Light Absorption in N-Acetonyl Quinolinium Iodide
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The absorption spectra of N-acetonyl quinolinium iodide in different solvents have been studied in the region 200 nm—1100 nm. Four bands have been observed in DMF, methanol, water and alkaline water. The bands have been assigned to different intramolecular transitions.

Recently the absorption spectra of some methiodides of styryl quinolines has been reported by the authors. Though the infrared absorption in N-acetonyl quinolinium iodide has been reported, its absorption in visible and ultraviolet regions has not been studied in details. The present communication reports the absorption spectra of N-acetonyl quinolinium iodide in four different solvents, DMF, methanol, water and alkaline water, assigning the bands in the light of the theoretical MO calculations of the parent molecule and computed spectroscopic parameters.

N-acetonyl quinolinium iodide has the following structure:

Experimental
The absorption measurements were carried out with Carl Zeiss Jena VSU-2 Spectrophotometer in the region 200 nm to 1100 nm at 25°C ± 0.1°C. The solvents were of highest purity available (A.R. or Spectro-grade).

Results
The plots of optical density (O.D.) vs wave number (cm⁻¹) for solvents DMF, methanol, water and alkaline water have been given in Fig. 1.

Four bands have been observed (Fig. 1). They have been classified as bands A, B, C and D starting from longest wavelength. The characteristics of the bands in different solvents have been collected in Table I. The values of molar extinction coefficient εₘₐₓ, oscillator strength f, dipole moment Dₘₙ, Einstein's coefficients Aₘₙ and Bₘₙ and lifetime of the excited state T have also been computed and included in Table I.

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Table I. Characteristics of bands A, B, C, and D of N-Acetonyl Quinolinium Iodide in different solvents.

<table>
<thead>
<tr>
<th>Solvent</th>
<th>Band</th>
<th>Band position [nm]</th>
<th>Intensity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>e_{\text{max}} [litres/mole-cm]</td>
<td>f</td>
</tr>
<tr>
<td>DMF</td>
<td>A</td>
<td>470</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>314</td>
<td>2900</td>
</tr>
<tr>
<td>Methanol</td>
<td>A</td>
<td>445</td>
<td>100</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>319</td>
<td>6900</td>
</tr>
<tr>
<td></td>
<td>C</td>
<td>235</td>
<td>3500</td>
</tr>
<tr>
<td></td>
<td>D</td>
<td>229</td>
<td>1000</td>
</tr>
<tr>
<td>Alkaline water</td>
<td>A</td>
<td>440</td>
<td>150</td>
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<tr>
<td></td>
<td>B</td>
<td>316</td>
<td>8300</td>
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<td></td>
<td>C</td>
<td>234</td>
<td>6000</td>
</tr>
<tr>
<td></td>
<td>D</td>
<td>228</td>
<td>1000</td>
</tr>
<tr>
<td>Water</td>
<td>A</td>
<td>430</td>
<td>200</td>
</tr>
<tr>
<td></td>
<td>B</td>
<td>316</td>
<td>8600</td>
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<tr>
<td></td>
<td>C</td>
<td>234</td>
<td>6000</td>
</tr>
<tr>
<td></td>
<td>D</td>
<td>228</td>
<td>2000</td>
</tr>
</tbody>
</table>

**Band A**

The band A is located at 470 nm in DMF. It exhibits a blue shift when the solvents are changed in the order DMF-methanol-alkaline water-water. The molar extinction coeff. (e_{\text{max}}), oscillator strength (f), dipole strength (D_{nm}), and Einstein's coeff. (A_{nm} and B_{nm}) suggest that the band is of low intensity.

The lifetime of the excited state varies between 2.5×10⁻⁶ to 5×10⁻⁶ sec. in case of different solvents.

**Band B**

The band is located at 314 nm in DMF. The band exhibits a blue shift when the solvents are changed in the order DMF-alkaline water-water-methanol. The estimated values of e_{\text{max}}, f, D_{nm}, A_{nm} and B_{nm} show that band is an intense one. The calculated value of lifetime of the excited state is ~10⁻⁸ sec. in different solvents.

**Band C**

The band is located at 234 nm. The effect of solvent on the energy of the band is very small. The estimated values of e_{\text{max}}, f, D_{nm}, A_{nm} and B_{nm} show that band is weak.

The estimated values of the lifetime of the excited state is ~10⁻⁸ seconds.

**Band D**

The band is located at 228 nm. The estimated values of e_{\text{max}}, f, D_{nm}, A_{nm} and B_{nm} show that band is very weak. The effect of solvent on the energy of the band is very small. The estimated values of lifetime of excited state are ~10⁻⁷ sec. in different solvents.

**Discussion**

The spectra of the compound may be interpreted by considering the transitions in parent molecules, quinoline and naphthalene. Naphthalene has D_{th} symmetry. Its ground state is 1^A_g. By substitution −N = for =CH − the symmetry is lowered to C_{s}.

**Assignment of Bands**

**Band A**

The observed solvent effect i.e. increase in energy of the band on changing the solvent DMF-methanol-alkaline water-water is of typical n→π* transition. Low energy and low intensity of the band also support this assignment. The non-bonding orbitals of carbonyl group are also involved in increasing the energy of n→π* transition. Consequently the band may be assigned to n→π* transition.

**Band B**

The position and intensity of band B agrees well with that of α-bands of quinoline (314 nm) and naphthalene (311 nm).
This shows that the substitution of aza group in naphthalene and bonding of CH\textsubscript{3} group to aza-group do not effect much the position of the band. Small blue shift is observed when solvents are changed in the order methanol-alkaline water-water. Hence the band may be assigned to transition corresponding to $^{1}L_0 \rightarrow ^{1}A$, $\pi \rightarrow \pi^*$ transition of naphthalene.

**Band C**

The intensity of this band resembles with that of $p$-bands of quinoline and naphthalene. The $n$ and $\pi$ orbitals both of carbonyl and methyl group are also involved in this transition. On the ground of intensity it may be assigned to the transition corresponding to $^{1}L_0 \rightarrow ^{1}A$, $\pi \rightarrow \pi^*$ transition of naphthalene.

**Band D**

Intensity of this band agree well with those of $\beta$-bands of naphthalene. The absorption band of iodide ion, which is loosely bonded to the nitrogen, is also expected to be superimposed on it. On ground of intensity the band may be assigned to $^{1}B_n \rightarrow ^{1}A$ transition of naphthalene.

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