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Electronic Supplementary Information for

Competition between Dispersion Interactions and Conventional Hydrogen Bonding: Insights from a Theoretical Study on Z-Arg-OH

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Table S1 Energy values (in kcal mol^{-1}) of the noncovalent interaction from the energy decomposition analysis between the three different parts: the guanidine group (P_1), the benzene group (P_3) and the middle part (P_2), including the peptide bond and the carboxylate group in conformer AT_{11} and AC_{12}.

		Electrostatic	Repulsion	Dispersion	Total
AT_{11}	P_1 and P_3	0.62	0.12	-1.03	-0.29
	P_1 and P_2	-10.84	7.00	-5.21	-9.06
AC_{12}	P_1 and P_3	-0.52	0.02	-0.37	-0.87
	P_1 and P_2	-7.89	8.19	-7.87	-7.56

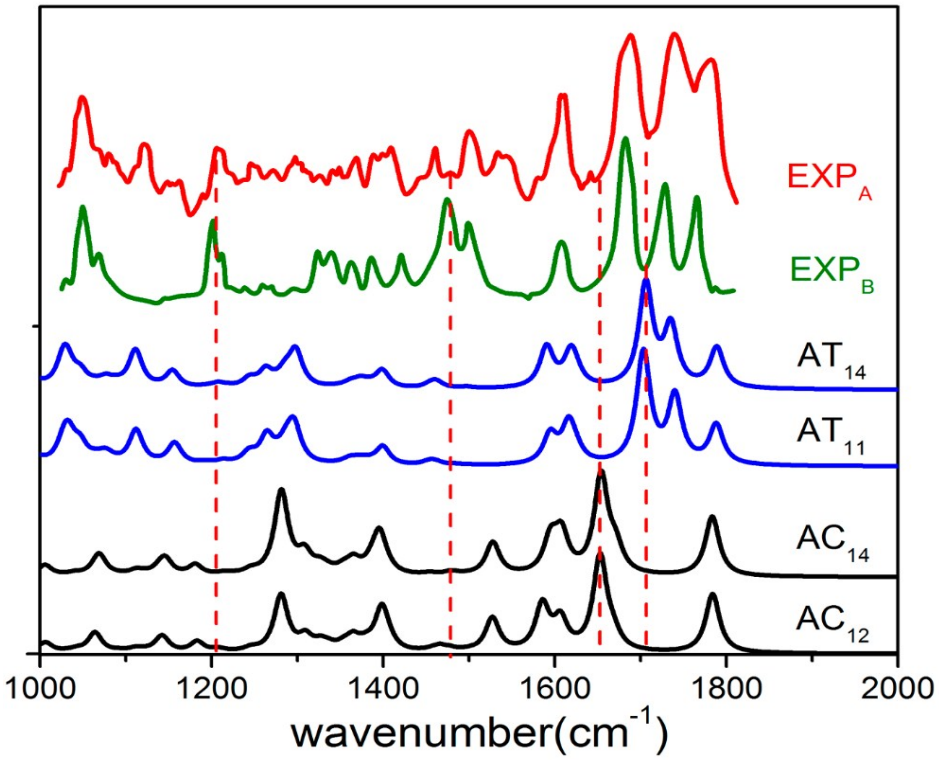

Fig. S1 Simulated IR spectra of the most stable folded structures AC_{12}, AC_{14}, AT_{11} and AT_{14} at the B3LYP-D3 level with experimental results EXP_A and EXP_B for comparison. A Lorentzian profile with a FWHM of 20 cm^{-1} is used to convolute the calculated spectra.

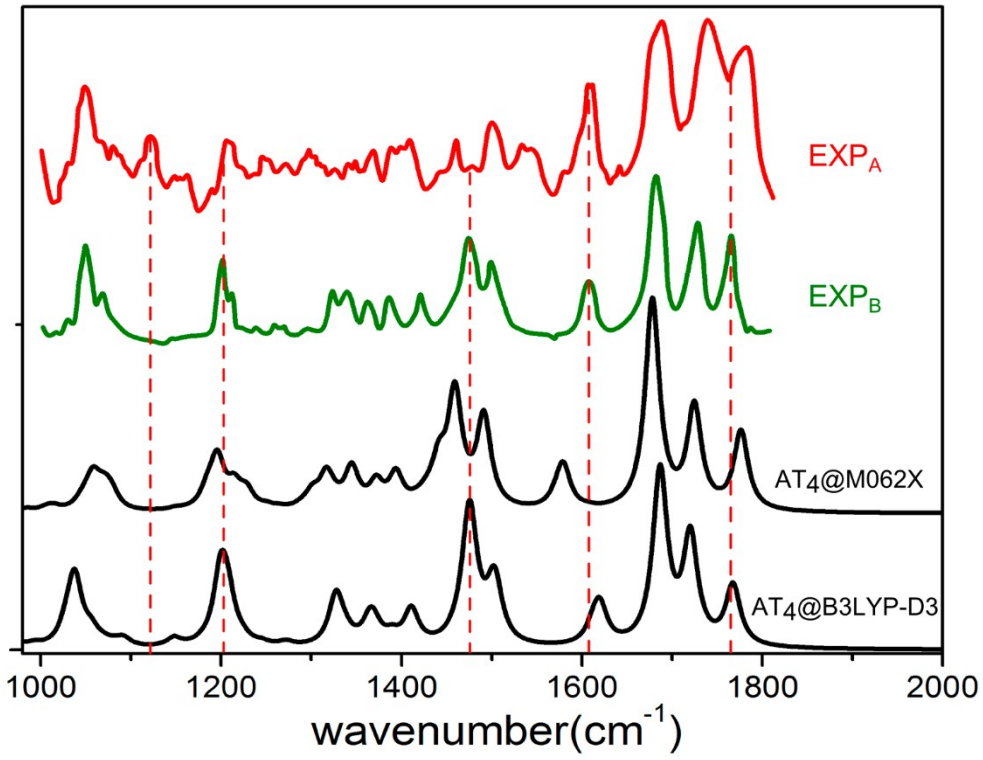

Fig. S2 Simulated IR spectra of conformer AT_4 at the B3LYP-D3 and M062X level with experimental results EXP_A and EXP_B for comparison. A Lorentzian profile with a FWHM of 20 cm^{-1} is used to convolute the calculated spectra.

Table S2 Conformers with low Gibbs free energy of the three different isomers (AC_1, AT_1-AT_5, AZ_1) of Z-Arg-OH, together with their respective percent abundances at four different temperatures: 350, 300, 250 and 200 K.

	Percent (%)			
conformer	350 K	300 K	250 K	200 K
AC_1	0.32	0.20	0.10	0.03
AT_1	19.57	22.18	25.22	29.23
AT_2	16.73	18.87	21.34	24.55
AT_3	11.57	13.18	15.07	17.59
AT_4	22.78	21.45	18.82	14.87
AT_5	20.92	19.25	16.37	12.40
AZ_1	0.80	0.40	0.20	0.05

Note: the abundances were calculated using the DSD-PBEP86-D3(BJ)/aug-cc-pVTZ electronic energies and Gibbs free energy corrections at the B3LYP-D3(BJ)/6-311++G (d, p) level of theory.

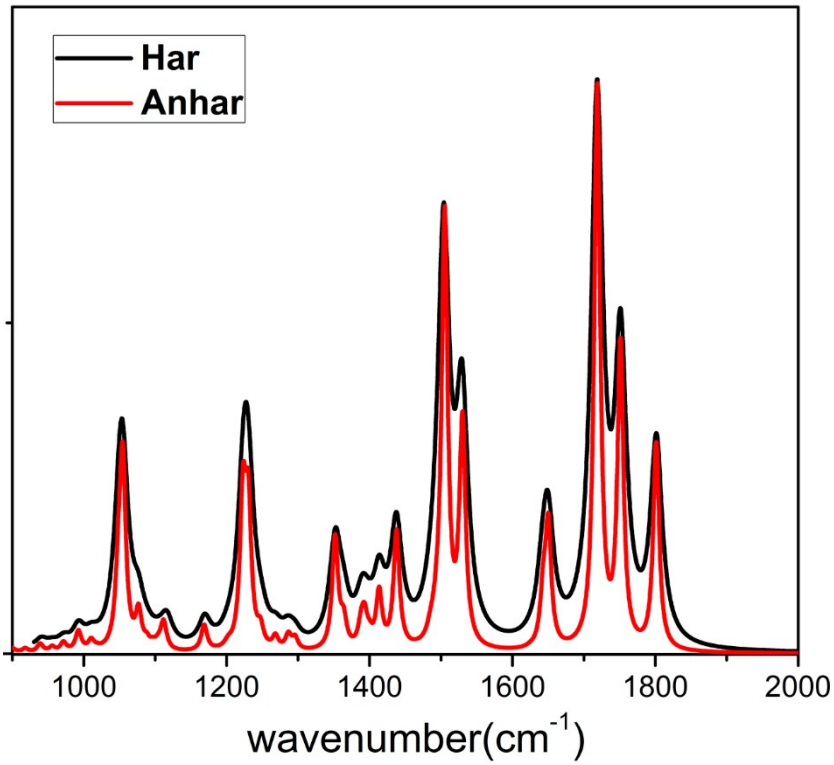

Fig. S3 The computed IR spectrum of representative conformer AT_1 in the anharmonic motion (red) and the calibrated harmonic motion (black, scaling factor: 0.9813) at the B3LYP(BJ)/6-311++G (d, p) level. A Lorentzian profile with a FWHM of 20 cm^{-1} is used to convolute the calculated spectra.

Table S3 Conformers with low Gibbs free energy of the three different isomers (AC_3, AT_1-AT_5, AZ_3) of Z-Arg-OH, together with their respective percent abundances at 498 K.

Conf.	AC_3	AT_1	AT_2	AT_3	AT_4	AT_5	AZ_3
Percent (%)	1.05	14.70	12.71	8.59	23.86	22.94	2.06

Note: the abundances were calculated using the DSD-PBEP86-D3(BJ)/aug-cc-pVTZ electronic energies and Gibbs free energy corrections at the B3LYP-D3(BJ)/6-311++G (d, p) level of theory.