Role of intramolecular hydrogen bonding on photoelectron circular dichroism: the diastereoisomers of 1-Amino-2-Indanol

Etienne Rouquet, ^{a) b)} Jennifer Dupont,^{a)} Julien Vincent,^{a)} Valéria Lepère,^{a)} Anne Zehnacker^{a)*}

Sebastian Hartweg^{b)} Gustavo A. Garcia,^{b)} Laurent Nahon^{b)}*

a) Institut des Sciences Moléculaires d'Orsay (ISMO), CNRS, Université Paris-Saclay,
F-91405 Orsay, France

b) Synchrotron Soleil, L'Orme des Merisiers, St. Aubin BP48, F-91192 Gif sur Yvette,
France

Corresponding Authors

* Anne Zehnacker <u>anne.zehnacker-rentien@universite-paris-saclay.franne.zehnacker-rentien@universite-paris-saclay.franne.zehnacker-rentien@universite-paris-saclay.fr</u>

* Laurent Nahon laurent.nahon@synchrotron-soleil.fr

Supplementary Information



Figure S1: Mass spectrum of *trans*-AI (a) and *cis*-AI (b) at 9, 10, 11, 12 and 13.5 eV photon energy.



Figure S2: TPES and TPEPICO spectra of a) *trans*-AI and b) *cis*-AI recorded between 8.3 and 11 eV. TPES (black) and TPEPICO spectra for the parent and different fragments. As expected, the TPES corresponds to the sum of all TPEPICO spectra. The dashed lines correspond to the orbital energies calculated for *trans*-AI, *cis*-AI_I and *cis*-AI_{II}. The X, A, B, C and D labels correspond to the experimental values of the orbital energies from which the electron is ejected, namely, HOMO to HOMO-3.



Figure S3: PES (solid line) and PECD spectra (line with error bars) of (1S,2S)-trans-AI (brown) and (1R,2S)-cis-AI (green) for a photon energy of 13.5 eV. The spectra are obtained by summing the PECD recorded at all masses.



Figure S4: $S_1 \leftarrow S_0$ electronic transition of *trans*-AI (left) and *cis*-AI (right) recorded my monitoring the total electron current. The bands corresponding to the transitions used for recording the PECD are the transition origins, indicated by 0-0, and the vibronic transition corresponding to the excitation of the puckering motion. The transition origin of *trans*-AI, *cis*-AI_I, *cis*-AI_{II}, are located at 37027, 36918, 36921 cm⁻¹, respectively.



Figure S5: Photoelectron spectra (full line) and PECD (squares) for (top) (1R,2R)-*trans*-AI excited at the origin transition (37027 cm⁻¹, 9.181 eV total ionisation energy) (black) and at the vibronic transition corresponding to the excitation of one quantum of the puckering motion (37106 cm⁻¹, 9.201 eV total ionisation energy) (blue). (bottom) (1R,2S)-*cis*-AI_{II} excited at the origin transition (36921 cm⁻¹, 9.155 eV total ionisation energy) (black) and at the vibronic transition corresponding to the excitation of the puckering motion (36989 cm⁻¹, 9.172 eV total ionisation energy) (blue). The PECD is defined as $2b_1$ -0.5 b₃ (see text).