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Comparison of the substituent effects in tetrazole systems and benzene. A computational study

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A R T I C L E I N F O

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Dedicated to Dr. John Shorter on the occasion of his 85 birthday and in recognition of his outstanding contribution to physical organic chemistry

A B S T R A C T

Natural Population Analysis of two tautomeric forms of 16 tetrazole derivatives substituted at carbon atom (AlH_2, BeH, BH_2, CCH, CF_3, CHO, Cl, CN, F, Me, NH_2, NO, NO_2, OH, SH, SiH_3) was carried out at B3LYP/6-31G(d,p) level of theory and compared with data for monosubstituted benzene derivatives. The individual occupancies of $2p_z$ orbitals at all atoms of the tetrazole and benzene derivatives were correlated with the sum of occupation overall $2p_z$ orbitals, named *pEDA*(*A*) or *pEDA*(*B*), respectively. These characteristics correlate well with the Hammett-like substituent constants. Acceptable correlations between the individual atom occupancies at the $2p_z$ orbital and *pEDA* were found for all atoms except N4.

1. Introduction

Azoles form an important class of molecules closely related to DNA nitrogen bases.[1,2] Due to the presence of amphiprotic nitrogen atoms in the ring, they demonstrate an inclination to undergo tautomeric reactions.[3] However, the position of the tautomeric proton depends on the substituents, and there is no clear explanation as to how the substituent influences the tautomeric equilibria. The different stabilization of tautomers by various substituents is related to the differences in the charge distribution in the azole ring. Since azoles are aromatic systems, the primary role is played by the substituent influence on the π-electron distribution, or in other words, on π-electron delocalization. In this respect, the transmission of the substituent effect in the azole ring, which is very different from that in the benzene ring, plays an important role. There are several factors involved. First of all, azole rings are five-membered so they are non-alternant like systems. Secondly, there are two types of atoms in the ring: carbon and nitrogen. And finally, there are two kinds of nitrogen atoms: one is a pyrrole-like nitrogen atom, which donates its lone pair to the aromatic sextet, and none or a few pyridine-like nitrogen atoms. The presence of the pyrrole-like nitrogen atom can introduce some kind of modification of the electron density in azole ring, dependent on the number of pyridine-like nitrogen atoms and their position in respect to the pyrrole-like nitrogen atom.[4] Modification of the electronic structure is also dependent on the substituent. Therefore, it is of interest to establish the relation of particular positions of the azole ring to *ortho*-, *meta*-, and *para*-positions of benzene and to analyze the dependence of the substituent on the occupation numbers of ring atoms in the azole moiety.

As a system to study we have chosen tetrazole derivatives substituted at the carbon atom, which exist as two tautomers[5] and have four nitrogen atoms in the ring. The $2p_z$ occupations on different ring atoms were estimated by the NBO approach.

2. Calculation

All calculations were done at the B3LYP/6-31G(d,p) level of theory by the use of Gaussian 03 software.[6] Geometry optimizations were followed by a frequency check to prove that the stationary points obtained are true energy minima. NBO analysis[7] was carried out by the use of the NBO 5.G program interfaced to Gaussian. The π-electron occupations of the ring carbon atoms were obtained as the occupations of the $2p_z$ Natural Atomic Orbitals (NAOs) for the ring of the molecule positioned in the xy plane. As a measure of deviations from the ideal sextet in the benzene ring we used the *pEDA* index,[8] for benzene molecule defined as the sum of occupations of all six ring $2p_z$ NAOs with subtracted number 6 (Eq. 1).

$$pEDA(B) = \sum_{i=1}^{6} \pi^{i}_{\text{benzene}} - 6 \tag{1}$$

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Where i index runs overall six benzene carbon atoms and π^{i}_{benzene} is the occupation of the i-th $2p_z$ NAO.

We also applied the *pEDA* index to study azoles in a way similar to that used in our previous study.[9] For the azole molecule the *pEDA* index is obtained by summing up the populations of $2p_z$ NAOs of all five ring atoms and subtracting the 'nominal' value of 6. Thus, *pEDA*(*A*)[Eq. 2] expresses the deviation from the 'nominal' or 'ideal' value of the electronic sextet in an azole molecule.

$$pEDA(A) = \sum_{i=1}^{5} \pi^{i}_{\text{azole}} - 6 \tag{2}$$

To compare the influence of the substituent on the π-electron structure of benzene and azoles, we employed 16 substituents of various π- and σ-donor/acceptor properties: AlH_2, BeH, BH_2, CCH, CF_3, CHO, Cl, CN, F, Me, NH_2, NO, NO_2, OH, SH, SiH_3.

3. Results

Substituent effects in benzene and its derivatives are the subject of a huge amount of papers, which have recently been discussed in two extensive reviews.[10,11] This is the reason why the data for azoles discussed in this study is presented in comparison with those for benzene. In most cases, some chemical, physicochemical or theoretically derived characteristics are plotted against substituent constants or quantities, which are equivalent measures of substituent electronic influence on a substituted system. In this paper we consider as a π-electron characteristic for benzene and tetrazole derivatives, the described earlier *pEDA*—a summation of occupation of $2p_z$ orbitals at all atoms in the ring, thus for the six-membered ring in benzene,[8] and the five member ring in azoles.[9] They represent a general consequence of the influence of substituent on the π-electron structure of the rings. Regression of the $2p_z$ occupation of individual carbon or nitrogen atoms plotted against *pEDA* gives and indication about the non-uniformity of substituent effects in particular positions leading to two pieces of information: (i) the slope describes sensitivity of the substituent effect on occupation at particular carbon or nitrogen atoms but presented in the same scale—the *pEDA* values, and (ii) the correlation coefficient describes a measure of how well $2p_z$ occupations on the individual atoms correlate with a general descriptor—thus giving some insight into mechanism of substituent effects on individual atoms in the ring.

3.1. Benzene derivatives

Benzene derivatives are discussed first, since the substituent effects in these systems are best known, and some rules can be firmly stated for these systems. As we see from Figs. 1 through 3, relations between the $2p_z$ occupation at the carbon atoms in the *para*- and *ortho*- positions correlate nicely with *pEDA*(*B*). It shows also that an increase of the overall occupation of the $2p_z$ orbitals at all carbon atoms in the ring, i.e., *pEDA*(*B*) value, is in line with an increase observed at the carbon atoms in the *ortho*- and *para*-positions, whereas for the *meta*-position, correlation is worse and with an opposite slope.

An increase in *pEDA*(*B*) is associated in this case with a decrease in the occupation at the *meta*-carbon atom. This may be a good illustration of a different substituent effect in *ortho*- and *para*- and then in the *meta*-position. For *ortho*- and *para*-interactions, single-excited resonance structures for monosubstituted benzene show (Scheme 1) that only two *ortho*- and one *para*-position may be charged positively if the substituent is electron accepting, and negatively if it is an electron donating one.

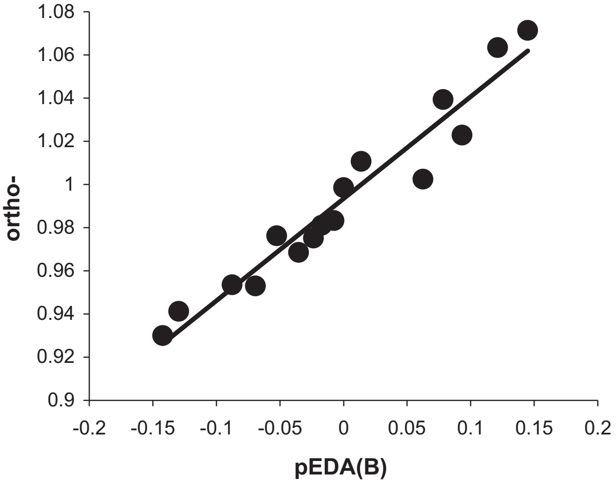


Fig. 1. Dependence of occupation of the $2p_z$ orbital at the *ortho*-carbon atom in substituted benzene derivatives. $cc=0.971$; $y=0.473x+0.993$.

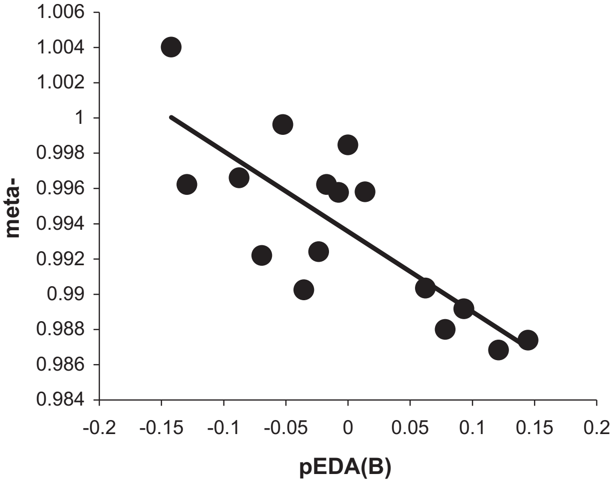


Fig. 2. Dependence of occupation of the $2p_z$ orbital at the *meta*-carbon atom in substituted benzene derivatives. $cc=-0.791$; $y=-0.046x+0.994$.

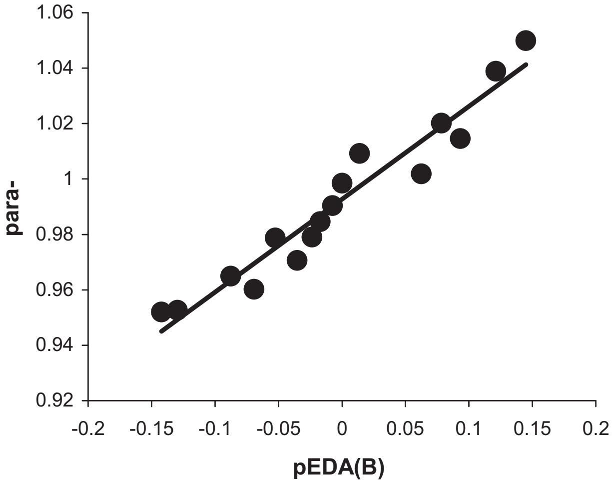


Fig. 3. Dependence of occupation of the $2p_z$ orbital at the *para*-carbon atom in substituted benzene derivatives. $cc=0.968$; $y=0.335x+0.993$.

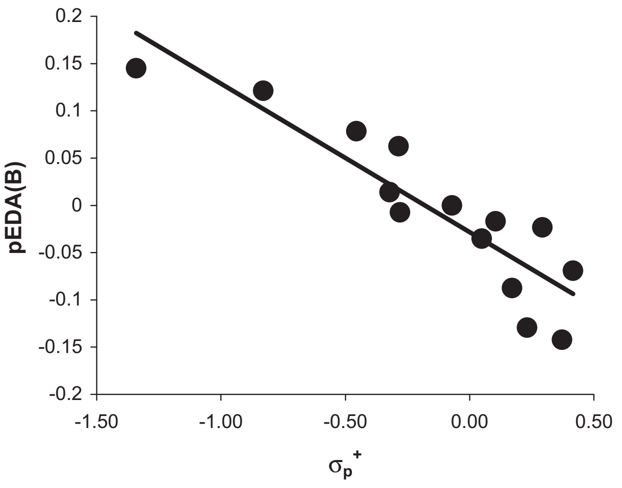
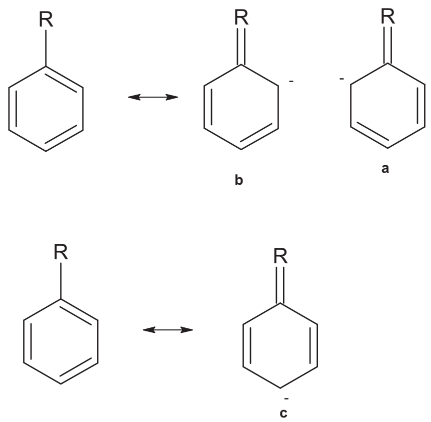


Fig. 4. Dependence of the occupation of *pEDA*(*B*) on the Hammett-like substituent constants σ_p^+.



Scheme 1. Resonance structures of the monosubstituted benzene molecule (with R electron-donating).

However, for single-excited resonance structures there is no possibility of resonance interactions with carbon atoms in the *meta*-position, where is required a higher energetic double excited resonance structure (for details see Ref. 12). Following the classical interpretation of substituent effects from the *meta*- and *para*-positions (for review see Refs. 13–16), the *meta*-position is more influenced by field effects, whereas the *para*- and *ortho*- by resonance. In consequence, $2p_z$ orbitals at the carbon atoms in the *meta*-positions are less sensitive to substituent effects than the *ortho*- and *para*-ones, and the slope is (as an absolute value) dramatically smaller and negative. When occupation of the $2p_z$ orbital at the *ortho*- and *para*-carbon atoms in substituted benzene derivatives are plotted each other, the regression is $\mathrm{Occ}_{ortho\text{-}}=1.397\mathrm{Occ}_{para\text{-}}-0.394$ with a very high *cc*=0.994. The slope shows that occupation at the *ortho*-position is almost 1.4 times greater than in *para*-, as could be expected due to a longer distance from the substituent.

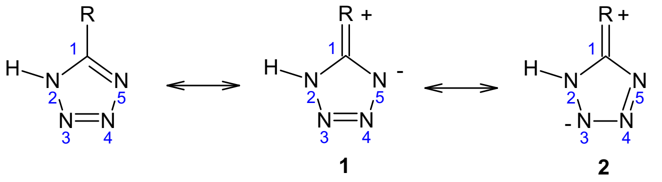
The *pEDA*(*B*) index itself correlates well with the Hammett-like substituent constant σ_p^+ (taken from[17]) as presented in Eq. 3.

$$pEDA = -0.157\sigma_p^+ - 0.028 \tag{3}$$

with correlation coefficient *cc*=0.90. This is understandable since substituent constants σ_p^+ describe the ability of substituents for electron donation to the substituted system, whereas *pEDA* measures an increase of π-electron occupation of all $2p_z$ orbitals in the ring.

3.2. 1*H*-Tetrazole

Now, let us look at the substituent effect on the occupation of the nitrogen atoms in 1*H* tetrazole. Scheme 2 shows the labeling of atoms and possible singly excited resonance structures, whereas Figs. 5 through 8 show the dependences of $2p_z$ occupation at the nitrogen atoms on *pEDA* values.



Scheme 2. Atom numbering and the resonance structures describing the electron donation by a donor substituent in the 1*H*-tetrazole ring.

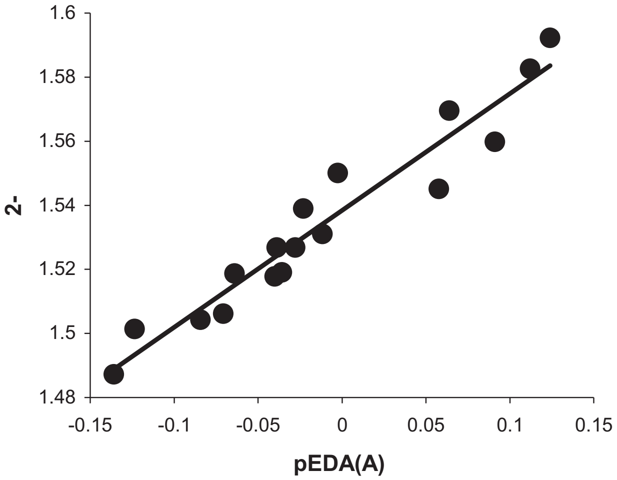


Fig. 5. Dependence of the occupation of the $2p_z$ orbital at N2 atom on *pEDA*. *cc*=0.965; *y*=0.365*x*+1.538.

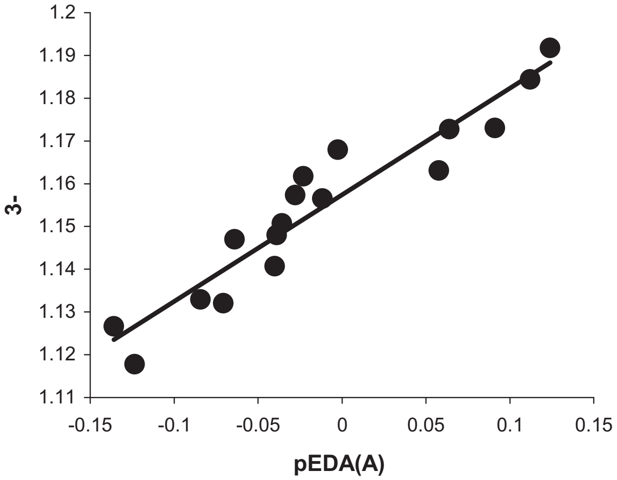


Fig. 6. Dependence of occupation of the $2p_z$ orbital at the N3 atom on *pEDA*. *cc*=0.949; *y*=0.249*x*+1.157.

Please note that the numbering of atoms is not in agreement with IUPAC nomenclature. We have choosen different scheme because we compare occupancies of similar positions in the ring so it is convenient to give them the same numbers for both tautomers

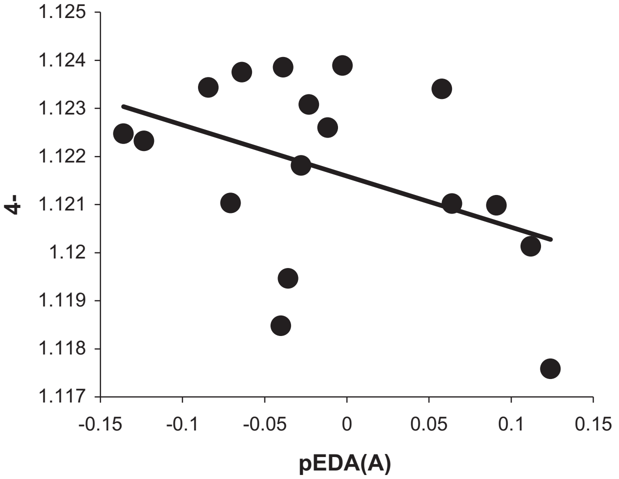


Fig. 7. Dependence of occupation of the $2p_z$ orbital at the N4 atom on *pEDA*. $cc=-0.429$; $y=-0.011x+1.122$.

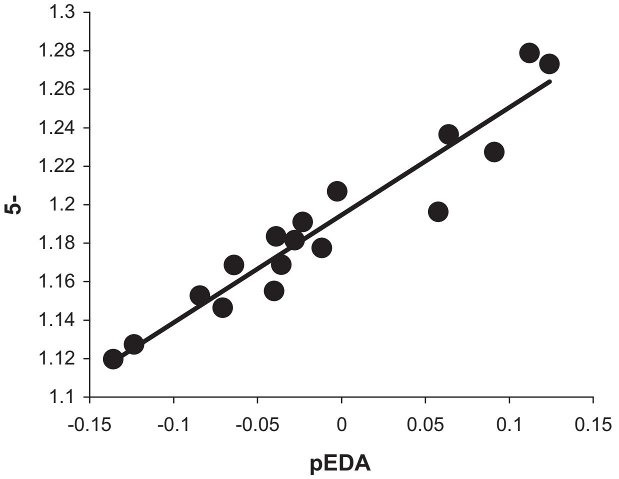
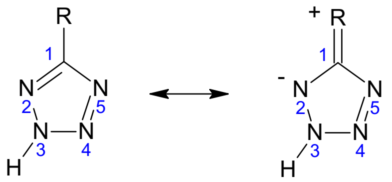


Fig. 8. Dependence of occupation of the $2p_z$ orbital at the N5 atom on *pEDA*. $cc=0.955$; $y=0.559x+1.195$.

1*H* and 2*H*. The *ipso*-carbon atom connected to the substituent is always number 1 and then numbering starts in the direction of the closest pyrrole-like nitrogen atom. Consecutive nitrogen atoms are incrementally numbered. The same comment applies to Scheme 3.



Scheme 3. Atom numbering and the resonance structures describing the electron donation by a donor substituent in 2*H*-tetrazole.

As can be seen, in both cases (N3 and N5) as predicted by simple canonical structures describing the substituent effects (Scheme 2) the dependences of occupation of the $2p_z$ orbital at the N3 and N5 atoms on *pEDA*(*A*) give good correlations with positive slopes, similar to those observed for the *ortho*- and *para*-carbon atoms in benzene derivatives. Looking at the resonance path, note that the route of the resonance omits the pyrrole-like nitrogen atom, N2, and acts along a longer path through atoms C1N5N4N3. Additionally, a good correlation is found for occupation at N2, i.e., at the nitrogen atom with a pair of π-electrons able to delocalization. The only nitrogen atom of which $2p_z$ occupation is not correlated at all with *pEDA* is N4 (Fig. 7). Interestingly, occupations at the nitrogen atoms in unsubstituted azole are diversified as shown in Table 1.

Table 1
$2p_z$ Occupation at all atoms in the ring of 1*H*-tetrazole

	1	2	3	4	5	*p*-Total	*pEDA*
1*H*	0.962	1.539	1.162	1.123	1.191	5.977	−0.023

Moreover, N4 is the least (apart from C1) populated at its $2p_z$ orbital. This is in line with the lack of a single-excited canonical structure for a substituted species (Scheme 2). Moreover, while looking at $2p_z$ occupancies in Table 1, we find that of the $2p_z$ electron pair of pyrrole-like nitrogen atoms, almost 0.5e is delocalized over three pyridine-like nitrogen atoms, increasing their original occupancies by 10–20%. This is in line with the well known properties of this kind of nitrogen atom which are electron attracting. The 3-position of pyridine is the most reactive for electrophilic substitution, but much less than in benzene and resembling that position of nitrobenzene.[18]

3.3. 2*H*-Tetrazole

Scheme 3 presents the labeling of atoms and possible singly excited resonance structures, whereas Figs. 9 through 12 show the dependences of $2p_z$ occupation at the nitrogen atoms on *pEDA* values.

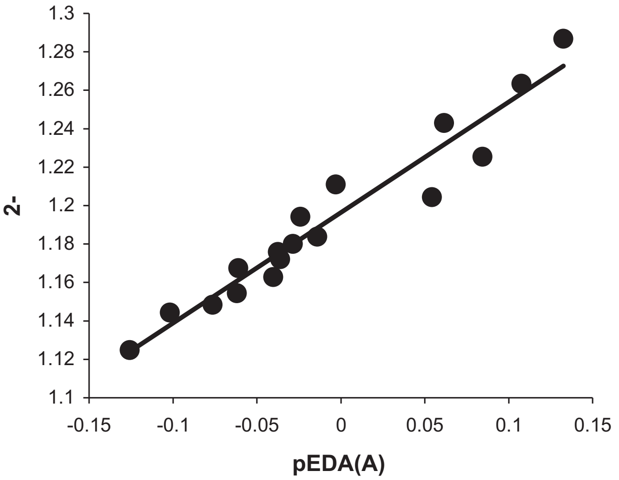


Fig. 9. Dependence of occupation of the $2p_z$ orbital at the N2 atom on *pEDA*. $cc=0.968$; $y=0.5754x+1.1964$.

As we see apart of a good correlation for $2p_z$ occupation at N2, there are also acceptable correlations of $2p_z$ orbitals at the N3 and N5 atoms, despite the fact that there are no available single excited canonical structures describing substituent effects (Scheme 3) in favor of these atoms. As in the case of 1*H*-tetrazole, only $2p_z$ occupation at N4 does not follow any correlation with *pEDA*. As shown in Table 2, the occupation of $2p_z$ orbital at N4 is again the lowest (except for C1) of all other pyridine-like nitrogen atoms.

4. Discussion

The dependences of the $2p_z$ orbital occupations at all nitrogen atoms in substituted derivatives of 2*H*-tetrazole on *pEDA* are partly similar to those observed in the case of substituted derivatives of

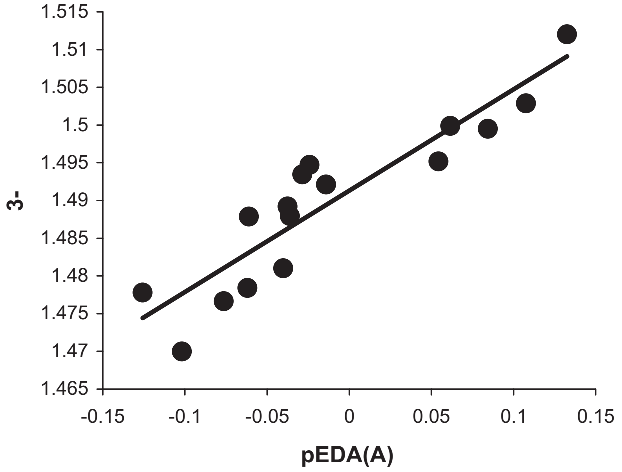


Fig. 10. Dependence of occupation of the $2p_z$ orbital at the N3 atom on *pEDA* (all substituents except Me). $cc=0.918$; $y=0.1343x+1.4913$.

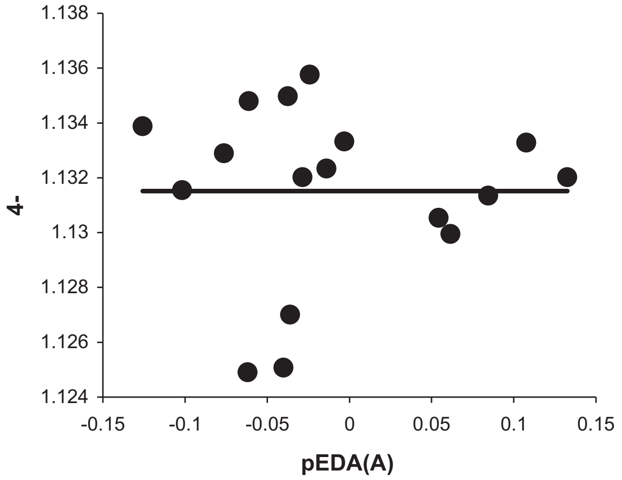


Fig. 11. Dependence of occupation of the $2p_z$ orbital at the N4 atom on *pEDA*. $cc=0.018$; $y=0.0006x+1.132$.

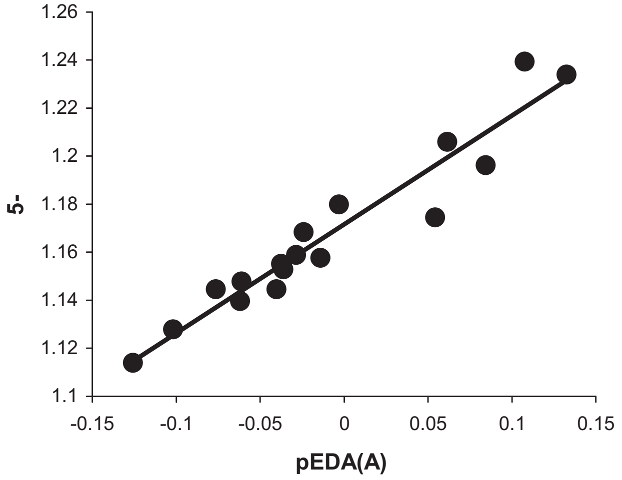


Fig. 12. Dependence of occupation of the $2p_z$ orbital at the N5 atom on *pEDA*. $cc=0.962$; $y=0.453x+1.172$.

Table 2
$2p_z$ Occupation at all atoms in the ring of 2*H*-tetrazole

	1	2	3	4	5	*p*-Total	*pEDA*
2*H*	0.983	1.194	1.495	1.1358	1.168	5.976	−0.024

tautomeric 1*H*-tetrazole. In both cases occupations at the $2p_z$ orbitals of all nitrogen except N4 (Figs. 7 and 11) correlate with *pEDA*. The difference between tautomers is, for 2*H*-tetrazole derivatives, the observed good correlations for N3 and N5 have no support by means of simple resonance theory with single-excited reference structures (Schemes 2 and 3). In both tautomeric tetrazoles, N4 has the lowest (except C1) occupation at the $2p_z$ orbital of all the nitrogen atoms, and $2p_z$ occupation on this atom never correlates with *pEDA*.

An interesting picture is also found for the dependences of *pEDA* values for both tautomers on the Hammett like substituent constants σ_p^+. For 1*H*-tetrazole derivatives, Eq. 4.

$$y = -0.146\sigma_p^+ - 0.034 \text{ with } cc = -0.905 \qquad (4)$$

and for 2*H*-tetrazole derivatives, Eq. 5

$$y = -0.141\sigma_p^+ - 0.031 \text{ with } cc = -0.924 \qquad (5)$$

The regressions have a form similar to that for benzene (Fig. 4). However, in the case of benzene, the slope is (as an absolute value) greater. This indicates a smaller sensitivity of the π-electron structure in azoles than in benzene. It may be explained by a difference in π-electron structure: benzene has six π-electrons delocalized over six carbon atoms, whereas in azoles there are six π-electrons, which are delocalized over five atoms. Also, the charge distribution in azoles is less uniform—the occupation of the $2p_z$ orbital on pyrrole-like atom is much larger (Tables 1 and 2). Thus, the ability to accept additional π electrons from the donating substituent seems to be weaker. As expected, the overall occupation of the $2p_z$ orbitals in the ring decrease with an increase in electron-attracting power of the substituent.

Furthermore, the individual occupations on the nitrogen atoms depend in a different way on substituent constants σ_p^+, as shown in Table 3. Approximately, the smaller the occupation at the $2p_z$ orbital (except the pyrrole-like nitrogen atom, which is donating π-electrons) the lower the correlation coefficient.

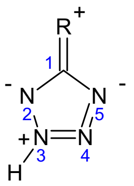
Table 3
Correlation coefficients for occupation on atoms (numbering of atoms see schemes 2 and 3) versus σ_p^+

cc	1	2	3	4	5
1*H*	0.697	0.941	0.889	0.383	0.923
2*H*	0.693	0.947	0.861	0.305	0.925

These results show that the best correlations between the $2p_z$ orbital occupation of the atoms and the substituent constants are found for both adjacent nitrogen atoms (independently whether they are pyrrole-like nitrogen atoms or otherwise).

Looking at the resonance structures in Schemes 2 and 3, we find out that for 2*H*-tetrazole a simple explanation via resonance structure does not work. Only one single-excited structure may be drawn and correlation of the $2p_z$ occupation at N5 on *pEDA* (Fig. 11) is out with this explanation. However, if double excited structure is taken into account (Scheme 4) then occupations at N5 follow the correlation with pEDA (Fig. 12).

Analogously, relatively good correlations of the occupation at the pyrrole-like nitrogen atom on *pEDA* are outside of the resonance structures scheme. There are at least two factors, which may



Scheme 4. Double excited resonance structure describing the electron donation by a donor substituent in 2*H*-tetrazole to position N5.

cause this kind of situation. Firstly, azole molecules are five-membered rings and their substituted molecules are not symmetrical. Secondly, one of the atoms in the ring possesses an electron pair at the $2p_z$ orbital. For these reasons a full analogy with alternant system like benzene may have a limited significance. However in order to find some qualitative rationalization of the correlations presented in Figs. 5 through 12 we will employ an observation made for 4-substituted derivatives of 1,2-benzoquinone.[19] For electron-donating substituents it was found that if the number of bonds between the electron-donating atom in the substituent and the electron-attracting *one in an affixed group is even*, *then the* π-*electron delocalization takes place*, *and the changes in acceptor group are significant*. *If this number is odd*, *then the mentioned changes are negligible*. Pyridine-like nitrogen atoms may be considered as electron attracting,[16] and hence in positions 3 and 5 of 1*H*-tetrazole, and in positions 2 and 5 of 2*H*-tetrazole, good correlations between the $2p_z$ occupation and *pEDA* are observed, since in all these cases the number of bonds between electron-donating D and the nitrogen atoms equals 2 or 4. According to the observation from Figs. 5–12 in counting the number of bonds, the path should exclude the pyrrole-like nitrogen atom, which is a donor of two π-electrons to the π-electron system of tetrazole, and behaves in a different way from all other nitrogen atoms.

5. Conclusions

pEDA as a measure of π-electron delocalization in benzene and tetrazole tautomers 1*H* and 2*H* allowed the study of substituent effects on the $2p_z$ occupation at nitrogen/carbon atoms and indicated approximately equal properties of them except two cases: *meta*-carbon atoms in benzene and N4 in both tetrazoles.

In both cases, tetrazole N4 atoms present the lowest $2p_z$ occupation of all nitrogen atoms, and also lack correlation with substituent constants for regression of $2p_z$ occupation on *pEDA*.

In all three cases: substituted benzene, 1*H*, and 2*H*-tetrazole derivatives, *pEDA* correlates with σ_p^+.

Acknowledgements

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