

Supplementary Information

A Time-Dependent Perspective for the Intramolecular Couplings of the N-H Stretches of Tryptophan

Alexander Kaiser,^a Bhumika Jayee,^b Yuxuan Yao,^b Xinyou Ma^{b,c}

Roland Wester,^a William L. Hase^b

^aInstitut für Ionenphysik and Angewandte Physik

Universität Innsbruck

Technikerstrasse 25

6020 Innsbruck, Austria

^bDepartment of Chemistry and Biochemistry

Texas Tech University

Lubbock, Texas, USA 79409

^cDepartment of Chemistry

University of Chicago

5735 S. Ellis Ave.

Chicago, Illinois 60637

Figure S1. Scaled displacement vectors for the calculated harmonic normal modes corresponding to NH(α), NH(β), and NH(γ) from left to right.

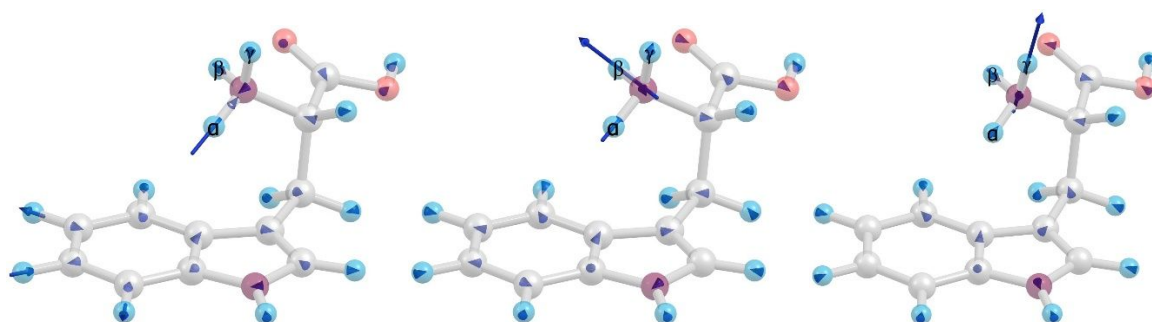


Table S1. Comparison of experimental and calculated vibrational frequencies in wavenumbers of the NH_3^+ , NH, and OH modes of protonated tryptophan.

	NH_3^+ sym	NH_3^+ asym	NH_3^+ asym	NH	OH	conformer
TrpH⁺						
Experiment ¹	3044	3094	3357	3503	3555	B
Experiment ¹	3044	3123	3339	3503	3555	A
Theory harmonic unscaled (this work)						
B3LYP/cc-pVDZ+Grimme D3	3178	3255	3502	3640	3681	B
B3LYP-631g(d,p)+Grimme D3	3202	3288	3522	3670	3735	B
MP2/6-31g(d,p)	3295	3423	3571	3715	3779	A
B3LYP-D3/6-31g(d,p)	3215	3323	3502	3669	3731	A
B3LYP/6-311++G(d,p)	3232	3359	3487	3650	3726	A
PBE1PBE/6-31g(d,p)+Grimme D3	3216	3329	3549	3711	3791	A
PBE1PBE/6-311++g(d,p)+Grimme D3	3221	3357	3533	3689	3780	A
RIMP2/cc-pVTZ (partial Hessian method) ²	3214	3350	3517	3648	3724	A
Theory harmonic scaled (this work)						
B3LYP/cc-pVDZ, Grimme D3, scaled with 0.966	3070	3144	3383	3516	3556	B
B3LYP/6-31G(d,p) GD3, scaled with 0.953	3065	3167	3339	3497	3556	A
Theory anharmonic						
DFT TOSH ³ (this work)	2917	3023	3253	3468	3588	A
DFT VPT2 ⁴ (this work)	2881	3002	3257	3478	3528	A
CCSD(T)/cc-pVTZ (VDPT2 on top of VSCF) ⁵	2980	3090	3330	3490	3540	B
MP2/cc-pVTZ (VDPT2 on top of VSCF) ⁵	2960	3110	3360	3490	3540	B

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