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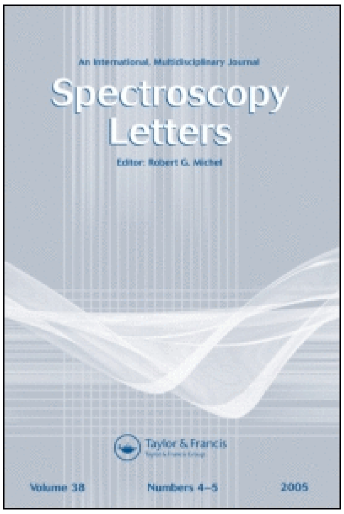

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The Intensity of the Secondary Transition of the Benzene Chromophore with Fused Rings. The New Vector Model

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THE INTENSITY OF THE SECONDARY TRANSITION OF THE BENZENE CHROMOPHORE WITH FUSED RINGS.
THE NEW VECTOR MODEL.

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It has been shown recently[1] that it is possible to calculate the intensity of the secondary transition (towards 260 nm) of the substituted benzene chromophore with better accuracy than it is possible with the simple Sklar vector model.[2-9] This new approach is based on MNDO calculations. It leads to a simple relationship, which is applied – for the time being – to π-donating substituents such as $-CH_3$, $-OH$, $-OCH_3$, since we are mainly involved in the study of natural products :

$$\varepsilon_{sm} = 4905\,(TS + V)$$

ε_{sm} is the maximum of the smoothed absorption curve, as it has been defined by BALLESTER and RIERA.[10] It avoids the problems linked to the vibrational fine structure which depend strongly on the relative importance of the two progressions of the secondary transition,[11] on the interactions of the molecule with the solvent,[12] etc. Our relationship has been tested for the values $0 < \varepsilon_{sm} < 3600$, for molecules with weak steric strain (no fused rings).

V is the vibrationnal component to the intensity. It is only of importance for the low values of intensity. It is based on BALLESTER and RIERA's work.[10]

S is related to the UV cross section of the molecule.

T is based on the combination of the moduli (t_1 and t_2) of two vectors : $\mathbf{t}_1$ and $\mathbf{t}_2$. $\mathbf{t}_1$ is the transition moment vector as defined by the simple vector model (Figure 1A). Nevertheless, the moduli of the component vectors related to each one of the six positions around the chromophore, and used to calculate $\mathbf{t}_1$, are given a MNDO basis. The modulus of a given component vector is assumed to be the same as the π bond order between the position to which it is related and the corresponding substituent (the first atom of the substituent). $\mathbf{t}_1$ strongly takes into account the whole part of the π system outside of the benzene moiety. t_2 is the modulus of the vector $\mathbf{t}_2$ obtained when using only the two π highest occupied orbitals in the ground state (corresponding to those which are degenerate in the free benzene molecule). These orbitals are those of the ground state which are mainly involved in the secondary transition. The evaluation of the modulus of each component vector is obtained by calculating the distorsion of the π density (the part related to these two orbitals) from what is observed in the benzene itself in the considered position of the ring. Thus, t_2 puts the emphasis on the highest energy electrons inside the benzene moiety. T, which is used in the calculations, is a combination of t_1 and t_2. The corresponding vectors ($\mathbf{t}_1$ and $\mathbf{t}_2$) should be colinear, since both of them are assumed to represent the transition moment, and both of them should be perfectly equal if these two approaches were perfectly equivalent. The angle between them is always low. To be simple we have used a combination of their moduli. Thus T is the modulus of the vector **T**. S also may be related to a vector **S** since it is also an approach to the transition moment emphasizing another way. All these vectors should be perfectly colinear if all these approach were perfectly equivalent.

The modulus of the transition moment, not taking into account the vibrational component to intensity, is proportional to $\mu = (TS)^{1/2}$.

THE RINGS FUSED TO THE BENZENE MOIETY

The strain induced by the rings fused to the benzene moiety distorts the structure of the chromophore. These rings can cause an alternation of the bond lengths towards a Kekulé-like structure (Mills-Nixon effect [13]), [14-15] as well as an alternation of the π bond orders. The π densities too are changed. The D_{6h} symmetry of the benzene chromophore being decreased, the secondary transition – which is electronically forbidden for a D_{6h} symmetry – becomes allowed. Its intensity increases under strain.

Surprisingly, neither t_1, nor t_2, is strongly modified compared to the non cyclic corresponding molecule (for example : indane or tetralin compared to 1,2-dimethylbenzene (orthoxylene) ; benzodioxole compared to 1,2-dihydroxybenzene (pyrocatechol)). The use of the two highest occupied orbitals is not sufficient to take into account the strain effects. We should have to use also deeper orbitals. This would strongly weighten the method. We choose to work on a more empirical basis.

The best results have been obtained when S is used to take into account the fused ring effect. Such an approach assumes that the strain effect increases the UV the cross section.

First of all, the calculation is done for the corresponding molecule with no fused ring : orthoxylene is used for indane or tetraline, pyrocatechol for benzodioxole etc. T, S, V are calculated. Then, the strain is taken into account as a vector increment **R** added to the resulting vector **S** : **S' = S + R**.

S is one of the possible approaches to the transition moment vector. Only its modulus has been calculated in our preceding work. Thus, **R** is given the direction of $\mathbf{t}_1$ – another approach to the transition moment vector – (whose direction has been calculated), since the two directions should have to be the same.

When considering the vector pattern, for π donating substituents (Figure 1A), one sees that, for a given fused ring (Figure 1B), the fused ring contribution **R** to S' points to the same direction as the resultant of the two component vectors of the two positions of substitutions. The direction of that resultant – and thus the direction of **R** (Figure 1B, 1C, 1D) – is related to the position of the fused ring on the chromophore. **R** can display two directions : from the chromophore towards the fused ring, or from the fused ring towards the chromophore. This depends on the direction which has been choosen for the vector pattern in figure 1A (the directions of the whole vectors could be reversed), and for the position of the fused ring. This fact leads to no trouble at all, provided the vector pattern of figure 1A being choosen, the internal consistency is not destroyed. The resulting vectors for a disubstitution pattern – for fused rings as well – display alternating directions as in figure 1E.

R is given an empirical value : 1.82 for an aliphatic five membered fused ring, 0.50 for an aliphatic six membered fused ring, 0.65 for a benzodioxole type fused ring (methylenedioxy fused rings). The vector addition being done, the value of T calculated for the molecule with no fused ring is used to calculate TS'. Then V (calculated for the molecule with no fused ring) is added to the result.

Using the molecule with no fused ring, for the calculation of the intensity of molecules with fused ring, is based on simplicity. Actually, many calculations on molecules with no fused ring have been done in our preceding work and the results for T are available. Furthermore, if some calculations have to be done, it is much more easier to reach a MNDO geometry optimization for two small substituents such as two methyles than for a fused ring. One could argue that geometries could be quite different, and the electronic densities, the π bond orders also. We are quite aware of such a problem, and some of our preceding works have shown the strong incidence of the strain induced by the fused rings on geometry, densities etc. [14-15] Nevertheless, as far as the intensity of the secondary transition is concerned, the perturbation induced by the fused rings can be taken into account as empirical standard vectors, that is to say : as an increase of the perturbation of the two substituents on the chromophore. In fact, MNDO calculation, with full optimization, on some molecules with fused rings, have been done and they have shown that the value obtained for T, when there is a fused ring, is not very far from the value obtained for the corresponding molecule with no fused ring.

INTENSITY CALCULATIONS

The greek letter ϕ inside an hexagone is used in figure 2 for the benzene chromophore. See figure 3 for the whole results. The straight line is what has been obtained in our preceding work. [1]

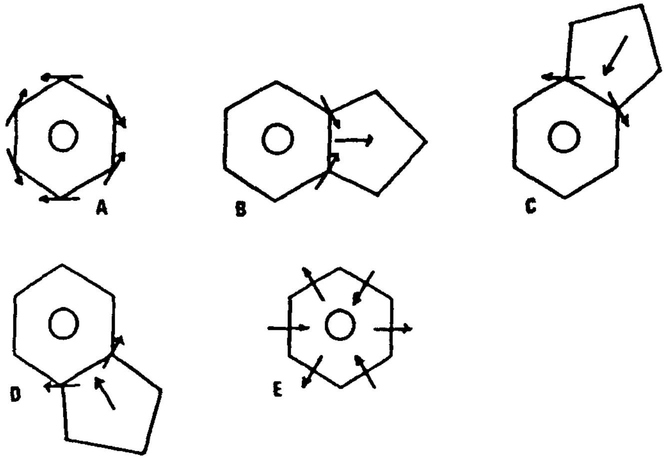

Figure 1 A) The simple Sklar's vector model. B) C) D) Examples with the tetraline molecule showing the direction of the strain contribution (**R**). The direction depends on the position of the fused ring around the benzene chromophore and on the direction of the vector pattern in A. E) The alternating directions for the strain contribution of the fused rings.

A) (Figure 2A, indane) Calculations are based on 1,2-dimethylbenzene (orthoxylene). From our preceding work [1] : T = 0.0857, S = 0.357, V = 0.024. The direction of S is given by these calculations, since it is the same as the direction of $\mathbf{t}_1$. **R** and S are colinear vectors since the fused ring is the only substituent on the chromophore. As R = 1.82, S' = S + R = 2.177. m = TS' + V = 0.211. ε_{sm} = 4905 (TS' + V) = 1035. The experimental value for ε_{sm} given by BALLESTER and RIERA is 1040.[10]

B) (Figure 2B). Calculations are based on 1,2,4,5-tetramethylbenzene (T = 0.1682, S = 0.5, V = 0.030, from our preceding work [1]). The two fused rings contributions are colinear vectors : S' = 0.5 + 1.82x2 = 4.14. Thus : m = TS' + V = 0.1682x4.14 + 0.030 = 0.726. ε_{sm} = 4905(TS' + V) = 3560. The experimental value for ε_{sm} is 3700. [10]

C) (Figure 2C, tetraline) Calculations are based on 1,2-dimethylbenzene (orthoxylene). T = 0.0857, and S = 0.357, V = 0.024, from our preceding work. [1] The direction of S is given by these preceding calculations. **R** and S are colinear vectors since the fused ring is the only substituent on the chromophore. R = 0.5, thus : S' = S + R = 0.357 + 0.5 = 0.857. m = TS' + V = 0.0974. ε_{sm} = 4905 (TS' + V) = 478. The experimental value for ε_{sm} is 465. [10]

D) (Figure 2D) Calculations are based on 1,2,4,5-tetramethylbenzene. T = 0.1682, S = 0.5, V = 0.030. [1] The contributions of the two fused rings are colinear vectors : S' = 0.5 + 0.5x2 = 1.5. Thus : m = TS' + V = 0.1682x1.5 + 0.030 = 0.282. ε_{sm} = 4905(TS' + V) = 1385. The experimental value is 1450. [10]

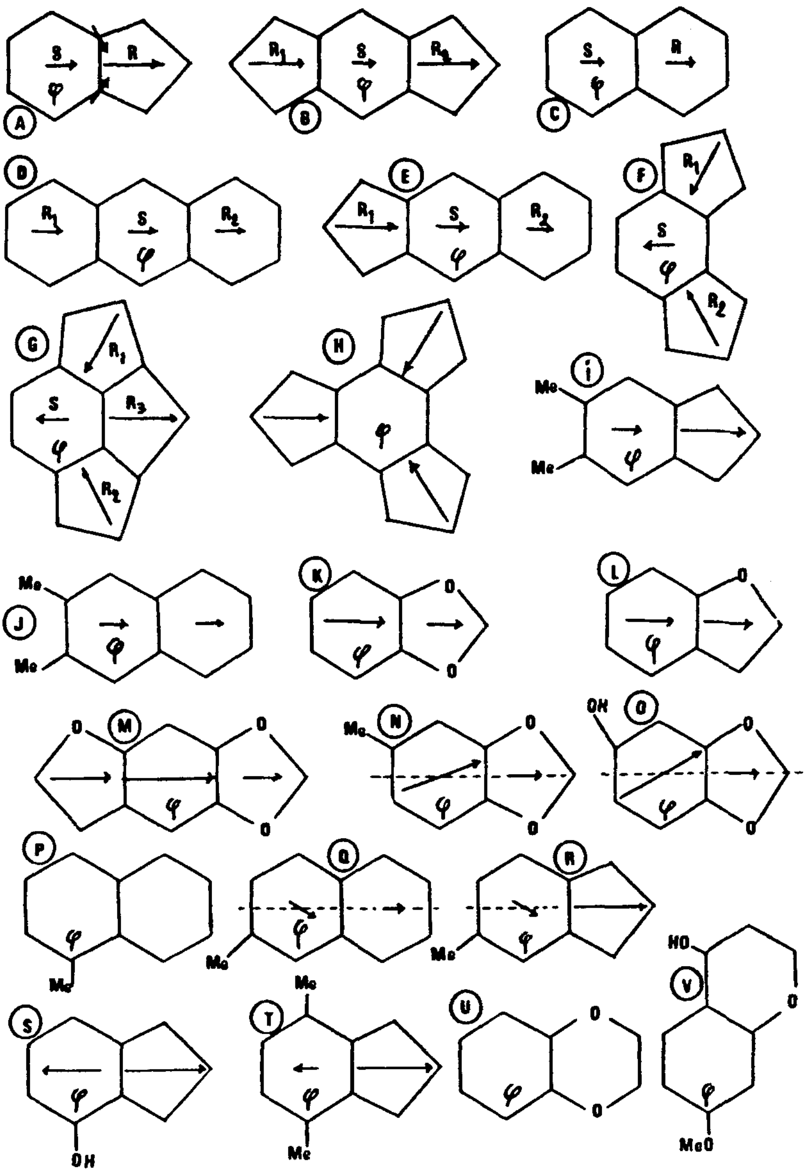

Figure 2 Molecules studied in that work. When there is the greek letter φ inside an hexagon, that hexagon represents the benzene chromophore.

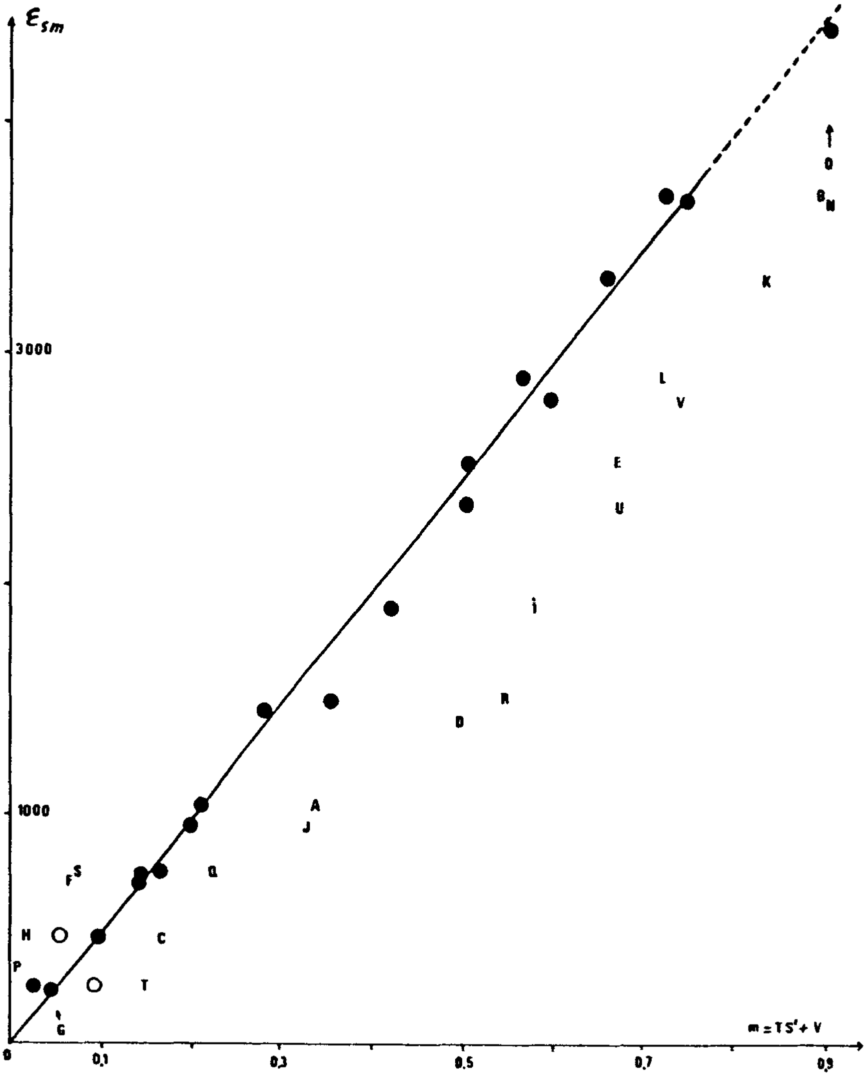

Figure 3 Intensity versus m = TS' + V

E) (Figure 2E) Calculations are based on 1,2,4,5-tetramethylbenzene. $T = 0.1682$, $S = 0.5$, $V = 0.030$. [1] The contributions of the two fused rings are colinear vectors : $S' = 0.5 + 0.5 + 1.82 = 2.82$. Thus : $m = TS' + V = 0.1682 \times 2.82 + 0.030 = 0.504$. $\varepsilon_{sm} = 4905(TS' + V) = 2472$. The experimental value is 2500-2550. [16]

F) (Figure 2F) Calculations are based on 1,2,3,4-tetramethylbenzene. $T = 0.0878$, $S = 0.5$, $V = 0.030$. Calculations give too high a value for T, since such a value leads to : $\varepsilon_{sm} = 4905(TS + V) = 362$, when the experimental value is only 265 (*API* n°129 [20]). It has been found, in our preceding work, [1] for such low intensities, some discrepancies (pentamethylbenzene). t_1 is perhaps too much taken into account compared to t_2 (t_1 is stronger than t_2). Knowing the experimental value of intensity for 1,2,3,4-tetramethylbenzene it is possible to determine an experimental value for T which will be used instead of the calculated T : $T_{exp} = [(\varepsilon_{sm}/4905) - V]/S = 0.048$. This leads to $S' = 0.5 + 1.82 = 2.32$ since in the vector addition the angle between the contributing vectors arising from the two rings is 120° : the length of the resulting vector is equal to the length of one of the two contributing vectors. Thus : $T_{exp}S' + V = 0.048 \times 2.32 + 0.030 = 0.141$. $\varepsilon_{sm} = 4905(T_{exp}S + V) = 692$. The experimental value for ε_{sm} given by BALLESTER and RIERA from RAPOPORT and SMOLENSKY's work [17] is 700.

G) (Figure 2G) The parentmolecule is hexamethylbenzene : $T = 0$, $V = 0.036$. The strained molecule displays a D_{3h} symmetry. The angles between the three vectors contributing to **R** are 120°, and their sum vanishes. Thus : $T = 0$, $\varepsilon_{sm} = 4905\ V = 4905 \times 0.036 = 177$. Experiment leads to 230. [10] At first glance it could seem that there is a strong discrepancy between experimental and calculated values. Calculated value is 24 % lower than the experimental one. In fact, for such low values it is difficult to evaluate accurately all the parameters that are involved. Our evaluation is within the range of what is obtained in classical intensity calculations. Nevertheless, as above, using a T_{exp} value ($\varepsilon_{sm} = 225$ for hexamethylbenzene [1]), and considering that $S' = S$ since the strain contribution vanishes, this leads to : $\varepsilon_{sm} = [[(225/4905) - 0.036]/S]S + 0.036 = 225$ (this is of course the same value as the hexamethylbenzene one) which is quite consistent with the experimental value : 230.

H) (Figure 2H). The parent molecule is 1,2,3,4-tetramethylbenzene (values given in **F**). The main point to take into account is the fact that the contribution **R** of the "sandwiched" fused ring is opposed to the contribution of the two vectors arising from the two fused rings already present in **F** (Figure 1E). The strain contribution vanishes : $S' = 0.5 + 1.82 - 1.82 = 0.5$. Using as above in **F** : $T_{exp} = 0.048$, this leads to : $m = 0.048 \times 0.5 + 0.030 = 0.054$. $\varepsilon_{sm} = 4905 \times 0.054 = 265$. Using the calculated value for T we should have obtained 363 which would have been closer to the experimental value : 470 (RAPOPORT and SMOLENSKY [17]). Nevertheless, this would have not been completely satisfactory. In fact, the value 1.82 used for the contribution of the sandwiched fused ring in the calculation of S' is not very good, since it is the value used for a five membered fused ring having no common part with another fused ring (the same could be said for the two other fused rings but to a smaller extent). The sandwiched fused ring is not the same as an ordinary fused ring because of its sandwiched position, and because it is not coplanar to the rest of the molecule. It should be less perturbating than the others. Furthermore, the others tend to distort the molecule towards a Kekulé like structure (Mills-Nixon effect [13]) [14-15] lengthening the bond to which they are fused, and shortening the adjacent bonds. The sandwiched fused ring tends to lengthen a bond which tends to be shortened by the two other rings : its contribution to S' cannot be as great as the others contribution. R should not vanish and the value should be much higher than what is calculated on a rough basis. This is what experiment shows. As our method is not built to take into account such effects, if we want to reach more accurate results we have to study the strain effects of each one of the two sorts of fused rings in that molecule, comparing F and H.

I) (Figure 2I). The parent compound is 1,2,4,5-tetramethylbenzene. The values for that molecule are those given for **D** and **E** ($T = 0.1682$, $S = 0.5$, $V = 0.030$). S and **R** are colinear : $S' = 0.5 + 1.82 = 2.32$. $m = TS' + V = 0.420$. $\varepsilon_{sm} = 4905x0.420 = 2060$. The experimental value is 1900. [10]

J) (Figure 2J). The parent compound still is 1,2,4,5-tetramethylbenzene. S and **R** are colinear. The length of **R** is 0.5 since the ring is a six membered one : $S' = 0.5 + 0.5 = 1$. $m = TS' + V = 0.1682x1 + 0.030 = 0.198$. $\varepsilon_{sm} = 4905x0.198 = 970$. The experimental value is 950. [10]

K) (Figure 2K) (benzodioxole). The parent compound is 1,2-dihydroxybenzene (pyrocatechol) : $T = 0.246$, $S = 1.786$, $V = 0.063$. As in indane (**A**) **R** and **S** are colinear. $R = 0.65$, since the fused ring is a methylenedioxy one. Thus : $S' = 1.786 + 0.65 = 2.436$. $m = TS' + V = 0.246x2.436 + 0.063 = 0.662$. $\varepsilon_{sm} = 4905x0.662 = 3247$. The experimental value is 3330. [18]

L) (Figure 2L) The parent compound is 1-methyl-2-hydroxybenzene ($T = 0.207$, $S = 1.2$, $V = 0.063$). The effect of the fused ring are considered as an average of the effects of the fused ring of indane and those of benzodioxole. In these two latter molecules the action of the fused ring is colinear to the C_2 symmetry axis. The contribution of the fused ring in the molecule **F** will be assumed to be the same for simplicity. Thus : $S' = 1.2 + (0.65 + 1.82)/2 = 2.435$. $m = TS' + V = 0.207x2.435 + 0.063 = 0.567$. $\varepsilon_{sm} = 4905x0.567 = 2781$. The experimental value is 2900. [18]

M) (Figure 2M) In fact, such a molecule is one of the two chromophores of pterocarpin, a natural product whose spectrum has been published in one of our preceding works. [19] The parent compound for the present calculation is 1-methyl-2,4,5-trihydroxybenzene. As that molecule has not been studied in our preceding work [1] devoted to the new vector model, we studied it here : $T = 0.324$, $S = 2.473$, $V = 0.069$. $S' = 2.473 + 0.65 + (0.65 + 1.82)/2 = 4.358$. The first 0.65 value is the value linked to the benzodioxole ring. $m = 0.324x4.358 + 0.069 = 1.481$. $\varepsilon_{sm} = 4905x1.481 = 7264$. The experimental value is 6600. One could notice the difference between experiment and calculation. In fact, that difference is only 10% of the experimental value which is quite good for intensity calculation.

Furthermore, the validity of our new vector model method has been checked only till ε_{sm} = 3600 in our preceding work. The intensity of the secondary transition of the present molecule is much higher, and the theory could have to be improved to fit to such experimental values.

N) (Figure 2N) The parent molecule is 1-methyl-3,4-dihydroxybenzene (T = 0.262, S = 1.986, V = 0.066). The angle between the transition moment vector and the C_2 axis of the benzodioxole moiety (the angle between **S** and **R**) is 19.2°, wich leads to : S' = 2.609. Thus : m = 0.262x2.609 + 0.066 = 0.749. ε_{sm} = 4905x0.749 = 3675. The experimental value is 3670. [18]

Neglecting the angle between the two components of **S'** would have led to : S' = 1.986 + 0.65 = 2.636, to : ε_{sm} = 4905(0.262x2.636 + 0.066) = 3711.

O) (Figure 2O) The parent molecule is 1,2,4-trihydroxybenzene (T = 0.297, S = 2.273, V = 0.066). The angle between **R** and **S** is : 28.2°. This leads to S' = 2.863. m = 0.297x2.863 + 0.066 = 0.916. ε_{sm} = 4905x0.916 = 4493. The experimental value is : 4400. [18] Neglecting the angle would lead to : 2.273 + 0.65 = 2.923 and ε_{sm} = 4905(0.297x2.923 + 0.066) = 4582.

P) (Figure 2P) The parent molecule is 1,2,3-trimethylbenzene (T = 0, V = 0.027). Since T = 0 there is no need to calculate S' : TS' will be 0. This leads to : m = TS' + V = 0.027. ε_{sm} = 4905x0.027 = 132. The experimental value is 250 (*API* n°752 [20]). If we use the experimental value of the intensity of 1,2,3-trimethylbenzene 170 – instead of 132 – is obtained. It is better, but somewhat too low. We have choosen to take into account the strain perturbation in modifying S and not T. Thus, when T = 0 for the parent compound, the only contribution to intensity is V. This is the vibrational component, which is not very accurately known.

Q) (Figure 2Q) The parent molecule is 1,2,4-trimethylbenzene (T = 0.148, S = 0.455, V = 0.027). The angle between **R** and **S** is : 30.1°. The vector addition leads to : S' = 0.922 . Thus : m = TS' + V = 0.148x0.922 + 0.027 = 0.163. ε_{sm} = 4905x0.163 = 800. Experiment leads to 760 (*API* n°753 [20]). Neglecting the angle would lead to : S' = 0.455 + 0.5 = 0.955 and ε_{sm} = 4905x0.168 = 825.

R) (Figure 2R) The parent molecule is 1,2,4-trimethylbenzene (**Q**). The vector addition leads to : S' = 2.226. m = TS' + V = 0.148x2.226 + 0.027 = 0.356. ε_{sm} = 4905x0.356 = 1745. The experimental value is 1490 (measured from *API* n°904 [20]), 1415 (measured from *API* n°873 [20]). Neglecting the angle would lead to : S' = 0.455 + 1.82 = 2.275 and : ε_{sm} = 1784.

S) (Figure 2S) The parent molecule is 1,2-dimethyl-3-hydroxybenzene (T = 0.162, S = 1.337, V = 0.066)[1]. The direction of **R** is almost opposed to that of S : S' = | 1.337 - 1.82| = 0.483. m = 0.162x0.483 + 0.066 = 0.144. ε_{sm} = 4905x0.144 = 705. The experimental value is 740. [21]

T) (Figure 2T) T, calculated from experiment (1,2,3,4-tetramethylbenzene), is 0.048 as it has been discussed here above. S = 0.5, V = 0.030. Owing to the symmetry of the molecule the vector **R** is opposed to **S'** : S' = | 0.5 - 1.82| = 1.32. m = 0.048x1.32 + 0.030 = 0.093. ε_{sm} = 4905x0.093 = 455. The experimental value is 250 (*API* n°615 [20]). Such a value is quite surprising since it is also 265 for 1,2,3,4-tetramethylbenzene (*API* n°129

20). The strain would have no visible effect. It is still possible that there is a mistake in the *API* spectrum. Nevertheless, we have already found some other discrepancies for low values. Owing to the questions which arise about the experiment, the molecule appears as a circle in figure 3 and not as a point.

U) (Figure 2U, benzodioxane) The modulus of the vector component taking into account the strain effect induced by a six membered ring is much lower (0.5 for tetraline) than the modulus of the corresponding vector concerning a five membered ring (1.82 for indane). Thus we should find for the fused ring of benzodioxane a much lower value than what is observed for benzodioxole (0.65). Experiment shows that such a value is so low that it can be neglected : no correction is necessary when using the unstrained molecule as a basis : T = 0.246, S = 1.786, V = 0.063. m = 0.246x1.786 + 0.063 = 0.502. ε_{sm} = 4905x0.502 = 2460. The experimental value is 2350. [18] Experiment and calculation are consistent. In fact, we lack of experimental values for such molecules.

Our calculations on the actual cyclic chromophores show that for benzodioxole and benzodioxane the T values obtained are lower than those which are obtained for the parent unstrained molecules. Using "actual" values, all along this work, would have been another approach to the problem. This would have led to slightly different parameters. It would also have led to a huge amount of calculations to obtain consistent geometries, when these calculations have already been done for the unstrained parent compounds.

V) (Figure 2V) This is the second chromophore of pterocarpine. The unstrained parent molecule leads to : T = 0.238, S = 1.986, V = 0.066. As in **I**, the fused ring is considered as the average of an alkyl fused ring and a benzodioxane type one : S' = 1.986 + (0 + 0.5)/2 = 2.236. m = 0.238x2.236 + 0.066 = 0.598. ε_{sm} = 2930. The experimental value is 2800. [19] Taking into account the vector nature of the correction leads to 2918 (T = 0.595).

CONCLUSION

Although the method studied in our preceding work would have to be improved for the lowest values of intensity, it has been quite unexpected to reach such an accuracy in applying it to the intensity of the secondary transition of strained molecules. Our aim now is to include nitrogen substituents (aniline type molecules) since we are mainly involved in the spectroscopy of natural products. Furthermore, it is necessary too to include -C=O substituents, but it could be difficult since π donating substituents and π withdrawing ones on the same benzene ring lead sometimes to interactions through the π system. These interactions are stronger in the excited state which till now, in our work, has been taken into account on an almost empirical basis. These interactions could lead to too a complex parametrization.

Our MNDO calculations have been done from La Réunion Island (France, Indian Ocean) on the Cyber 960 computer of the "Centre Interuniversitaire de l'Information" of Lille (France, Europe), *via* the TRANSPAC world satellite network.

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