Dynamics of the $\text{O} + \text{H}_2^+ \rightarrow \text{OH}^+ + \text{H}, \text{OH} + \text{H}^+$ proton and hydrogen atom transfer reactions on the two lowest potential energy surfaces

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Table S1. Cross sections

| Property | $v_0=0$ | $v_0=1$ |
|----------|---------|---------|
| $E_{col}$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ |
| $\sigma$ (Å$^2$) | 181.3 | 60.8 | 41.4 | 182.6 | 62.1 | 41.3 | 181.3 | 60.0 | 39.8 | 167.9 | 58.6 | 39.7 | 175.3 | 60.2 | 40.2 | 175.1 | 58.2 | 38.8 |
| $b_{max}$/Å | 7.81 | 4.86 | 4.01 | 7.73 | 4.93 | 4.11 | 7.73 | 4.93 | 4.08 | 7.84 | 4.89 | 4.05 | 7.74 | 4.98 | 4.15 | 7.74 | 4.96 | 4.09 |
| Probability | 0.95 | 0.82 | 0.82 | 0.97 | 0.81 | 0.78 | 0.97 | 0.79 | 0.76 | 0.87 | 0.78 | 0.77 | 0.93 | 0.77 | 0.74 | 0.93 | 0.75 | 0.74 |

Table S2. Average energy fractions

| Property | $v_0=0$ | $v_0=1$ |
|----------|---------|---------|
| $E_{col}$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ |
| $<f_T>$ | 0.23 | 0.25 | 0.26 | 0.21 | 0.25 | 0.25 | 0.21 | 0.23 | 0.24 | 0.21 | 0.22 | 0.23 | 0.20 | 0.22 | 0.22 | 0.19 | 0.21 | 0.21 |
| $<f_V>$ | 0.52 | 0.50 | 0.50 | 0.53 | 0.50 | 0.50 | 0.54 | 0.52 | 0.51 | 0.56 | 0.55 | 0.56 | 0.56 | 0.54 | 0.55 | 0.58 | 0.55 | 0.55 |
| $<f_R>$ | 0.25 | 0.25 | 0.24 | 0.26 | 0.25 | 0.25 | 0.25 | 0.25 | 0.25 | 0.23 | 0.22 | 0.24 | 0.24 | 0.24 | 0.23 | 0.23 | 0.24 | 0.24 |

| $E_{col}$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ | $0.05$ | $0.25$ | $0.50$ |
| $<f_T>$ | 0.30 | 0.30 | 0.34 | 0.29 | 0.30 | 0.32 | 0.29 | 0.30 | 0.30 | 0.28 | 0.30 | 0.32 | 0.28 | 0.30 | 0.31 | 0.29 | 0.29 | 0.30 |
| $<f_V>$ | 0.41 | 0.41 | 0.38 | 0.42 | 0.40 | 0.38 | 0.42 | 0.40 | 0.39 | 0.44 | 0.42 | 0.40 | 0.44 | 0.40 | 0.40 | 0.43 | 0.41 | 0.40 |
| $<f_R>$ | 0.29 | 0.29 | 0.28 | 0.29 | 0.30 | 0.30 | 0.29 | 0.30 | 0.31 | 0.28 | 0.28 | 0.28 | 0.28 | 0.30 | 0.29 | 0.28 | 0.30 | 0.30 |
Table S3. Average properties of the J, l' and j’ vectors for H$_2^+$(v=0, j=0)

Ground PES (1$^2$A$''$)

| $E_{\text{col}}$/eV | 0.05  | 0.15  | 0.30  | 0.50  |
|---------------------|-------|-------|-------|-------|
| $<\cos(J l')>$     | 0.267 | 0.382 | 0.413 | 0.444 |
| $\langle \frac{l'}{J} \rangle$ | 0.729 | 0.591 | 0.566 | 0.516 |
| $<\cos(Jj')>$      | 0.770 | 0.838 | 0.857 | 0.886 |
| $\langle \frac{j'}{J} \rangle$ | 1.093 | 0.994 | 0.969 | 0.955 |
| $<\cos(l'j')>$     | $-1.0 \times 10^{-2}$ | $-8.6 \times 10^{-3}$ | $4.2 \times 10^{-3}$ | $-6.2 \times 10^{-3}$ |
| $\langle \frac{l'}{j'} \rangle$ | 0.850 | 0.717 | 0.711 | 0.633 |

Excited PES (1$^2$A$'$)

| $E_{\text{col}}$/eV | 0.05  | 0.15  | 0.30  | 0.50  |
|---------------------|-------|-------|-------|-------|
| $<\cos(J l')>$     | 0.218 | 0.219 | 0.268 | 0.373 |
| $\langle \frac{l'}{J} \rangle$ | 0.982 | 0.696 | 0.574 | 0.487 |
| $<\cos(Jj')>$      | 0.658 | 0.802 | 0.868 | 0.894 |
| $\langle \frac{j'}{J} \rangle$ | 1.241 | 1.110 | 1.065 | 0.994 |
| $<\cos(l'j')>$     | $-3.5 \times 10^{-4}$ | $-5.7 \times 10^{-3}$ | $-2.6 \times 10^{-3}$ | $-8.0 \times 10^{-3}$ |
| $\langle \frac{l'}{j'} \rangle$ | 1.183 | 0.810 | 0.608 | 0.535 |
Figure S1

Product vibrational distributions

Ground PES ($1^2A''$)

Excited PES ($1^2A'$)
Figure S2

Product rotational distributions

Ground PES (1^2A'')

|       | 0.05 eV | 0.25 eV | 0.50 eV |
|-------|---------|---------|---------|
| v=0 j=0 | ![Graph](image1) | ![Graph](image2) | ![Graph](image3) |
| v=0 j=2 | ![Graph](image4) | ![Graph](image5) | ![Graph](image6) |
| v=0 j=4 | ![Graph](image7) | ![Graph](image8) | ![Graph](image9) |
| v=1 j=0 | ![Graph](image10) | ![Graph](image11) | ![Graph](image12) |
Figure S2 (cont.)

Product rotational distributions

Excited PES (1^2A')
Figure S3

Angular distributions (kk’)

Ground PES ($1^2\text{A}''$)

| Energy (eV) | 0.05 eV | 0.25 eV | 0.50 eV |
|------------|---------|---------|---------|
| $\Delta^2$ PES, Ecol = 0.05 eV | ![Graph](image1.png) | ![Graph](image2.png) | ![Graph](image3.png) |
| $\Delta^2$ PES, Ecol = 0.25 eV | ![Graph](image4.png) | ![Graph](image5.png) | ![Graph](image6.png) |
| $\Delta^2$ PES, Ecol = 0.50 eV | ![Graph](image7.png) | ![Graph](image8.png) | ![Graph](image9.png) |

Excited PES ($1^2\text{A}'$)

| Energy (eV) | 0.05 eV | 0.25 eV | 0.50 eV |
|------------|---------|---------|---------|
| $\Delta^2$ PES, Ecol = 0.05 eV | ![Graph](image10.png) | ![Graph](image11.png) | ![Graph](image12.png) |
| $\Delta^2$ PES, Ecol = 0.25 eV | ![Graph](image13.png) | ![Graph](image14.png) | ![Graph](image15.png) |
| $\Delta^2$ PES, Ecol = 0.50 eV | ![Graph](image16.png) | ![Graph](image17.png) | ![Graph](image18.png) |
Figure S4

Angular distributions (kj')

Ground PES (1^2A'')

| Energy (eV) | Plot |
|------------|------|
| 0.05       | ![Plot](image1) |
| 0.25       | ![Plot](image2) |
| 0.50       | ![Plot](image3) |

Excited PES (1^2A')

| Energy (eV) | Plot |
|------------|------|
| 0.05       | ![Plot](image4) |
| 0.25       | ![Plot](image5) |
| 0.50       | ![Plot](image6) |
Figure S5

Angular distributions (k’j’)

Ground PES (1^2A'')

| 0.05 eV | 0.25 eV | 0.50 eV |
|---------|---------|---------|
| ![Graph](image) | ![Graph](image) | ![Graph](image) |

Excited PES (1^2A')

| 0.05 eV | 0.25 eV | 0.50 eV |
|---------|---------|---------|
| ![Graph](image) | ![Graph](image) | ![Graph](image) |
Figure S6

Angular distributions (kk’j’)

Ground PES (1^2A'')

| Energy (eV) | Angle Distribution |
|------------|--------------------|
| 0.05 eV    | ![Diagram](image)  |
| 0.25 eV    | ![Diagram](image)  |
| 0.50 eV    | ![Diagram](image)  |

Excited PES (1^2A')

| Energy (eV) | Angle Distribution |
|------------|--------------------|
| 0.05 eV    | ![Diagram](image)  |
| 0.25 eV    | ![Diagram](image)  |
| 0.50 eV    | ![Diagram](image)  |
Allowed vector modules of the couple \((l', j')\) for the average \(J\) value* and \(H_2^+(v=0, j=0)\)

**Ground PES \(1^2\)A''**

**Excited PES \(1^2\)A'**

*The average \(J\) values for \(E_{col} = 0.05, 0.15, 0.30\) and 0.50 eV are the following (units of \(\hbar\)): 33.3, 41.2, 45.6 and 51.5, respectively (ground PES) and 18.4, 27.4, 35.7 and 43.3, respectively (excited PES).
Movie 1

Time evolution of an example of direct reactive trajectory (mpg file, 65 kB).

Movie 2

As movie 1 but for a non-direct reactive trajectory (mpg file, 163 kB).

Movie 3

As movie 1 but for a collision-complex forming reactive trajectory (mpg file, 163 kB).