>1.55</td>
<td>2.07</td>
<td>2.58</td>
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<td>1.79</td>
<td>2.39</td>
<td>2.99</td>
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<tr>
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<td>1.26</td>
<td>1.89</td>
<td>2.52</td>
<td>3.15</td>
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<tr>
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<tr>
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<td>2.25</td>
<td>3.37</td>
<td>4.49</td>
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Table S13. Increase (in percent) of the rate constant of Reaction 1 plus Reaction 2 at different temperatures (T in Kelvin), and relative humidity (%RH).

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<th>60%RH</th>
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<th>100%RH</th>
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<td>7.35</td>
<td>9.18</td>
</tr>
<tr>
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<td>4.17</td>
<td>6.26</td>
<td>8.33</td>
<td>10.41</td>
</tr>
<tr>
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<td>11.34</td>
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<td>300.00</td>
<td>2.33</td>
<td>4.66</td>
<td>6.99</td>
<td>9.30</td>
<td>11.61</td>
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<td>7.75</td>
<td>10.32</td>
<td>12.88</td>
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<td>6.03</td>
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### Table S14. Absolute energies, enthalpy and free energy corrections (in hartree) and ZPE (in Kcal/mol) and S (in Cal/Mol·Kelvin) \(^{a,b}\)

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<td>64.3</td>
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</tr>
</tbody>
</table>

\(^{a}\) Geometries optimized and characterized at QCISD/6-311+G(2df,2p). The ZPE and enthalpic and entropic corrections are obtained at this level of theory.

\(^{b}\) B1 stands for aug-cc-pVTZ; B2 stands for aug-cc-pVQZ basis sets.
Table S15. Absolute energies, enthalpy and free energy corrections (in hartree) and ZPE (in Kcal/mol) and S (in Cal/Mol·Kelvin) a,b

<table>
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<tr>
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a) Geometries optimized and characterized at BH&HLYP/6-311+G(2df,2p). The ZPE and enthalpic and entropic corrections are obtained at this level of theory.

b) B1 stands for aug-cc-pVTZ; B2 stands for aug-cc-pVQZ basis sets.
**Table S16.** Cartesian coordinates (in Å) optimized at QCISD(6-311+G(2df,2p)

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**ATS1b**

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Table S17 Cartesian coordinates (in Å) optimized at BH&HLYP/6-311+G(2df,2p)

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H     0.869295    -1.080552    -0.888216

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ATS1b

H  0.356297   0.016805   0.005209
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ATS2a

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ACP2

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CH₃OOH···H₂O

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H  0.232599  -1.758560  -0.762530
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TSBCR1BCR2

C -0.104997  0.167100  0.020481
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| H  | -0.863008 | 1.695593 | 3.987062 |
| O  | -0.043145 | 0.126410 | 4.489544 |
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O  -0.735518  -0.397870  -2.277981
H  -0.266901  -1.213974  -2.024558
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