Electronic Spectra of Acridine and Phenazine

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In the first papar[1] of our studies on the electronic structure and spectra of nitrogen heterocycles, some semiquantitative treatments on the electronic spectra of acridine and phenazine have been given, on the basis of the results obtained for nitrogen heterobenzenes employing the Hartree-Fock SCF theory including the limited amount of configuration interactions. In the present report, we shall apply the perturbation method developed in the third paper[2] to these three-ring nitrogen heterocycles, and give more detailed and quantitative interpretations on the electronic structure and spectra of these molecules.

Electronic Spectra of Anthracene as a Basis of the Perturbation Calculation

As a first step, we have regarded the naive MO's of anthracene as a good approximation to the MO's of these three ring nitrogen heterocycles. As pointed out by Dewar and Longuet-Higgins[3] in their semiquantitative discussions on the general feature of aromatic hydrocarbon spectra, the naive MO's of these aromatic hydrocarbons may be good approximate solutions of the Hartree-Fock self-consistent field equations or close to the best MO's available for constructing the excited state wave functions, owing to the uniformity of electron distribution in these molecules.

In our theoretical work[4] on the electronic spectra of some unsaturated hydrocarbons, it has been clearly indicated, that, for example, employing our semiempirical parameters,[1,5] the naive MO's of naphthalene interpret the experimental spectra almost equally well as the Hartree-Fock self-consistent field MO's and also the approximate self-consistent field MO's obtained by neglecting the non-diagonal matrix elements of Fock's Hamiltonian in terms of AO's, $F_{\mu\nu}$, when μ and ν are apart each other further than the nearest neighbor. Thus, in this case, naive MO's are very satisfactory for the description of electronic spectra, although they give a wrong prediction about the bond orders in the ground state.

The naive MO's of anthracene also give a satisfactory explanation of the experimental spectra as in the following cases.

In view of the approximate nature of our treatment, the geometrical structure of the molecule has been assumed to be a condensed regular hexagon, the nearest neighbor bond distance of which has been taken as 1.402_7 Å. This value is a weighted mean of five different bond distances determined by X-ray diffraction[6]. The same geometrical structure as anthracence, has been assumed also for acridine and phenazine treated in a latter paragraph.

The MO's and MO energies of anthra-

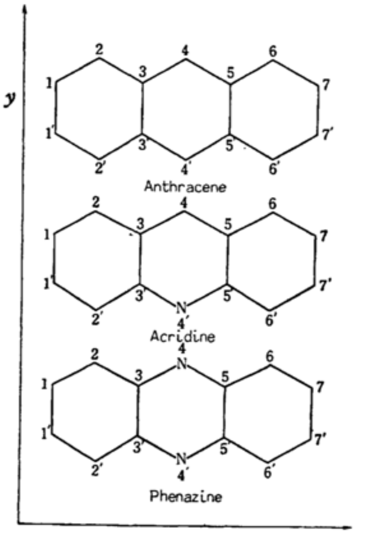

Fig. 1. The numbering of atoms and the coordinate of symmetry operation.

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[1] N. Mataga and K. Nishimoto, *Z. Phys. Chem.* N. F., in press.

[2] N. Mataga, to be published in this Bulletin.

[3] M. J. S. Dewar and H. C. Longuet-Higgins, *Proc. Phys. Soc.*, **67A**, 795 (1954).

[4] N. Mataga and K. Nishimoto, to be published elsewhere.

[5] N. Mataga, to be published in this Bulletin.

[6] J. M. Robertson, "Organic Crystals and Molecules", Cornell University Press, 1953.

TABLE I

MO'S AND MO ENERGIES OF ANTHRACENE

Symmetry	$\varepsilon_i (e.v.)$	
b_{1g}	-10.4865	$\phi_6 = 0.3535\sigma_6 + 0.3535\sigma_7$
b_{3g}	-8.8987	$\phi_7 = 0.3109\sigma_8 + 0.2199\sigma_9 + 0.0911\sigma_{10} - 0.4397\sigma_{11}$
b_{2u}	-3.1013	$\phi_8 = 0.3109\sigma_1 - 0.2199\sigma_2 + 0.0911\sigma_3 - 0.4397\sigma_4$
a_{1u}	-1.5135	$\phi_9 = -0.3535\sigma_{13} + 0.3535\sigma_{14}$

$$\sigma_1 = (\phi_6 + \phi_{6'} + \phi_2 + \phi_{2'}), \quad \sigma_2 = (\phi_7 + \phi_{7'} + \phi_{1'} + \phi_1), \quad \sigma_3 = (\phi_{3'} + \phi_3 + \phi_5 + \phi_{5'}), \quad \sigma_4 = (\phi_4 + \phi_{4'})$$

$$\sigma_8 = (\phi_6 - \phi_{6'} + \phi_2 - \phi_{2'}), \quad \sigma_6 = (\phi_7 + \phi_{7'} - \phi_{1'} - \phi_1), \quad \sigma_7 = (\phi_{3'} + \phi_3 - \phi_5 - \phi_{5'}), \quad \sigma_{11} = (\phi_4 - \phi_{4'})$$

$$\sigma_9 = (\phi_7 - \phi_{7'} - \phi_{1'} + \phi_1), \quad \sigma_{10} = (\phi_{3'} - \phi_3 - \phi_5 + \phi_{5'}),$$

$$\sigma_{13} = (\phi_7 - \phi_{7'} + \phi_{1'} - \phi_1), \quad \sigma_{14} = (\phi_{3'} - \phi_3 + \phi_5 - \phi_{5'}),$$

TABLE II*

THE EXCITED STATE WAVE FUNCTIONS, ENERGIES OF CONFIGURATIONS AND THE VALUES OF INTERCONFIGURATIONAL MATRIX ELEMENTS OF ANTHRACENE

$$\Psi({}^1B^+{}_{1u}) = 0.9875\,{}^1\chi_{7\to8} + 0.1576\,{}^1\chi_{6\to9}, \qquad E({}^1\chi_{7\to8}) = 3.5549,$$

$$\Psi({}^1B^-{}_{1u}) = 0.1576\,{}^1\chi_{7\to8} - 0.9875\,{}^1\chi_{6\to9}, \qquad E({}^1\chi_{6\to9}) = 6.3681,$$

$$\Psi({}^3B^+{}_{1u}) = 0.9986\,{}^3\chi_{7\to8} + 0.0516\,{}^3\chi_{6\to9}, \qquad E({}^3\chi_{7\to8}) = 1.6999,$$

$$\Psi({}^3B^-{}_{1u}) = 0.0516\,{}^3\chi_{7\to8} - 0.9986\,{}^3\chi_{6\to9}, \qquad E({}^3\chi_{6\to9}) = 4.8158.$$

$$(78 \mid G \mid 78) = 4.0975, \qquad (78 \mid G \mid 87) = 0.9275, \qquad (68 \mid G \mid 79) = 0.1616,$$

$$(69 \mid G \mid 69) = 4.1572, \qquad (69 \mid G \mid 96) - 0.7761, \qquad (68 \mid G \mid 97) = -0.1496.$$

$$\Psi({}^1B^+{}_{3u}) = \frac{1}{\sqrt{2}}({}^1\chi_{6\to8} + {}^1\chi_{7\to9}), \qquad E({}^1\chi_{6\to8}) = E({}^1\chi_{7\to9}) = 4.5470$$

$$\Psi({}^1B^-{}_{3u}) = \frac{1}{\sqrt{2}}({}^1\chi_{6\to8} - {}^1\chi_{7\to9}),$$

$$\Psi({}^3B^+{}_{3u}) = \frac{1}{\sqrt{2}}({}^3\chi_{6\to8} + {}^3\chi_{7\to9}), \qquad E({}^3\chi_{6\to8}) = E({}^3\chi_{7\to9}) = 3.7472$$

$$\Psi({}^3B^-{}_{3u}) = \frac{1}{\sqrt{2}}({}^3\chi_{6\to8} - {}^3\chi_{7\to9}),$$

$$(68 \mid G \mid 68) = (79 \mid G \mid 79) = 3.6380, \qquad (68 \mid G \mid 86) = (79 \mid G \mid 97) = 0.3999,$$

$$(78 \mid G \mid 69) = (68 \mid G \mid 79), \qquad (78 \mid G \mid 96) = (68 \mid G \mid 86).$$

$$({}^1\chi_{7\to8} \mid \mathbf{H} \mid {}^1\chi_{6\to9}) = ({}^1\chi_{6\to8} \mid \mathbf{H} \mid {}^1\chi_{7\to9}) = -0.4608.$$

$$({}^3\chi_{7\to8} \mid \mathbf{H} \mid {}^3\chi_{6\to9}) = ({}^3\chi_{6\to8} \mid \mathbf{H} \mid {}^3\chi_{7\to9}) = -0.1616.$$

* in units of *e.v.*

cene, which concern the electronic transitions to lower excited states are given in Table I.

The numbering of atoms and the coordinate of symmetry operation are shown in Fig. 1. In the approximation of naive MO theory, $\psi_6(b_{1g})$ and $\psi_5(a_{1u})$ are degenerate accidentally in the occupied orbitals as well as $\psi_9(a_{1u})$ and $\psi_{10}(b_{1g})$ in the vacant orbitals. The inclusion of electron interaction, however, removes this accidental degeneracy, and a_{1u} is the lower both in occupied and vacant orbitals. The excited state wave functions, energies of configurations and the values of interconfigurational matrix elements are given in Table II.

The calculated excitation energies and oscillator strengths are collected in Table III, in comparison with the observed values. By an inspection of this table, one may be allowed to say that the theoretical predictions are in very good agreement with the experimental observation, in view of the approximate nature of our calculation.

TABLE III

CALCULATED AND OBSERVED EXCITATION ENERGIES AND OSCILLATOR STRENGTHS OF ANTHRACENE

Symmetry		Excitation Energy (*e.v.*)		Oscillator Strength	
Group theory	Platt	Calcd.	Obsd.	Calcd.	Obsd.[a]
${}^1B^+{}_{1u}$	${}^1L_a$	3.4813	3.30[a]	0.39	~0.1
${}^1B^-{}_{3u}$	${}^1L_b$	3.9087	3.50[a]	0.00	~0
${}^1B^+{}_{3u}$	${}^1B_b$	5.1853	4.80[a]	3.00	2.20
${}^1B^-{}_{1u}$	${}^1B_a$	6.4416	5.64[a]	0.81	0.65
${}^3B^+{}_{1u}$	${}^3L_a$	1.6915	1.8[b]	0.00	—
${}^3B^+{}_{3u}$	${}^3B_b$	3.5856	—	0.00	—
${}^3B^-{}_{3u}$	${}^3L_b$	3.9087	—	0.00	—
${}^3B^-{}_{1u}$	${}^3B_a$	4.8241	—	0.00	—

a) H. B. Klevens and J. R. Platt, *J. Chem. Phys.* **17**, 470 (1949).

b) G. N. Lewis and M. Kasha, *J. Am. Chem. Soc.*, **66**, 2100 (1944); McGlynn, Padhye and Kasha, *J. Chem. Phys.*, **23**, 593 (1955).

Now, let us examine the spectra of heterocycles, on the basis of these results.

Acridine and Phenazine

The orbital energies for acridine and phenazine are collected in Table IV, and Tables V and VI correspond to Tables II and III of the preceding paragraph respectively.

TABLE IV.

ORBITAL ENERGIES OF ACRIDINE AND PHENAZINE

i	$\varepsilon_i(e.v.)$	
	acridine	phenazine
6	-10.4865	-10.4865
7	-9.3459	-9.7924
8	-3.9069	-3.7815
9	-1.5135	-1.5135

The agreement between the calculated and the observed values of excitation energies and oscillator strengths is fairly good in general, although the error between calculated and observed energies of ^1L_a band of phenazine is considerable. About this inconsistency, a more detailed treatment is given in the latter part of this paper. The behavior of ^1L_b band, however, is well comprehended with the above results.

The cause of the intensification of ^1L_b band has been ascribed to the inequality of the coefficients a and b in Eq. 1, in the case of nitrogen heterobenzenes[1,5] and monoazanaphthalenes[2].

$$\Psi(^1L_b)=a\,^1\chi_{i\to k}+b\,^1\chi_{j\to l} \tag{1}$$

The ratio of the coefficients in Eq. 1 is correlated to the energies of configurations and the interconfigurational matrix element by

$$\frac{a}{b}=\frac{2(^1\chi_{i\to k}\mid \mathbf{H}\mid {}^1\chi_{j\to l})}{[\{E(^1\chi_{i\to k})-E(^1\chi_{j\to l})\}^2+4(^1\chi_{i\to k}\mid \mathbf{H}\mid {}^1\chi_{j\to l})^2]^{1/2}-\{E(^1\chi_{i\to k})-E(^1\chi_{j\to l})\}} \tag{2}$$

TABLE V*

THE EXCITED STATE WAVE FUNCTIONS, ENERGIES OF CONFIGURATIONS AND THE VALUES OF INTERCONFIGURATIONAL MATRIX ELEMENTS OF ACRIDINE AND PHENAZINE

$\Psi(^1A^+{}_1)=0.9892\,^1\chi_{7\to8}+0.1461\,^1\chi_{6\to9}$, $E(^1\chi_{7\to8})=3.2367$,
$\Psi(^1A^-{}_1)=0.1461\,^1\chi_{7\to8}-0.9892\,^1\chi_{6\to9}$, $E(^1\chi_{6\to9})=6.3681$,
$\Psi(^3A^+{}_1)=0.9990\,^3\chi_{7\to8}+0.0450\,^3\chi_{6\to9}$, $E(^3\chi_{7\to8})=1.2357$,
$\Psi(^3A^-{}_1)=0.0450\,^3\chi_{7\to8}-0.9990\,^3\chi_{6\to9}$, $E(^3\chi_{6\to9})=4.8158$.
$(78\mid G\mid 78)=4.2033$, $(78\mid G\mid 87)=1.0005$, $(68\mid G\mid 79)=0.1616$,
$(69\mid G\mid 69)=4.1572$, $(69\mid G\mid 96)=0.7761$, $(68\mid G\mid 97)=-0.1556$.
$(^1\chi_{7\to8}\mid \mathbf{H}\mid {}^1\chi_{6\to9})=-0.4728$, $(^3\chi_{7\to8}\mid \mathbf{H}\mid {}^3\chi_{6\to9})=-0.1616$.
$\Psi(^1B^+{}_1)=0.3870\,^1\chi_{6\to8}+0.9221\,^1\chi_{7\to9}$, $E(^1\chi_{6\to8})=3.7182$,
$\Psi(^1B^-{}_1)=0.9221\,^1\chi_{6\to8}-0.3870\,^1\chi_{7\to9}$, $E(^1\chi_{7\to9})=4.6170$,
$\Psi(^3B^+{}_1)=0.9920\,^3\chi_{6\to8}+0.1259\,^3\chi_{7\to9}$, $E(^3\chi_{6\to8})=2.9184$,
$\Psi(^3B^-{}_1)=0.1259\,^3\chi_{6\to8}-0.9920\,^3\chi_{7\to9}$, $E(^3\chi_{7\to9})=4.1712$.
$(68\mid G\mid 68)=(79\mid G\mid 79)=3.6612$, $(78\mid G\mid 96)=(68\mid G\mid 86)$,
$(68\mid G\mid 86)=(79\mid G\mid 97)=0.3999$, $(78\mid G\mid 69)=(68\mid G\mid 79)$.
$(^1\chi_{6\to8}\mid \mathbf{H}\mid {}^1\chi_{7\to9})=0.6382$, $((^3\chi_{6\to8}\mid \mathbf{H}\mid {}^3\chi_{7\to9})=-0.1616$.

Phenazine

$\Psi(^1B^+{}_{1u})=0{\cdot}9831\,^1\chi_{7\to8}+0.1828\,^1\chi_{6\to9}$, $E(^1\chi_{7\to8})=3.8507$,
$\Psi(^1B^-{}_{1u})=0.1828\,^1\chi_{7\to8}-0.9831\,^1\chi_{6\to9}$, $E(^1\chi_{6\to9})=6.3681$,
$\Psi(^3B^+{}_{1u})=0.9986\,^3\chi_{7\to8}+0.0517\,^3\chi_{6\to9}$, $E(^3\chi_{7\to8})=1.7025$,
$\Psi(^3B^-{}_{1u})=0.0517\,^3\chi_{7\to8}-0.9986\,^3\chi_{6\to9}$, $E(^3\chi_{6\to9})=4.8158$.
$(78\mid G\mid 78)=4.3084$, $(78\mid G\mid 87)=1.0741$, $(68\mid G\mid 79)=0.1616$,
$(69\mid G\mid 69)=4.1572$, $(69\mid G\mid 96)=0.7761$, $(68\mid G\mid 97)=-0.1616$.
$(^1\chi_{7\to8}\mid \mathbf{H}\mid {}^1\chi_{6\to9})=-0.4849$, $(^3\chi_{7\to8}\mid \mathbf{H}\mid {}^3\chi_{6\to9})=-0.1616$.
$\Psi(^1B^+{}_{3u})=0.3341\,^1\chi_{6\to8}+0.9425\,^1\chi_{7\to9}$, $E(^1\chi_{6\to8})=3.8205$,
$\Psi(^1B^-{}_{3u})=0.9425\,^1\chi_{6\to8}-0.3341\,^1\chi_{7\to9}$, $E(^1\chi_{7\to9})=5.3944$,
$\Psi(^3B^+{}_{3u})=0.9949\,^3\chi_{6\to8}+0.1011\,^3\chi_{7\to9}$, $E(^3\chi_{6\to8})=3.0207$,
$\Psi(^3B^-{}_{3u})=0.1011\,^3\chi_{6\to8}-0.9949\,^3\chi_{7\to9}$, $E(^3\chi_{7\to9})=4.5946$.
$(68\mid G\mid 68)=(79\mid G\mid 79)=3.6843$, $(78\mid G\mid 96)=(68\mid G\mid 86)$,
$(68\mid G\mid 86)=(79\mid G\mid 97)=0.3999$, $(78\mid G\mid 69)=(68\mid G\mid 79)$.
$(^1\chi_{6\to8}\mid \mathbf{H}\mid {}^1\chi_{7\to9})=0.6382$, $(^3\chi_{6\to8}\mid \mathbf{H}\mid {}^3\chi_{7\to9})=-0.1616$.

* in units of $e.v.$

TABLE VI

CALCULATED AND OBSERVED EXCITATION ENERGIES AND OSCILLATOR STRENGTHS OF ACRIDINE AND PHENAZINE

Symmetry		Excitation Energy ($e.v.$)		Oscillator Strength	
Group throry	Platt	Calcd.	Obsd.	Calcd.	Obsd.
		Acridine			
${}^1A^+{}_1$	${}^1L_a$	3.1669	3.18[a)]	0.36	*
${}^1B^-{}_1$	${}^1L_b$	3.4504	3.50[a)]	0.29	*
${}^1B^+{}_1$	${}^1B_b$	5.2389	4.96[a)]	2.61	*
${}^1A^-{}_1$	${}^1B_a$	6.4379	5.82[a)]	0.79	*
${}^3A^+{}_1$	${}^3L_a$	1.2284	—	0.00	—
${}^3B^+{}_1$	${}^3B_b$	2.8979	—	0.00	—
${}^3B^-{}_1$	${}^3L_b$	4.1917	—	0.00	—
${}^3A^-{}_1$	${}^3B_a$	4.8231	—	0.00	—
		Phenazine			
${}^1B^+{}_{1u}$	${}^1L_a$	3.7605	3.09[b)]	0.39	*
${}^1B^-{}_{3u}$	${}^1L_b$	3.5942	3.40[b)]	0.38	*
${}^1B^+{}_{3u}$	${}^1B_b$	5.6206	4.95[b)]	2.66	*
${}^1B^-{}_{1u}$	${}^1B_a$	6.4583	5.88[b)]	0.85	*
${}^3B^+{}_{1u}$	${}^3L_a$	1.6941	—	0.00	—
${}^3B^+{}_{3u}$	${}^3B_b$	3.0043	—	0.00	—
${}^3B^-{}_{3u}$	${}^3L_b$	4.6110	—	0.00	—
${}^3B^-{}_{1u}$	${}^3B_a$	4.8241	—	0.00	—

a) V. Zanker, *Z. physikal. Chem.* N. F., **2**, 52 (1954).

b) H. H. Perkampus, ibid., **6**, 18 (1956) and N. Mataga, unpublished.

* The oscillator strengths of these molecules are uncertain. The intensification of ${}^1L_b$ band due to hetero-replacement is remarkable, and the oscillator stength of ${}^1L_b$ band may be almost equal to that of ${}^1L_a$ band, in its order of magnitude, and the oscillator strengths of ${}^1B_b$ and ${}^1B_a$ bands are approximately equal to those of anthracene, respectively.

When $({}^1\chi_{i\to k}\mid \mathbf{H}\mid {}^1\chi_{j\to l})$ is constant, the inequality of a and b becomes more remarkable, the larger the difference of $E({}^1\chi_{i\to k})$ and $E({}^1\chi_{j\to l})$. This was the case in the series of benzene, pyridine and pyrazine[1)], the inequality being increased in this order. Moreover, it is characteristic that, the larger the difference between $(\varepsilon_k-\varepsilon_i)$ and $(\varepsilon_l-\varepsilon_j)$, the greater is the $\{E({}^1\chi_{j\to l})-E({}^1\chi_{j\to l})\}$, viz., $2(ik\mid G\mid ki)-(ik\mid G\mid ik)$ is nearly equal to $2(jl|\mathrm{G}|lj)-(jl|\mathrm{G}|jl)$. It was assumed that, this circumstance in nitrogen heterobenzenes might also prevail in the ${}^1L_b$ bands of anthracene, acridine and phenazine. On this assumption, the observed intensities of ${}^1L_b$ bands in this series of molecules were discussed qualitatively.[1)]

From Tables II, V and VI, it is evident that, our previous assumption is almost exactly valid in the approximation of the present calculation, and accordingly the observed intensities are well comprehended by such a consideration. In contradistinction to ${}^1L_a$ band, which suffers the red shift by the heteroreplacement, the position of ${}^1L_b$ band is almost invariable in this series of molecules. This situation can be interpreted similarly to the case of nitrogen heterobenzenes.[1,5)] The two configurations ${}^1\chi_{6\to 8}$ and ${}^1\chi_{7\to 9}$ are degenerate in anthracene, although they are split in the case of acridine and phenazine, the degree of splitting being larger in phenazine. As shown in Tables II, III, V and VI, however, the energy depression due to the configuration interaction is most remarkable in the case of anthracene and it becomes smaller in acridine and phenazine in this order causing the approximate invariance of the excitation energy of ${}^1L_b$ band in this series of molecules. Thus, the observed excitation energy and oscillator strength of ${}^1L_b$ band in these molecules are well interpreted by the present calculation. Now, the cause of the reversal of the relative order in the calculated energy of ${}^1L_a$ and ${}^1L_b$ states, in the case of phenazine, may probably be attributable to the inadequacy of the MO's used.

As is pointed out previously,[1,5)] the Hartree-Fock self-consistent field MO's of nitrogen heterobenzenes are fairly close to the naive MO's obtained by putting α_N, the Coulomb integral at the nitrogen atom, to be equal to $\alpha+0.5\beta$. Extending this result to the present case, we have calculated the naive MO's of phenazine as shown in Table VII, where only the MO's concerning the lower excited states are indicated.

In terms of these MO's, the excitation

TABLE VII*

MO's AND MO ENERGIES OF PHENAZINE ($\alpha_N=\alpha+0.5\beta$)

Symmetry	$\varepsilon_i(e.v.)$	
b_{1g}	−10.6821	$\phi_6=0.3535\sigma_6+0.3535\sigma_7$
b_{3g}	− 9.5282	$\phi_7=0.3557\sigma_8+0.2244\sigma_9+0.0162\sigma_{10}-0.3816\sigma_{11}$
b_{2u}	− 3.6398	$\phi_8=0.2636\sigma_1-0.2182\sigma_2+0.1632\sigma_3-0.4609\sigma_4$
a_{1u}	− 1.7233	$\phi_9=-0.3535\sigma_{13}+0.3535\sigma_{14}$

* The definitions of σ's are the same as those of anthracene.

energies, and oscillator strengths have been computed. The results are collected in Table VIII.

TABLE VIII

CALCULATED EXCITATION ENERGIES AND OSCILLATOR STRENGTHS OF PHENAZINE

(MO's: $\alpha_N = \alpha + 0.5\beta$)

Symmetry		Excitation Energy (*e.v.*)	Oscillator Strength
Group theory	Platt		
$^1B^+_{1u}$	^1L_a	3.5142	0.34
$^1B^-_{3u}$	^1L_b	3.9122	0.20
$^1B^+_{3u}$	^1B_b	5.2439	2.84
$^1B^-_{1u}$	^1B_a	6.4294	0.80
$^3B^+_{1u}$	^3L_a	1.6958	0.00
$^3B^+_{3u}$	^3B_b	3.2523	0.00
$^3B^-_{3u}$	^3L_b	4.2029	0.00
$^3B^-_{1u}$	^3B_a	4.8087	0.00

As indicated in Table VIII, ^1L_a and ^1L_b bands are put in their right order, thus making the agreement with the experimental observation more satisfactory.

Eventually, the electronic spectra of acridine and phenazine, as well as those of quinoline and isoquinoline in the previous report[2], are well interpreted by our perturbation calculation, and the assignment of the spectra of three-ring nitrogen heterocycles, which was made in the first paper, has been given a more rigorous basis.

Summary

The electronic spectra of three-ring nitrogen heterocycles have been calculated by the perturbation method based on the Hartree-Fock self-consistent field theory. There is a satisfactory agreement in general between the calculated the and observed excitation energies and oscillator strengths, and the mechanism of the electronic transitions in these molecules has been discussed in detail.

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