MAPPING THE CONFORMATION SPACE OF α-PROLINE BY MATRIX-ISOLATION IR SPECTROSCOPY COMBINED WITH NIR LASER INDUCED CONFORMATIONAL CHANGE AND STATE-OF-THE-ART AB INITIO COMPUTATIONS

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The conformers of α-proline were studied by matrix-isolation IR spectroscopy. In order to group the vibrational bands to different conformers, conformational changes were induced by NIR laser irradiations, by exciting the OH stretching overtone of a selected conformer. For identification, the single conformer spectra were compared to state-of-the-art ab initio computations. Infrared spectra and anharmonic thermodynamic corrections have been computed by means of second order vibrational perturbation theory (VPT2), with GVPT2 and HDCPT2 models, respectively. A hybrid force-field was developed by addition of the cubic and semi-diagonal quartic B3LYP-D3/SNSD force constants to the (harmonic quadratic) B2PLYP-D3/maug-cc-pVTZ results. As the result of the spectrum analysis, seven conformers could be identified. Four of these conformers were present in the as-deposited matrix, two of them were generated by the NIR laser irradiation, and found to be stable in Ar matrix. The seventh conformer could also be produced upon the NIR laser irradiation, and it decays by H-atom tunneling to a lower energy form on the sub-second and minute timescales in Ar and N_2 matrices, respectively.