

# Role of sulfur in proton-induced collisions of RNA prebiotic precursors

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## Supplementary information

Fig. S1: a) Adiabatic potential energy curves of the  $^1A$  states in the collision of a proton on 2-aminooxazole in the  $z$  direction. Black, entrance channel  $H^+ + 2\text{-aminooxazole}$   $\{\{p_{xy}^N\}^2 \{\pi_2\}^2 \{\pi_{CC}\}^2\}$ ; red, charge transfer channel  $\{\{p_{xy}^N\}^2 \{\pi_2\}^2 \{\pi_{CC}\} 1s_H\}$  with singly excitation to the  $1s_H$  orbital on hydrogen; green, charge transfer channel  $\{\{p_{xy}^N\} \{\pi_2\}^2 \{\pi_{CC}\}^2 1s_H\}$ ; blue, charge transfer channel  $\{\{p_{xy}^N\}^2 \{\pi_2\} \{\pi_{CC}\}^2 1s_H\}$ ; magenta, charge transfer channel  $\{\{p_{xy}^N\} \{\pi_2\}^2 \{\pi_{CC}\} \{\pi_{nb}\} 1s_H\}$ . b) Adiabatic potential energy curves of the  $^1A$  states in the collision of a proton on 2-aminooxazole towards  $C=C$ . Black, entrance channel  $H^+ + 2\text{-aminooxazole}$   $\{\{\pi_2\}^2 \{p_{xy}^N\}^2 \{\pi_{CC}\}^2\}$ ; red, charge transfer channel  $\{\{\pi_2\}^2 \{p_{xy}^N\} \{\pi_{CC}\} 1s_H\}$ ; green, charge transfer channel  $\{\{\pi_2\}^2 \{p_{xy}^N\} \{\pi_{CC}\}^2 1s_H\}$ ; blue, charge transfer channel  $\{\{\pi_2\} \{p_{xy}^N\}^2 \{\pi_{CC}\}^2 1s_H\}$ .

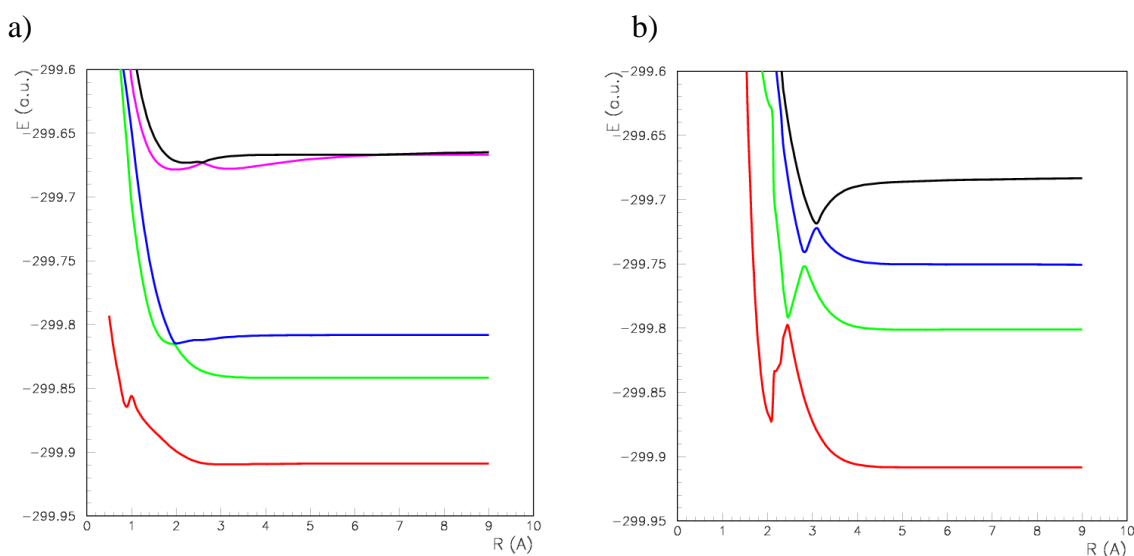


Fig. S2: Main molecular orbitals involved in the charge transfer process in collision of a proton on 2-aminooxazole

