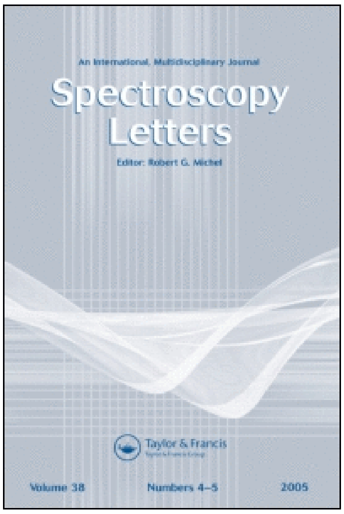

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INTENSITY BEHAVIOUR IN THE NEAR ULTRAVIOLET SPECTRA OF CHLORO AND FLUORO DERIVATIVES OF THE BENZENE CHROMOPHORE

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ABSTRACT

The *Interaction Vector Model* (IVM) is used to understand the behaviour of the intensity of the secondary transition of chloro derivatives of the benzene chromophore, extending the work to some fluoro derivatives. These latter molecules show a surprising result: the ortho and meta interaction vectors for fluoro disubstituted molecules point in directions opposed to what has been observed in the whole preceding works.

INTRODUCTION

Chlorinated benzene molecules, apart from their interest to test the range of application of the *Interaction Vector Model* [1-8] (IVM, a model for the intensity of the secondary transition of the benzene chromophore), are used as pesticides.[9] Considering their possible incidence on health, our knowledge of their physical properties, particularly their spectrocopic ones, needs to be bettered [9].

In the IVM [1-8], as in the Sklar's approach[10], a basis vector **n** [1,2] is attributed to each position of substitution (Figure 1). The new *interaction vector* concept takes into account the interaction of substituents. The directions of the interaction vectors are given in Figure 1. A photonic *cross section* S (and $\sigma = S^{1/2}$) has been introduced as: $S = \Sigma_X h_X n_X/(4.8 + 0.2n_X^2)$; n_X is the number of substituents of

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the X type. A small vibrational contribution V is used. Intensities are given as the molar extinction coefficients of the smoothed graph of the secondary transition (ε_{sm}) [11], so ε_{sm} is close to integrated intensities. ε_{calc} is the calculated value for ε_{sm}.

EXPERIMENTAL

Chloro substituted benzene chromophore

The smoothed intensities are the same for chlorobenzene (ε_{sm} = 190), and for toluene (ε_{sm} = 192).[1] Thus, the set of parameters should be similar for the two substituents : $\mathbf{n_{Cl} = 0.098}$; S = 0.2 [which imposes : $h_{Cl} = 1$; $S_{Cl} = h_{Cl}\, n_{Cl}/(4.8 + 0.2n_{Cl}^2)$], and $\sigma = 0.447$, assuming, as it is the case for many substituents[8], that the contribution to V is the same as that of methyls, and that the interaction vectors are also the same. Thus, the moduli of the ortho interaction vector, and of the meta one are : $\mathbf{n_{ortho,ClCl} = n_{meta,ClCl} = 0.0060}$; the modulus of the para interaction vector is $\mathbf{n_{para,ClCl} = 0.012}$.[1]

These values lead to: ε_{calc} = 250 for dichloro-1,2-benzene. The experiment gives: ε_{sm} = 265 [13g] (235 for the dimethyl derivative). The difference between calculation and experiment, taking experiment as a reference, is: $\Delta = -5.7$ %. In preceding works, calculations have been considered satisfactory when Δ is within the range of ± 10%.[1-8]

For dichloro-1,3-benzene (ε_{sm} = 245 [13h]) : ε_{calc} = 250 ($\Delta = +2.0$ %) (235 for the dimethyl derivative). For dichloro-1,4-benzene : ε_{calc} = 425 ; experiment : ε_{sm} = 315 [13i] and 375 ($\Delta = +13.3$%)[14d]. The experiment could be questioned, since the corresponding methyl derivative gives : 425.

For trichloro-1,2,4-benzene : ε_{calc} = 425, ε_{sm} = 395 [13j] ($\Delta = +7.6$ %) (for the methyl derivative, ε_{sm} = 440 [1]). The two values are consistent.

As concerns tetrachloro-1,2,3,5-benzene : ε_{calc} = 245, experiment: 945.[13k] The experiment is not consistent with the well known fact that for symmetry reasons intensity should be strongly forbidden.

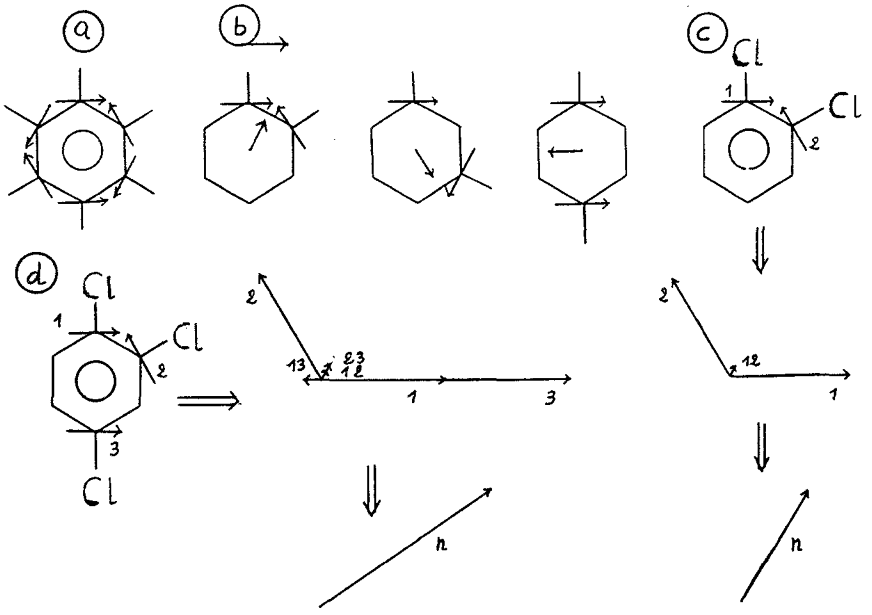

Figure 1. a) The Sklar's vectors scheme. When there is a substituent on a given position, the corresponding basis vector (contribution to the transition moment vector) is effective. Its length depends on the efficiency of the perturbation on the π_ϕ system. b) Basis vectors for ortho, meta, para substitutions. The direction of the interaction vector is shown in the center of the ring. For ortho and meta substituents this vector lies on the bisectrix of the angle between the two basis vectors. It points in the same direction as the projections of the two basis vectors on the bisectrix (fluoro substitutions excepted). For para substitutions it points in the direction opposed to the basis vectors. The circle (showing conjugation) in the center of the ring has been omitted for clarity. For fluoro substitutions the directions of the orto and meta interaction vectors should be reversed. c) Example showing the vector pattern in dichloro-1,2-benzene. (12) is the interaction vector. n is the resulting vector. d) Example showing the vector pattern for trichloro-1,2,4-benzene.

When n is very weak, there is a contribution $q^{1\text{-}2}$ for -OR or methyl substituents. Owing to the similarity between a chloro and a methyl substitution, *intensity for the 1,3,5 derivative should be* $\varepsilon_{calc} = 160$. *The experiment gives : 200* (for the methyl derivative : 170 [1]), and 160 for the 1,2,3-trichlorobenzene (the methyl derivative : 170 [1]). Calculations are only indicative since these low intensity cases have not been under thorough examination.

For the methyl-chloro derivatives, the two types of substituents, although they display the same effects, are different ; will be considered as providing two separate contributions to S.

Owing to the similarity Cl-methyl the methyl interaction vectors lengths are used for Cl :

$n_{ortho,Cl\ Met} = 0.006$, $n_{meta,Cl\ Met} = 0.006$, $n_{para,Cl\ Met} = 0.012$.

Thus, calculations lead to the same results for chloro-1-methyl-2-benzene[13l] and chloro-1-methyl-3-benzene[13m] : $\varepsilon_{calc} = 256$. The experiment gives : $\varepsilon_{sm} = 245$, for the first[13l] ($\Delta = + 4.5$ %) (235 for the dimethyl derivative,[1] 265 for the dichloro derivative (as above)). The experiment gives 170 [13m] for the second (235 for the dimethyl derivative,[1] 245 for the dichloro derivative (here above)). This latter value is very surprising since it is lower than the values obtained for the mono derivatives (chlorobenzene, toluene).

For chloro-1-methy-l-4-benzene, calculation gives : $\varepsilon_{calc} = 435$, experiment : $\varepsilon_{sm} = 425$ [13n] (corrected from overlap)($\Delta = + 2.4$ %), 405 [15], and the surprising value : 945[14d], which will not be considered.

Note that $\varepsilon_{calc} = 440$, and $\varepsilon_{sm} = 365$ [13o] ($\Delta = + 20.5$ %), for chloro-1-dimethyl-3,6-benzene. Also, $\varepsilon_{calc} = 440$ for dichloro-1,3-methyl-6-benzene, and $\varepsilon_{sm} = 490$ [13p] ($\Delta = - 10.2$ %), which is almost satisfactory.

As concerns dichloro-1,3-methyl-2-benzene, calculations lead to : $\varepsilon_{calc} = 160$, and experimental : $\varepsilon_{sm} = 170$, taking into account q.[2]

Three data for ortho derivatives involving Cl and -OR, are known : $\varepsilon_{sm} = 1830$ [13w] for chloro-1-hydroxy-2-benzene, 2100 [13x] for the methoxy derivative, and 1800 [13y] for the ethoxy derivative. These values should be very close. The methoxy derivative displays too high a value. The average of the others is : $\varepsilon_{sm} = 1815$. The basis value of V is $V = 0.060$ when there is an -OR group [1] : $\varepsilon_{calc} = 1645$ ($\Delta = - 9.4$ %).

As concerns the meta substitution pattern, the experiment for the methoxy derivative is only known : $\varepsilon_{sm} = 1720$ [13z], and calculation gives : $\varepsilon_{calc} = 1550$ ($\Delta = - 9.9$ %).

Three molecules are known displaying the para substitution pattern : the hydroxy derivative : $\varepsilon_{sm} = 1800$ [13α], the methoxy derivative : $\varepsilon_{sm} = 1580$ [13β], and the ethoxy derivative : $\varepsilon_{sm} = 1650$ [13γ] (average 1677) Calculation gives : $\varepsilon_{calc} = 1780$ ($\Delta = + 6.1$ %).

For dichloro-1,3-hydroxy-6-benzene : $\varepsilon_{sm} = 2430$ [13δ], $\varepsilon_{calc} = 1855$ ($\Delta = -24$ %). This is a strong discrepancy. The same arises for dichloro-1,3-hydroxy-5-benzene whose experiment leads to : $\varepsilon_{sm} = 2250$ [13ε], and calculation gives : $\varepsilon_{calc} = 1315$. For dichloro-1,3-dihydroxy-2,5-benzene : $\varepsilon_{sm} = 1710$ [13ζ], and : $\varepsilon_{calc} = 3070$. This experiment is surprising. This latter value is far lower than what is obtained for the para disubstituted hydroxy or methoxy derivatives (roughly : $\varepsilon_{sm} = 3000$ [1]). When checking ε_{sm} from the published concentrations, one does not find 1710, but 4250, which is as much surprising.

For dichloro-1,3-methoxy-2-benzene, the experiment gives the next surprising result : $\varepsilon_{sm} = 435$ [13η], and calculation : $\varepsilon_{calc} = 1315$.

When considering chloro substituted phenoxyacetic acid (ϕ-O-CH_2-CO_2H) molecules [9], one needs to determine the parameters for the substituent -O-CH_2-CO_2H. -CO_2H is σ electron attracting. Phenoxyacetic acid (ϕ-O-CH_2-CO_2H) has been studied, [7] obtaining : S = 0.9014, σ = 0.9494, n = 0.3593 and V = 0.05229, for -O-CH_2-CO_2H. These values are lower than those obtained for an alkoxy substituent. Actually, the intensity of the secondary transition is only $\varepsilon_{sm} = 1260$ ($\varepsilon_{max} = 1510$, methanol) for phenoxyacetic acid when it is 1450-1500 for the phenol or alkoxy derivatives.[1] Such a decrease is linked to the fact that the $p_{z,O}$ orbital and the -CH_2- group plays the part of a bridge between the σ effect of the -CO_2H and the π_ϕ system, through an extended hyperconjugative effect. -CO_2H withdraws a part of the π_ϕ electrons, decreasing the perturbation on the π_ϕ system imposed by the -OR substituent, and partly restoring the D_{6h} symmetry.

Nevertheless, as -O-CH_2-CO_2H is near to a pure -OR substituent, and as the interaction vectors display contributions much lower than basis vectors, the lengths

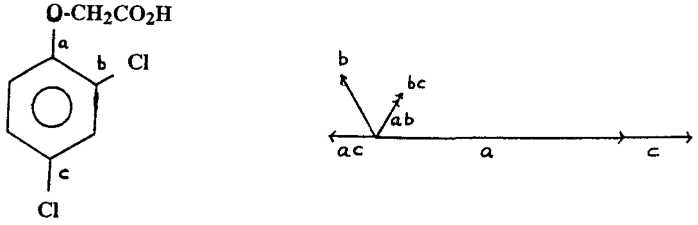

Figure 2. Vector pattern for the (dichloro-2,4-phenoxy)-2-ethanoic acid molecule

of the interaction vectors have been kept the same as those used between -Cl and -OR substituents :

$$\mathbf{n_{ortho,Cl,OR} = 0.052,\ n_{meta,Cl,OR} = 0.024,\ n_{para,Cl,OR} = 0.063}$$

Chloro-2-phenoxyacetic acid displays a substitution pattern similar to that of the chloro-1-hydroxy-2-benzene molecule, thus : $\varepsilon_{calc} = 1400$, $\varepsilon_{max} = 1585$ 1b (hexane), and $\varepsilon_{sm} = 1450$ ($\Delta = -3.4$ %).

The chloro-3-phenoxyacetic is similar to chloro-1-hydroxy-3-benzene, thus : $\varepsilon_{calc} = 1310$. $\varepsilon_{sm} = 1300$ 1b (hexane) ($\Delta = 0$).

The molecule of (dichloro-2,4-phenoxy)-2-ethanoic acid (or : 2,4-D) [see Figure 2] is similar to dichloro-1,3-hydroxy-6-benzene : $\varepsilon_{calc} = 1645$. The experiment gives : $\varepsilon_{sm} = 1800$ 1b ($\varepsilon_{max} = 1860$, 0.1 $mol{\cdot}l^{-1}$, HCl) ($\Delta = -7.6$ %). The value obtained for the corresponding phenol derivative is : $\varepsilon_{sm} = 2430$. The two values, although different, should be close. They are not. This shows that 2430 is certainly too high.

Fluoro substituted benzene chromophore

Studying fluorobenzenes, one lacks data to calculate values for the basis vectors. It is not possible to deduce these values from the -OR series which displays a different intensity pattern. Actually, going from the fluorobenzene molecule, to the ortho difluoro derivative, then to the meta, and the para derivative,

ε_{sm} is 660,[12] ; 605,[13a] ; 580,[13b,14a] ; 1700, [13c,14b] when it is 1500, 2500, 2000, 3000 for the -OR derivatives. [1]

A change of medium from hexane to methanol acts mainly on the widths of the transitions, and on their ε_{max}, keeping constant ε_{sm}. Thus, the greater difference between the two series (F and -OR) lies on the intensity change along the series. In the -OR series ortho and meta interactions, increase intensity ; in the fluoro derivatives they decrease it. This imposes, for the interaction vectors in the fluoro derivatives, directions <u>opposed</u> to those observed in the alkoxy ones.

Interpolating the ε_{sm} of the mono substituted chromophores, for the already studied substituents (methyl, -CO_2R, -OR, -O^- (phenolate)), against the modulus n of the basis vectors, leads to the basis parameters of the fluoro substituent. These parameters should be :

$$\mathbf{S = 0.545,\ \sigma = 0.7382\ (\sigma = S^{1/2}),\ n_F = 0.2378,\ V = 0.0325}$$

This is near to the benzoic acid values: n = 0.2517 and S = 0.5830, and: ε_{sm} = 725. This ε_{sm} is the nearest value to fluorobenzene (ε_{sm} = 660), among those already observed. [7]

The general formula for S simplifies for a mono fluoro chromophore: $S = h_F n_F/(4.8 + 0.2n_F^2)$. The above empirical comparison with benzoic acid and other substituted chromophores gives: S = 0.545 for the fluorobenzene molecule. Then one calculates: h_F = 2.725 for F, and: S = 0.9732, σ = 0.9865, for two fluorine substituents.

Using the above values for F (n = 0.2378), one calculates, from the difluoro-1,2-benzene spectrum, the modulus of the interaction vector for the ortho derivative: $n_{ortho,FF}$ = 0.0508.

Contrary to what has been observed till now, the ortho interaction vector in difluoro-1,2-benzene must lie in the direction <u>opposed</u> to the projections of the basis vectors on their bisectrix (Figure 3). As concerns the difluoro-1,3-benzene molecule: $n_{meta,FF}$ = 0.0578, this interaction too is opposed to the projections of the basis vectors on their bisectrix. For the difluoro-1,4-benzene molecule:

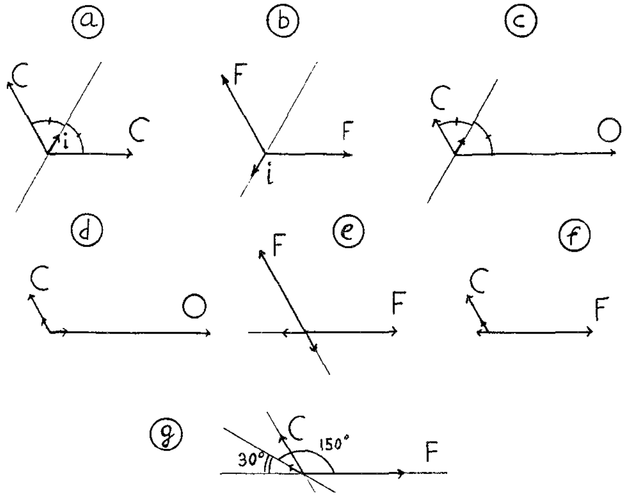

Figure 3. Vectors are not proportional to their lengthes. a) The interaction vector **i** between two ortho or meta substituents such as alkyl substituents (or OR ones etc.) : **C**. This vector lies on the bisectrix of the two basis vectors **C**, in the same direction as their projections on their bisectrix. b) The interaction vector between two ortho or meta fluoro substitutions. This vector points in the direction opposed to the projection of the basis vectors on their bisectrix. c) The classical interaction vector between two different ortho or meta substituents such as methyl and -OR. It lies on the bisectrix of the two basis vectors. d) A similar pattern which leads to the same result, since two vectors of length n displaying a 120° angle give a resulting vector of length n. For the para substi-tutions there is no need to use two partial interaction vectors. Nevertheless, for the sake of consistency, since the para interaction vector is colinear to the two basis vectors of para substituents, taking two partial interaction vectors impose that the sum of these two partial interaction vectors be equal to the complete interaction vector, each one of the two partial interaction vectors should display half the length of the complete interaction vector. e) The same as in d for two fluoro substitutions. f) Considering two substituents in ortho or meta positions, say a methyl C, and a fluorine atom F, the partial interaction vector of C should point in the same direction as the corresponding basis vector, and the partial interaction vector of F should point in the direction opposed to the direction of the basis vector F, to take into account the fact that interaction vectors between two fluoro substitutions point in the direction opposed to the projections of the basis vectors on their bisectrix. As two partial interaction vectors display the same length, the resultant will lie on their bisectrix. The angle between the resultant and the direction of the basis vector F is 150°. Calculating the length of the resultant (the actual interaction vector) is explained in the text.

$n_{para,FF}$ = 0.0250. The para interaction vector, in the molecules already studied, is opposed to the basis vectors. This is still the case.

The above calculations have used a 0.0030 increase of V for each substituent [1-8]. Thus, V = 0.035 for the disubstituted fluoro derivatives.

For trifluoro-1,2,4-benzene : ε_{calc} = 1100, ε_{sm} = 1350 [14c]. This is disturbing: Δ = - 18 %. It is the only published data concerning three fluoro substitituents, not considering the higly symmetric molecules, such as trifluoro-1,3,5-benzene, for which intensity is very low (IVM is not designed to fit with these latter cases). One lacks possibilities to test further the method on fluorobenzenes bearing only F substituents.

It has been possible to study monomethyl monofluoro benzenes. For fluoro-1-methyl-2-benzene : ε_{sm} = 600,[13d] for fluoro-1-methyl-3-benzene : ε_{sm} = 575,[13e], for fluoro-1-methyl-4-benzene : ε_{sm} = 870,[13f] (toluene gives : 192 [1]). A question arises related to the direction of the interaction vector of two ortho or meta fluoro substituents: how to choose the direction for alkyl⇔F interactions ?

The interaction vector has been parted in two. The sum of the two parts is the actual interaction vector. $\mathbf{n}_{1,interac}$ is a part related to, and colinear to, the basis vector of the first substituent. $\mathbf{n}_{2,interac}$ is for the second substituent ($\mathbf{n}_{interac} = \mathbf{n}_{1,interac} + \mathbf{n}_{2,interac}$) (Figure 3). One should notice that the sum of two vectors displaying the same given length, and a 120° angle, displays that same given length. Thus, as far as a 120° angle is concerned between the two partial vectors, each one of these vectors, by virtue of vector addition, has to display a length equal to the length of the actual interaction vector. For alkoxy or alkyl substituents, the partial interaction vectors for the ortho and meta positions are directed to the same direction as the projections of the corresponding basis vectors on their bisectrix. Using two interaction vectors, as we are doing here, will not impose changes in calculations already performed (see Fig. 3 for the methyl⇔-OR case).

For the methyl⇔F interaction, owing to the specific behaviour of fluorine, the partial interaction vector of fluorine points in the direction opposed to the direction of the fluorine basis vector. Then, the two partial interaction vectors will not display a 120° angle but a 60° one (Figure 3). As the two partial vectors display the same length, their vector sum will lie on the bisectrix of the two interaction vectors, pointing in a direction displaying a 30° angle with the methyl basis vector, and a 150° angle with the fluoro basis vector.

As concerns the length of the actual methyl⇔F interaction vector, one uses the standard process (only the direction of the vector is a problem). As it has already been established, [1] one has to start from the length of the interaction vectors of two fluoro substituents (n_{FF}) and of two methyl substituents (n_{CC}), and find the value which converges, after an iterative process, the geometric average and the arithmetic average of the successive average values. First step : $(n_{FF}\cdot n_{CC})^{1/2} = n_1$; $(n_{FF}+n_{CC})/2 = n_2$. Second step : $(n_1\cdot n_2)^{1/2} = n'_1$; $(n_1+n_2)/2 = n'_2$ etc. Convergence is quite readily obtained.

For a methyl⇔F ortho interaction, the values being : 0.0508 (F), and 0.0060 (methyl [1-8]): $n_{ortho,FC} = 0.0228$. For a meta disubstitution (0.0578 for F, 0.0060 for methyl [1-8]): $n_{meta,FC} = 0.0250$. For a para disubstitution (0.025 for F, 0.012 for methyl [1-8]): $n_{para,FC} = 0.0179$.

For fluoro-1-methyl-2-benzene ($\varepsilon_{sm} = 600$ [13d]) : $n = 0.1945$. The fluoro substituent contribution to S being 0.545, as above calculated, and the methyl contribution being 0.2 [2-9] : $S = 0.545 + 0.2 = 0.745$, $\sigma = 0.8631$, $V = 0.0325 + 0.003 = 0.0355$, thus: $\varepsilon_{calc} = 585$ ($\Delta = -2.6$ %).

For fluoro-1-methyl-3-benzene ($\varepsilon_{sm} = 575$ [13e]) : $n = 0.1934$, $\sigma = 0.86311$ $V = 0.0355$, and : $\varepsilon_{calc} = 580$ ($\Delta = +1.0$ %).

For fluoro-1-methyl-4-benzene ($\varepsilon_{sm} = 870$ [13f]): $n = 0.3179$, $\sigma = 0.8631$, $V = 0.0355$, $\varepsilon_{calc} = 1014$ ($\Delta = +16.6$ %).

Interaction vectors being the same for Cl⇔F as for F⇔methyl interactions, the results are the same as those obtained for F and methyl substituents. Thus, for chloro-1-fluoro-2-benzene : $\varepsilon_{calc} = 585$ when : $\varepsilon_{sm} = 610$ (corrected from overlap) [13q] ($\Delta = -4.1$%). For chloro-1-fluoro-3-benzene : $\varepsilon_{calc} = 580$, $\varepsilon_{sm} = 585$ (corrected from overlap) [13r] ($\Delta = -1$ %), the para derivative is not available. For dichloro-1,2-fluoro-4-benzene ($\varepsilon_{sm} = 925$ [13s]), calculations lead to $n = 0.2704$,

$\sigma = 0.9498$, $V = 0.0385$: $\varepsilon_{calc} = 890$ and ($\Delta = -3.8$ %). For chloro-1-fluoro-3-methyl-6-benzene : $\varepsilon_{calc} = 900$, $\varepsilon_{sm} = 1050$ [13t] ($\Delta = -14$ %).

As concerns fluoro-1-hydroxy-2-benzene ($\varepsilon_{sm} = 1500$ [13u]), the length of the interaction vector : $n_{ortho,F,OR} = 0.05673$ (for two F : 0.0508 ; for two -OR ortho substituents : 0.1330 [2]). This leads to : $\varepsilon_{calc} = 1425$ ($\Delta = -4.9$ %). The meta derivative is not available.

For fluoro-1-hydroxy-4-benzene ($\varepsilon_{sm} = 2650$ [13v]), the interaction vector displays the length : $n_{para,F,OR} = 0.0839$ (0.1800 [2] for two OH substituents in para positions, and 0.025 for two F). Calculations lead to $S = 1 + 0.545$, $\sigma = 1.2430$, $n = 0.5434$, $V = 0.063$. $\varepsilon_{calc} = 2575$ ($\Delta = -2.8$ %).

CONCLUSION

All our calculations, when compared to the experimental data, seem not to be completely successful. In fact, as far as halogeno (F, Cl) benzenes are concerned, some published data in the literature should be revisited. Furthermore, apart from some discrepancies, when accurate data can be obtained, the IVM is able to fit with the experimental data. This makes us confident with the model.

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