Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for "**Reactive Quenching of NO ($A^2\Sigma^+$) with H_2O Leads to HONO: A Theoretical Analysis of the Reactive and Nonreactive Electronic Quenching Mechanisms**"

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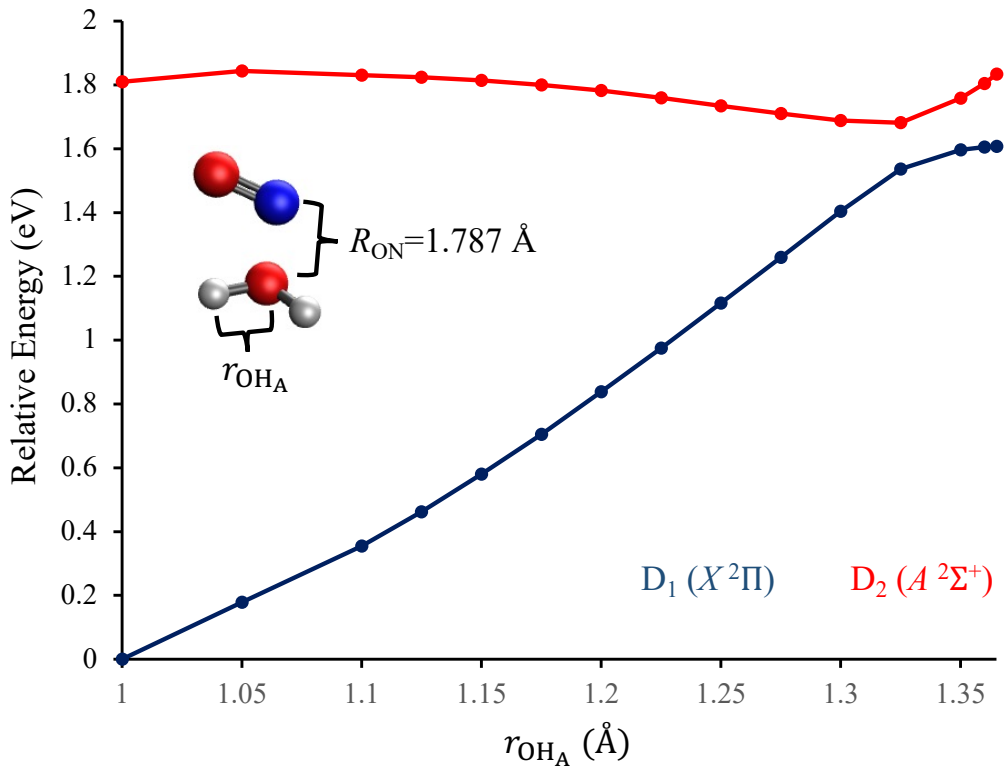

Figure S1. Cuts of the adiabatic PESs for NO+H_2O as a function of the O-H bond length that is nearly perpendicular to the NO, r_{OH_A} at a fixed R_{ON} = 1.787 Å. The geometries are the same as in Figure 10. The energies were calculated using (9,9) NEVPT2/aug-cc-pVTZ. These calcualtions were built off a CASSCF refence wave function with a 9 electrons in 9 orbitals active space and a state-averaging over 3 states. Dynamic electron correlation was included using N-electron valence state perturbation theory. The energies are reported relative to that of D_1 at r_{OH_A}=1.0 Å. The calculations were performed using ORCA 5.0.3.[1,2]

The cuts of the PESs shown above are similar to those presented in Figure 10. Specifically, the energy of the D_1 state increases rapidly as r_{OH_A} increases. In contrast, the energy of D_2 exhibits a much weaker dependence on r_{OH_A}, slightly increasing and then decreasing as the bond is stretched. The D_1 and D_2 electronic states grow closer together as r_{OH_A} increases. Finally, at $r_{OH_A} = 1.0$ Å, $E_{D_2} - E_{D_1}$ is 1.81 eV at the (9,9) NEVPT2/aug-cc-pVTZ level of theory versus 1.90 eV at the EOM-EA-CCSD/aug-cc-pVTZ level of theory.

Figures 10 and S1 are not in perfect agreement. The D_2 PES reaches a maximum at a significantly smaller value of r_{OH_A} for (9,9) NEVPT2/aug-cc-pVTZ than for EOM-EA-CCSD/aug-cc-pVTZ. Moreover, Figure S1 does not exhibit a conical intersection but rather an avoided crossing, which we confirmed by analyzing the electronic character of the adiabats above and below $r_{OH_A} = 1.35$ Å. Because $E_{D_2} - E_{D_1}$ is strongly affected by both R_{ON} and r_{OH_A}, the data in Figure S1 suggests that a D_2-D_1 conical intersection exists at the (9,9) NEVPT2/aug-cc-pVTZ level of theory but at a slightly different value of R_{ON}.

Overall, the application of multireference electronic structure methods does not fundamentally

change the mechanistic picture from that presented in Figure 10. Increasing $r_{\mathrm{OH_A}}$ is feasible on D_2 because it does not significantly increase E_{D_2}. Moreover, stretching this O-H bond significantly reduces the D_2-D_1 energy gap. Figure S1 displays an avoided crossing between D_2 and D_1, with a D_2-D_1 conical intersection likely occurring at a slightly different value of R_{ON}.

Finally, it is worth noting that Figure S1 is not necessarily more accurate than Figure 10. While a multireference approach was used in Figure S1, dynamic electron correlation was only approximately captured via second-order perturbation theory. EOM-EA-CCSD includes higher-order dynamic electron correlation for states which have dominant single-excitation character from the reference. As discussed in the main text, we verified that this is true for all of the states considered in this study.

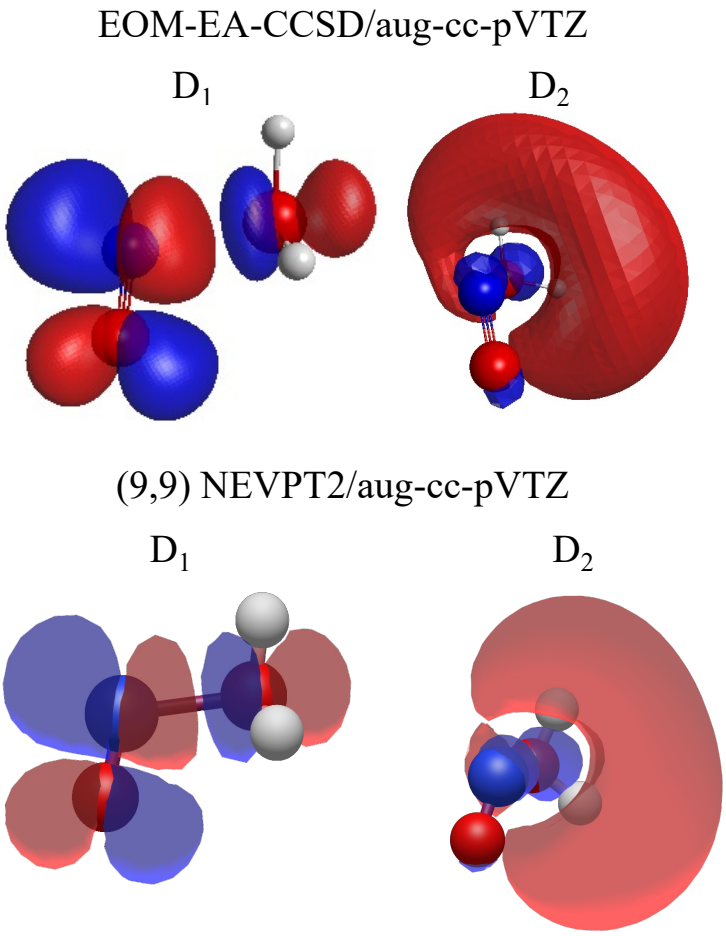

Figure S2. Singly occuppied molecular orbitals (SOMOs) of D_1 and D_2 as calculated using the EOM-EA-CCSD/aug-cc-pVTZ and (9,9) NEVPT2/aug-cc-pVTZ levels of theory at an EOM-EA-CCSD/aug-cc-pVTZ optimized geometry with R_{ON}=1.787 Å and $r_{\mathrm{OH_A}} = 1.0$ Å. For the EOM-EA-CCSD data, the SOMOs were obtained using natural transition orbital analysis and plotted using wxMacMolPlt.[3,4] For the (9,9) NEVPT2/aug-cc-pVTZ data, the SOMOs were plotted using Avogadro.[5] Note that the electronic characters of D_1 and D_2 are identical for both methods. In particular, the SOMO for the D_2 state is consistent with electron transfer from the NO and to the H_2O.

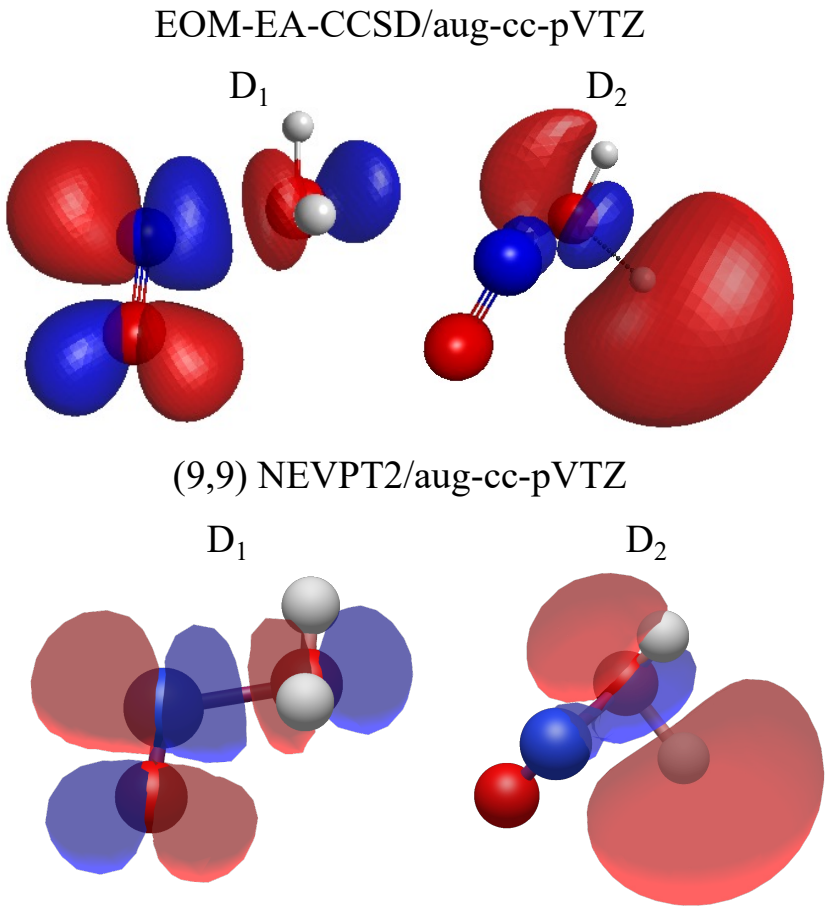

Figure S3. Singly occuppied molecular orbitals (SOMOs) of D_1 and D_2 as calculated using the EOM-EA-CCSD/aug-cc-pVTZ and (9,9) NEVPT2/aug-cc-pVTZ levels of theory at an EOM-EA-CCSD/aug-cc-pVTZ optimized geometry with R_{ON}=1.787 Å and $r_{OH_A} = 1.30$ Å. For the EOM-EA-CCSD data, the SOMOs were obtained using natural transition orbital analysis and plotted using wxMacMolPlt.[3,4] For the (9,9) NEVPT2/aug-cc-pVTZ data, the SOMOs were plotted using Avogadro.[5] Note that the electronic characters of D_1 and D_2 are identical for both methods. In particular, the SOMO for the D_2 state is consistent with electron transfer from the NO and to the H_2O.

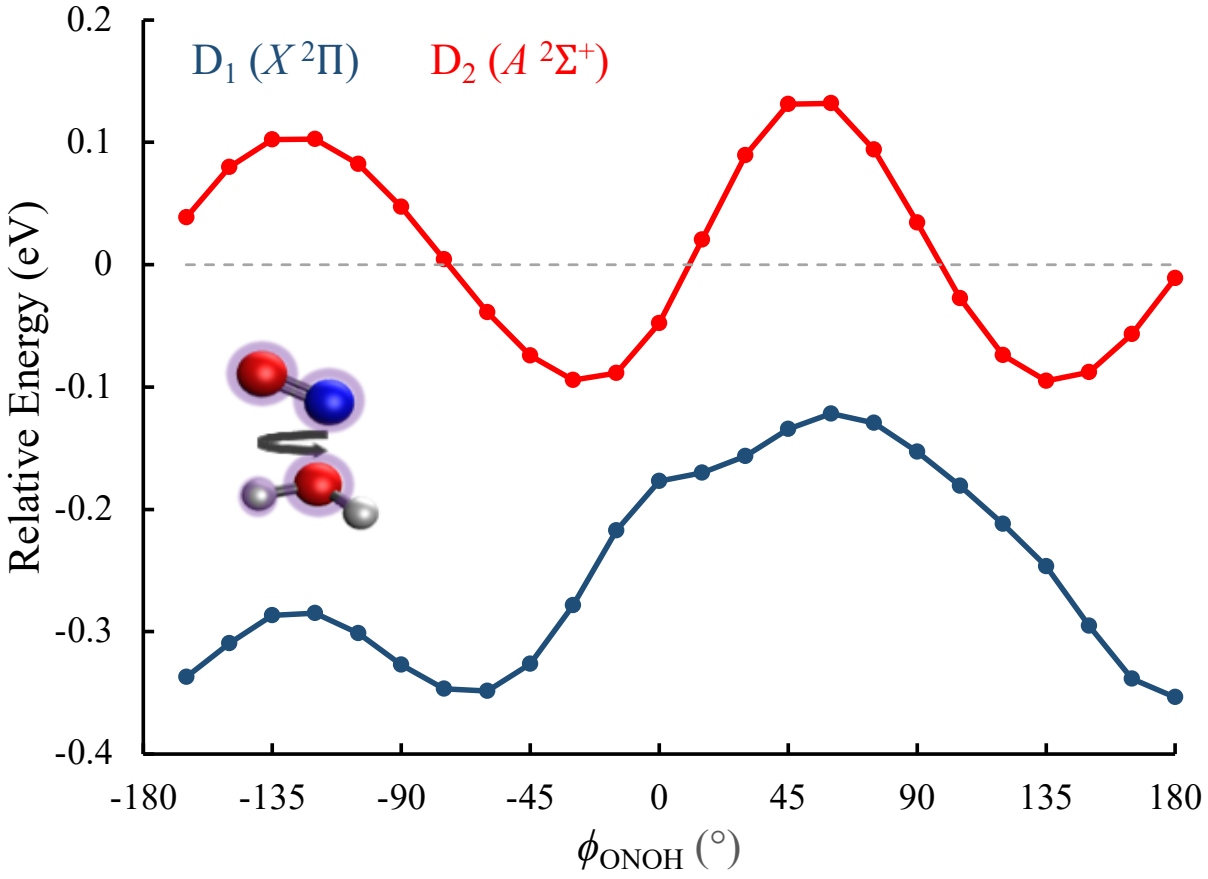

Figure S4. Cuts of the adiabatic PESs of the D_2 ($A^2\Sigma^+$) and D_1 ($X^2\Pi$) states for ON+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 1.56 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

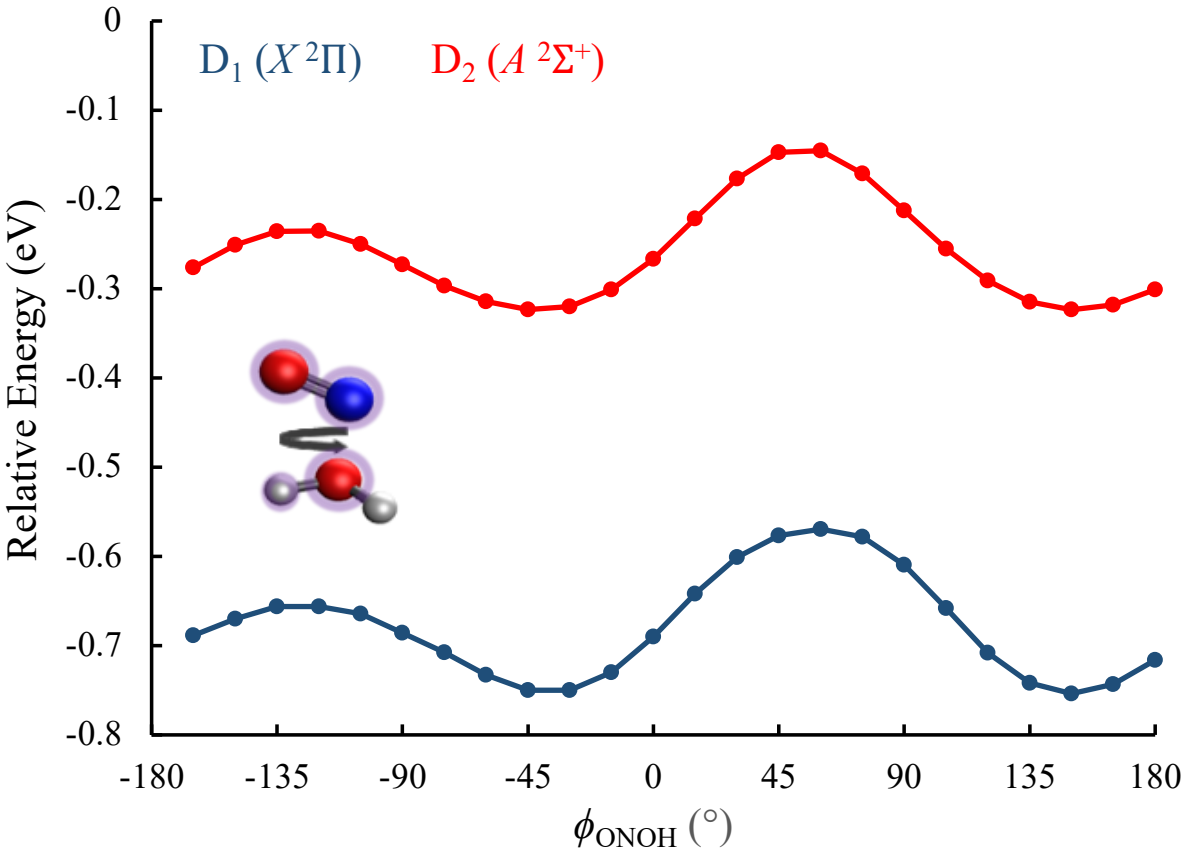

Figure S5: Cuts of the adiabatic PESs of the D_2 ($A^2\Sigma^+$) and D_1 ($X^2\Pi$) states for ON+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 1.61 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

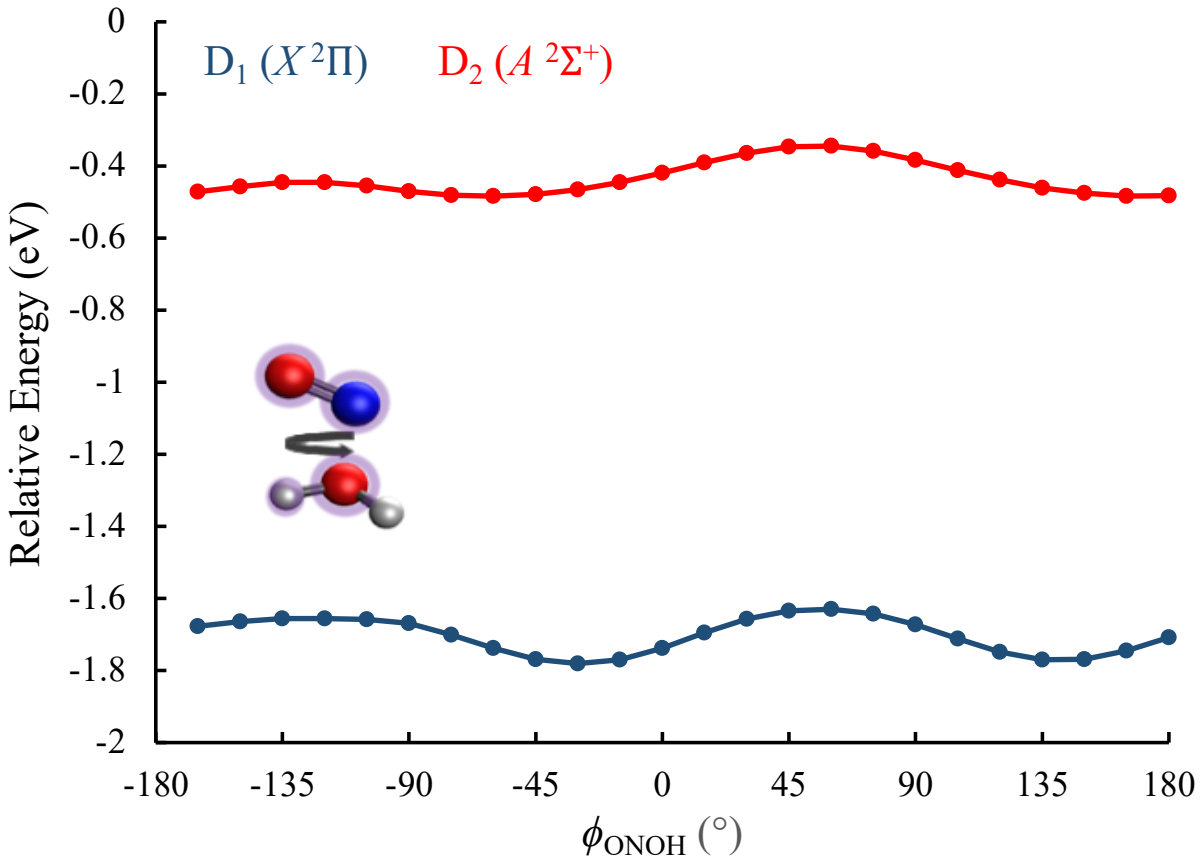

Figure S6: Cuts of the adiabatic PESs of the D_2 ($A^2\Sigma^+$) and D_1 ($X^2\Pi$) states for ON+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 1.71 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

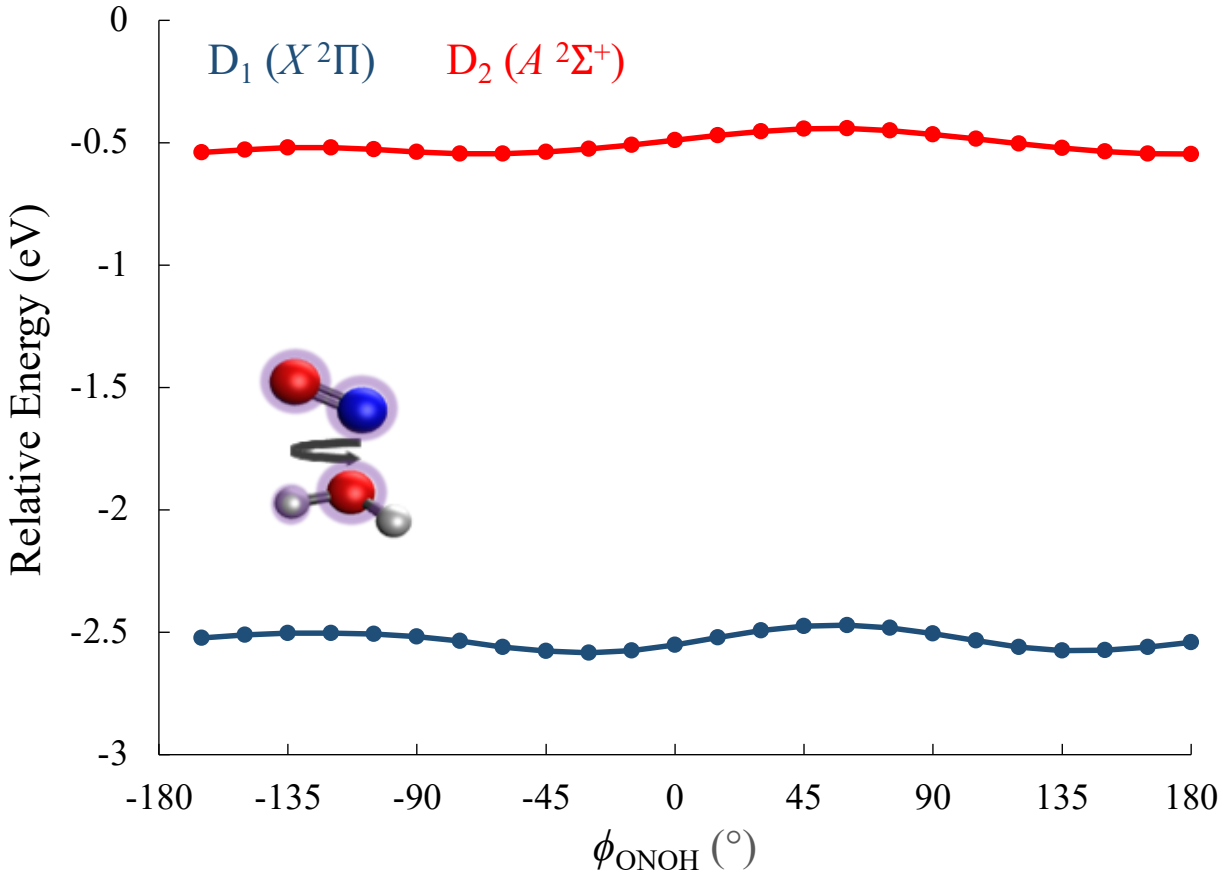

Figure S7: Cuts of the adiabatic PESs of the D_2 ($A^2\Sigma^+$) and D_1 ($X^2\Pi$) states for ON+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 1.81 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

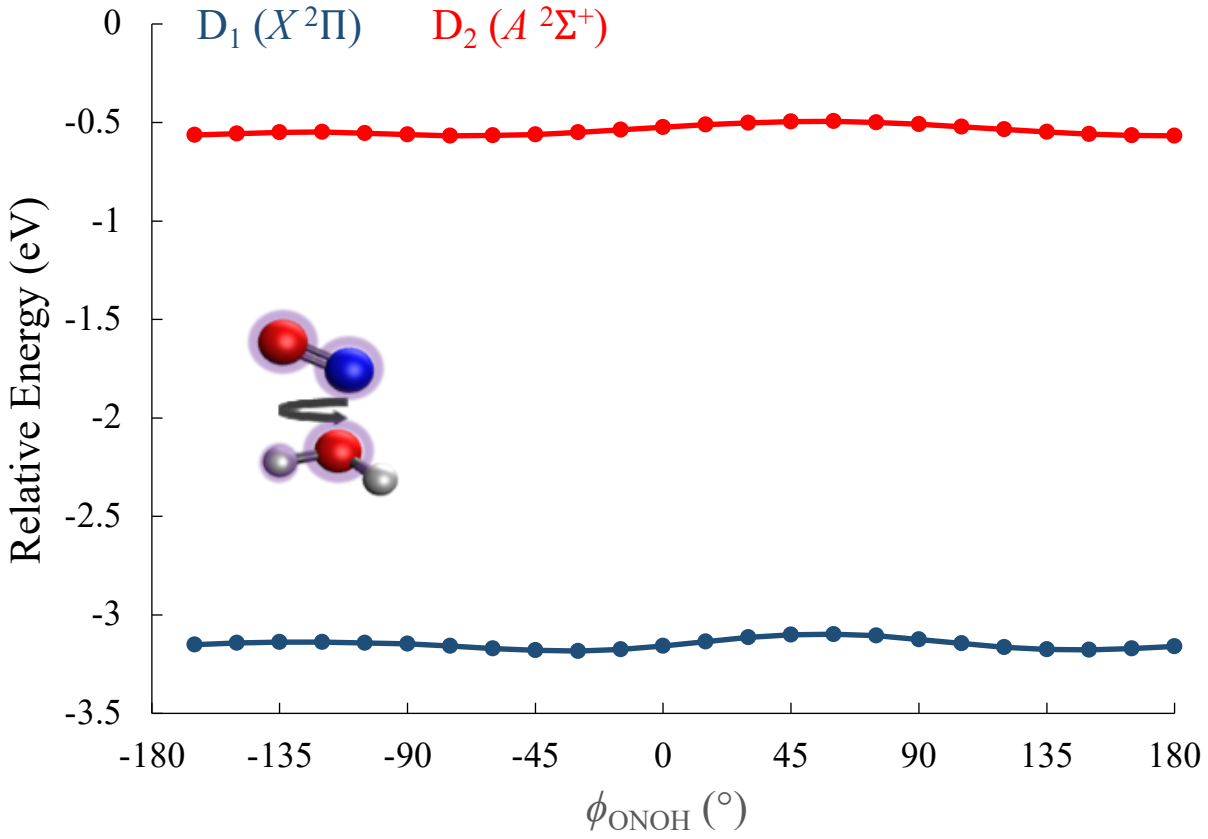

Figure S8: Cuts of the adiabatic PESs of the D_2 ($A^2\Sigma^+$) and D_1 ($X^2\Pi$) states for ON+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 1.91 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

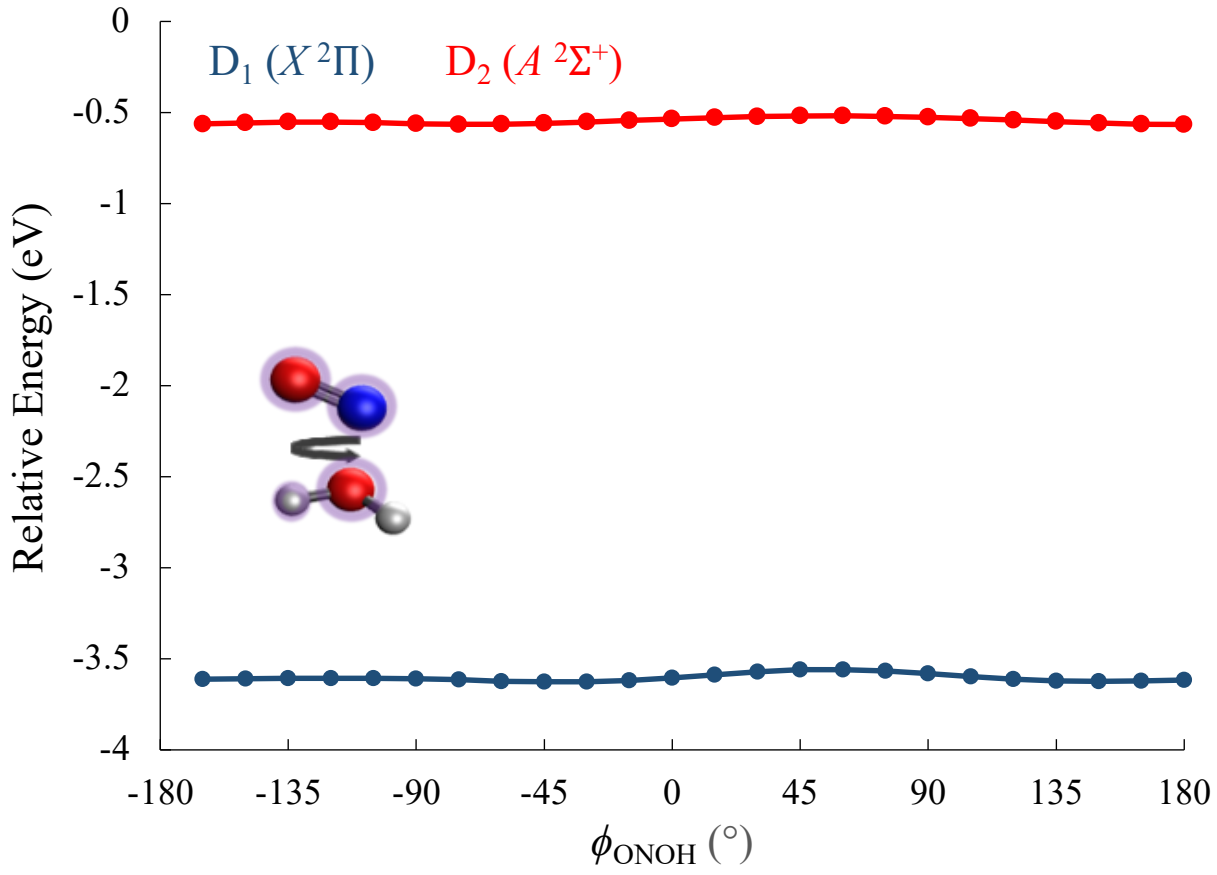

Figure S9: Cuts of the adiabatic PESs of the D_2 ($A^2\Sigma^+$) and D_1 ($X^2\Pi$) states for ON+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 2.01 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

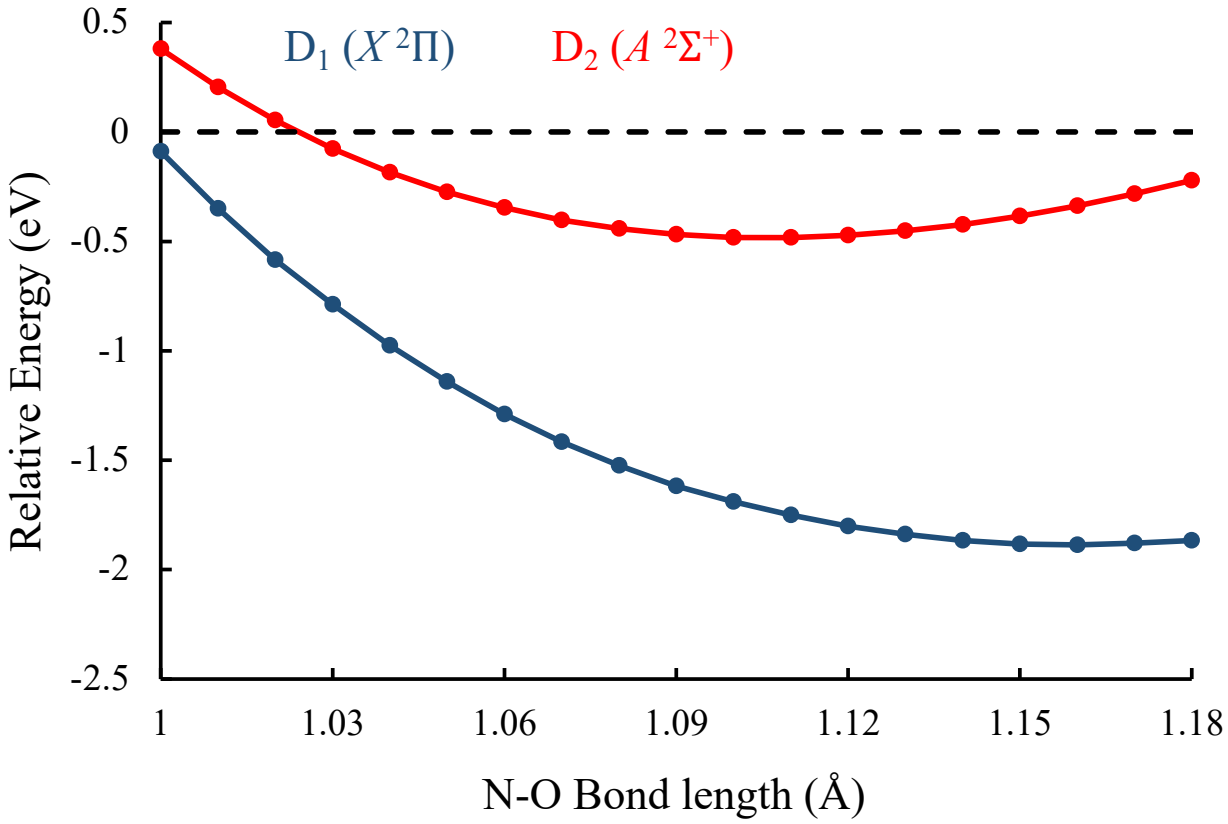

Figure S10: Cuts of the adiabatic PESs of the D_1 ($X^2\Pi$) and D_2 ($A^2\Sigma^+$) states for $NO+H_2O$ as a function of N-O bond length at a fixed intermolecular distance R_{ON} = 1.71 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

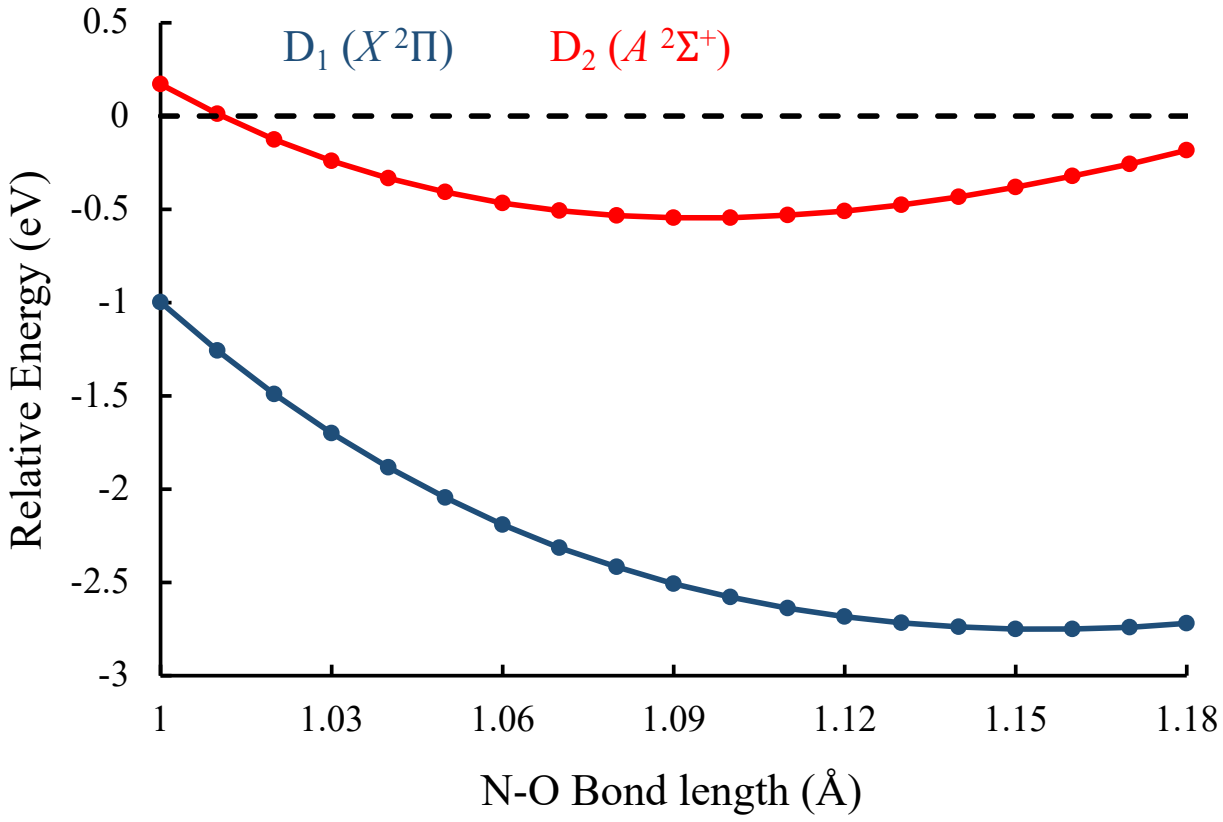

Figure S11: Cuts of the adiabatic PESs of the D_1 ($X^2\Pi$) and D_2 ($A^2\Sigma^+$) states for NO+H_2O as a function of N-O bond length at a fixed intermolecular distance R_{ON} = 1.81 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

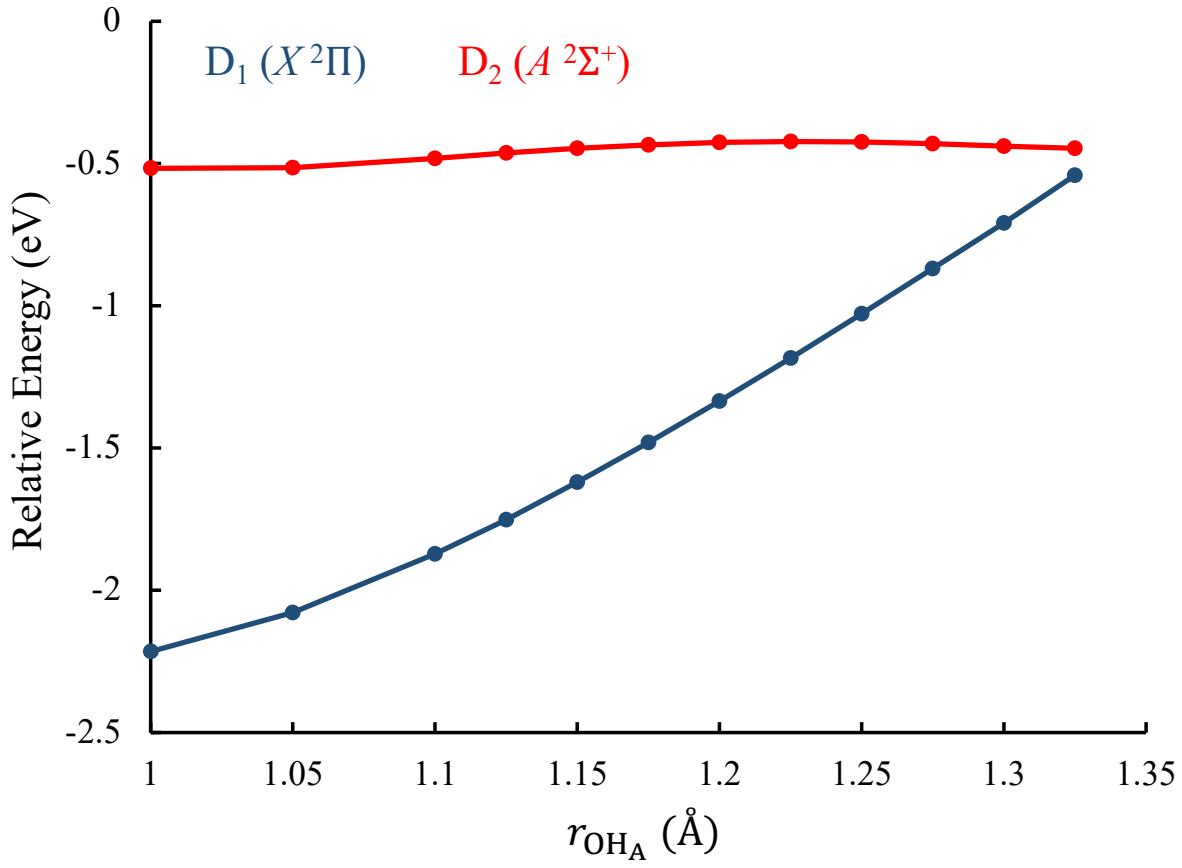

Figure S12. Cuts of the adiabatic PESs of the D_1 ($X^2\Pi$) and D_2 ($A^2\Sigma^+$) states for NO+H_2O as a function of the O-H bond length that is nearly perpendicular to the NO, r_{OH_A} at a fixed R_{ON} = 1.76 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

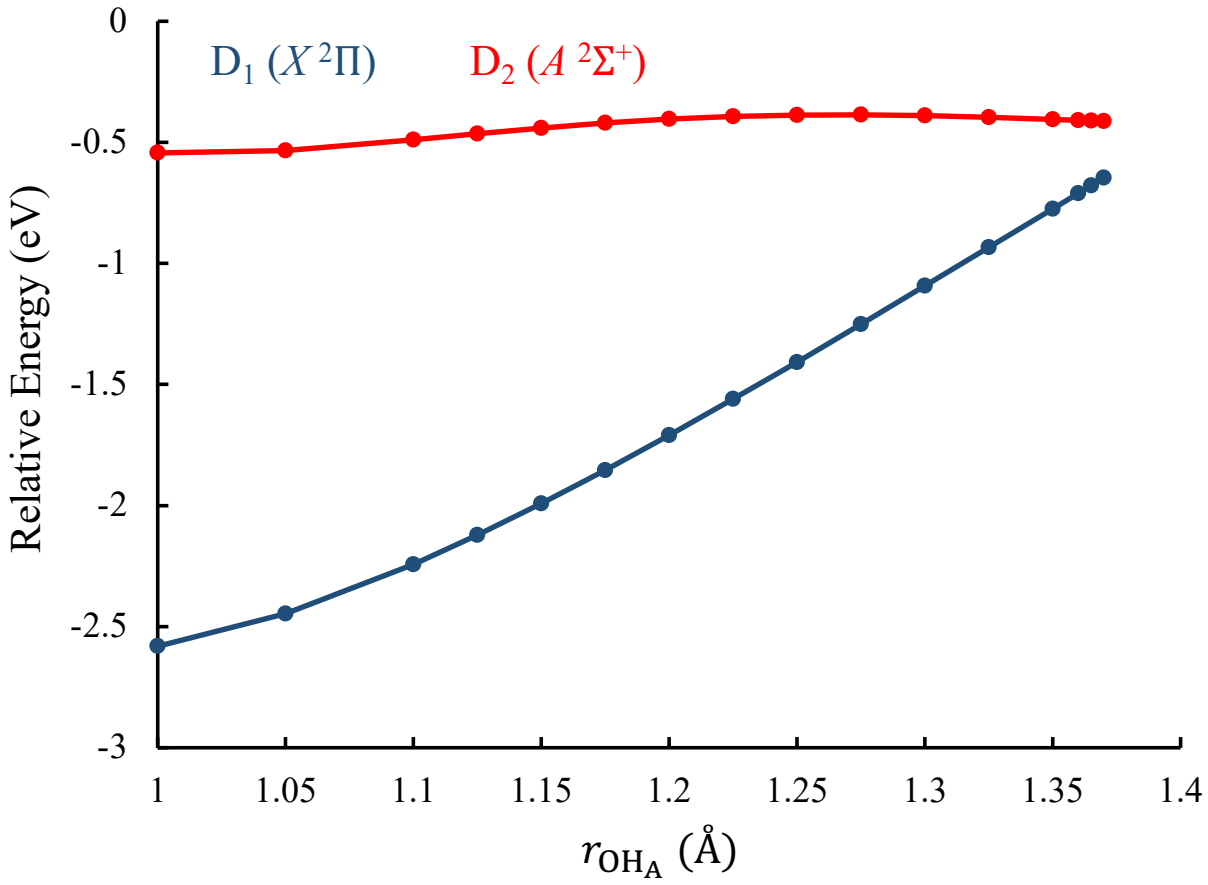

Figure S13. Cuts of the adiabatic PESs of the D_1 ($X^2\Pi$) and D_2 ($A^2\Sigma^+$) states for NO+H_2O as a function of the O-H bond length that is nearly perpendicular to the NO, r_{OH_A} at a fixed R_{ON} = 1.81 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

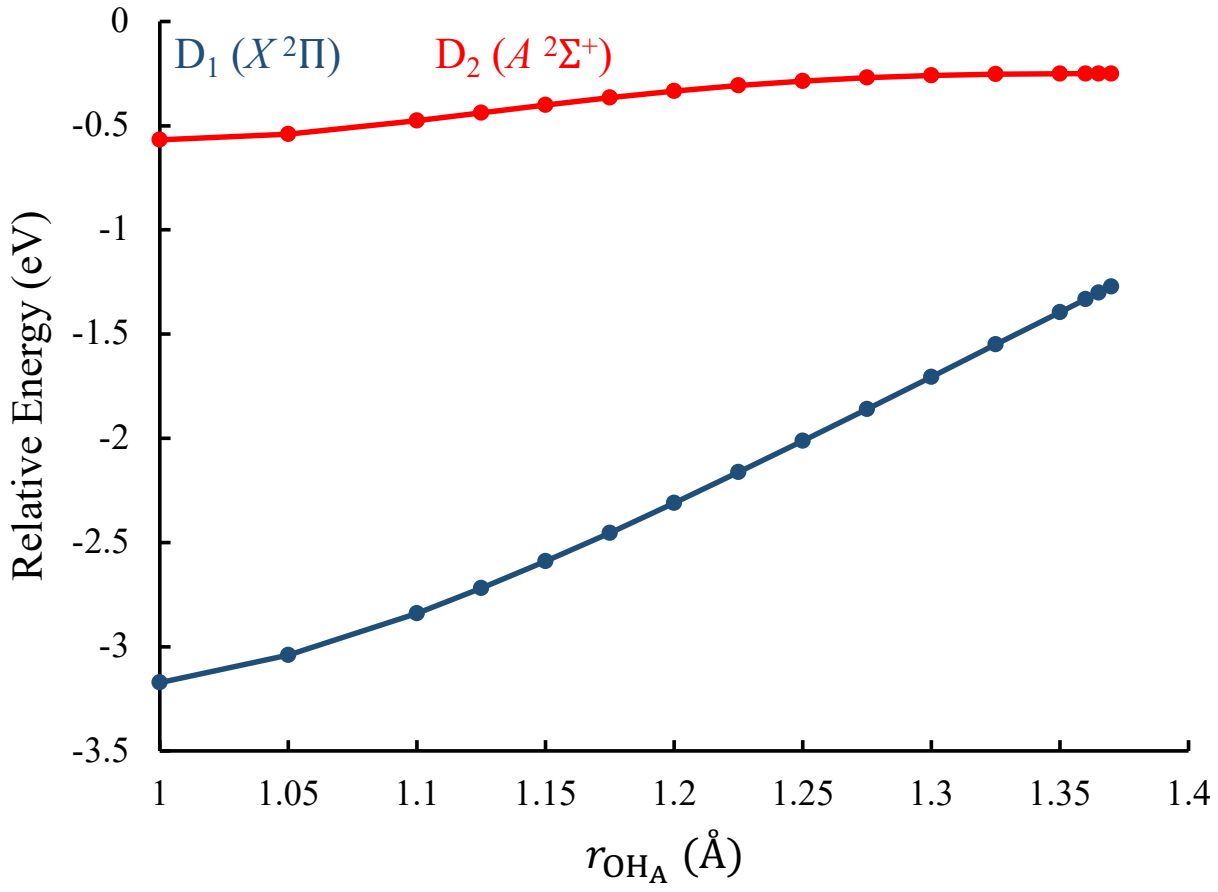

Figure S14. Cuts of the adiabatic PESs of the D_1 ($X^2\Pi$) and D_2 ($A^2\Sigma^+$) states for $NO+H_2O$ as a function of the O-H bond length that is nearly perpendicular to the NO, r_{OH_A} at a fixed R_{ON} = 1.91 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

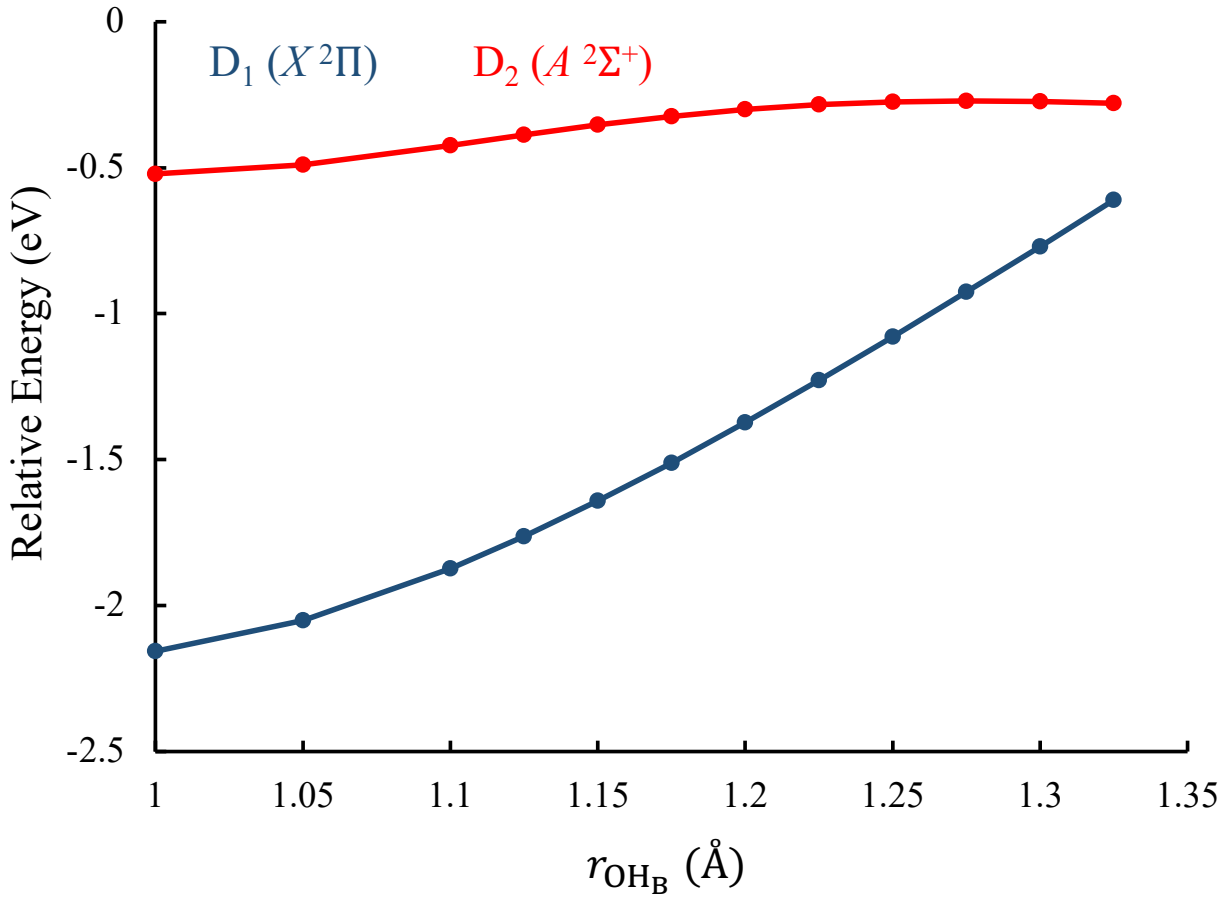

Figure S15. Cuts of the adiabatic PESs of the D_1 ($X^2\Pi$) and D_2 ($A^2\Sigma^+$) states for NO+H_2O as a function of the O-H bond length that is nearly parallel to the NO, r_{OH_B} at a fixed R_{ON} = 1.76 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

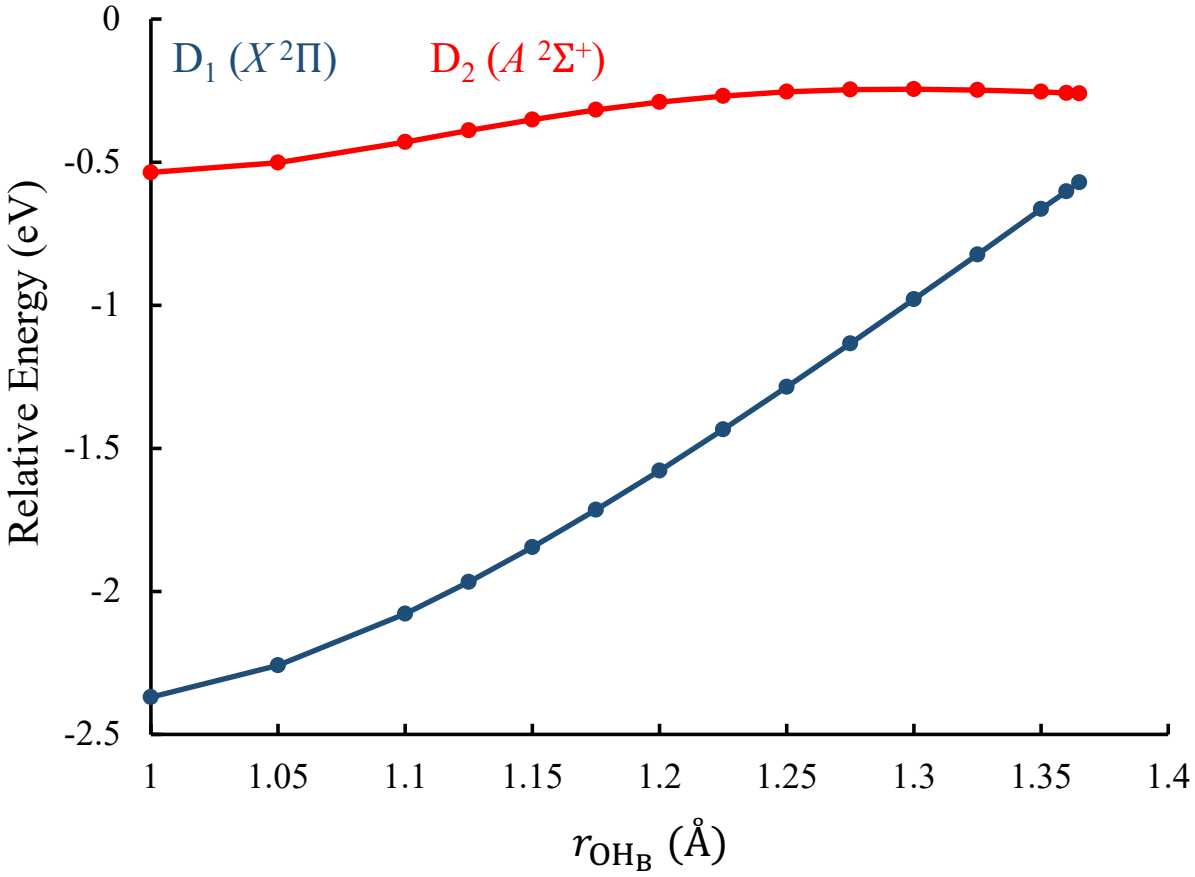

Figure S16. Cuts of the adiabatic PESs of the D_1 ($X^2\Pi$) and D_2 ($A^2\Sigma^+$) states for NO+H_2O as a function of the O-H bond length that is nearly parallel to the NO, r_{OH_B} at a fixed R_{ON} = 1.787 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

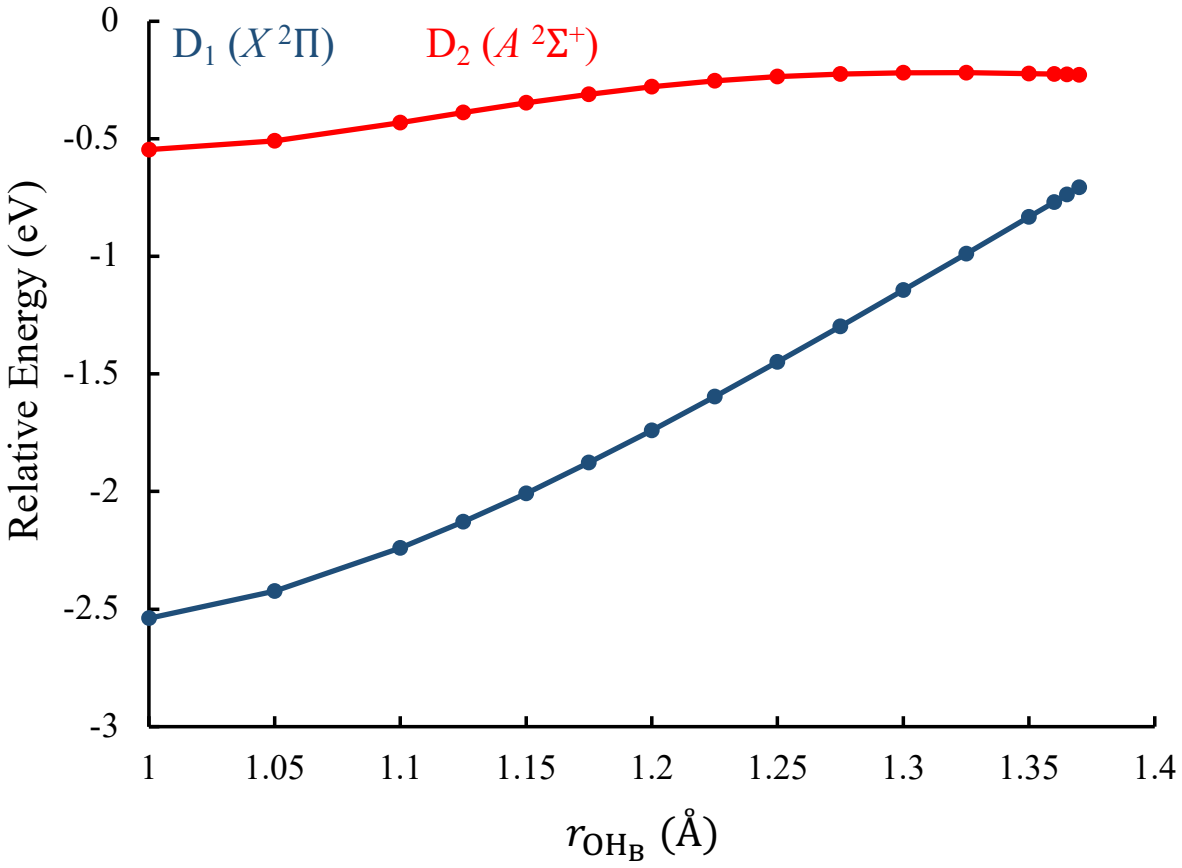

Figure S17. Cuts of the adiabatic PESs of the D_1 ($X^2\Pi$) and D_2 ($A^2\Sigma^+$) states for NO+H_2O as a function of the O-H bond length that is nearly parallel to the NO, r_{OH_B} at a fixed R_{ON} = 1.81 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

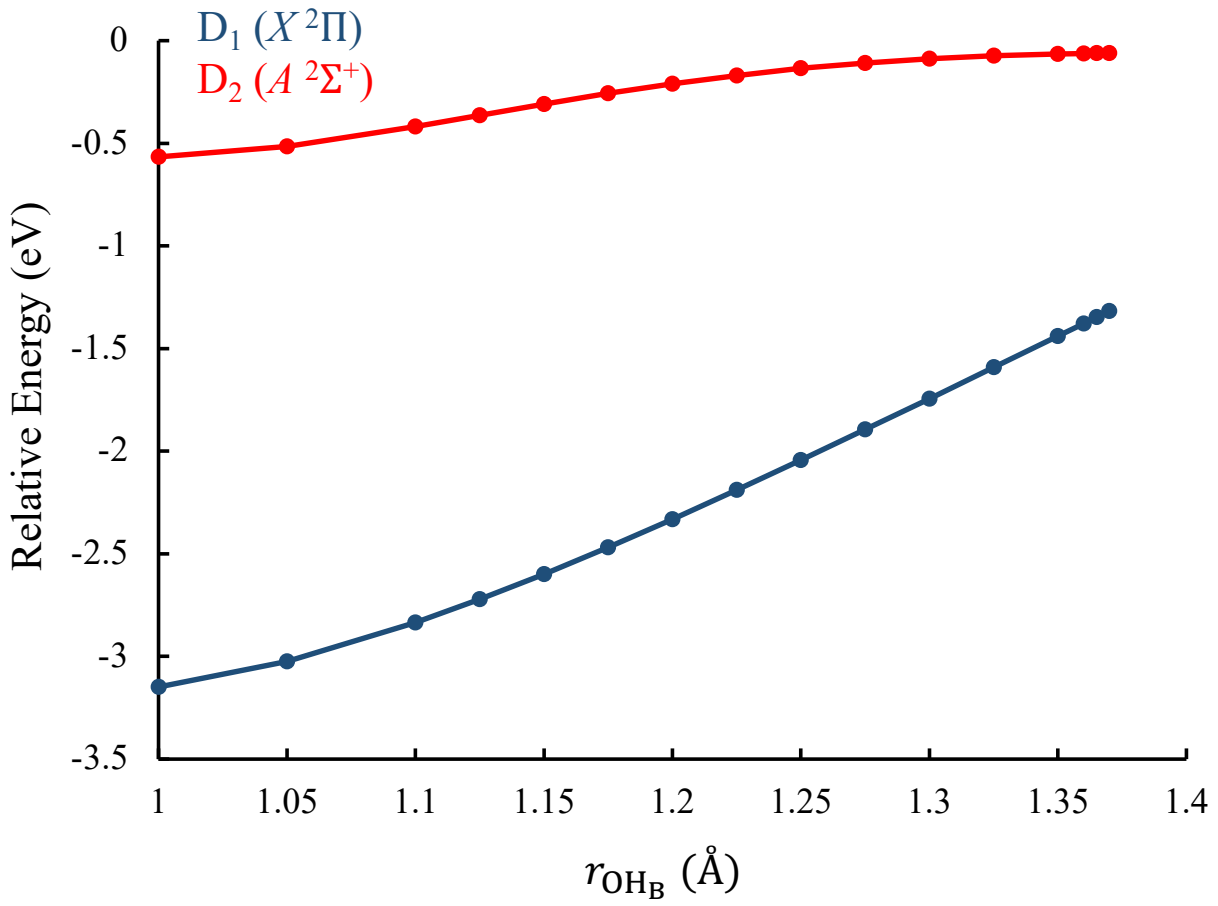

Figure S18. Cuts of the adiabatic PESs of the D_1 ($X^2\Pi$) and D_2 ($A^2\Sigma^+$) states for NO+H_2O as a function of the O-H bond length that is nearly parallel to the NO, r_{OH_B} at a fixed R_{ON} = 1.91 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

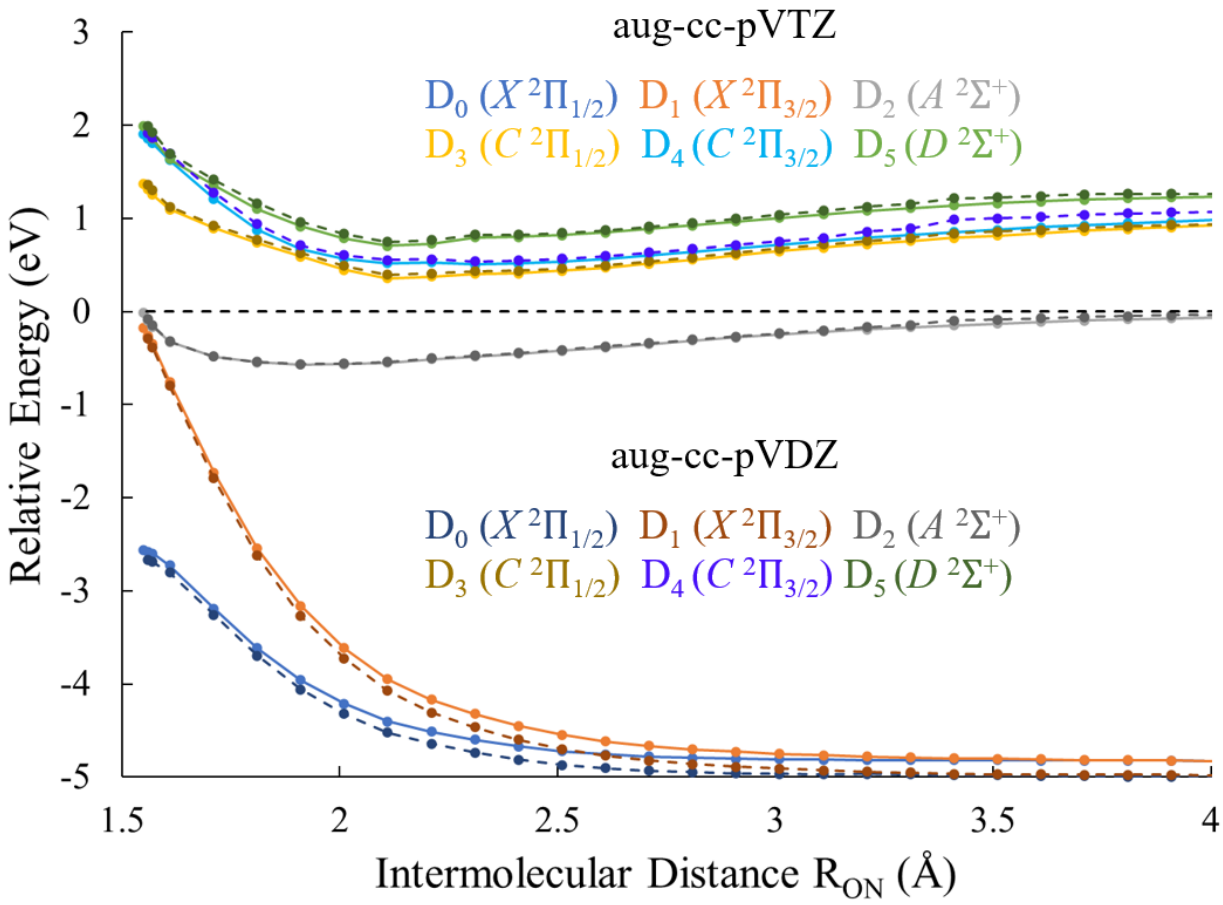

Figure S19: Cuts of the adiabatic PESs of the first six lowest electronic states for NO+H_2O as a function of intermolecular distance, R_{ON}. The PESs represent benchmarking between two different basis sets used for the geometry optimizations. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory for the solid curves and at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVDZ level of theory for the dashed curves.

Table S1: Relative electronic energies of the first six electronic states for NO+H_2O as a function of the distance between the N of NO and the O of H_2O, R_{ON}. This intermolecular distance is the only constraint for these geometry optimizations; all other degrees of freedom were optimized on D_2. These states are labeled based on their electronic character at RON = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVDZ level of theory.

R_{ON} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.51	-1.93	0.29	0.43	2.17	2.61	2.68
1.515	-2.30	0.05	0.37	1.79	2.26	2.35
1.52	-2.52	-0.03	0.30	1.60	2.10	2.22
1.53	-2.60	-0.07	0.19	1.52	2.05	2.16
1.54	-2.64	-0.13	0.09	1.47	2.01	2.11
1.545	-2.65	-0.17	0.04	1.45	1.99	2.08
1.56	-2.67	-0.29	-0.08	1.36	1.92	1.99
1.57	-2.69	-0.39	-0.15	1.30	1.87	1.93
1.61	-2.80	-0.80	-0.32	1.13	1.69	1.70
1.71	-3.26	-1.79	-0.48	0.92	1.28	1.42
1.81	-3.70	-2.62	-0.54	0.77	0.94	1.16
1.91	-4.06	-3.27	-0.56	0.63	0.71	0.97
2.01	-4.32	-3.73	-0.56	0.49	0.61	0.84
2.11	-4.52	-4.07	-0.54	0.39	0.55	0.75
2.21	-4.64	-4.31	-0.50	0.41	0.56	0.77
2.31	-4.74	-4.47	-0.48	0.43	0.54	0.82
2.41	-4.82	-4.60	-0.45	0.44	0.55	0.83
2.51	-4.87	-4.70	-0.41	0.46	0.57	0.85
2.61	-4.91	-4.77	-0.38	0.50	0.60	0.87
2.71	-4.93	-4.82	-0.34	0.54	0.63	0.91
2.81	-4.95	-4.86	-0.30	0.58	0.67	0.95
2.91	-4.96	-4.89	-0.27	0.63	0.71	1.00
3.01	-4.97	-4.91	-0.23	0.68	0.75	1.04
3.11	-4.97	-4.93	-0.20	0.72	0.79	1.08
3.21	-4.97	-4.94	-0.17	0.76	0.86	1.12
3.31	-4.97	-4.95	-0.15	0.79	0.89	1.15
3.41	-4.98	-4.97	-0.10	0.84	0.99	1.22
3.51	-4.98	-4.97	-0.09	0.86	1.00	1.23
3.61	-4.99	-4.97	-0.07	0.88	1.02	1.24
3.71	-4.99	-4.97	-0.06	0.90	1.04	1.26
3.81	-4.99	-4.98	-0.05	0.92	1.05	1.26
3.91	-5.00	-4.98	-0.04	0.93	1.07	1.27
4.01	-5.00	-4.98	-0.04	0.94	1.07	1.26
10.00	-4.98	-4.98	0.00	1.02	1.03	1.12

Table S2: Relative electronic energies of the first six electronic states for NO+H_2O as a function of the distance between the N of NO and the O of H_2O, R_{ON}. This intermolecular distance is the only constraint for these geometry optimizations; all other degrees of freedom were optimized on D_2. These states are labeled based on their electronic character at RON = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

R_{ON} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.51	-2.27	0.07	0.41	1.73	2.18	2.28
1.515	-2.43	0.01	0.36	1.59	2.07	2.19
1.53	-2.53	-0.06	0.18	1.48	1.99	2.10
1.54	-2.55	-0.11	0.08	1.43	1.95	2.05
1.545	-2.56	-0.14	0.03	1.40	1.93	2.02
1.55	-2.57	-0.18	-0.02	1.37	1.91	1.99
1.56	-2.58	-0.26	-0.10	1.31	1.86	1.92
1.57	-2.60	-0.35	-0.16	1.26	1.81	1.86
1.61	-2.73	-0.75	-0.32	1.10	1.63	1.64
1.71	-3.19	-1.73	-0.48	0.90	1.21	1.36
1.81	-3.62	-2.55	-0.55	0.74	0.88	1.10
1.91	-3.96	-3.16	-0.57	0.59	0.67	0.91
2.01	-4.21	-3.62	-0.57	0.45	0.57	0.79
2.11	-4.40	-3.95	-0.55	0.36	0.52	0.71
2.21	-4.51	-4.17	-0.51	0.38	0.53	0.73
2.31	-4.60	-4.32	-0.49	0.40	0.51	0.80
2.41	-4.67	-4.45	-0.46	0.41	0.52	0.80
2.51	-4.72	-4.55	-0.42	0.44	0.54	0.82
2.61	-4.76	-4.62	-0.39	0.47	0.57	0.85
2.71	-4.78	-4.67	-0.35	0.51	0.60	0.89
2.81	-4.80	-4.70	-0.31	0.56	0.64	0.92
2.91	-4.80	-4.73	-0.28	0.60	0.68	0.97
3.01	-4.81	-4.75	-0.25	0.65	0.72	1.01
3.11	-4.81	-4.77	-0.22	0.69	0.76	1.05
3.21	-4.82	-4.78	-0.19	0.73	0.79	1.08
3.31	-4.82	-4.79	-0.17	0.76	0.82	1.11
3.41	-4.82	-4.80	-0.15	0.79	0.85	1.14
3.51	-4.82	-4.81	-0.13	0.82	0.88	1.16
3.61	-4.82	-4.81	-0.11	0.84	0.90	1.18
3.71	-4.82	-4.82	-0.10	0.87	0.93	1.20
3.81	-4.82	-4.82	-0.08	0.89	0.95	1.21
3.91	-4.82	-4.82	-0.07	0.91	0.97	1.22
4.01	-4.83	-4.83	-0.06	0.92	0.98	1.23
10.00	-4.82	-4.82	0.00	1.02	1.02	1.13

Table S3: Relative electronic energies, of the first 6 electronic states, for NO+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 1.56 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

ϕ_{ONOH} (°)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
-165	-2.62	-0.34	0.04	1.27	1.85	1.99
-150	-2.60	-0.31	0.08	1.31	1.87	2.04
-135	-2.59	-0.29	0.10	1.34	1.88	2.08
-120	-2.58	-0.28	0.10	1.35	1.88	2.08
-105	-2.59	-0.30	0.08	1.32	1.88	2.06
-90	-2.61	-0.33	0.05	1.29	1.87	2.02
-75	-2.62	-0.35	0.00	1.26	1.86	1.97
-60	-2.63	-0.35	-0.04	1.25	1.84	1.92
-45	-2.63	-0.33	-0.07	1.26	1.83	1.90
-30	-2.60	-0.28	-0.09	1.30	1.84	1.91
-15	-2.55	-0.22	-0.09	1.34	1.89	1.95
0	-2.53	-0.18	-0.05	1.38	1.96	2.01
15	-2.57	-0.17	0.02	1.40	2.00	2.08
30	-2.61	-0.16	0.09	1.43	2.04	2.15
45	-2.62	-0.13	0.13	1.46	2.07	2.21
60	-2.62	-0.12	0.13	1.47	2.08	2.22
75	-2.59	-0.13	0.09	1.46	2.07	2.19
90	-2.57	-0.15	0.03	1.44	2.04	2.13
105	-2.55	-0.18	-0.03	1.40	1.99	2.05
120	-2.55	-0.21	-0.07	1.36	1.93	1.98
135	-2.57	-0.25	-0.09	1.32	1.87	1.93
150	-2.60	-0.30	-0.09	1.28	1.83	1.90
165	-2.63	-0.34	-0.06	1.24	1.82	1.89
180	-2.63	-0.35	-0.01	1.24	1.83	1.93

Table S4: Relative electronic energies, of the first 6 electronic states, for NO+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 1.61 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

ϕ_{ONOH} (°)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
-165	-2.72	-0.69	-0.28	1.11	1.66	1.78
-150	-2.72	-0.67	-0.25	1.13	1.65	1.81
-135	-2.71	-0.66	-0.24	1.15	1.65	1.83
-120	-2.71	-0.66	-0.24	1.15	1.65	1.83
-105	-2.71	-0.66	-0.25	1.14	1.66	1.83
-90	-2.72	-0.69	-0.27	1.12	1.67	1.79
-75	-2.73	-0.71	-0.30	1.10	1.66	1.75
-60	-2.74	-0.73	-0.31	1.09	1.65	1.69
-45	-2.73	-0.75	-0.32	1.09	1.63	1.65
-30	-2.71	-0.75	-0.32	1.11	1.63	1.64
-15	-2.69	-0.73	-0.30	1.13	1.66	1.67
0	-2.68	-0.69	-0.27	1.17	1.71	1.74
15	-2.68	-0.64	-0.22	1.20	1.77	1.84
30	-2.69	-0.60	-0.18	1.23	1.81	1.92
45	-2.70	-0.58	-0.15	1.25	1.83	1.97
60	-2.70	-0.57	-0.15	1.26	1.84	1.98
75	-2.68	-0.58	-0.17	1.26	1.83	1.96
90	-2.66	-0.61	-0.21	1.24	1.81	1.90
105	-2.66	-0.66	-0.26	1.20	1.76	1.81
120	-2.68	-0.71	-0.29	1.16	1.69	1.72
135	-2.71	-0.74	-0.31	1.12	1.65	1.66
150	-2.73	-0.75	-0.32	1.10	1.63	1.64
165	-2.74	-0.74	-0.32	1.08	1.64	1.67
180	-2.73	-0.72	-0.30	1.09	1.65	1.73

Table S5: Relative electronic energies, of the first 6 electronic states, for NO+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 1.71 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

ϕ_{ONOH} (°)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
-165	-3.17	-1.68	-0.47	0.90	1.23	1.41
-150	-3.17	-1.66	-0.46	0.91	1.22	1.42
-135	-3.18	-1.66	-0.45	0.92	1.21	1.43
-120	-3.18	-1.66	-0.45	0.93	1.21	1.43
-105	-3.17	-1.66	-0.46	0.92	1.22	1.43
-90	-3.16	-1.67	-0.47	0.91	1.24	1.42
-75	-3.18	-1.70	-0.48	0.90	1.23	1.39
-60	-3.19	-1.74	-0.48	0.90	1.21	1.35
-45	-3.20	-1.77	-0.48	0.90	1.19	1.32
-30	-3.19	-1.78	-0.47	0.92	1.18	1.31
-15	-3.18	-1.77	-0.45	0.94	1.20	1.34
0	-3.16	-1.74	-0.42	0.96	1.25	1.40
15	-3.15	-1.70	-0.39	0.98	1.30	1.47
30	-3.15	-1.66	-0.36	1.00	1.34	1.53
45	-3.16	-1.63	-0.35	1.01	1.36	1.57
60	-3.15	-1.63	-0.34	1.01	1.37	1.58
75	-3.15	-1.64	-0.36	1.01	1.36	1.56
90	-3.14	-1.67	-0.38	1.00	1.33	1.51
105	-3.15	-1.71	-0.41	0.98	1.28	1.44
120	-3.17	-1.75	-0.44	0.96	1.23	1.38
135	-3.18	-1.77	-0.46	0.94	1.20	1.34
150	-3.19	-1.77	-0.48	0.92	1.19	1.32
165	-3.19	-1.75	-0.48	0.90	1.21	1.34
180	-3.18	-1.71	-0.48	0.90	1.22	1.38

Table S6: Relative electronic energies, of the first 6 electronic states, for NO+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 1.81 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

ϕ_{ONOH} (°)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
-165	-3.62	-2.52	-0.54	0.74	0.88	1.12
-150	-3.62	-2.51	-0.53	0.74	0.87	1.13
-135	-3.62	-2.50	-0.52	0.75	0.85	1.14
-120	-3.62	-2.50	-0.52	0.76	0.85	1.14
-105	-3.62	-2.51	-0.53	0.75	0.87	1.14
-90	-3.62	-2.52	-0.54	0.74	0.88	1.13
-75	-3.61	-2.54	-0.55	0.74	0.88	1.11
-60	-3.62	-2.56	-0.55	0.74	0.87	1.09
-45	-3.62	-2.58	-0.54	0.76	0.86	1.07
-30	-3.61	-2.58	-0.53	0.78	0.86	1.07
-15	-3.60	-2.58	-0.51	0.79	0.87	1.09
0	-3.59	-2.55	-0.49	0.80	0.91	1.14
15	-3.58	-2.52	-0.47	0.81	0.95	1.20
30	-3.58	-2.49	-0.45	0.82	0.98	1.25
45	-3.58	-2.47	-0.44	0.83	1.01	1.28
60	-3.58	-2.47	-0.44	0.83	1.01	1.29
75	-3.57	-2.48	-0.45	0.83	1.00	1.27
90	-3.57	-2.51	-0.47	0.83	0.97	1.23
105	-3.58	-2.53	-0.48	0.82	0.94	1.18
120	-3.59	-2.56	-0.50	0.81	0.90	1.13
135	-3.60	-2.57	-0.52	0.80	0.88	1.09
150	-3.61	-2.57	-0.54	0.77	0.87	1.08
165	-3.62	-2.56	-0.54	0.75	0.88	1.09
180	-3.62	-2.54	-0.55	0.74	0.88	1.11

Table S7: Relative electronic energies, of the first 6 electronic states, for NO+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 1.91 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

ϕ_{ONOH} (°)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
-165	-3.96	-3.15	-0.56	0.58	0.65	0.92
-150	-3.97	-3.14	-0.56	0.59	0.64	0.93
-135	-3.97	-3.14	-0.55	0.59	0.63	0.93
-120	-3.97	-3.14	-0.55	0.59	0.63	0.93
-105	-3.97	-3.14	-0.55	0.59	0.64	0.93
-90	-3.96	-3.15	-0.56	0.59	0.65	0.93
-75	-3.96	-3.16	-0.57	0.59	0.66	0.92
-60	-3.95	-3.17	-0.57	0.60	0.67	0.91
-45	-3.95	-3.18	-0.56	0.61	0.67	0.89
-30	-3.94	-3.18	-0.55	0.62	0.68	0.90
-15	-3.94	-3.18	-0.54	0.64	0.68	0.92
0	-3.93	-3.16	-0.52	0.67	0.69	0.96
15	-3.92	-3.14	-0.51	0.69	0.70	1.01
30	-3.92	-3.11	-0.50	0.69	0.73	1.05
45	-3.91	-3.10	-0.50	0.70	0.75	1.08
60	-3.91	-3.10	-0.49	0.70	0.75	1.08
75	-3.91	-3.11	-0.50	0.70	0.74	1.07
90	-3.91	-3.12	-0.51	0.70	0.72	1.03
105	-3.92	-3.15	-0.52	0.69	0.70	0.99
120	-3.93	-3.16	-0.53	0.66	0.70	0.94
135	-3.94	-3.18	-0.55	0.63	0.69	0.91
150	-3.95	-3.18	-0.56	0.62	0.68	0.90
165	-3.95	-3.17	-0.57	0.60	0.68	0.91
180	-3.96	-3.16	-0.57	0.59	0.67	0.92

Table S8: Relative electronic energies, of the first 6 electronic states, for NO+H_2O as a function of torsion angles -165° ≤ ϕ_{ONOH} ≤ 180° at a fixed intermolecular distance of R_{ON} = 2.01 Å. All energies are reported relative to D_2 ($A^2\Sigma^+$) at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

ϕ_{ONOH} (°)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
-165	-4.22	-3.61	-0.56	0.44	0.55	0.79
-150	-4.23	-3.61	-0.56	0.43	0.54	0.79
-135	-4.23	-3.61	-0.55	0.42	0.53	0.79
-120	-4.23	-3.61	-0.55	0.42	0.53	0.79
-105	-4.23	-3.61	-0.56	0.43	0.54	0.79
-90	-4.22	-3.61	-0.56	0.44	0.55	0.79
-75	-4.22	-3.62	-0.57	0.44	0.56	0.79
-60	-4.21	-3.62	-0.56	0.45	0.58	0.78
-45	-4.20	-3.63	-0.56	0.46	0.59	0.77
-30	-4.20	-3.63	-0.55	0.47	0.60	0.78
-15	-4.19	-3.62	-0.54	0.49	0.60	0.80
0	-4.18	-3.60	-0.54	0.51	0.60	0.84
15	-4.18	-3.59	-0.53	0.54	0.60	0.88
30	-4.17	-3.57	-0.52	0.56	0.60	0.92
45	-4.17	-3.56	-0.52	0.57	0.60	0.94
60	-4.17	-3.56	-0.52	0.58	0.60	0.94
75	-4.17	-3.57	-0.52	0.57	0.61	0.93
90	-4.17	-3.58	-0.53	0.55	0.61	0.90
105	-4.18	-3.60	-0.53	0.52	0.61	0.86
120	-4.19	-3.61	-0.54	0.50	0.61	0.82
135	-4.19	-3.62	-0.55	0.48	0.61	0.79
150	-4.20	-3.62	-0.56	0.47	0.60	0.78
165	-4.21	-3.62	-0.56	0.46	0.59	0.78
180	-4.21	-3.62	-0.57	0.45	0.57	0.79

Table S9: Relative electronic energies of the first six electronic states for NO+H_2O as a function of the N-O bond length for R_{ON}=1.61 Å. All energies are reported relative to the D_2 state at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{NO} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.06	-2.08	-0.19	-0.07	1.31	1.71	1.74
1.07	-2.23	-0.32	-0.15	1.23	1.66	1.68
1.08	-2.36	-0.44	-0.22	1.17	1.62	1.65
1.09	-2.47	-0.53	-0.26	1.14	1.60	1.62
1.1	-2.56	-0.62	-0.30	1.11	1.60	1.61
1.11	-2.65	-0.69	-0.32	1.10	1.60	1.62
1.12	-2.72	-0.74	-0.32	1.09	1.62	1.63
1.13	-2.77	-0.79	-0.32	1.10	1.65	1.66
1.14	-2.82	-0.82	-0.31	1.12	1.69	1.70
1.15	-2.85	-0.84	-0.28	1.15	1.74	1.74
1.16	-2.87	-0.85	-0.25	1.19	1.79	1.80
1.17	-2.88	-0.86	-0.21	1.23	1.85	1.86
1.18	-2.89	-0.85	-0.17	1.29	1.92	1.93

Table S10: Relative electronic energies of the first six electronic states for $NO+H_2O$ as a function of the N-O bond length for R_{ON}=1.71 Å. All energies are reported relative to the D_2 state at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{NO} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.06	-2.71	-1.29	-0.35	0.99	1.23	1.38
1.07	-2.85	-1.42	-0.40	0.95	1.20	1.35
1.08	-2.96	-1.53	-0.44	0.91	1.18	1.33
1.09	-3.06	-1.62	-0.47	0.90	1.18	1.33
1.1	-3.14	-1.69	-0.48	0.89	1.20	1.34
1.11	-3.21	-1.75	-0.48	0.90	1.23	1.37
1.12	-3.27	-1.80	-0.47	0.92	1.26	1.40
1.13	-3.31	-1.84	-0.45	0.95	1.31	1.44
1.14	-3.34	-1.87	-0.42	0.99	1.36	1.49
1.15	-3.36	-1.88	-0.38	1.03	1.42	1.55
1.16	-3.36	-1.89	-0.34	1.09	1.50	1.62
1.17	-3.36	-1.88	-0.28	1.15	1.58	1.69
1.18	-3.35	-1.87	-0.22	1.22	1.66	1.77

Table S11: Relative electronic energies of the first six electronic states for NO+H_2O as a function of the N-O bond length for R_{ON}=1.81 Å. All energies are reported relative to the D_2 state at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{NO} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.06	-3.25	-2.19	-0.47	0.79	0.88	1.11
1.07	-3.38	-2.32	-0.51	0.75	0.86	1.09
1.08	-3.49	-2.42	-0.53	0.74	0.86	1.09
1.09	-3.58	-2.51	-0.55	0.74	0.87	1.09
1.1	-3.65	-2.58	-0.54	0.75	0.89	1.12
1.11	-3.71	-2.64	-0.53	0.77	0.93	1.15
1.12	-3.75	-2.68	-0.51	0.80	0.98	1.19
1.13	-3.79	-2.72	-0.48	0.85	1.03	1.24
1.14	-3.81	-2.74	-0.43	0.90	1.10	1.31
1.15	-3.82	-2.75	-0.38	0.96	1.17	1.38
1.16	-3.81	-2.75	-0.32	1.02	1.25	1.45
1.17	-3.80	-2.74	-0.26	1.10	1.34	1.54
1.18	-3.78	-2.72	-0.18	1.18	1.44	1.63

Table S12: Relative electronic energies of the first six electronic states for $NO+H_2O$ as a function of the N-O bond length for R_{ON}=1.91 Å. All energies are reported relative to the D_2 state at R_{ON} = 10 Å. The calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{NO} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.06	-3.68	-2.88	-0.52	0.60	0.68	0.92
1.07	-3.80	-3.00	-0.55	0.58	0.66	0.90
1.08	-3.90	-3.11	-0.57	0.58	0.66	0.91
1.09	-3.99	-3.19	-0.57	0.60	0.67	0.92
1.1	-4.06	-3.26	-0.55	0.62	0.70	0.95
1.11	-4.11	-3.32	-0.53	0.66	0.74	1.00
1.12	-4.15	-3.36	-0.50	0.71	0.79	1.05
1.13	-4.17	-3.39	-0.45	0.76	0.86	1.11
1.14	-4.19	-3.41	-0.40	0.83	0.93	1.18
1.15	-4.19	-3.41	-0.34	0.90	1.01	1.26
1.16	-4.18	-3.41	-0.27	0.98	1.10	1.35
1.17	-4.16	-3.40	-0.19	1.07	1.19	1.44
1.18	-4.13	-3.37	-0.11	1.16	1.30	1.54

Table S13: Relative electronic energies of the first six electronic states for NO+H_2O as a function of r_{OH_A} at a fixed R_{ON} = 1.76 Å. All energies are reported relative to D_2 at R_{ON} = 10 Å and the calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{OH_A} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.00	-3.45	-2.22	-0.52	0.79	0.99	1.18
1.05	-3.34	-2.08	-0.51	0.87	1.11	1.30
1.10	-3.15	-1.87	-0.48	1.03	1.29	1.50
1.125	-3.03	-1.75	-0.46	1.13	1.41	1.61
1.15	-2.91	-1.62	-0.45	1.23	1.53	1.74
1.175	-2.77	-1.48	-0.43	1.35	1.67	1.88
1.20	-2.63	-1.33	-0.43	1.47	1.81	2.02
1.225	-2.48	-1.18	-0.42	1.60	1.96	2.17
1.25	-2.33	-1.03	-0.42	1.73	2.11	2.32
1.275	-2.18	-0.87	-0.43	1.87	2.27	2.48
1.30	-2.02	-0.71	-0.44	2.02	2.43	2.64
1.325	-1.86	-0.54	-0.45	2.18	2.61	2.82

Table S14: Relative electronic energies of the first six electronic states for NO+H_2O as a function of r_{OH_A} at a fixed R_{ON} = 1.787 Å. All energies are reported relative to D_2 at R_{ON} = 10 Å and the calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{OH_A} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.00	-3.56	-2.42	-0.53	0.75	0.91	1.12
1.05	-3.44	-2.28	-0.53	0.84	1.03	1.24
1.10	-3.25	-2.08	-0.49	1.00	1.21	1.44
1.125	-3.14	-1.96	-0.47	1.10	1.33	1.56
1.15	-3.01	-1.83	-0.45	1.21	1.45	1.68
1.175	-2.88	-1.69	-0.43	1.32	1.59	1.82
1.20	-2.74	-1.54	-0.42	1.45	1.73	1.96
1.225	-2.59	-1.39	-0.41	1.57	1.87	2.11
1.25	-2.44	-1.24	-0.41	1.71	2.02	2.26
1.275	-2.29	-1.08	-0.41	1.84	2.18	2.42
1.30	-2.13	-0.92	-0.41	1.98	2.33	2.57
1.325	-1.98	-0.76	-0.42	2.12	2.49	2.73
1.35	-1.82	-0.60	-0.43	2.27	2.66	2.90
1.36	-1.75	-0.53	-0.44	2.34	2.73	2.97
1.365	-1.72	-0.50	-0.44	2.37	2.77	3.01

Table S15: Relative electronic energies of the first six electronic states for NO+H_2O as a function of r_{OH_A} at a fixed R_{ON} = 1.81 Å. All energies are reported relative to D_2 at R_{ON} = 10 Å and the calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{OH_A} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.00	-3.64	-2.58	-0.54	0.72	0.85	1.07
1.05	-3.53	-2.45	-0.53	0.82	0.96	1.19
1.10	-3.33	-2.24	-0.49	0.98	1.15	1.39
1.125	-3.22	-2.12	-0.46	1.08	1.26	1.51
1.15	-3.09	-1.99	-0.44	1.19	1.39	1.64
1.175	-2.96	-1.85	-0.42	1.31	1.52	1.77
1.20	-2.82	-1.71	-0.40	1.43	1.66	1.92
1.225	-2.67	-1.56	-0.39	1.56	1.81	2.06
1.25	-2.53	-1.41	-0.39	1.69	1.96	2.21
1.275	-2.37	-1.25	-0.39	1.82	2.11	2.37
1.30	-2.22	-1.09	-0.39	1.96	2.26	2.52
1.325	-2.06	-0.93	-0.40	2.10	2.42	2.68
1.35	-1.91	-0.78	-0.41	2.24	2.58	2.84
1.36	-1.85	-0.71	-0.41	2.30	2.64	2.90
1.365	-1.81	-0.68	-0.41	2.33	2.67	2.93
1.37	-1.78	-0.65	-0.41	2.36	2.70	2.96

Table S16: Relative electronic energies of the first six electronic states for NO+H_2O as a function of r_{OH_A} at a fixed R_{ON} = 1.91 Å. All energies are reported relative to D_2 at R_{ON} = 10 Å and the calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{OH_A} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.00	-3.97	-3.17	-0.57	0.58	0.66	0.90
1.05	-3.84	-3.04	-0.54	0.71	0.76	1.03
1.10	-3.65	-2.84	-0.48	0.90	0.93	1.23
1.125	-3.53	-2.72	-0.44	1.02	1.04	1.35
1.15	-3.40	-2.59	-0.40	1.13	1.16	1.48
1.175	-3.27	-2.45	-0.36	1.25	1.30	1.62
1.20	-3.13	-2.31	-0.33	1.38	1.44	1.76
1.225	-2.99	-2.16	-0.31	1.50	1.59	1.91
1.25	-2.79	-2.01	-0.29	1.76	2.15	2.65
1.275	-2.69	-1.86	-0.27	1.77	1.90	2.21
1.30	-2.54	-1.71	-0.26	1.90	2.05	2.37
1.325	-2.38	-1.55	-0.25	2.04	2.20	2.52
1.35	-2.23	-1.40	-0.25	2.17	2.36	2.67
1.36	-2.17	-1.33	-0.25	2.23	2.42	2.74
1.365	-2.14	-1.30	-0.25	2.26	2.45	2.77
1.37	-2.11	-1.27	-0.25	2.28	2.48	2.80

Table S17: Relative electronic energies of the first six electronic states for NO+H_2O as a function of r_{OH_B} at a fixed R_{ON} = 1.76 Å. All energies are reported relative to D_2 at R_{ON} = 10 Å and the calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{OH_B} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.00	-3.41	-2.16	-0.52	0.81	1.03	1.23
1.05	-3.31	-2.05	-0.49	0.85	1.13	1.32
1.10	-3.14	-1.87	-0.42	0.95	1.30	1.49
1.125	-3.03	-1.76	-0.39	1.02	1.41	1.60
1.15	-2.91	-1.64	-0.35	1.10	1.53	1.71
1.175	-2.79	-1.51	-0.32	1.20	1.66	1.84
1.20	-2.65	-1.37	-0.30	1.30	1.80	1.98
1.225	-2.51	-1.23	-0.28	1.41	1.94	2.12
1.25	-2.37	-1.08	-0.27	1.52	2.09	2.27
1.275	-2.22	-0.93	-0.27	1.65	2.24	2.42
1.30	-2.06	-0.77	-0.27	1.77	2.39	2.57
1.325	-1.91	-0.61	-0.28	1.90	2.55	2.72

Table S18: Relative electronic energies of the first six electronic states for NO+H_2O as a function of r_{OH_B} at a fixed R_{ON} = 1.787 Å. All energies are reported relative to D_2 at R_{ON} = 10 Å and the calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{OH_B} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.00	-3.52	-2.37	-0.54	0.77	0.95	1.16
1.05	-3.42	-2.26	-0.50	0.81	1.05	1.26
1.10	-3.24	-2.08	-0.43	0.92	1.23	1.43
1.125	-3.13	-1.97	-0.39	0.99	1.34	1.54
1.15	-3.02	-1.85	-0.35	1.08	1.46	1.66
1.175	-2.89	-1.72	-0.32	1.17	1.59	1.79
1.20	-2.75	-1.58	-0.29	1.27	1.73	1.92
1.225	-2.61	-1.43	-0.27	1.38	1.87	2.06
1.25	-2.47	-1.29	-0.25	1.50	2.02	2.21
1.275	-2.32	-1.13	-0.25	1.62	2.17	2.36
1.30	-2.17	-0.98	-0.25	1.74	2.32	2.51
1.325	-2.02	-0.82	-0.25	1.87	2.47	2.66
1.35	-1.86	-0.66	-0.25	2.01	2.63	2.81
1.36	-1.80	-0.60	-0.26	2.06	2.69	2.87
1.365	-1.77	-0.57	-0.26	2.09	2.72	2.91

Table S19: Relative electronic energies of the first six electronic states for NO+H_2O as a function of r_{OH_B} at a fixed R_{ON} = 1.81 Å. All energies are reported relative to D_2 at R_{ON} = 10 Å and the calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{OH_B} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.00	-3.61	-2.54	-0.55	0.74	0.88	1.11
1.05	-3.50	-2.42	-0.51	0.79	0.99	1.21
1.10	-3.33	-2.24	-0.43	0.90	1.17	1.39
1.125	-3.22	-2.13	-0.39	0.97	1.28	1.49
1.15	-3.10	-2.01	-0.35	1.06	1.40	1.61
1.175	-2.97	-1.88	-0.31	1.15	1.53	1.74
1.20	-2.84	-1.74	-0.28	1.25	1.67	1.88
1.225	-2.70	-1.60	-0.25	1.36	1.81	2.02
1.25	-2.55	-1.45	-0.24	1.48	1.96	2.17
1.275	-2.40	-1.30	-0.22	1.60	2.11	2.32
1.30	-2.25	-1.14	-0.22	1.72	2.27	2.47
1.325	-2.10	-0.99	-0.22	1.85	2.42	2.62
1.35	-1.95	-0.83	-0.22	1.98	2.57	2.77
1.36	-1.88	-0.77	-0.22	2.04	2.64	2.83
1.365	-1.85	-0.74	-0.23	2.06	2.67	2.86
1.37	-1.82	-0.71	-0.23	2.09	2.70	2.89

Table S20: Relative electronic energies of the first six electronic states for NO+H_2O as a function of r_{OH_B} at a fixed R_{ON} = 1.91 Å. All energies are reported relative to D_2 at R_{ON} = 10 Å and the calculations were performed at the EOM-EA-CCSD/d-aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{OH_B} (Å)	D_0 (eV)	D_1 (eV)	D_2 (eV)	D_3 (eV)	D_4 (eV)	D_5 (eV)
1.00	-3.95	-3.15	-0.57	0.59	0.68	0.93
1.05	-3.83	-3.03	-0.51	0.67	0.79	1.04
1.10	-3.64	-2.83	-0.42	0.80	0.97	1.22
1.125	-3.53	-2.72	-0.36	0.88	1.09	1.34
1.15	-3.41	-2.60	-0.31	0.97	1.21	1.46
1.175	-3.28	-2.47	-0.26	1.07	1.35	1.59
1.20	-3.15	-2.33	-0.21	1.17	1.49	1.73
1.225	-3.01	-2.19	-0.17	1.29	1.63	1.87
1.25	-2.86	-2.04	-0.14	1.40	1.78	2.02
1.275	-2.71	-1.89	-0.11	1.53	1.93	2.17
1.30	-2.57	-1.74	-0.09	1.65	2.09	2.32
1.325	-2.41	-1.59	-0.07	1.78	2.24	2.47
1.35	-2.26	-1.44	-0.06	1.91	2.39	2.63
1.36	-2.20	-1.38	-0.06	1.96	2.46	2.69
1.365	-2.17	-1.35	-0.06	1.99	2.49	2.72
1.37	-2.14	-1.32	-0.06	2.02	2.52	2.75

Table S21: Relative electronic energies of the D_1 and D_2 electronic states for NO+H_2O as a function of r_{OH_A} at a fixed R_{ON} = 1.787 Å. All energies are reported relative to D_1 at r_{OH_A}=1.0 Å. The calculations were performed at either the (9,9) NEVPT2/aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory or the EOM-EA-CCSD/aug-cc-pVTZ//EOM-EA-CCSD/aug-cc-pVTZ level of theory.

r_{OH_B} (Å)	D_1 (eV) NEVPT2	D_2 (eV) NEVPT2	D_1 (eV) EOM-EA-CCSD	D_2 (eV) EOM-EA-CCSD
1.00	0.00	1.81	0.00	1.90
1.05	0.18	1.84	0.14	1.91
1.10	0.36	1.83	0.34	1.95
1.125	0.46	1.82	0.46	1.97
1.15	0.58	1.81	0.59	1.99
1.175	0.70	1.80	0.73	2.00
1.20	0.84	1.78	0.88	2.01
1.225	0.98	1.76	1.03	2.02
1.25	1.12	1.73	1.18	2.02
1.275	1.26	1.71	1.34	2.02
1.30	1.40	1.69	1.50	2.01
1.325	1.54	1.68	1.66	2.00
1.35	1.60	1.76	1.82	1.99
1.36	1.61	1.80	1.89	1.99
1.365	1.61	1.83	1.93	1.99

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