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

Electronic Supporting Information

Stereochemistry-dependent structures of hydrogen-bonded protonated dimers: The case of 1-amino-2-indanol

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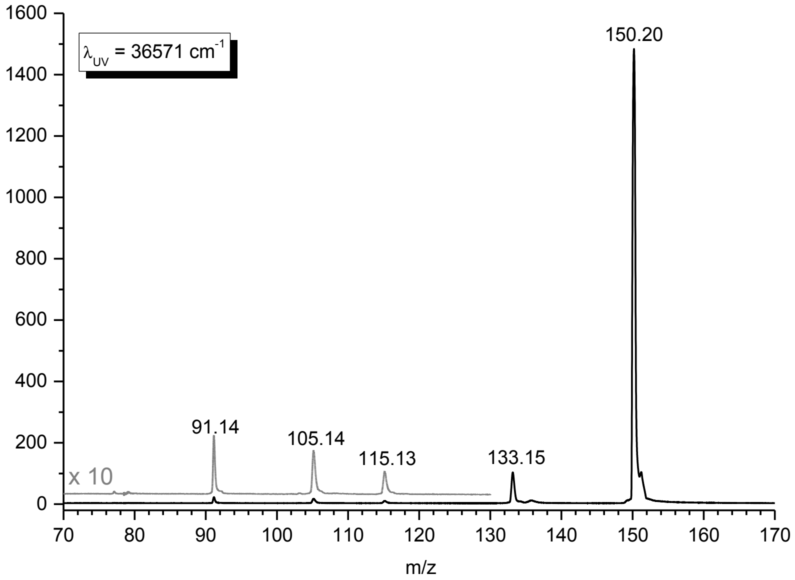
(R,S)-*cis*-AIH$^+$



(R,R)-*trans*-AIH$^+$

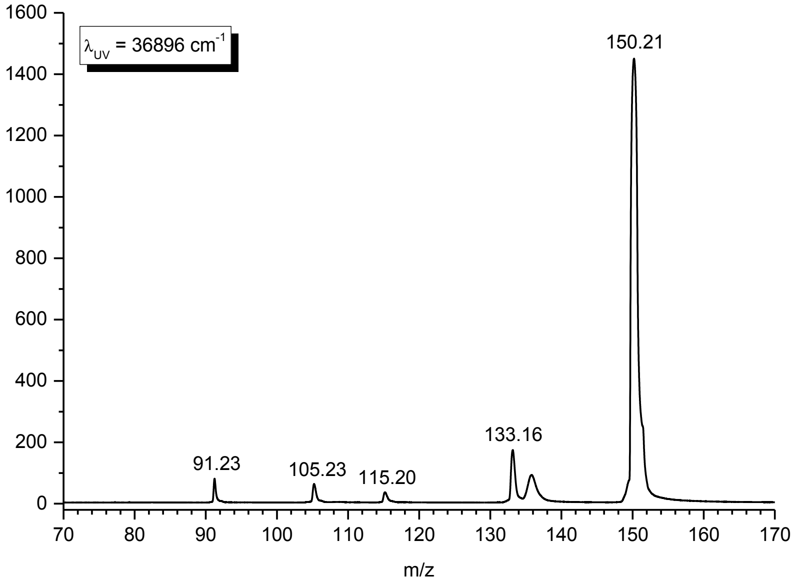


Figure S1: UV photodissociation (UVPD) mass spectra of *c*-AIH$^+$ and *t*-AIH$^+$ monomers, with the laser set at the most intense UV transition. The signal observed at *m/z* ~136 comes from CID occurring after the ion trap. This signal is thus not recorded at the right time in the TOF and should be ignored for the analysis.

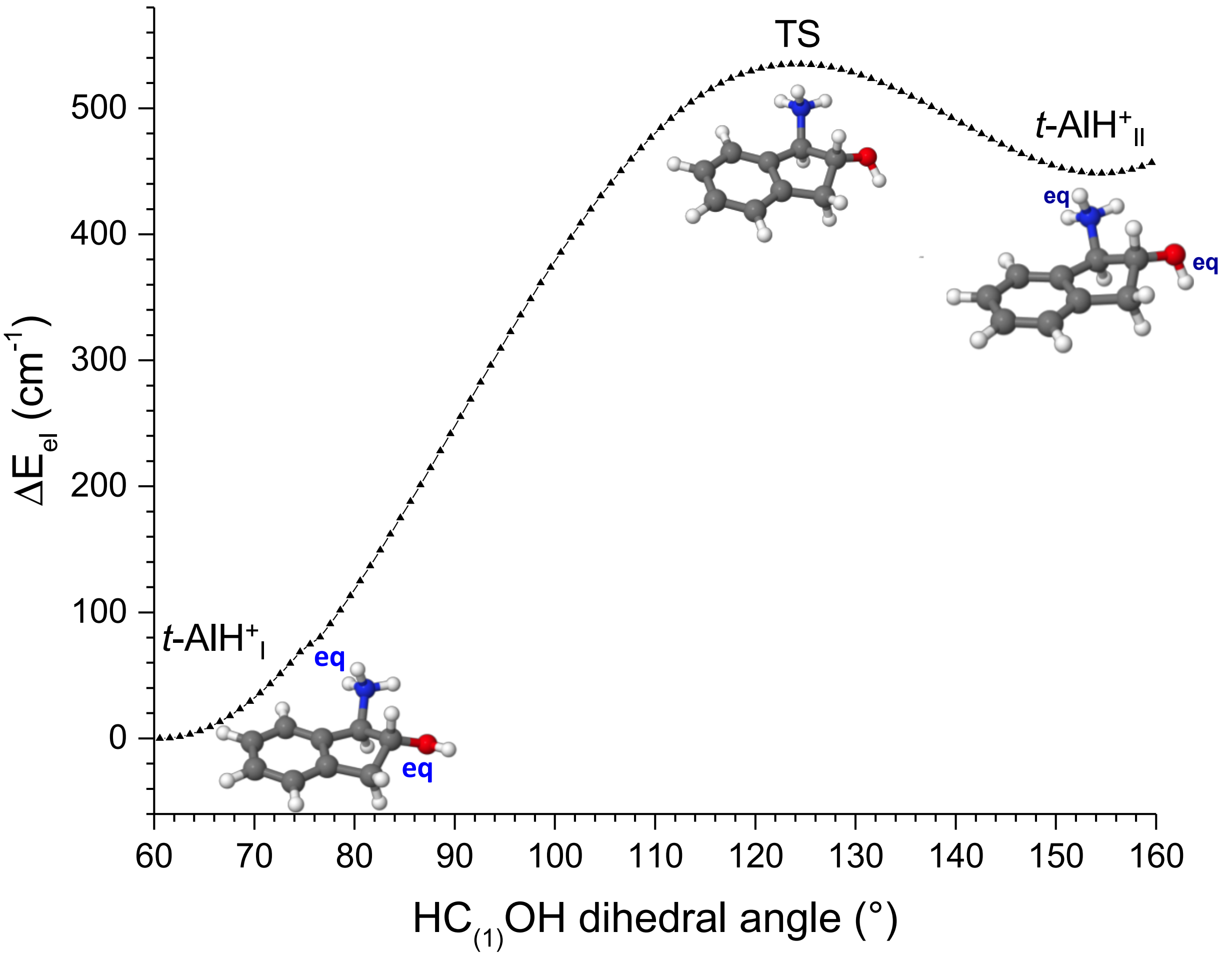


Figure S2: Relaxed potential energy surface scan and transition state identification between t-AIH$^+_{I}$ and t-AIH$^+_{II}$ (OH rotation) calculated at the B3LYP-D3/6-31G++(d,p) level. The structures shown on the graph are all optimized at the same level of theory.

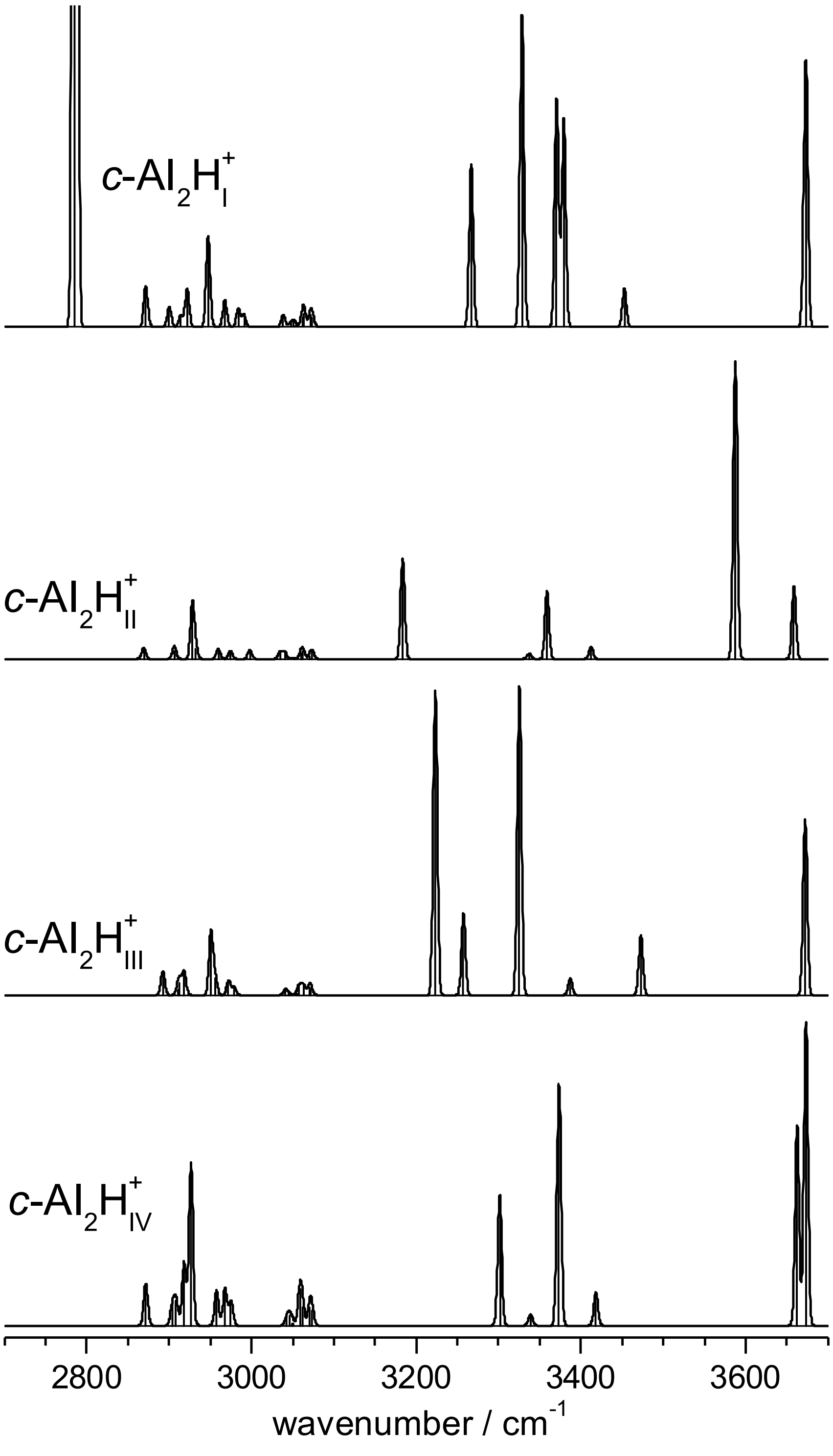


Figure S3: IR absorption spectra of the four most stable conformers of c-Al_2H^+ predicted at the B3LYP-D3/6-31G++(d,p) level. Corresponding geometries are given in Figure 4 and relative energies in Table 3.

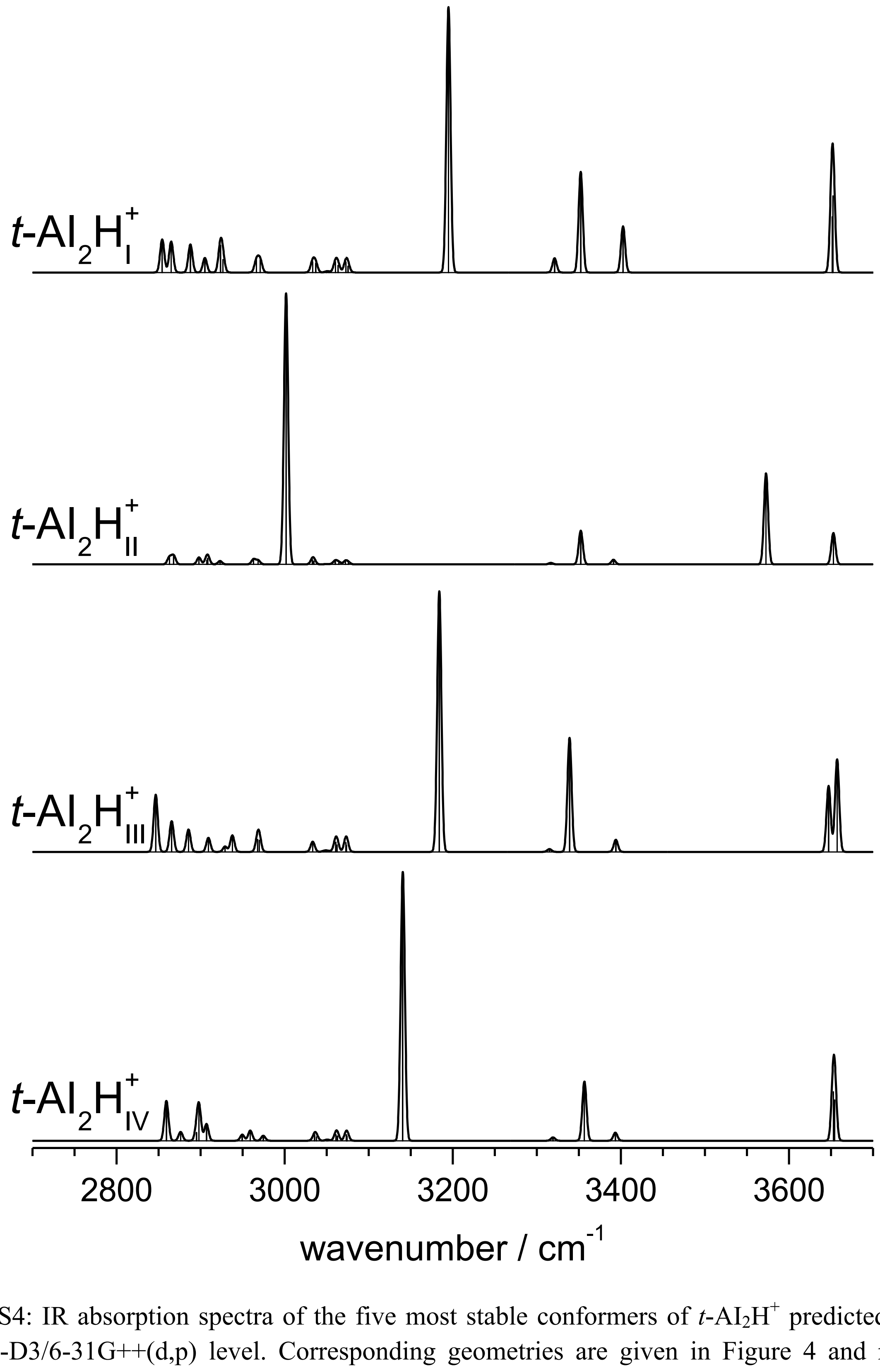


Figure S4: IR absorption spectra of the five most stable conformers of t-AI_2H^+ predicted at the B3LYP-D3/6-31G++(d,p) level. Corresponding geometries are given in Figure 4 and relative energies in Table 3.

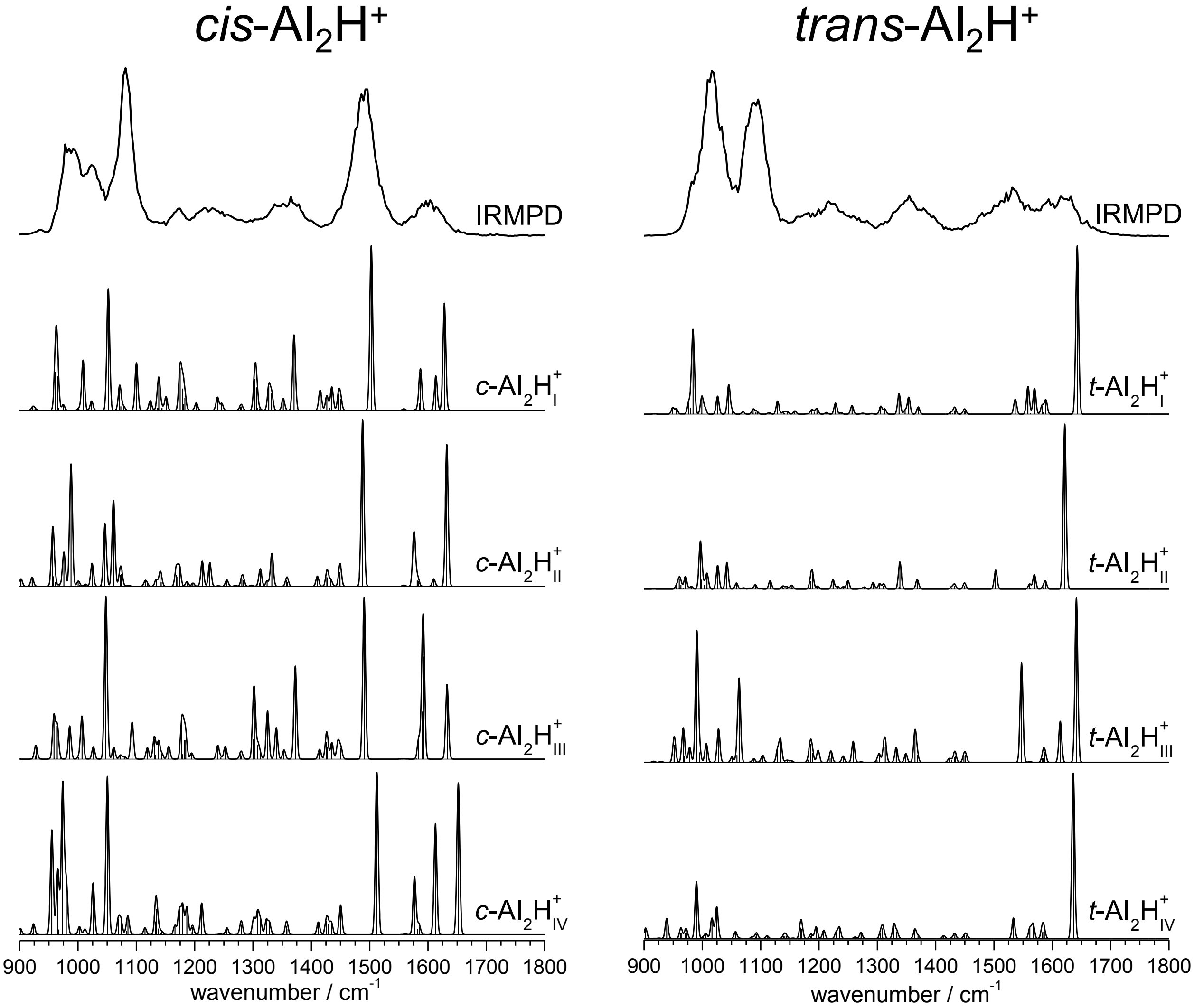


Figure S5: IR multiple photon (IRMPD) spectra of c-AI$_2$H$^+$ (top left) and t-AI$_2$H$^+$ (top right) in the fingerprint range (900-1800 cm^{-1}) compared to the IR absorption spectra of the most stable corresponding conformers calculated at the B3LYP-D3/6-31G++(d,p) level. The IRMPD spectra are recorded in a Fourier-transform ion cyclotron resonance (FT-ICR) mass spectrometer equipped with an electrospray ion source and coupled to the IR beamline of a tunable free electron laser (FEL) at the CLIO (Centre Laser Infrarouge d'Orsay) facility in Orsay. The fragmentation channel observed upon IRMPD of c-AI$_2$H$^+$ and t-AI$_2$H$^+$ (*m/z* 299) is *m/z* 150, corresponding to loss of the neutral monomer. Further details on the experimental setup and acquisition conditions can be found in the experimental section of Reference 35.

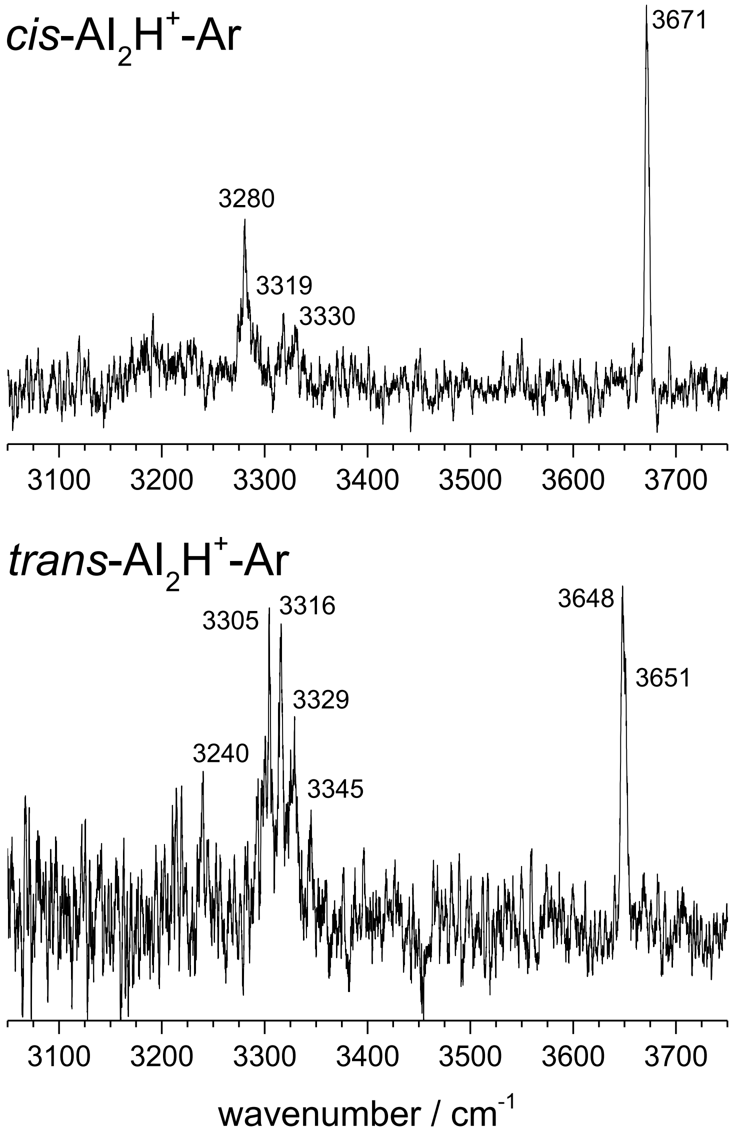


Figure S6: IR photodissociation (IRPD) spectra of *c*-AI$_2$H$^+$-Ar (top) and *t*-AI$_2$H$^+$-Ar (bottom) in the X-H stretching range (X=O, N, C, 3050-2750 cm^{-1}). These spectra are recorded using the messenger technique by single photon IRPD spectroscopy of mass-selected *c*-/*t*-AI$_2$H$^+$-Ar cluster ions in a tandem quadrupole mass spectrometer at TU Berlin, which is coupled to an electron impact ionization source. The only fragmentation channel observed upon IRPD of *c*-/*t*-AI$_2$H$^+$-Ar (*m/z* 339) is *m/z* 299, corresponding to loss of the Ar ligand. Further details on the experimental setup and acquisition conditions can be found in the experimental section of Reference 35.