Journal of Physics: Conference Series **635** (2015) 032053 doi:10.1088/1742-6596/635/3/032053

Interactions of amino acid enantiomers with chiral target in high and low energy collisions

O. Rebrov*[1], K. Kulyk*[2], M. Ryding[†], M. Stockett[‡], J. Alexander*, H. Zettergren*, H. Schmidt*, H. Cederquist*, R. D. Thomas*, E. Uggerud[†], M. Larsson*

[*] Stockholm University, Department of Physics, SE-106 91 Stockholm, Sweden
[†] Department of Chemistry, University of Oslo, N - 0315 Oslo, Norway
[‡] Department of Physics and Astronomy, Aarhus University, DK-8000 Aarhus, Denmark

Synopsis The study is focused on investigation of stereospecific interaction of amino acid enantiomers with chiral targets in collisions of 1 keV and ~1 eV energy using tandem mass spectrometry.

Investigation of stereospecific biomolecular interactions is an active area of research nowadays. Chiral forms of molecules can experience different interactions in chiral environment and thereby trigger different reaction mechanisms. Homochirality of amino acid and sugar enantiomers in living organisms results in stereospecificity of biomolecular processes. Therefore it is crucial in particular for pharmaceutics and drug discovery to be able to detect and separate optical isomers. The lack of theoretical basis able to describe processes that lead to enantioselectivity constitutes the need of fundamental research in this area.

Our study is focused on investigating interactions between singly protonated and neutral chiral molecules in the gas phase using tandem mass spectrometry. High and low energy collisional activation of L- and D-forms of amino acid cations with chiral and achiral target gases were studied. In order to make stereospecific interactions more feasible the amino acids with bulky side chain groups namely Phe, Trp and Met were utilized. The chiral (S)-(+)-2-butanol, racemic (+/-)-2-butanol and Argon were used as target gases. For collisions of 1 keV in a center-of-mass frame, the amount of transferred energy was sufficient to induce fragmentation via multiple channels. For all measured amino acids the most abundant products were produced due to the loss of NH_3 and combined loss of H_2O + CO. The fragmentation pathways and abundances of fragments revealed no difference for both amino acid enantiomers with all gases used. The collision energy was found to be too high to observe any kind of chiral effects. Thus the study of low energy collisions of around 1 eV in the center-of-mass energy with (S)-(+)-2-butanol and racemic (+/-)-2-butanol was performed. Additional to the main fragments that correspond to the loss of NH_3 and H_2O + CO, complexes of amino acids and 2-butanols were detected. The possible chiral impact in fragmentation and efficiency of adduct formation was elaborately investigated.

[1] E-mail: oleksii.rebrov@fysik.su.se

[2] E-mail: Kostiantyn.kulyk@fysik.su.se

Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.
Published under licence by IOP Publishing Ltd