

Chirality of Peptide Molecules

dedicated to the late Jon T. Hougen

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Several new experimental methods such as flash photolysis, lasers, and so on, appeared in 1950's and 60's and generated hitherto-unknown exotic molecules, which led to a new category in molecular structure and spectroscopy for classifying them. Such epoch-making movements in molecular science could be brought about by young bright peoples; they gathered at a few centers of research in the world. Just after getting PhD from Professor Moffitt at Harvard, Jon Hougen joined Gerhard Herzberg (GH)'s group at NRC, Canada in 1960, where he set up theoretical frameworks for molecules newly detected by the GH group, as described in detail in the GH's third volume: *Molecular Spectra and Molecular Structure*. Symbols, notations, classifications, and so on for new molecules were invented by scientists who investigated the new species, and Jon was one of such pioneer peoples. After these brilliant experiences in Ottawa for seven years, he returned to one of the other best molecular spectroscopy centers in the US: National Bureau of Standards (NBS), which is now National Institute of Standards and Technology (NIST), where he spent the rest of his lifetime as a leader in molecular spectroscopy and molecular structure all over the World. His interest has been spread over on most fundamental aspects of molecular sciences, particularly on the couplings between the overall rotation and low-frequency and/or large-amplitude motions like internal rotation, inversion, puckering, and so on.

Jon and his associates at NIST and Yoshiyuki Kawashima, Nobukimi Ohashi, and their collaborators in Japan focused particular attention to molecules which act as the central backbone units in biological systems and related areas, such as those named peptide molecules XC=O-NHY with either X - C and N - Y in *trans* or *cis*. It should be pointed out that the simplest peptide molecule: formamide is planar at the equilibrium, with the lowest-frequency out-of-plane bending mode accompanied by an anomalously large anharmonicity, and is hence achiral, in spite of the fact that it is regarded as a most typical "biological" molecule. In order to obtain chiral systems, we need to extend the molecular skeleton; one example is *N*-acetyl-alanine *N'*-methylamide: $\text{CH}_3\text{CONH-C}(\text{CH}_3)\text{-CONHCH}_3$. We may also link two or more peptide molecules to generate helix chains. See the following paper for more details:

Y. Kawashima, T. Usami, N. Ohashi, R. D. Suenram, J. T. Hougen, and E. Hirota, *Acc. Chem. Res.* **39**, 216-220 (2006).