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Excited state of peptide nanorings TETSUO YAMADA, HIROSHI MIYAZAKI, HAJIME OKAMOTO, KYOZABURO TAKEDA, Waseda University
— Peptide nanorings (PNRs) has a closed ring form composed of alternating D- and L-α-amino acid residues. Much interest has been attracted owing to their function as a selective ion receptor. Here, based on *ab initio* molecular orbital theory, the excited as well as the ground state structures have been theoretically studied and discussed how the photo-excitation changes the ion-capturing ability with regarding on the two ring skeletons of Extended (E)- and Bound (B)-type PNR geometries. Because the HOMO-LUMO transition is optically allowed, we took into account this single excitation via the unrestricted Hartree-Fock (UHF/6-31G**) calculations. Our results reveal that the HOMO-LUMO single electron transition expands the bore of E-type PNR while narrows that of B-type one. This *ad hoc* treatment, however, causes an overestimation, because the electronic states both near the HOMO and LUMO are *pseudo*-degenerated. An inclusion of other configurations due to the single electron excitation (CIS) relaxes the above geometrical changes predicted by the UHF HOMO-LUMO single excitation. Thus, the ring molecular geometry in the first optical excitation is rather indistinguishable compared with that in the ground state.

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