

# UV-spectrum and photodecomposition of peroxynitrous acid in the troposphere: supplemental material

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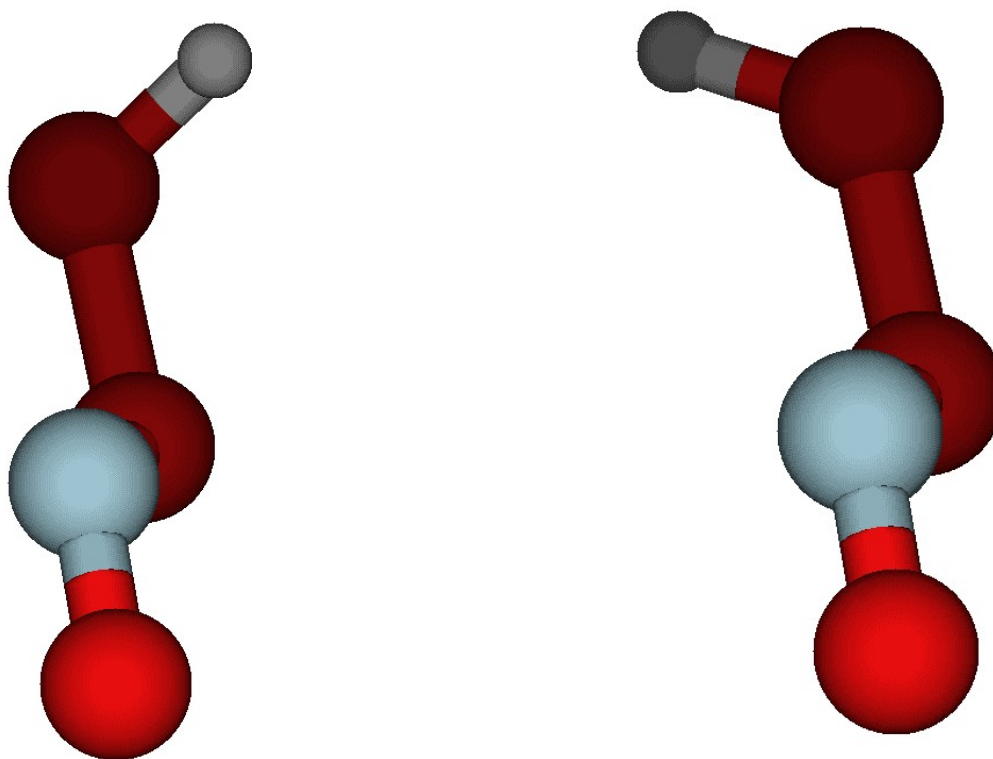


Figure 1: The two enantiomers of the trans-perp conformer

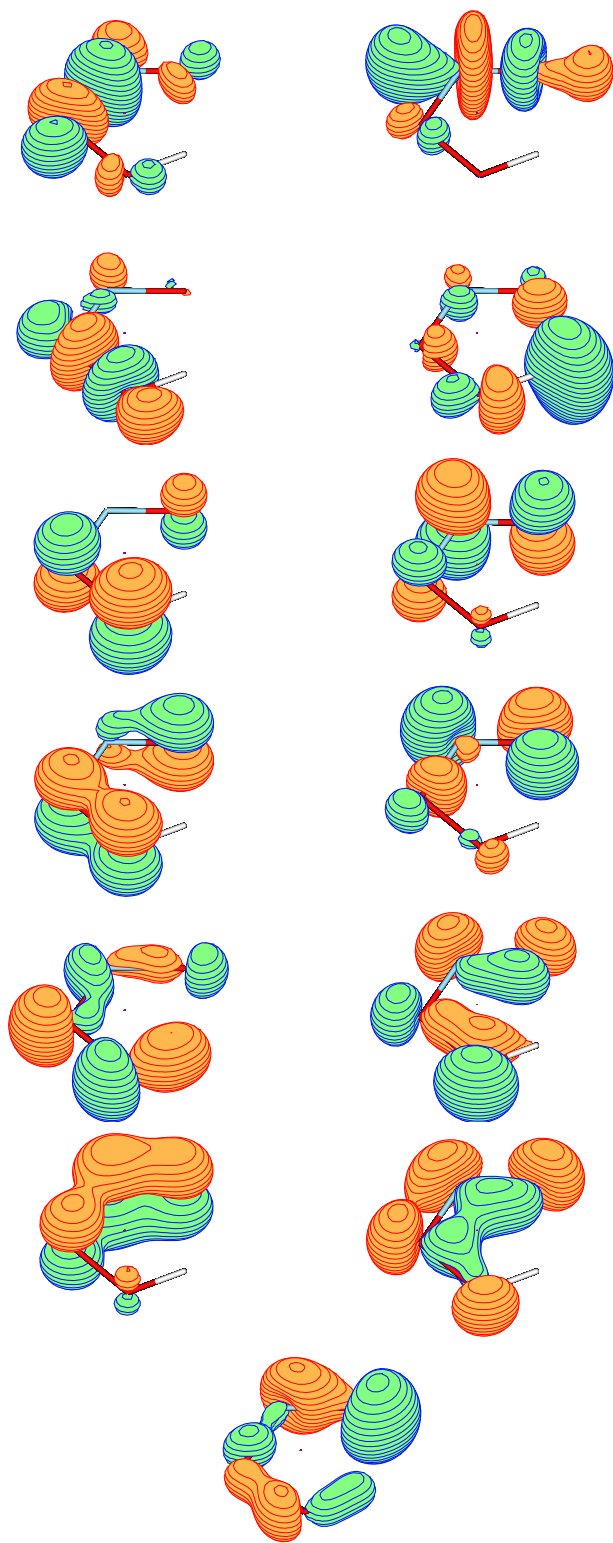


Figure 2: Active space (16e/13o) orbitals of the cis-cis conformer. Order from upper left to lower right is [20, 21], [18, 19], [16 (HOMO), 17 (LUMO)], [14, 15], [12, 13], [10, 11], [9]. The lowest eight molecular orbitals are linear combinations of the N, O 1s and 2s orbitals and were kept inactive.

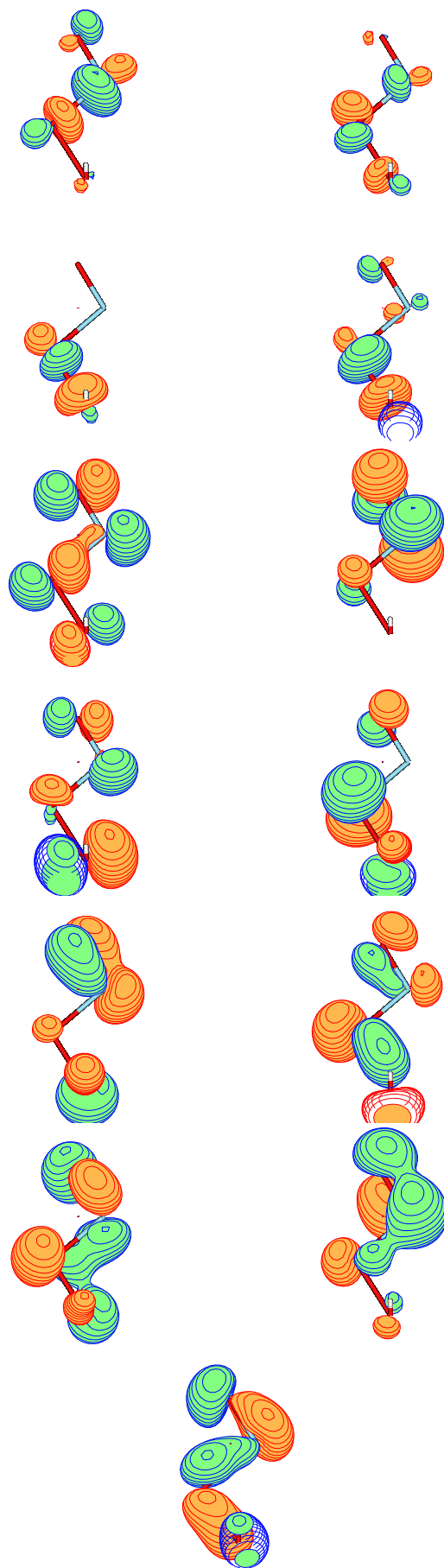


Figure 3: Active space (16e/13o) orbitals of the trans-perp conformer. Order from upper left to lower right is [20, 21], [18, 19], [16 (HOMO)], 17 (LUMO)], [14, 15], [12, 13], [10, 11], [9]. The lowest eight molecular orbitals are linear combinations of the N, O 1s and 2s orbitals and were kept inactive.