

Circular dichroism and absorption spectroscopy with SAC-CI method

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Circular dichroism (CD) [1] spectroscopy gives us useful information for chiral molecules and it is used for determination of absolute configuration of the complicated molecules such as DNA and RNA. The SAC/SAC-CI method is a useful established method for studying ground, excited, ionized and electron attached states of molecules [2-4]. It is widely distributed through Gaussian03 [5]. We have calculated the rotatory strength of CD spectra by SAC-CI method with velocity form, which is independent for gauge origin.

Three-membered ring

Figure 1 shows the experimental and SAC-CI CD spectra of R-methyloxirane (RMO). The SAC-CI CD spectrum is in good agreement with the experimental one. The peak around 7.7 eV is the excitation of $n - p$ Rydberg and $\sigma - s$ rydberg. This results show the excitation from σ orbital is important in RMO.

DNA

Figure 2 shows the experimental and SAC-CI spectra of anti-dA. In the UV spectrum, the oscillator strength of $\pi - \pi^*$ is strong but the one of $n - \pi^*$ is weak. But in the CD spectrum, the $n - \pi^*$ has strong rotatory strength as well as the $\pi - \pi^*$. The CD spectra give the additional information, which can not be obtained in UV spectra.

We will make study the CD spectra of other three-membered rings and DNA (figure) by the SAC-CI method.

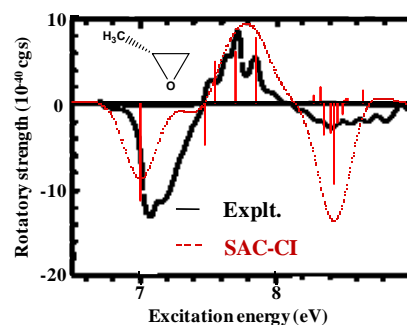
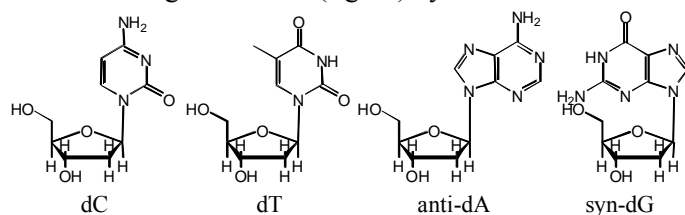


Figure 1. CD spectra of RMO

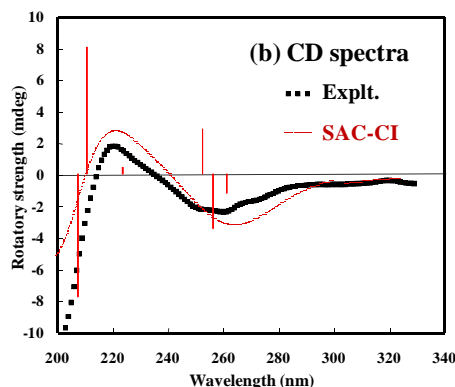
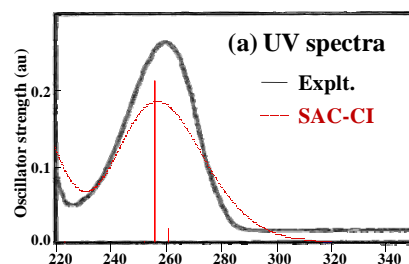


Figure 2. Experimental and SAC-CI (a) UV spectra and (b) CD spectra of anti-dA.

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