



Supporting Information

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Base-Assisted Conversion of Protonated D-Fructose to 5-HMF: Searching for Gas-Phase Green Models

Anna Troiani,* Giulia de Petris, Federico Pepi, Stefania Garzoli, Chiara Salvitti, Marzio Rosi, and Andreina Ricci*©2019 The Authors. Published by Wiley-VCH Verlag GmbH & Co. KGaA. This is an open access article under the terms of the Creative Commons Attribution Non-Commercial NoDerivs License, which permits use and distribution in any medium, provided the original work is properly cited, the use is non-commercial and no modifications or adaptations are made.

Author Contributions

A.R. Conceptualization:Lead; Investigation:Equal; Methodology:Lead; Writing - Original Draft:Lead; Writing - Review & Editing:Lead

A.T. Data curation:Equal; Investigation:Equal; Writing - Original Draft:Lead; Writing - Review & Editing:Equal

G.d. Data curation:Lead; Writing - Original Draft:Lead; Writing - Review & Editing:Equal

F.P. Data curation:Equal; Writing - Original Draft:Supporting

M.R. Investigation:Equal

S.G. Data curation:Equal

C.S. Data curation:Equal; Formal analysis:Equal

Supporting Information

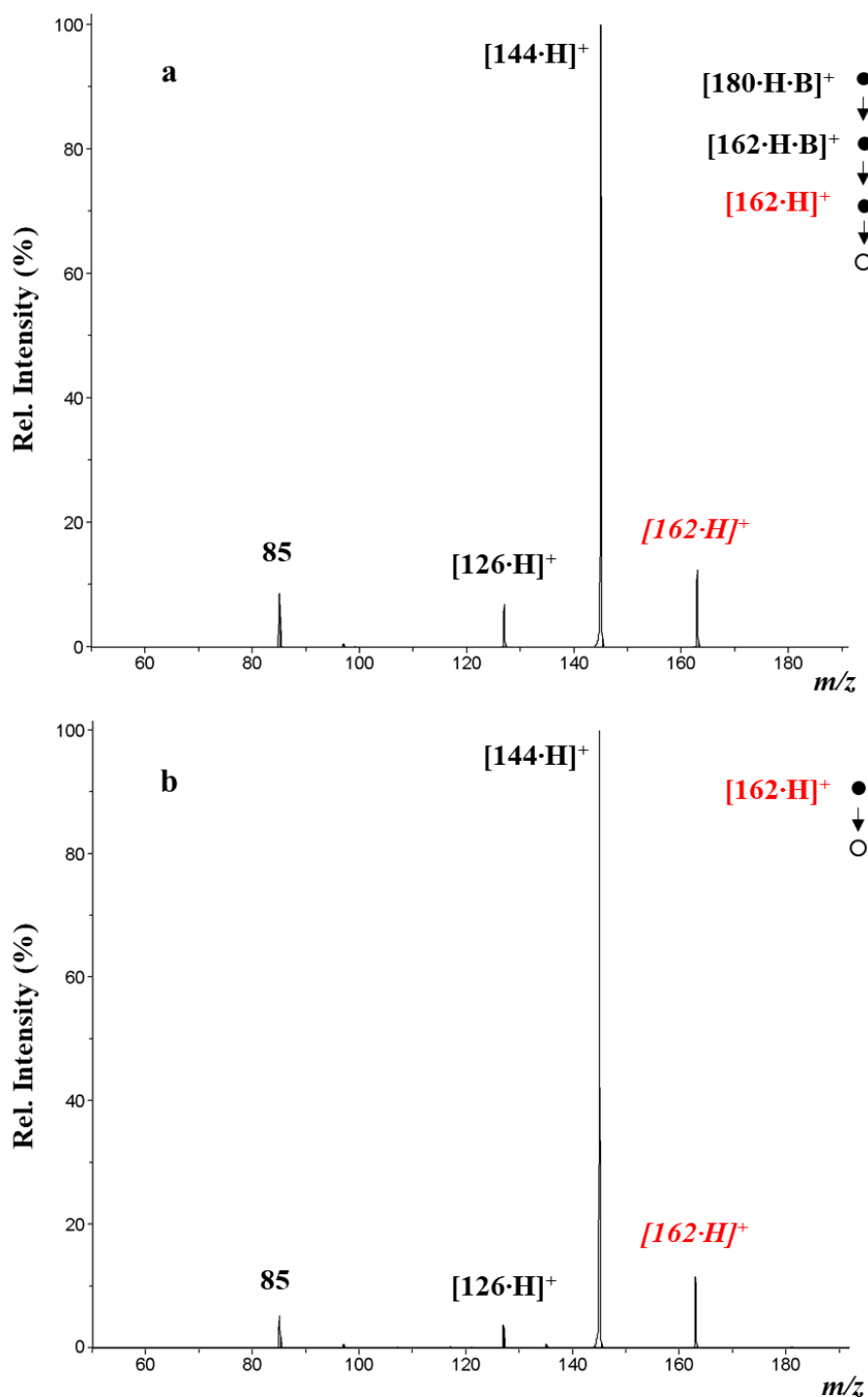


Fig. 1S. (a) CAD spectrum of $[162\cdot\text{H}]^+$ ions at m/z 163 (in red) isolated from the sequence $[180\cdot\text{H}\cdot\text{B}]^+ \rightarrow [162\cdot\text{H}\cdot\text{B}]^+ \rightarrow [162\cdot\text{H}]^+$. (b) CAD spectrum of isolated $m/z = 163$ ions (in red) obtained from the acid catalyzed dehydration of D-fructose (D-fructose dissolved in H_2O /methanol, 0.1% formic acid).

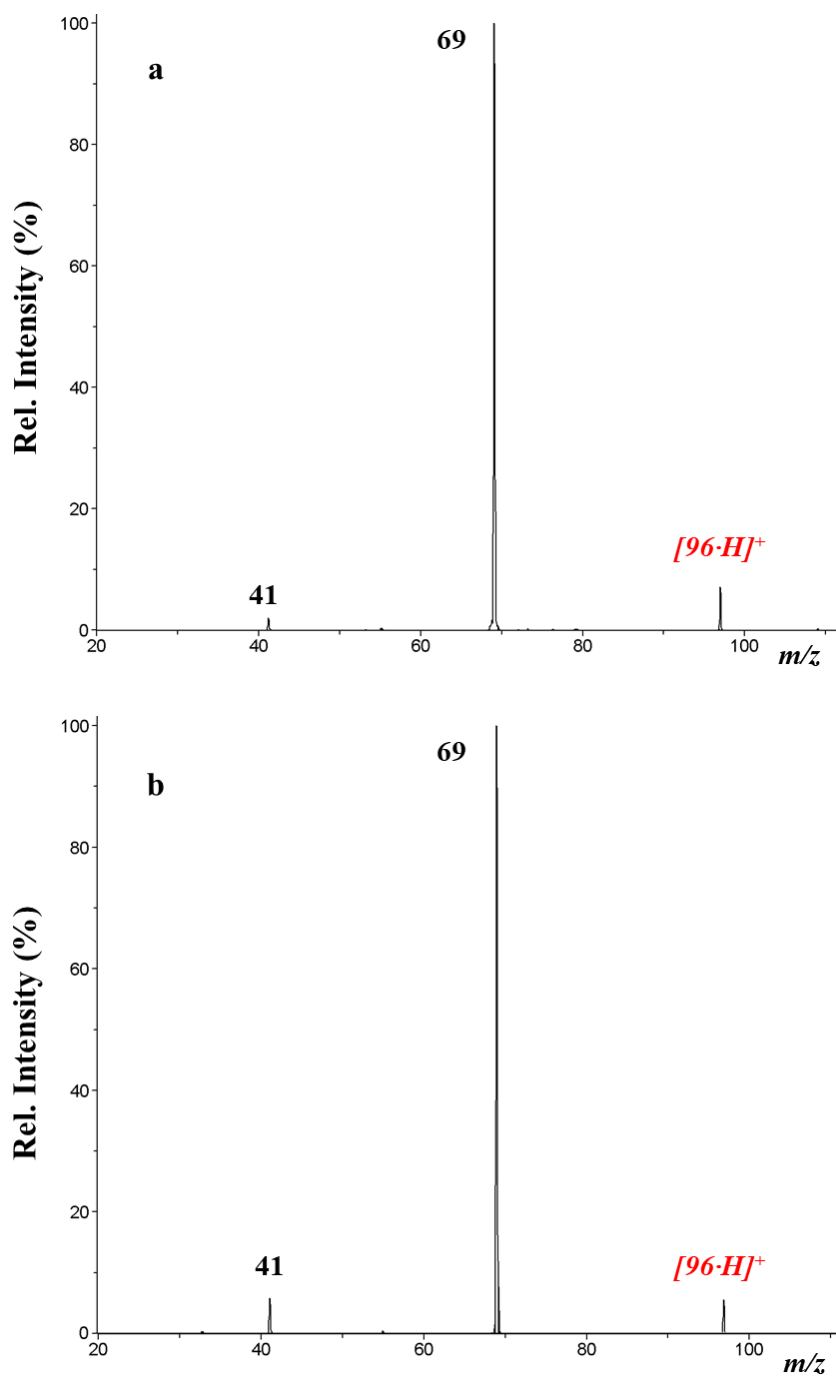


Fig. 2S. (a) CAD spectrum of $[96\cdot H]^+$ ions at m/z 97 (in red) isolated from a solution containing the D-fructose/ NH_3 protonated adduct, $[180\cdot H\cdot NH_3]^+$. (b) CAD spectrum of isolated $[96\cdot H]^+$ ions at $m/z = 97$ (in red) obtained from the standard protonated 2-furaldehyde, $[2\text{-FA}]\text{H}^+$.

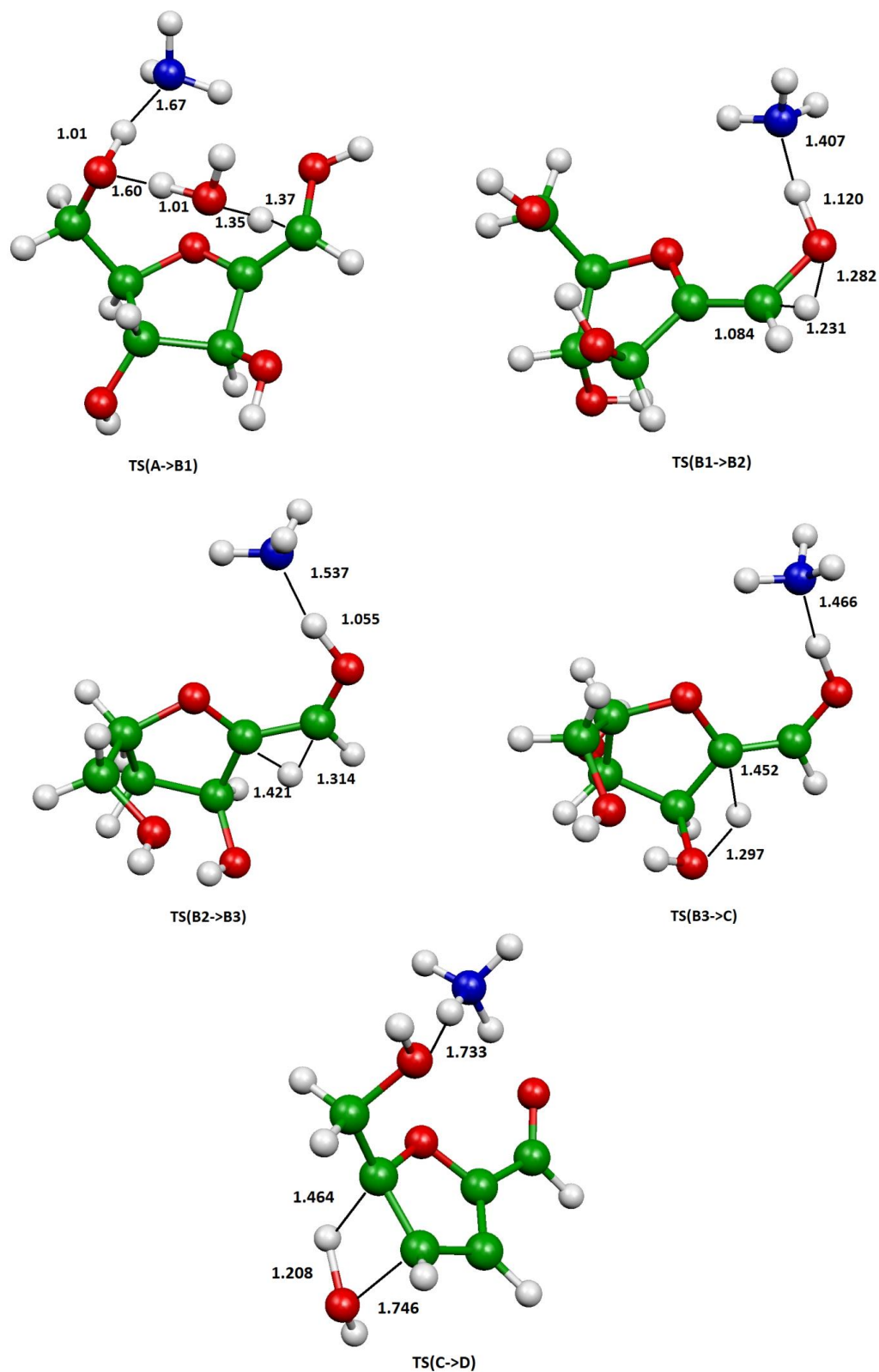


Fig. 3S. Optimized geometries at the B3LYP/6-31G(2df,p) level of theory of the transition states identified on the potential energy surface of the protonated D-fructose dehydration assisted by ammonia. Bond lengths in angstroms.

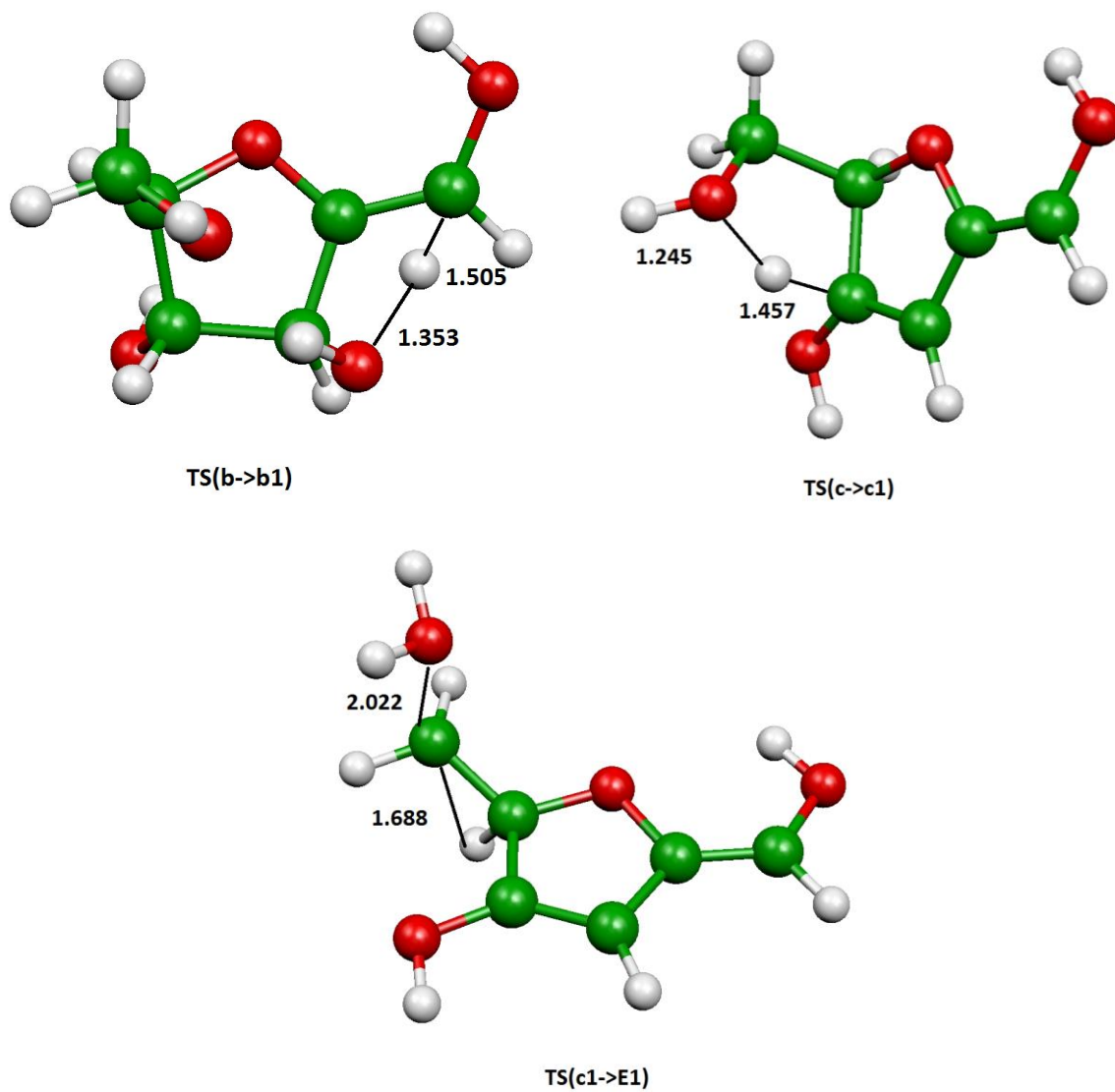


Fig. 4S. Optimized geometries at the B3LYP/6-31G(2df,p) level of theory of the transition states identified on the potential energy surface of the protonated D-fructose dehydration after ammonia loss (path 3). Bond lengths in angstroms.