

# Towards physical interpretation of Hammett constants: charge transferred between active regions of substituents and a functional group

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**Abstract** The charges transferred between substituents and two functional groups: nitroso and *N,N*-dimethylamine in disubstituted benzene rings, were calculated at the B3LYP/cc-pVDZ level, using Natural Population Analysis. They were compared with the charges transferred between active regions of the substituents and of the groups. The transferred charge was well correlated with the Hammett constants, but only when the charges were calculated for the corresponding active regions instead of being calculated for the substituents and functional groups themselves. The results were compared for substituents introduced at the *para* and *meta* position to the NO and N(CH<sub>3</sub>)<sub>2</sub> groups.

**Keywords** Hammett constants · Nitrosobenzenes · *N,N*-dimethylanilines · Transferred charge · Substituent active region

## Introduction

The effects of substituents on the chemical and physico-chemical properties of *meta*- and *para*-substituted benzene and analogous compounds are most frequently treated by means of the Hammett equation [1–5]. They were successfully applied to a huge number of aromatic [6] and even non-aromatic systems [7].

The Hammett constants have been continuously used to quantify electron perturbation in substituted molecules, resulting in the modification of the reactivity and physicochemical properties of substituted molecules: only the papers are selected which appeared from 2002 to just now [8–32]. In parallel with the studies focused on the elucidation of reaction rates, equilibria and mechanisms, with the help of substituent constants, there have been scores of reports aimed at understanding a physical meaning of the constants. Introduction of the constants was based on chemical intuition: “a substituent alters the average density of electron charge in every part of the molecule” [33] but nowadays, armed with the computational facilities offered by the widespread programs rooted in quantum chemistry, chemists try to substitute the empirical constants with the well-defined physical properties of the substituents themselves or of the substituted molecules, which can easily be computed in no matter which chemical environment. The constants correlated with many properties calculated for the isolated molecules. Among them, one can mention:

- electron densities at *p*- and *m*-positions in monosubstituted benzenes [34]
- electrostatic potential values at the ring carbon atoms [28, 35, 36]
- electrostatic potential values at atoms of a reaction center [28, 37]
- topography of electrostatic potential near the molecular surface [38–42]
- hyperpolarizability [43]
- a complexed metal chemical shift [44, 45]
- energy of the highest occupied orbital ( $E_{\text{HOMO}}$ ) [46, 47]
- energy of the lowest unoccupied orbital ( $E_{\text{LUMO}}$ ) [16]
- ionization potential [48]

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- electrophilicity, being a measure of stabilization in energy when the system acquires an additional electronic charge  $\Delta N$  from the environment [28, 49, 50]
- core electron binding energy shifts [51, 52]
- intramolecular charge transfer between oxygen or sulfur lone pair and an adjacent orbital, both within the reaction active center [53, 54]
- the so-called quantum chemical topology descriptors constructed using properties of the bond critical points, BCP, where BCP is the saddle points in the electron density [55–58]
- charge of the reaction active site [42, 47, 59, 60]
- energy of  $\pi$ -conjugation [61]
- charge of the substituent active space [58, 62–64].

The sole reason behind occurrence of differences of electronic properties (e.g., potential and charge distribution) in the individual molecules is the electric charge (or more generally, electronic properties) of their substituents. The substituent constants were frequently correlated with the properties of atoms and bonds in the nearest vicinity of the reaction center [34–39, 41, 42, 47, 53–60], e.g., the hydrogen atom when dissociation of the COOH group was considered [37, 58, 63]. The Hammett constants were also correlated with properties characterizing whole molecules [16, 43, 46–52].

It might also be expected that the substituent constants correlate some way with the electronic properties of the substituents. However, it was found in the course of investigations of dissociation ability of organic acids that the substituent charges were uncorrelated with the Hammett constants [63]. Likewise, no such correlation was found for monosubstituted benzenes [62]. Nevertheless it appeared that the idea that the substituent charges may be quantitatively correlated with other molecular properties does not have to be abandoned. Namely, it was found that the replacement of the substituent charges by charges of the so-called substituent active regions SARs (where SAR is a unit composed of a substituent and the carbon atom,  $C_{\text{ipso}}$ , to which the substituent is attached) allowed to correlate a property related to substituents with Hammett constants. For example, good correlations of the SAR charges with the Hammett constants and with charges of acidic H in COOH functional group were obtained, for five classes of substituted aromatic carboxylic acids [58].

To the best of our knowledge, the charges of SAR (qSAR) are the sole property, correlating with Hammett constants, which are directly related to the substituent charges. However, there are no quantitative data which might relate charge transferred between the substituents and a functional group (or between their active regions) to the group reactivity or to the substituent Hammett constant.

Therefore, the present investigation was aimed at calculation of the amount of charge transferred between the substituent X and the functional group Y. Two functional groups lying near the opposite ends of the Hammett constants scale were taken: nitroso and *N,N*-dimethylamine groups. The substituents were introduced to nitrosobenzene or to *N,N*-dimethylaniline in *p*- and *m*-position.

To be more precise, we aimed to investigate how qX and qSAR(X) are related to qY and qSAR(Y) and also to appropriate substituent constants.

## Theoretical method

All calculations reported in the present study were carried out using the density functional theory (DFT) and the Becke three-parameter exchange functional combined with the dynamic (non-local) Lee–Yang–Parr correlation functional (B3LYP), as implemented in the Gaussian 03 package [65]. The initial three-dimensional structures of the compounds were built using Spartan Pro software [66], followed by a preliminary semi-empirical geometry optimization at the Austin model version 1 (AM1) level. Subsequently, geometries were optimized and energies calculated using the Dunning's valence double zeta cc-pVDZ basis set, followed by the calculation of vibrational frequencies at the same level.

The atomic charges were calculated by applying Natural Population Analysis (NPA). This is a Class II method of determination of partial atomic charges, according to the Cramer classification [67] (which involves direct partitioning of the molecular wave function into atomic contributions). The charge of a molecular fragment was calculated as the sum of individual charges of the atoms of which it was composed. The set of substituents comprised: NO<sub>2</sub>, CN, CF<sub>3</sub>, Br, Cl, F, H, CH<sub>3</sub>, NH<sub>2</sub>, NC, N(CH<sub>3</sub>)<sub>2</sub>, SiH<sub>3</sub>, NO, Si(CH<sub>3</sub>)<sub>3</sub>, OH, OCH<sub>3</sub>, CH<sub>2</sub>Cl, CHO, COCH<sub>3</sub>, N<sub>3</sub>, COOCH<sub>3</sub>, NHCH<sub>3</sub>, C<sub>2</sub>H<sub>5</sub>, CHCH<sub>2</sub>, SH, COF, COCl, CCH, CHF<sub>2</sub>, and COOH. The Hammett constants were taken from the compilation of Taft et al. [68].

## Results and discussion

It was previously shown that charges of the substituent active region, qSAR(X), correlated fairly well with the Hammett constants in monosubstituted benzenes [62], carboxylic acids [58, 63], and substituted tetrazoles [64]. On the other hand, the constants correlated well with the properties of reaction sites, e.g., with the charges and potentials at H atoms of COOH group [58].

Presently, similar dependencies were also checked in the substituted nitrosobenzenes and *N,N*-dimethylamines.

**Table 1** Correlation coefficients of linear regressions of Hammett's constants with charges of substituents (X), of the NO functional group, or their active regions and on the difference qSAR(X)–qSAR(NO), in *para*-substituted nitrosobenzenes

	q(X)	qSAR(X)	q(NO)	qSAR(NO)	qSAR(X)–qSAR(NO)
$\sigma_p$	–0.108	–0.938	0.954	0.955	–0.940

**Table 2** Correlation coefficients of linear regressions of Hammett's constants with charges of substituents (X), of the NO functional group, or their active regions and on the difference qSAR(X)–qSAR(NO), in *meta*-substituted nitrosobenzenes

	q(X)	qSAR(X)	q(NO)	qSAR(NO)	q(SAR(X)–qSAR(NO)
$\sigma_m$	–0.317	–0.772	0.939	0.719	–0.810

However, we took a step forward trying to find direct correlations of the Hammett constants with the substituent (X) and functional group (Y) properties at the same time. To this aim we calculated portions of the transferred charge between active regions of X and Y groups, qSAR(X)–qSAR(NO) and qSAR(X)–qSAR(N(CH<sub>3</sub>)<sub>2</sub>) and correlated the values with  $\sigma_p$  and  $\sigma_m$ . The results were compared with the correlations of the qSAR(X), q(NO), and qSAR(NO) for substituted nitrosobenzenes and with the correlations of the qSAR(X), q(N(CH<sub>3</sub>)<sub>2</sub>), and qSAR(N(CH<sub>3</sub>)<sub>2</sub>) for substituted *N,N*-dimethylamines. Tables 1, 2, 3, and 4 display the results.

As shown in Tables 1 and 3, i.e., in cases of *p*-substituted compounds, the charges of the functional groups, Y, as well as the charges of the corresponding active regions qSAR(X) and qSAR(Y), as well as the differences between the two latter variables are well correlated to the substituent constants  $\sigma_p$ . In contrast, inspection of the Tables 2 and 4 shows that except of the correlations of q(Y) with  $\sigma_m$ , given in the fourth columns of the tables, other correlation coefficients are significantly lower. Explanation of the reason of this behavior can be provided by analysis of variance [69]. Results of the analysis show that for the regressions shown in columns 3, 5, and 6 of Tables 1, 2, 3, and 4, the residual variance (due to scattering of the points) is several times larger for the *meta* than for the *para* set.

Only in the case of regression of q(NO) and q((NCH<sub>3</sub>)<sub>2</sub>) in the *meta* sets on  $\sigma_m$ , the residual variance (scattering) is comparable with those of the similar regression of the charges in the *para* set on  $\sigma_p$ . As a result, the correlation coefficients for the *meta* set remain high.

Of the correlations shown in Tables 1, 2, 3, and 4, those between the differences of two SARs and the Hammett constants (last columns of the tables) seem to us to be especially interesting because they offer an account of the cause (substituent with its specific electronic properties) and effect (perturbation of the electronic properties of a functional group present in the molecule).

To obtain a better understanding of the redistribution of electronic density in nitrosobenzenes and *N,N*-dimethylanilines following the impact of substituents, we supplemented the investigation of various regressions with the calculated amounts of the transferred charges. Table 5 presents the charge which is transferred between X and Y=NO groups and between their substituent active regions in *p*- and *m*-compounds.

Inspection of the table reveals that for *para* compounds the largest (positive) values of the transferred charge between the two active spaces (shown in bold) fall to the same substituents for which the (negative) Hammett constants are the larger. On the other hand, the largest values of the transferred charge between X and groups NO (also shown in bold) appear for quite different substituents. It may thus be stated that the Hammett constants in *para*-substituted nitrosobenzenes mirror the transfer of charge not between substituents and the NO functional group but between the corresponding active regions. For *meta*-nitrosobenzenes, the situation is similar. Namely, for three substituents: NHCH<sub>3</sub>, N(CH<sub>3</sub>)<sub>2</sub>, and NH<sub>2</sub>, the largest transferred positive charge between the SARs is joined with the largest (negative) Hammett constants. Figure 1 displays plots of the transferred charge between the SAR(X) and SAR(NO) in *p*-nitrosobenzenes, and the transferred charge between X and NO groups in the compounds.

Table 6 presents similar data as Table 5 but for Y=N(CH<sub>3</sub>)<sub>2</sub>.

**Table 3** Correlation coefficients of linear regressions of Hammett's constants with charges of substituents (X), of the (N(CH<sub>3</sub>)<sub>2</sub>) functional group, or their active regions and on the difference qSAR(X)–qSAR(N(CH<sub>3</sub>)<sub>2</sub>), in *para*-substituted *N,N*-dimethylanilines

	q(X)	qSAR(X)	q(N(CH <sub>3</sub> ) <sub>2</sub> )	qSAR(N(CH <sub>3</sub> ) <sub>2</sub> )	q(SAR(X)–qSAR(N(CH <sub>3</sub> ) <sub>2</sub> ))
$\sigma_p$	–0.112	–0.917	0.958	0.953	–0.931

**Table 4** Correlation coefficients of linear regressions of Hammett's constants with charges of substituents (X), of the (N(CH<sub>3</sub>)<sub>2</sub>) functional group, or their active regions and on the difference qSAR(X)–qSAR(N(CH<sub>3</sub>)<sub>2</sub>), in *meta*-substituted *N,N*-dimethylanilines

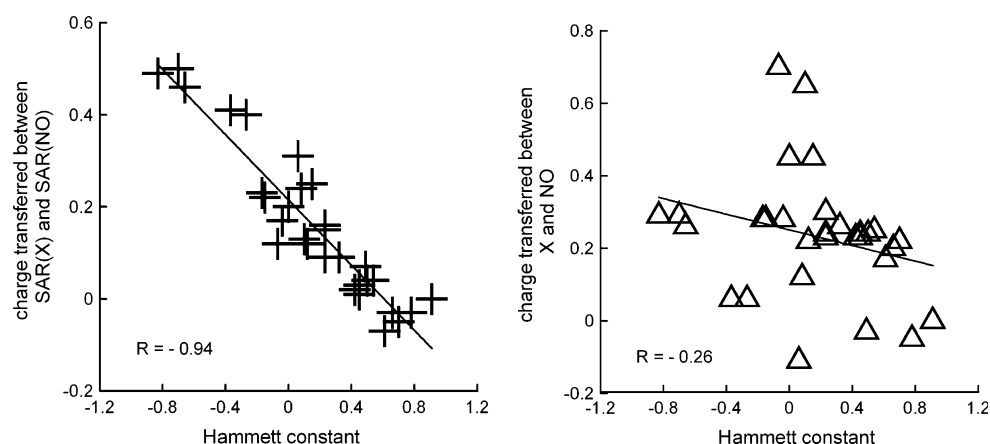
	q(X)	qSAR(X)	q(N(CH <sub>3</sub> ) <sub>2</sub> )	qSAR(N(CH <sub>3</sub> ) <sub>2</sub> )	q(SAR(X)–qSAR(N(CH <sub>3</sub> ) <sub>2</sub> ))
$\sigma_m$	–0.349	–0.767	0.969	0.819	–0.811

**Table 5** Comparison of the transferred charge between X and NO groups and between their active spaces SAR(X) and SAR(NO), in *p*-X-C<sub>6</sub>H<sub>4</sub>-NO and *m*-X-C<sub>6</sub>H<sub>4</sub>-NO

	<i>p</i> -NO-C <sub>6</sub> H <sub>4</sub> -X			<i>m</i> -NO-C <sub>6</sub> H <sub>4</sub> -X		
	qX-qNO	qSAR(X)-qSAR(NO)	$\sigma_p$	qX-qNO	qSAR(X)-qSAR(NO)	$\sigma_m$
NO	0.00	0.00	0.91	<b>0.53</b>	0.00	0.62
NO <sub>2</sub>	-0.05	-0.03	0.78	<b>0.63</b>	-0.04	0.71
COF	0.22	-0.05	0.70	0.13	-0.05	0.55
CN	0.20	-0.03	0.66	0.18	-0.05	0.56
COCl	0.17	-0.07	0.61	0.22	-0.06	0.51
CF <sub>3</sub>	0.25	0.04	0.54	0.02	0.01	0.43
COCH <sub>3</sub>	0.24	0.04	0.5	0.03	0.04	0.38
NC	-0.03	0.07	0.49	<b>0.57</b>	0.02	0.48
COOCH <sub>3</sub>	0.24	0.03	0.45	0.07	0.01	0.37
COOH	0.23	0.01	0.45	0.09	0.00	0.37
CHO	0.23	0.02	0.42	0.06	0.02	0.35
CHF <sub>2</sub>	0.26	0.09	0.32	-0.04	0.06	0.29
Br	<b>0.30</b>	0.15	0.23	-0.10	0.09	0.39
Cl	0.23	0.16	0.23	0.03	0.10	0.37
CCH	0.24	0.09	0.23	0.07	0.04	0.21
SH	<b>0.45</b>	0.25	0.15	-0.39	0.15	0.25
CH <sub>2</sub> Cl	0.22	0.12	0.12	0.04	0.08	0.11
SiH <sub>3</sub>	<b>0.65</b>	0.13	0.1	-0.82	0.10	0.05
N <sub>3</sub>	0.12	0.24	0.08	0.23	0.15	0.37
F	-0.11	0.31	0.06	<b>0.58</b>	0.23	0.34
H	<b>0.45</b>	0.20	0	-0.01	0.16	0
CHCH <sub>2</sub>	0.28	0.17	-0.04	-0.05	0.12	0.06
SiMe <sub>3</sub>	<b>0.70</b>	0.12	-0.07	-0.99	0.15	-0.04
C <sub>2</sub> H <sub>5</sub>	0.28	0.22	-0.15	-0.11	0.17	-0.07
CH <sub>3</sub>	0.28	0.23	-0.17	-0.11	0.17	-0.07
OCH <sub>3</sub>	0.06	<b>0.40</b>	<b>-0.27</b>	0.27	0.28	0.12
OH	0.06	<b>0.41</b>	<b>-0.37</b>	0.26	0.29	0.12
NH <sub>2</sub>	0.26	<b>0.46</b>	<b>-0.66</b>	-0.06	<b>0.30</b>	<b>-0.25</b>
NHCH <sub>3</sub>	0.29	<b>0.50</b>	<b>-0.70</b>	-0.09	<b>0.31</b>	<b>-0.21</b>
NCH <sub>3</sub>	0.29	<b>0.49</b>	<b>-0.83</b>	-0.09	<b>0.31</b>	<b>-0.16</b>

The largest (positive) values of the transferred charge (columns 2, 3, 5, 6) and the largest (negative) Hammett constants (columns 4 and 7) are shown in bold

**Fig. 1** *Para*-nitrosobenzenes: plots of the charge transferred between active regions of substituents and of NO functional group (*left*) and the charge transferred between substituents and the NO functional group themselves (*right*)



It can be stated that the data lead to the parallel conclusions as those for Y=NO in Table 5. Namely, for the *p*-, as well as for *m*-derivatives, five entries indicating the most

negative values (marked in bold) of the charge difference between the corresponding SARs occur for the same substituents, for which Hammett constants (be  $\sigma_p$  or  $\sigma_m$ ) are

**Table 6** Comparison of the transferred charge between X and N(CH<sub>3</sub>)<sub>2</sub> groups and between their active spaces SAR(X) and SAR(N(CH<sub>3</sub>)<sub>2</sub>) in *p*-X-C<sub>6</sub>H<sub>4</sub>-N(CH<sub>3</sub>)<sub>2</sub> and *m*-X-C<sub>6</sub>H<sub>4</sub>-N(CH<sub>3</sub>)<sub>2</sub>

	<i>p</i> -X-C <sub>6</sub> H <sub>4</sub> -N(CH <sub>3</sub> ) <sub>2</sub>			<i>m</i> -X-C <sub>6</sub> H <sub>4</sub> -N(CH <sub>3</sub> ) <sub>2</sub>		
	qX– qN(CH <sub>3</sub> ) <sub>2</sub>	qSAR(X)– qSAR(NCH <sub>3</sub> ) <sub>2</sub>	σ <sub>p</sub>	qX– qN(CH <sub>3</sub> ) <sub>2</sub>	qSAR(X)– qSAR(NCH <sub>3</sub> ) <sub>2</sub>	σ <sub>m</sub>
NO	<b>–0.29</b>	<b>–0.49</b>	<b>0.91</b>	<b>–0.19</b>	<b>–0.31</b>	<b>0.62</b>
NO <sub>2</sub>	<b>–0.30</b>	<b>–0.49</b>	<b>0.78</b>	<b>–0.23</b>	<b>–0.35</b>	<b>0.71</b>
COF	–0.02	<b>–0.50</b>	<b>0.70</b>	0.04	<b>–0.35</b>	<b>0.55</b>
CN	–0.03	<b>–0.47</b>	<b>0.66</b>	0.01	<b>–0.35</b>	<b>0.56</b>
COCl	–0.09	<b>–0.55</b>	<b>0.61</b>	–0.01	<b>–0.37</b>	<b>0.51</b>
CF <sub>3</sub>	0.06	–0.38	0.54	0.08	–0.29	0.43
COCH <sub>3</sub>	0.00	–0.42	0.5	0.06	–0.28	0.38
NC	<b>–0.24</b>	–0.36	0.49	<b>–0.22</b>	–0.28	0.48
COOCH <sub>3</sub>	0.01	–0.43	0.45	0.06	–0.29	0.37
COOH	0.00	–0.44	0.45	0.06	–0.31	0.37
CHO	–0.01	–0.44	0.42	0.05	–0.30	0.35
CHF <sub>2</sub>	0.06	–0.33	0.32	0.09	–0.23	0.29
Br	0.09	–0.25	0.23	0.08	–0.21	0.39
Cl	0.02	–0.24	0.23	0.02	–0.20	0.37
CCH	0.01	–0.36	0.23	0.04	–0.26	0.21
SH	0.14	–0.28	0.15	0.20	–0.15	0.25
CH <sub>2</sub> Cl	0.01	–0.32	0.12	0.04	–0.23	0.11
SiH <sub>3</sub>	0.45	–0.29	0.1	0.47	–0.20	0.05
N <sub>3</sub>	–0.12	–0.20	0.08	–0.11	–0.16	0.37
F	<b>–0.29</b>	–0.07	0.06	<b>–0.31</b>	–0.06	0.34
H	0.29	–0.18	0	0.28	–0.12	0
CHCH <sub>2</sub>	0.04	–0.28	–0.04	0.07	–0.19	0.06
SiMe <sub>3</sub>	0.53	–0.24	–0.07	0.54	–0.16	–0.04
C <sub>2</sub> H <sub>5</sub>	0.09	–0.18	–0.15	0.09	–0.13	–0.07
CH <sub>3</sub>	0.09	–0.17	–0.17	0.09	–0.13	–0.07
OCH <sub>3</sub>	<b>–0.15</b>	–0.02	–0.27	<b>–0.17</b>	–0.02	0.12
OH	<b>–0.15</b>	0.01	–0.37	<b>–0.16</b>	–0.01	0.12
NH <sub>2</sub>	0.00	0.01	–0.66	–0.01	0.00	–0.25
NHCH <sub>3</sub>	0.01	0.01	–0.70	0.00	0.01	–0.21
NCH <sub>3</sub>	0.00	0.00	–0.83	0.00	0.00	–0.16

The largest (negative) values of the transferred charge (columns 2, 3, 5, 6) and the largest (positive) Hammett constants (columns 4 and 7) are shown in bold

the higher. At the same time, the transferred charge is larger for the *p*- than for the *m*-compounds in all cases (except five substituents, N(CH<sub>3</sub>)<sub>2</sub>, NH<sub>2</sub>, OH, OCH<sub>3</sub>, and NHCH<sub>3</sub>, for which there is no X–N(CH<sub>3</sub>)<sub>2</sub> charge transfer). In contrast, the charges transferred between X and Y groups do not correlate with the Hammett constants.

Tables 5 and 6 and Fig. 1 enable comparison of the accuracy of representing the transferred charges by the Hammett constants. It clearly shows that the charge transfer qSAR(X)–SAR(Y) is much better correlated with the Hammett constants than the charge transfer q(X)–q(Y) is. These data offer a new interpretation of the Hammett constants, as equivalents to the transferred charges between substituent active regions of varying substituents (X) and of a functional group (Y).

## Conclusions

A coherent interpretation of the meaning of the Hammett constants was achieved: their values correspond with the amount of the charge transferred between SARs of the X and Y groups. The correlations, however, were weaker in the *meta* than in the *para* sets. In contrast, they do not correlate with the quantities of the charge transferred between the X and Y groups themselves.

It is also worth noticing that in all four classes of compounds, correlations of the Hammett constants with the NPA charge of the functional group (NO, N(CH<sub>3</sub>)<sub>2</sub>) were equally good in spite of the fact that the range of charges of the groups, situated in *para* position to substituent, 0.1 (NO) and 0.1 (N(CH<sub>3</sub>)<sub>2</sub>) charge units, was 2.5 times larger

than the analogous range of charges of the groups in *meta* position, 0.04 for both groups.

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