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Supporting Information

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

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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

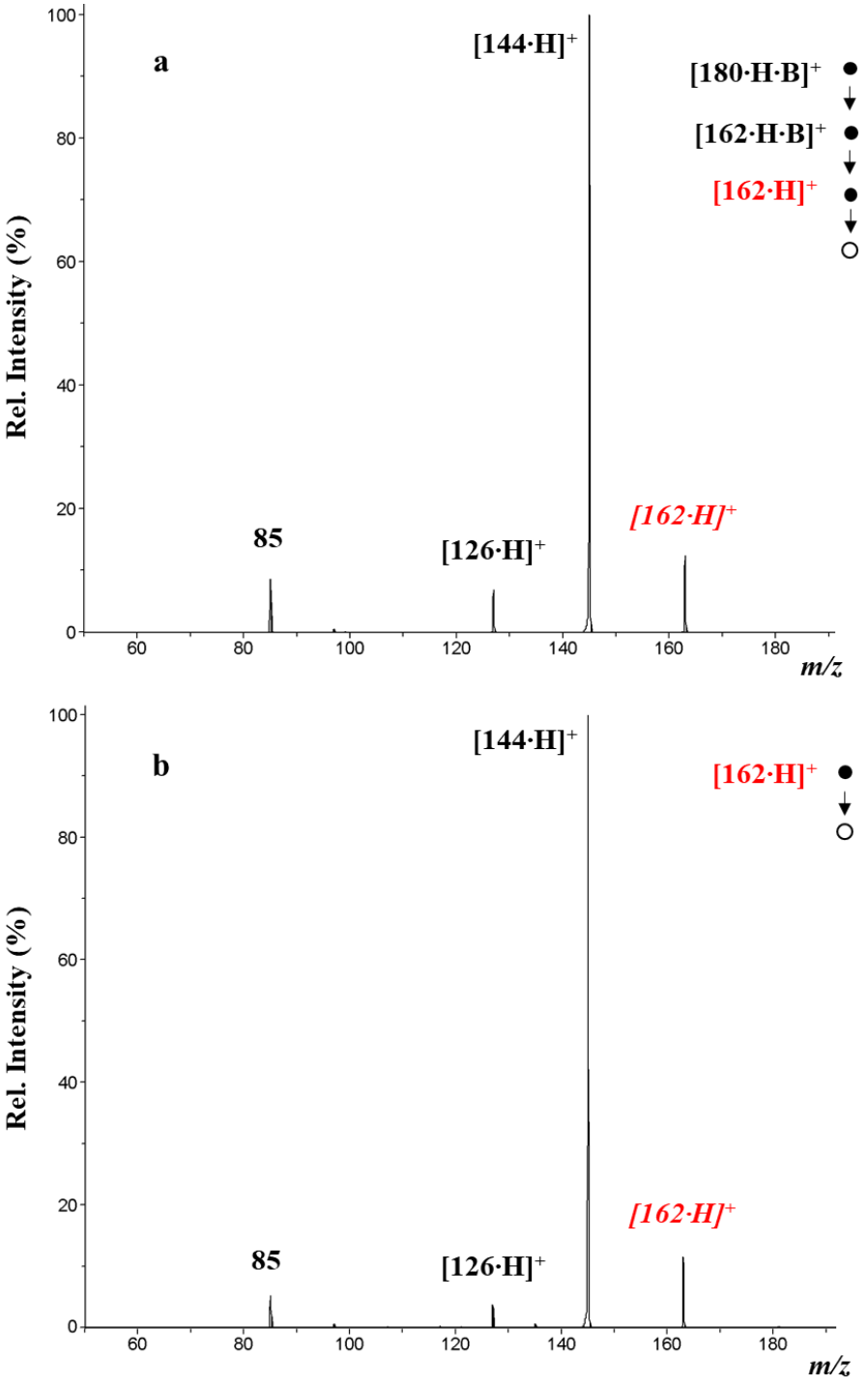

Fig. 1S. (a) CAD spectrum of $[162•H]^+$ ions at m/z 163 (in red) isolated from the sequence $[180•H•B]^+ \rightarrow [162•H•B]^+ \rightarrow [162•H]^+$. (b) CAD spectrum of isolated m/z = 163 ions (in red) obtained from the acid catalyzed dehydration of D-fructose (D-fructose dissolved in H_2O/methanol,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

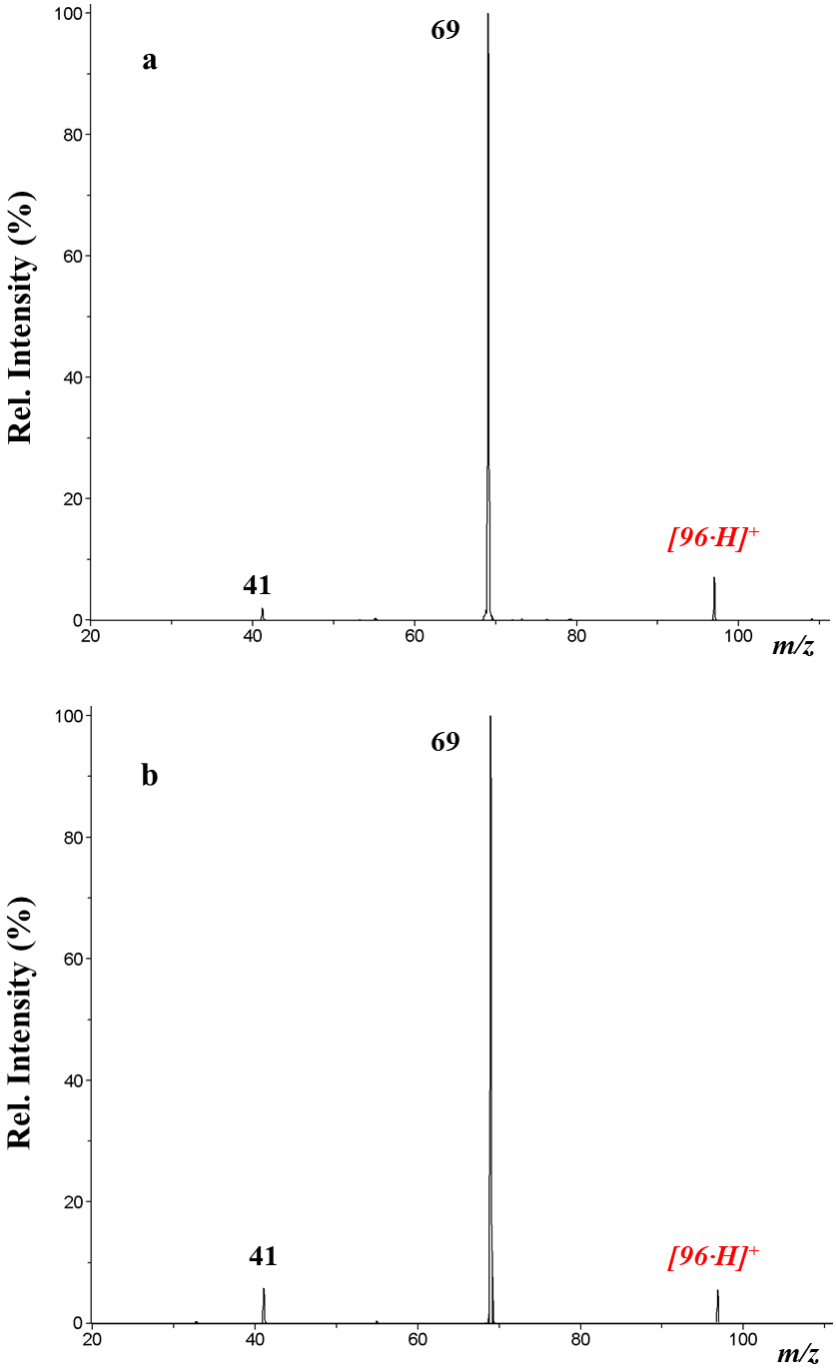

Fig. 2S. (a) CAD spectrum of $[96•H]^+$ ions at m/z 97 (in red) isolated from a solution containing the D-fructose/NH_3 protonated adduct, $[180•H•NH_3]^+$. (b) CAD spectrum of isolated $[96•H]^+$ ions at m/z = 97 (in red) obtained from the standard protonated 2-furaldehyde, $[2\text{-FA}]H^+$.

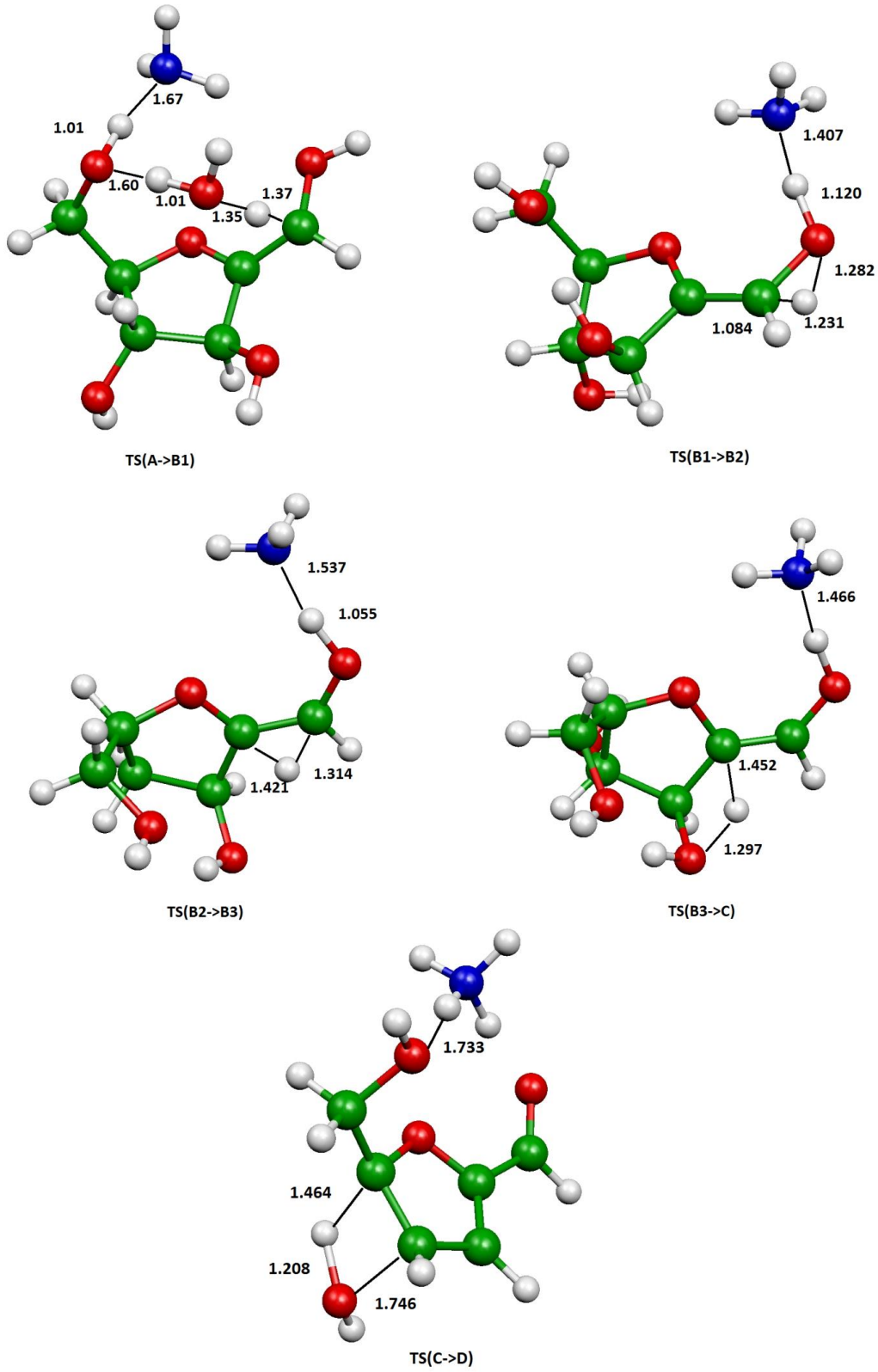

Fig. 3S. Optimized geometries at the B3LYP/6-31G(2df,p) level of theory of the transition states identified on the potential energy surface of the protonated D-fructose dehydration assisted by ammonia. Bond lengths in angstroms.

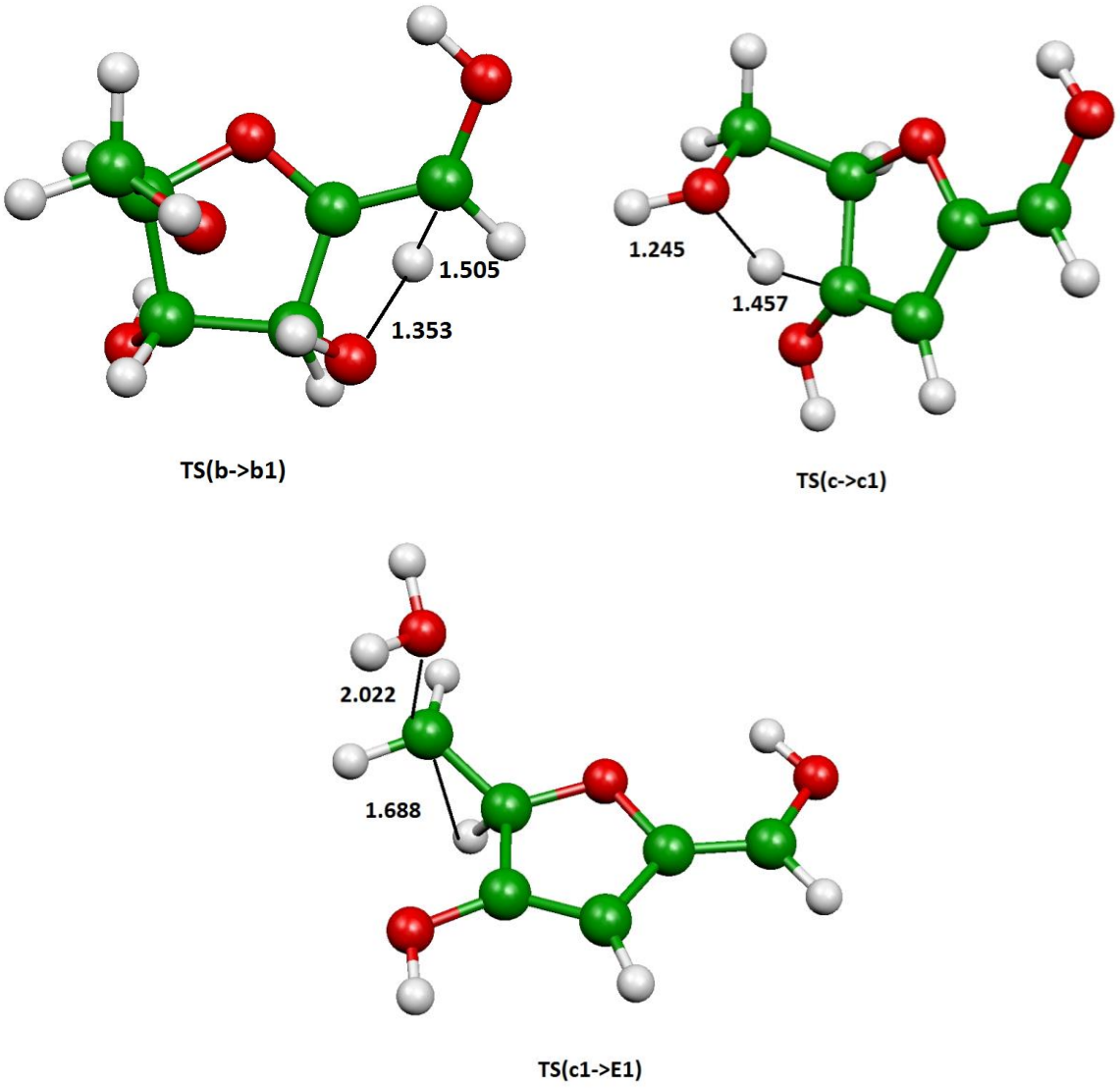

Fig. 4S. Optimized geometries at the B3LYP/6-31G(2df,p) level of theory of the transition states identified on the potential energy surface of the protonated D-fructose dehydration after ammonia loss (path 3). Bond lengths in angstroms.