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The application of Windows 95/98/NT for PPP MO (Pariser-Parr-Pople molecular orbital) calculation was developed by using the Inprise C++ builder. The novel two-center electron repulsion integral (new-γ), the concept of spectrochemical softness parameter *krs* for PPP calculation, was introduced in this application. The user can perform quickly the modeling of π-conjugated compounds on a PC monitor and select many suitable parameters (for example, ionization potentials, resonance integrals *etc.*) for the PPP calculation. The SCF calculation was momentarily performed and oscillator strength and LCAO coefficients of HOMO, LUMO or others were displayed. The calculations gave satisfactory results for the prediction of the electronic absorption spectra of polycyclic aromatic hydrocarbons(PAHs), symmetric cyanins and so on.

Keywords: PPP-Calculation; New-γ; Spectrochemical softness

1 INTRODUCTION

It is known that the PPP MO calculation is useful in order to predict electronic spectra of various functional dyes[1]. In our previous papers[2], we reported the software PPP-PC (MS-DOS version)[3], the PPP calculation software for personal computers. However, the most popular operating system for recent personal computers is MS-Windows. In this study, the Windows application (WIN-PPP) was transferred from

the previous one by using the Inprise C++ builder. The novel two center electron repulsion integrals new-γ proposed by Nishimoto[4], was introdued in the WIN-PPP.

2 HARDWARE AND COMPILER

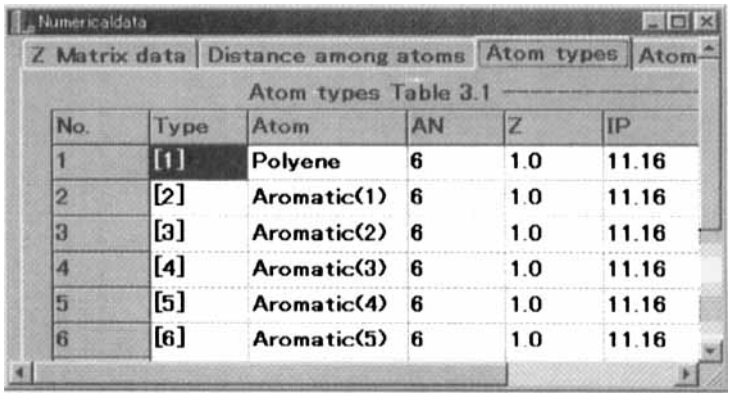
The WIN-PPP runs on the machine installed Windows 95/98/NT. It is recommended that the machine has Intel Pentium processor for fast execution of the program. At least 32 MB of RAM, a color monitor, and a printer are also required. The WIN-PPP was written by Inprise C++ Builder Ver. 1.0 in which includes useful codes for basic MS-Windows operation. As C++ of the compiler was a complete object oriented language, the development term was extremely shortened and the program debug was easily performed. A reliability of the program was also enhanced by the variables capsulation caused by class objects of C++.

3 DATA FILES FOR THE PPP MO CALCULATION

3.1 MODELING OF MOLECULES

The modeling was executed after loading a data file for a typical molecule and adding a proper unit of substituent. The data file stores a compound name, number of atoms, the atom type number of each atom, Cartesian (x, y, z) coordinates and bond information. The atom type numbers were identifiers used to refer to empirical values of IP (ionization potential), G (one center repulsion integral), Z (core charge) and Hx (coulomb integral for HMO calculation). The data files (*.PPP files) of typical organic colorants, for example, polyene, cyanine, azobenzene, indigo, *etc.*, were saved on a hard disk in advance. The user can see the π-framework of these compounds on the PC monitor and add

various substituent groups at the desired position by mouse–controlled interactive graphical input. As the π-framework drawing was displayed in the main window according to rotation and translation operations, the modeling of aromatic compounds could be quickly performed and saved as a new *.PPP file . Another window with page tab controls as shown in FIGURE 1, can pop up on the main window.



No.	Type	Atom	AN	Z	IP
1	[1]	Polyene	6	1.0	11.16
2	[2]	Aromatic(1)	6	1.0	11.16
3	[3]	Aromatic(2)	6	1.0	11.16
4	[4]	Aromatic(3)	6	1.0	11.16
5	[5]	Aromatic(4)	6	1.0	11.16
6	[6]	Aromatic(5)	6	1.0	11.16

FIGURE 1 The pop up window for the certification of empirical parameters of the atom type number, IP, Z and bond length etc., during π-framework modeling.

The user can make sure distance among atoms, atom type numbers and atomic coordinates *etc.*, and also edit these parameters.

3.2 SELECTION OF CALCULATION PARAMETERS

The user can execute the PPP-calculation with various mode ordered by the parameter input dialog window (FIGURE 2). If the user select new-γ, core resonance integrals (β) and γ are changed each iteration cycle of SCF calculation. The user can also decide the initial bond order

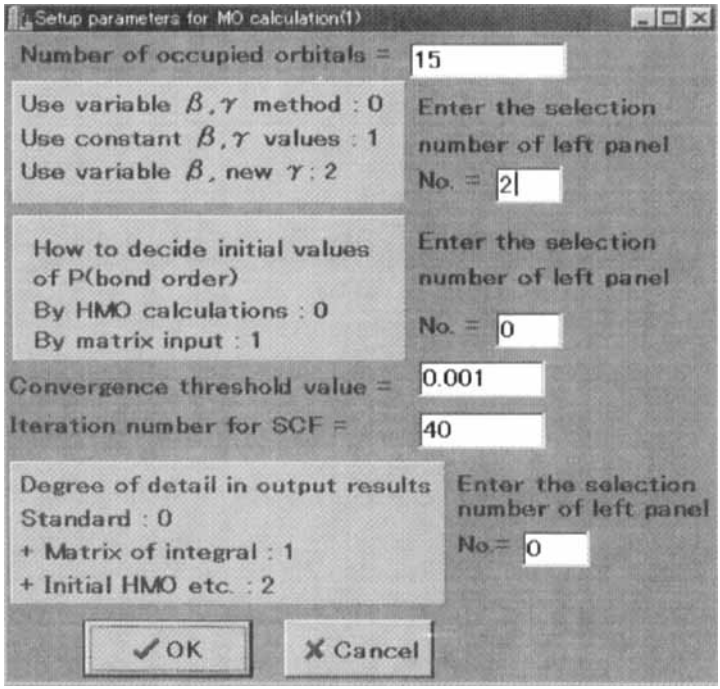


FIGURE 2 Dialog window for selection of PPP calculation method

(P) in Fock matrix either by HMO calculations or by data input and select the convergence conditions of SCF calculation, the details in the output file. In the spectra calculation section, the methods of configuration interaction (CI), upper limit of transition energy, lower limit and the calculation of triplet state can be selected by the another similar dialog window. After these input dialogs are closed, a data file (*.dat) stored the above-mentioned parameters is saved on a hard disk.

4 GRAPHICAL REPRESENTATION

The calculation and graphical output of popular coloring materials are

momentarily executed. Orbital energies, set of atomic orbital coefficients for the molecular orbitals, bond order matrices, dipole moments, absorption maxima and oscillator strengths are available as a numerical output file. The calculated atomic orbital coefficients for the molecular orbital are visually displayed as circle with radius proportional to the value on the π-framework drawing (FIGURE 3).

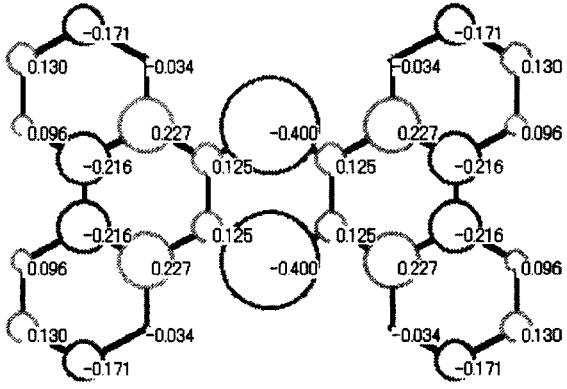


FIGURE 3 Example of LCAO coefficients of HOMO of Tetrabenzanthracene

The simulated spectra, which were built up by a shape of Gaussian function with constant half band width (FIGURE 4). As the background colors of all output figures can be easily changed by the color dialog window which supports 24 bit true colors and modified via various paint tools of MS-Windows, this application is a useful tool for presentations as well. By mouse-controlled interactive graphical input, the WIN-PPP showed remarkable advancement in operations of the modeling π-framework and the selection of IP, G, Z, Hx parameters. The calculated

spectra of PAHs agreed with the observed one by using the improved parameter new-γ[5].

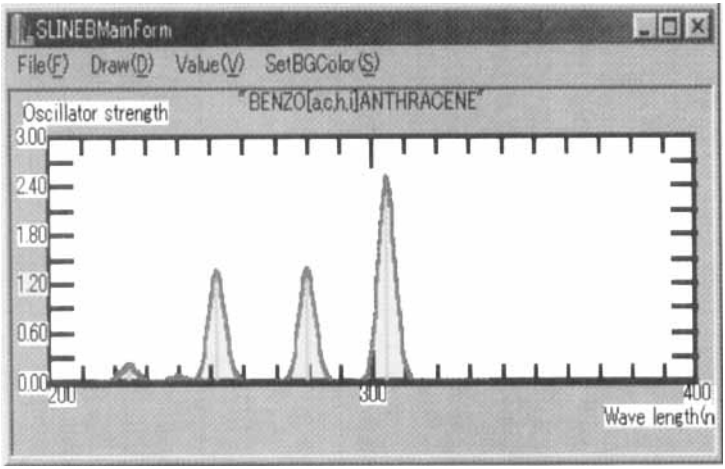


FIGURE 4 Calculated electronic spectra. (Example) Tetrabenzanthracene

5 SUMMARY

The PPP MO calculation program WIN-PPP was developed by C++ programming. The WIN-PPP showed remarkable advancement in the modeling operations of π-framework. By using the novel two-center electron repulsion (New-γ), the calculated absorption spectra of PAHs are in excellent agreement with the observed values.

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