Electronic Supplementary Information for

Identification of the protonation site of gaseous triglycine: the cis-peptide bond conformation as the global minimum

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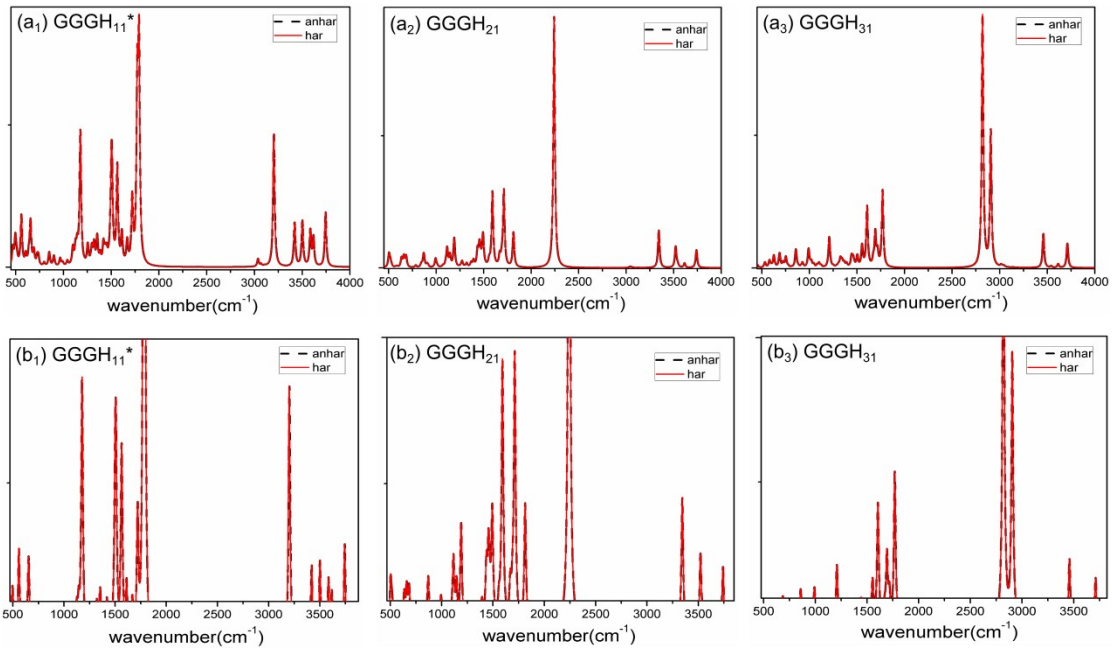

Fig. S1 Comparison of the theoretical IR spectra of the most stable conformer of each isomer of protonated triglycine (a_1) $GGGH_{11}^*$, (a_2) $GGGH_{21}$, (a_3) $GGGH_{31}$ and the corresponding enlarged small peaks (b_1-b_3) at 298 K, simulated by anharmonic (anhar) and unscaled harmonic (har) frequency calculations at the B3LYP/6-311++G(d, p) level of theory. A Lorentzian profile with a FWHM of 20 cm^{-1} is used to convolute the calculated spectra.

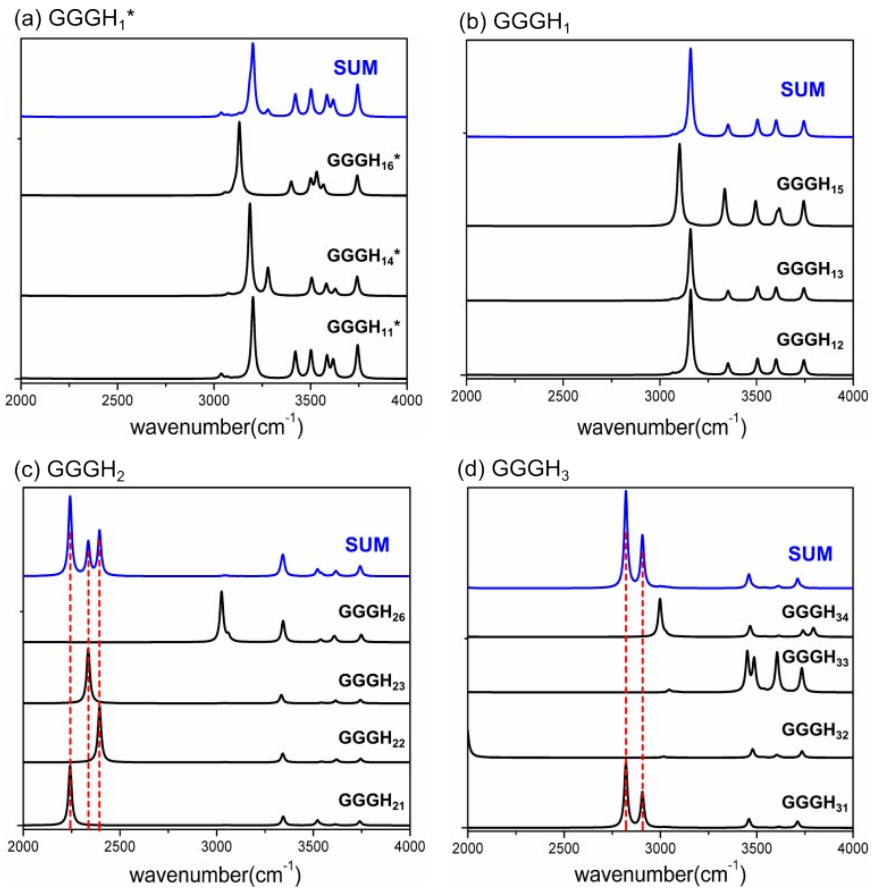

Fig. S2 Simulated IR spectra (2000-4000 cm^{-1} region) of dominant conformers in the four isomers of protonated triglycine (a) $GGGH_1^*$, (b) $GGGH_1$, (c) $GGGH_2$, (d) $GGGH_3$ at 298 K, calculated at the B3LYP/6-311++G(d, p) level of theory, as well as their summations (SUM) calculated using the percentage abundances listed in Table 3. A Lorentzian profile with a FWHM of 20 cm^{-1} is used to convolute the calculated spectra.

Table S1. Conformers with low Gibbs free energy of protonated triglycine, together with their respective percent abundances at 498, 298, 250 and 198 K. The abundances were calculated using CCSD/6-31++G (d, p) electronic energies and Gibbs free energy corrections at the B3LYP/6-311++G (d, p) level of theory.

	$GGGH_{11}^{*}$	**$GGGH_{12}$**	**$GGGH_{13}$**	**$GGGH_{14}^{*}$**	**$GGGH_{15}$**	**$GGGH_{21}$**	**$GGGH_{22}$**	**$GGGH_{23}$**
498 K	25.60%	12.65%	12.53%	13.00%	-	10.01%	9.04%	7.73%
298 K	60.44%	11.11%	10.95%	8.89%	0.60%	3.99%	2.38%	1.65%
250 K	73.45%	8.37%	8.23%	5.98%	0.30%	2.04%	1.01%	0.63%
198 K	-	45.52%	44.56%	-	0.84%	5.81%	2.11%	1.13%