改良CNDO/Sによる有機化合物の電子スペクトル計算：一中心電子反発積分を改良した新しいCNDO/S計算

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Improved CNDO/S Calculation of Electronic Spectra of Organic Compounds. I. New CNDO/S Calculation by Using an Improved Method of One-Center Electron Repulsion Integral

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ABSTRACT : The NM-γ CNDO/S program previously developed by our group was modified by the introduction of a new one-center electron repulsion integral γ_{AA}^{NEW} approximation, namely, the γ_{AA}^{NEW} CNDO/S method. The value of this γ_{AA}^{NEW} was evaluated according to the product values of the coefficient C with the γ_{AA} value proposed in our previous paper. This method using a new γ_{AA} was also found to improve the two-center electron repulsion integral γ_{AA} value with respect to the chemical softness proposed by Nishimoto and co-workers, together with the difference between HOMO and LUMO orbital energies. The results calculated by the present improved γ_{AA}^{NEW}-CNDO/S method demonstrated that not only the calculated absorption maxima wavelengths and ionization potentials, but also the order and the assignment of orbitals coincided very well with those based on the results of experiments investigating a variety of polyenes, cyanynes, and polycyclic aromatic hydrocarbons.

抄録　従来のCNDO/Sに新しい一中心電子反発積分の評価法を導入することにより改良CNDO/Sを開発した。様々なポリエン類、シアニン類や芳香族炭化水素に対する改良CNDO/Sにより得られた結果は、吸収極大波長やイオン化ポテンシャルの値だけでなく、軌道の帰属やその順序なども実測値をよく再現した。

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