Supplementary Material for PCCP

SUPPORTING INFORMATION

Spectroscopic Investigation of H Atom Transfer in a Gas-phase Dissociation Reaction: McLafferty Rearrangement of Model Gas-phase Peptide Ions

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Figure S1. Tandem mass spectra for the dissociation of (a) $(BetGOtBu)^+$ and (b) $(BetGOH)^+$ generated using multiple-stage CID in the quadrupole ion trap mass spectrometer.

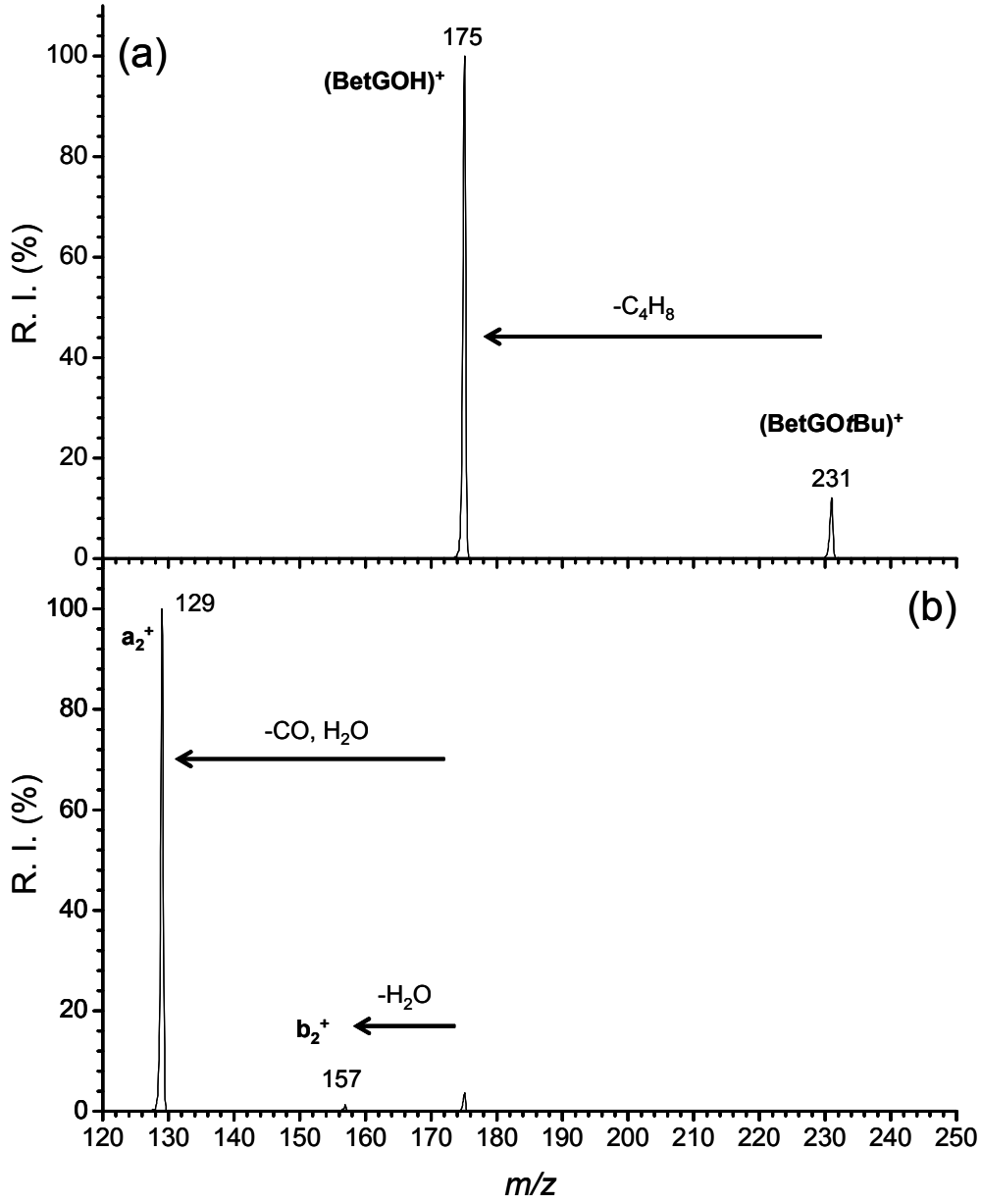

Figure S2. Tandem mass spectra generated from fully deuterium-exchanged betaine-glycine-*tert*-butyl ester using the quadrupole ion trap mass spectrometer: (a) dissociation of $(M)^+$, d_1-BetGO*t*Bu; (b) dissociation (MS^3 stage) of $(M)^+$, d_1-$(BetGOH)^+$, product resulting from McLafferty rearrangement.

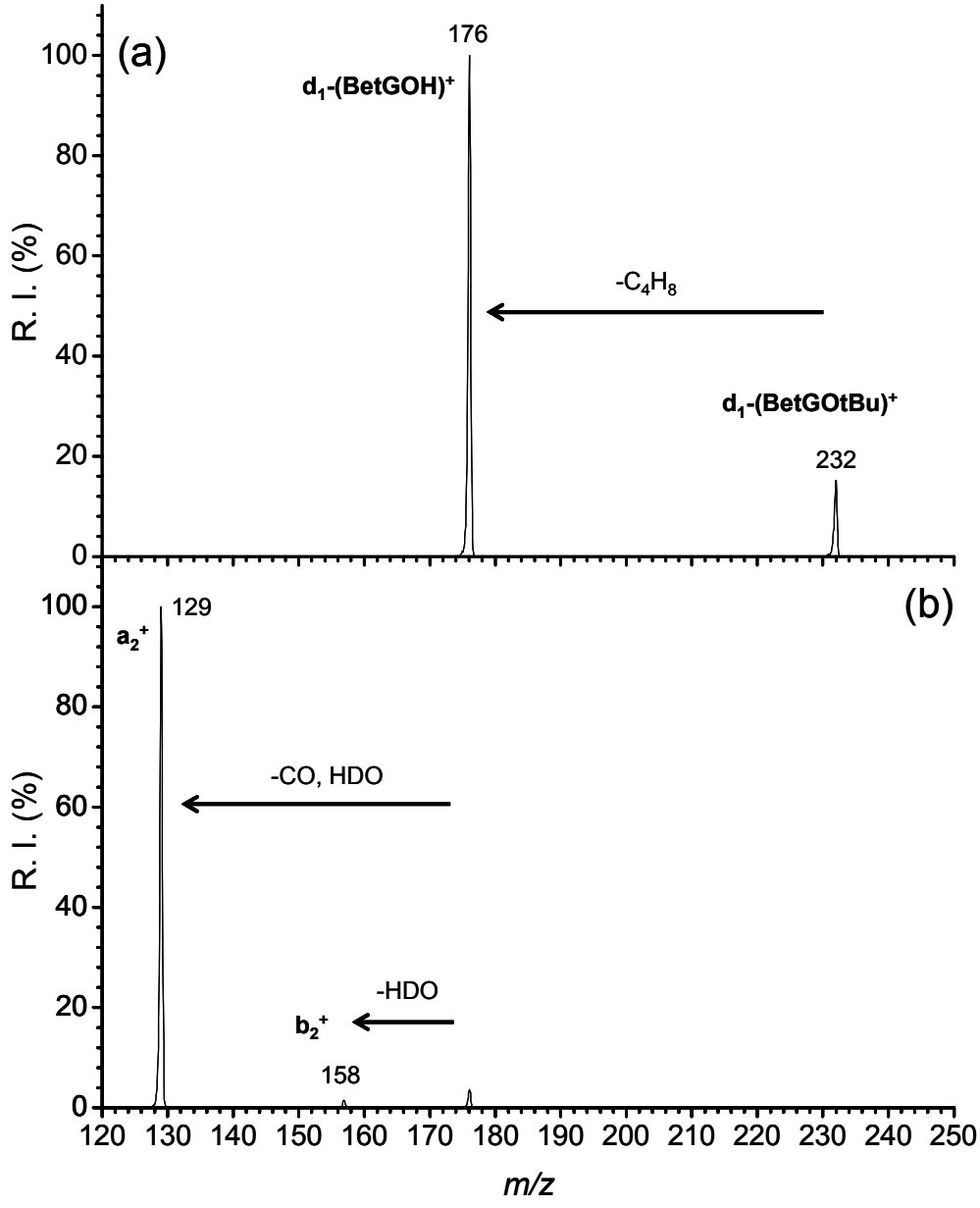

Figure S3. Comparison between IRMPD spectrum generated from (NicGGOH+H)+ (a) and theoretical spectra based on DFT calculations for structures (b) Nic_e, (c) Nic_f, (d) Nic_g, (e) Nic_h and (f) Nic_i. Conformations of the respective isomers are provided in figure 4 of the manuscript.