Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Material

For

Infrared Multiple Photon Dissociation Spectroscopy of Protonated Unsymmetrical Dimethylhydrazine, Proton-bound Hydrazine Dimer and Unsymmetrical Dimethylhydrazine Dimer

Christopher P. McNary,[a] Maria Demireva,[a,†] Jonathan Martens,[b] Giel Berden,[b] Jos Oomens,[b,c] L. A. Hamlow,[d] M. T. Rodgers,[d] and P.B. Armentrout*[a]

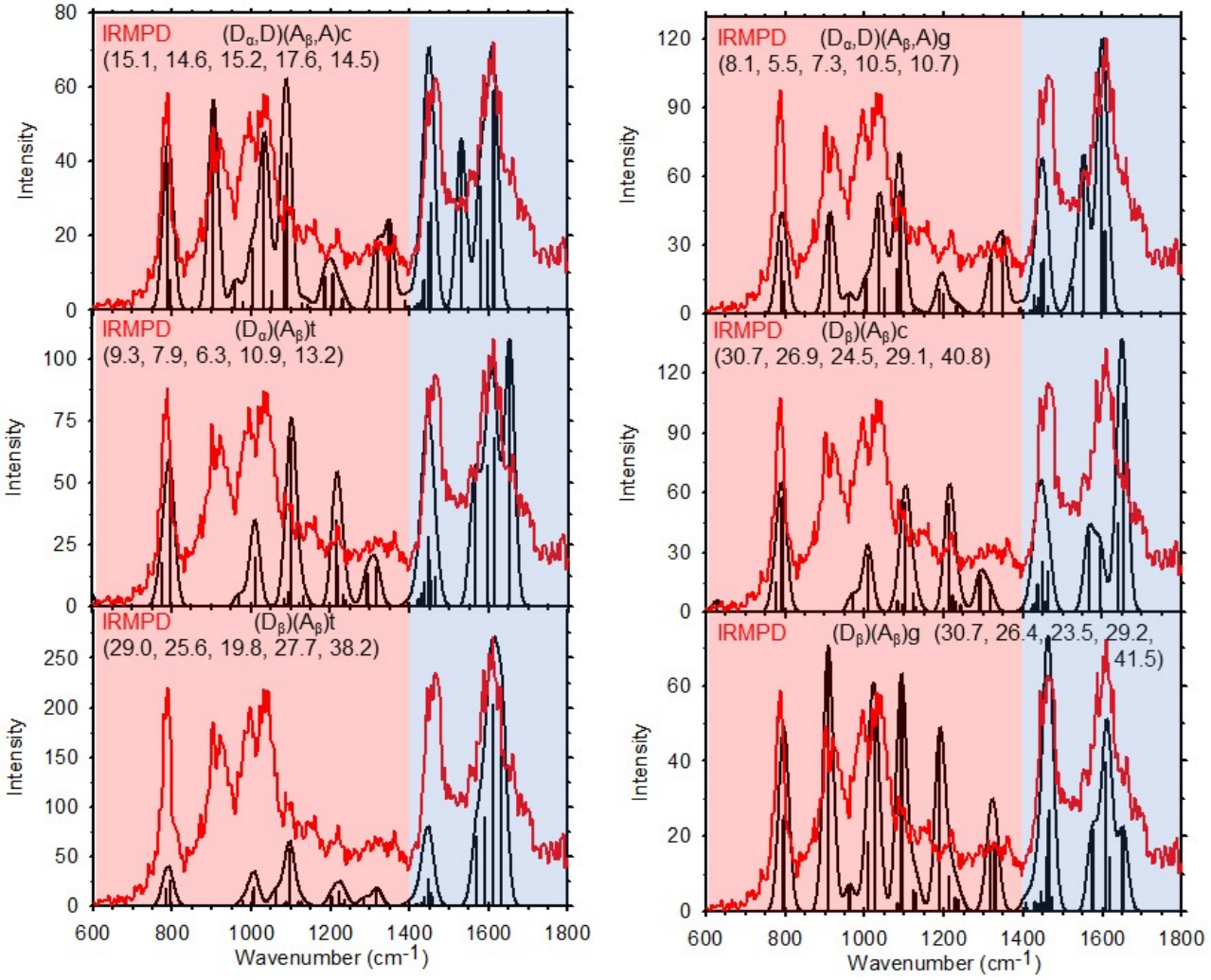

Figure S1. IRMPD spectrum of $(UDMH)_2H^+$ compared to the IR spectra of six higher-lying isomers of $(UDMH)_2H^+$. Relative 298 K Gibbs energies in kJ/mol at the B3LYP, M06, mPW1PW91, PBE0, and MP2 levels are also provided. Two scaling factors were used: 0.975 for frequencies below 1400 cm^{-1} (red) and 0.965 for frequencies above 1400 cm^{-1} (blue). Structures are shown in Figure S2.

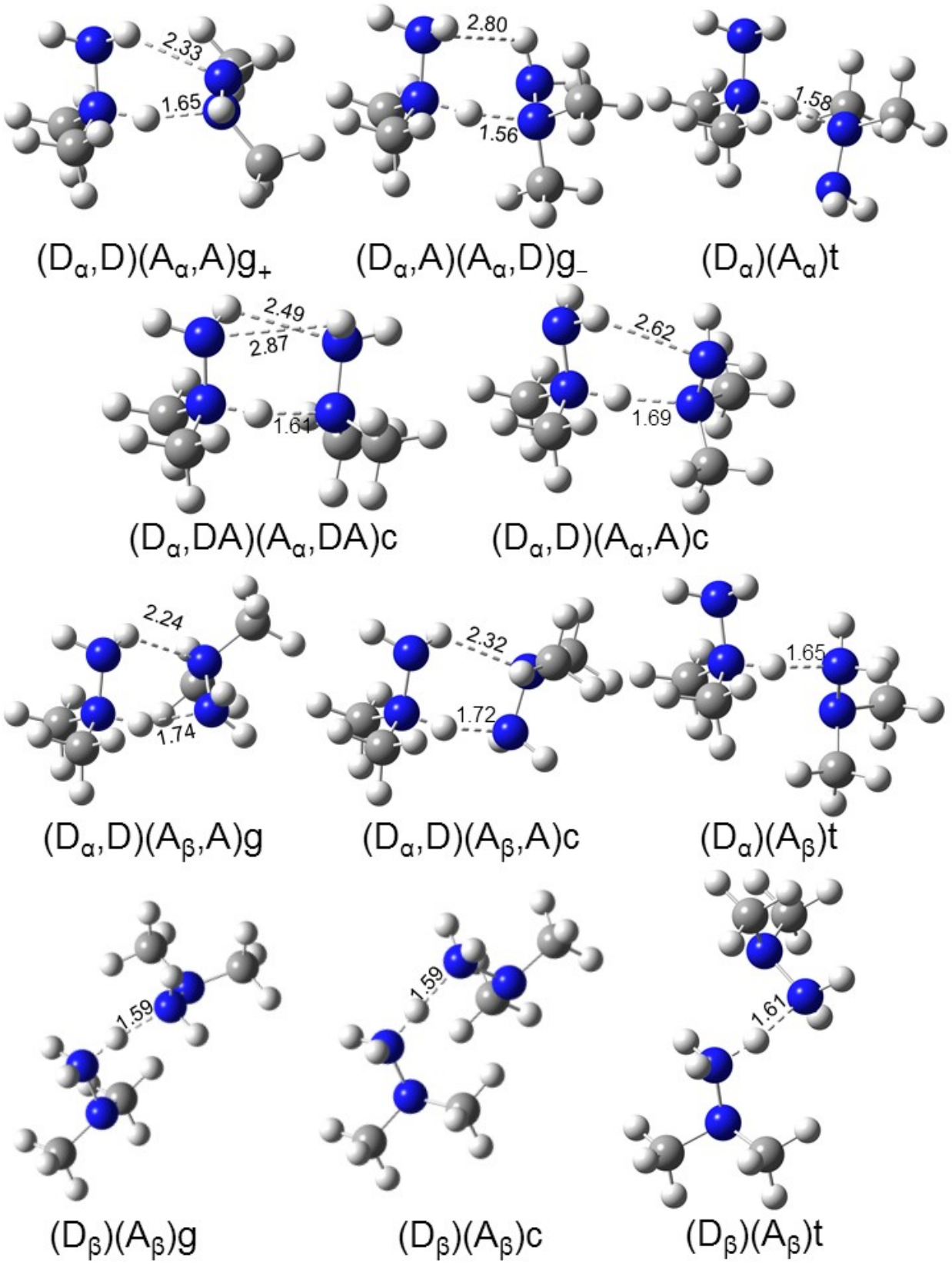

Figure S2. Structures of all $(UDMH)_2H^+$ species determined at the B3LYP-GD3BJ level of theory. Hydrogen bond lengths are provided in Å.