Supporting Information

for

The Conical Intersection Dominates the Generation of Tropospheric Hydroxyl Radical from NO₂ and H₂O

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Section 1: Tables

Table S1 The absolute energies (a.u.) for NO₂ along MEPs of photo-physical processes at CASSCF(9e/6o) and CASSCF(9e/6o)/CASPT2 computational levels, respectively.

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Table S2. The absolute energies (a.u.) for NO₂-H₂O complex along MEPs of photo-physical processes and hydrogen abstraction at CASSCF(13e/9o) and CASSCF(13e/9o)/CASPT2 computational levels, respectively.

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Table S3 The energies (au) of NO₂-H₂O complex for hydrogen abstraction at the B3LYP/6-31G** level of theory.

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Section 2: Cartesian coordinates

S2.1 Cartesian coordinates of NO₂ along MEPs of photo-physical processes at CASSCF(9e/6o)/6-31G** level of theory.
$$X^{2}A_1-179.9$$

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$\tilde{X}^2{A_1}$-130

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**S2.3** Cartesian coordinates of NO$_2$-H$_2$O complex MEP of hydrogen abstraction at B3LYP/6-32G** computational level.

### $S_0$ minimum

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