Supplementary information for:

Trapping intermediates of the NO_2 hydrolysis reaction on ice.

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Evolution of the NO stretching vibrational frequencies for the planar and non-planar conformers of *c*-$ONONO_2$ in *c*-$ONONO_2{\cdot}(H_2O)_n$ (Figure S1). Evolution of the intramolecular NO and NN bond lengths in $NO_2{\cdot}(H_2O)_n$ and $O_2NNO_2{\cdot}(H_2O)_n$ (Figure S2), in *t*-$ONONO_2{\cdot}(H_2O)_n$ (Figure S3), and in the planar and non-planar conformers of *c*-$ONONO_2$ in *c*-$ONONO_2{\cdot}(H_2O)_n$ (Figure S4).

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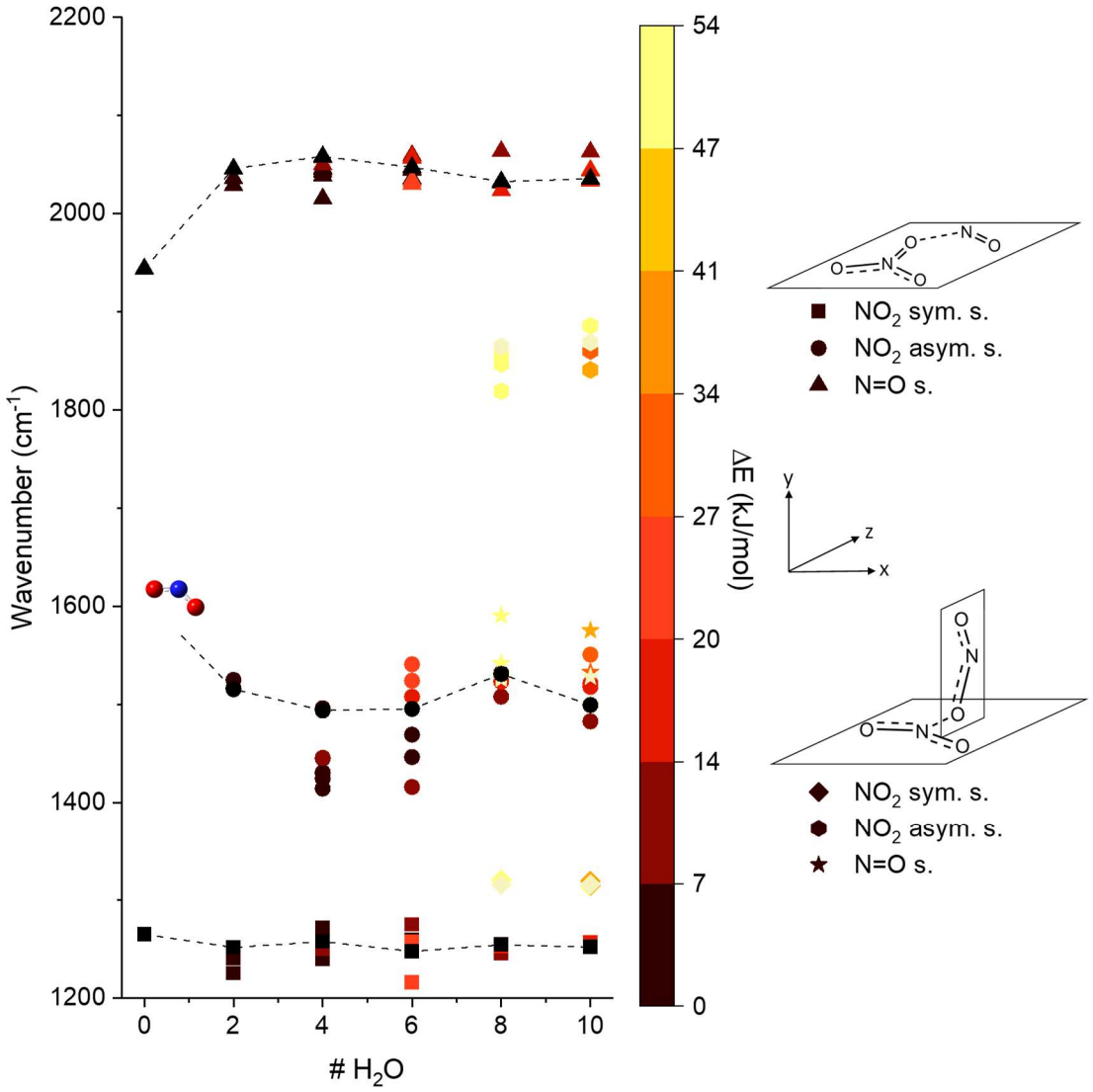

Figure S1 - (A) Vibrational frequencies for the planar and non-planar conformers of *c*-ONONO$_2$ in *c*-ONONO$_2$·(H$_2$O)$_n$ with n = 0-10. Vibrational frequencies are calculated using B3LYP/6-311g++(3df,3dp) and are scaled by 0.976 to account for their anharmonicity.[73] The symmetric and asymmetric ONO stretching modes are labeled by squares and circles, respectively, while the N=O stretching modes are labeled by triangles. Symbols for the individual isomers are color-coded to account for their energy relative to the most stable isomer for each n using the scale provided as insets.

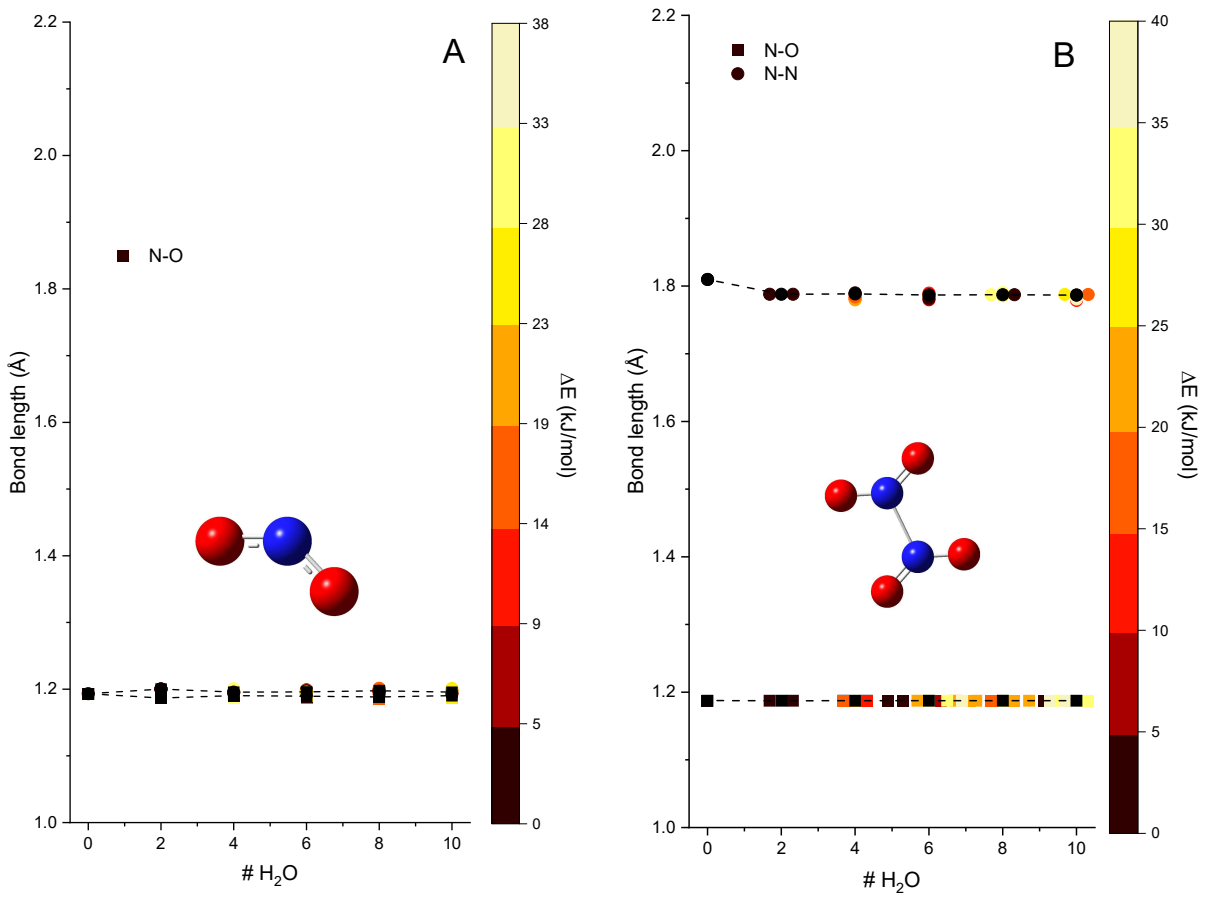

Figure S2 - (A) Intramolecular NO bond lengths for $NO_2 \cdot (H_2O)_n$ with n = 0-10; (B) Intramolecular NO and NN bond lengths for $O_2NNO_2 \cdot (H_2O)_n$ with n = 0-10. Structures are optimized using B3LYP/6-311g++(3df,3dp). NO and NN bond lengths are labeled by squares and circles, respectively. Symbols for the individual isomers are color-coded to account for their energy relative to the most stable isomer for each n using the scale provided as insets.

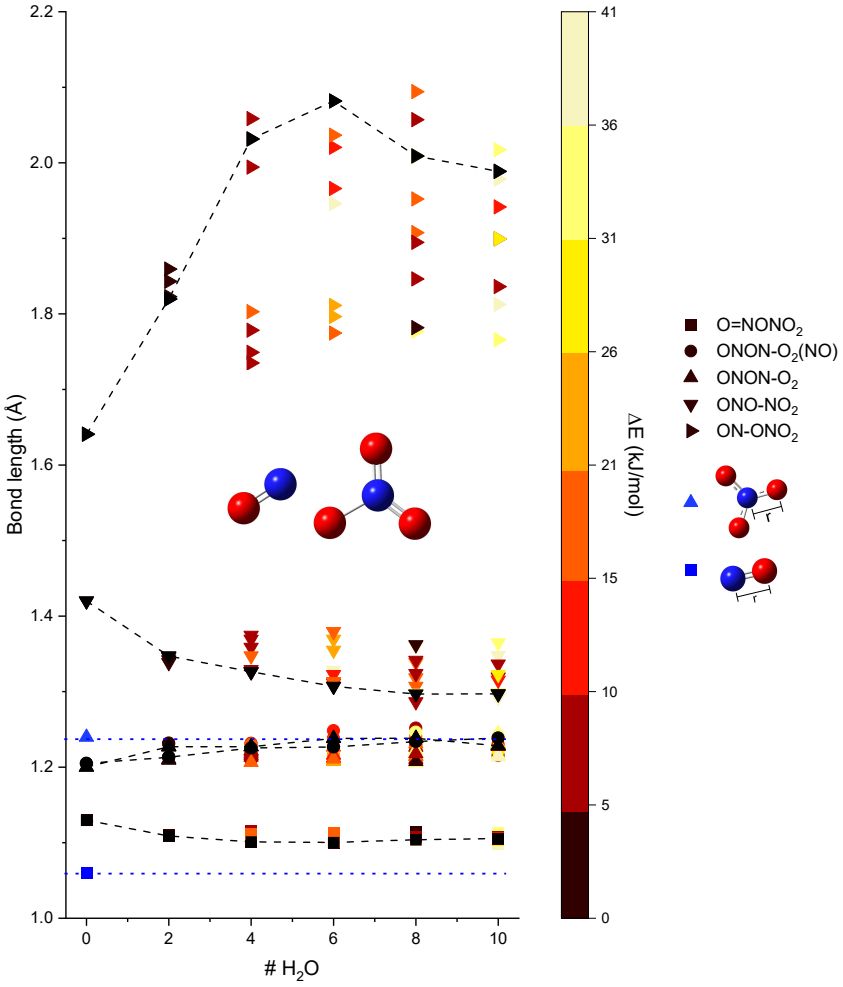

Figure S3 - Intramolecular NO bond lengths for *t*-$ONONO_2 \cdot (H_2O)_n$ with n = 0-10. Structures are optimized using B3LYP/6-311g++(3df,3dp). Symbols for the different NO bond lengths are defined in the legend. Symbols for the individual isomers are color-coded to account for their energy relative to the most stable isomer for each n using the scale provided as insets. The NO bond lengths for NO_3^- and NO^+ are indicated by blue triangles and squares, respectively.

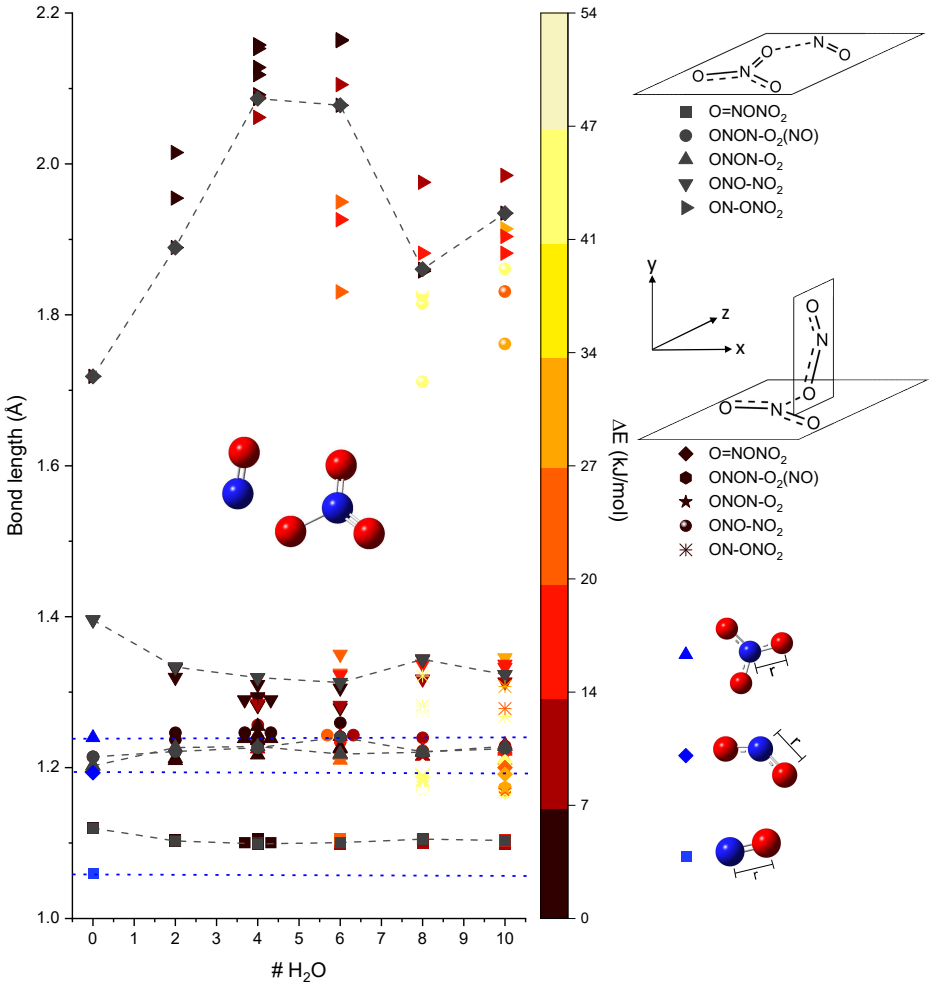

Figure S4 - Intramolecular NO bond lengths for the planar and non-planar isomers of *c*-$ONONO_2 \cdot (H_2O)_n$ with n = 0-10. Structures are optimized using B3LYP/6-311g++(3df,3dp). Symbols for the different NO bond lengths are defined in the legend. Symbols for the individual isomers are color-coded to account for their energy relative to the most stable isomer for each n using the scale provided as insets. The NO bond lengths for NO_3^-, NO_2, and NO^+ are indicated by blue triangles, diamonds, and squares, respectively.