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Density functional theory study of the regio and stereoselectivity in 1,3-dipolar cycloaddition reactions between *N*-methyl methylenenitrone and fluorinated dipolarophiles

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ABSTRACT

A DFT study of the reactivity, regio-, and stereoselectivity of 1,3-dipolar cycloaddition of *N*-methyl-methylenenitrone **1** with (E and Z)-2,4-diethoxy-5-(perfluoroprop-1-en-1-yl)pyrimidine **2E**, **2Z** and (E and Z)-(perfluoroprop-1-en-1-yl)benzene, **3E**, **3Z** in the gas phase and in toluene, has been carried out by using density functional theory (DFT)-based reactivity indices and activation energy calculations at B3LYP/6-31G (d) level of theory. Four reactive channels associated with the 5- and 4-regio and *endo* and *exo* stereoselective approach modes of the pyrimidine or phenyl group of these fluorinated vinyls relative to nitrone **1** have been explored and characterized. IRC calculations show that these cycloadditions follow an asynchronous concerted mechanism with a low polar character, displaying 5-regioselectivity and it is found that the *endo* pathway is preferred, therefore the formation of product with 5-regio and *endo* pathway is dominant. Also, DFT-based reactivity indices clearly predict the experimental regiochemistry.

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1. Introduction

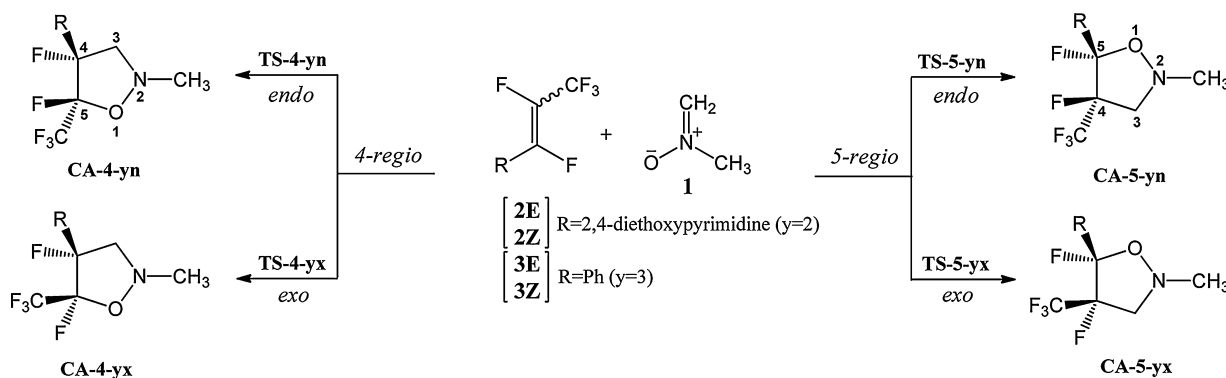
The 1,3-dipolar cycloaddition (1,3-DC) is a chemical reaction between a 1,3-dipole and a dipolarophile to form a five-membered ring [1]. These reactions are one of the most important processes with both synthetic and mechanistic interest in organic chemistry. Nitrones are useful and multipurpose compounds that are widely used in organic chemistry for many applications, i.e. reaction with other molecules (Grignard reagents) [2], trap of free radicals [3], precursors of nitroxides [4], etc. Their reactivity is principally caused by the presence of the carbon–nitrogen double bond, which makes them marvelous 1,3-dipoles in dipolar cycloaddition reactions [5]. In fact, nitrones are capable of reacting with a great variety of dipolarophiles giving rise to a wide range of nitrogen-containing compounds, which are often biologically active species such as antibiotics, alkaloids, amino sugars, etc. Moreover, the 1,3-DC reactions dominate several interesting attributes, especially, reactivity, regio and stereo selectivity. Reactivity descriptors based

on the density functional theory (DFT), like Fukui indices, local softnesses and local electrophilicity, have been widely used for the forecasting of the regio and stereochemistry. For instance, several treatments of 1,3-DC reactions of nitrones with various dipolarophiles can be found in the literature [6–8]. The 1,3-DC reactions of nitrones with alkenes is an important method for preparing isoxazolidines in a regioselective and stereoselective way [9]. Experimentally, it has been found that the cycloaddition reactions of *N*-methyl methylenenitrone **1** with (E and Z)-2,4-diethoxy-5-(perfluoroprop-1-en-1-yl)pyrimidine **2E**, **2Z** and (E and Z)-(perfluoroprop-1-en-1-yl)benzene, **3E**, **3Z** give only 4,5-difluoro-2-methyl-5-substituted-4-(trifluoromethyl)isoxazolidine (5-regioisomer) shown in Scheme 1. In addition, the *endo* pathway is preferred [10]. In continuation of our studies on the mechanism and regioselectivity of the 1,3-DC reactions [11–19], we became interested to study these reactions based on activation energy calculations and DFT-based reactivity indices.

2. Computational details

All calculations were carried out with GAUSSIAN03 program suite [20]. Geometry optimization of the reactants was carried out

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Scheme 1. The regio and stereoisomeric pathways for 1,3-dipolar cycloadditions.

using DFT methods at the B3LYP/6-31G (d) level of theory [21]. The transition states (TSs) for the 1,3-DC reactions have been localized at the B3LYP/6-31G (d) level of theory. Frequency calculations characterized the stationary points to verify that the TSs had one and only one imaginary frequency. The intrinsic reaction coordinates (IRC) [22] calculation was performed in forward and backward path to identify that each saddle point connects to the two associated minima using the second-order González-Schlegel integration method [23,24]. Solvent effects were considered at the B3LYP/6-31G (d) level of theory by geometry optimization of the gas-phase structures using a self-consistent reaction field (SCRF) [25] based on the polarizable continuum model (PCM) of Tomasi's group [26]. Because the studied cycloaddition reactions were carried out in toluene, we selected its dielectric constant at 298.0 K, $\epsilon = 2.38$.

Reactivity indices, chemical potential (μ) and softness (S) were evaluated within the finite difference approximation, using Eqs. (1) and (2) [27]:

$$\mu = \frac{-(IP + EA)}{2} \quad (1)$$

$$S = (IP - EA)^{-1} \quad (2)$$

where IP and EA are the vertical ionization potential and electron affinity, achieved by energy difference of the neutral with the cation and anion, respectively.

The global electrophilicity ω for dipoles and dipolarophile was evaluated using Eq. (3) [28]:

$$\omega = \frac{\mu^2}{2(IP - EA)} \quad (3)$$

Domingo et al. has introduced an empirical (relative) nucleophilicity index [29], N , based on the HOMO energies obtained within the Kohn–Sham scheme [28], and defined as

$$\varepsilon_{\text{HOMO}}(Nu) - \varepsilon_{\text{HOMO}}(\text{TCE}) \quad (4)$$

This nucleophilicity scale is referred to tetracyanoethylene (TCE) taken as a reference.

Very recently, Domingo proposed two new electrophilic, P_k^+ , and nucleophilic, P_k^- , Parr functions based on the atomic spin density distribution at the radical anion and at the radical cation of a neutral molecule [30]. The electrophilic, P_k^+ , and nucleophilic, P_k^- , Parr functions, were obtained through the analysis of the Mulliken atomic spin density of the radical anion and the radical cation by single-point energy calculations over the optimized neutral geometries using the unrestricted UB3LYP formalism for radical species. The local electrophilicity indices, ω_k [31], the local nucleophilicity indices, N_k [32] and local softness [33], s were

calculated using the following equations:

$$\omega_k = \omega P_k^+ \quad (5)$$

$$N_k = N P_k^- \quad (6)$$

$$s^+ = S P_k^+ \quad (7)$$

$$s^- = S P_k^- \quad (8)$$

where P_k^+ and P_k^- are the electrophilic and nucleophilic Parr functions [30], respectively.

The atoms in a molecule are open subsystems interchanging energy and electrons, thus the natural thermodynamic quantity is the grand potential $\Omega = E - N\mu$, where E is the energy. Suppose the cycloaddition of molecules A and B to give AB . The interaction of atom i of A with atom k of B is [8]

$$\Delta \Omega_i^k = -\frac{1}{2}(\mu_A - \mu_B)2 \frac{S_{Ai}S_{Bk}}{S_{Ai} + S_{Bk}} \quad (9)$$

and illustrates the stabilization owing to the charge transfer between Ai and Bk . Because cycloadditions are concerted reaction, the stabilization upon reactive encounter is owing to two bond-forming interactions $Ai \leftrightarrow Bk$ and $Aj \leftrightarrow Bl$ and is written as $\Delta \Omega_{ij}^{kl} = \Delta \Omega_i^k + \Delta \Omega_j^l$. For the opponent regioisomer, the stability is $\Delta \Omega_{ij}^{lk} = \Delta \Omega_i^l + \Delta \Omega_j^k$ [8].

3. Results and discussion

Our theoretical analyzes of the regio and stereochemistry of these 1,3-DC reactions will be based on activation energy calculations and DFT-based reactivity indices.

3.1. Activation energy calculations

The transition states have been localized for both cyclization modes. In this work, 4/5 and n/x , denote 4/5-regio- and endo/exo stereoselectivity, while, $y = 2$ and $y = 3$ are used for **2** (**E**, **Z**) and **3** (**E**, **Z**) ethenes, respectively (see Scheme 1). The corresponding activation barriers and structures are given in Table 1 and Fig. 1, respectively. An analysis of the geometries at the TS structures, given in Fig. 1, shows that they correspond to asynchronous bond formation processes. The extent of bond formation along a reaction pathway is provided by the concept of bond order (BO) [34]. The BO (Wiberg indices) values of the C–O and C–C forming bonds at TSs are shown in brackets in Fig. 1. These values are within the range of 0.29 to 0.37. These results show that the TS-5-2n and TS-5-2x are more asynchronous than the TS-4-2n and TS-4-2x, the TS-5-3n and TS-5-3x are more asynchronous than the TS-4-3n and TS-4-3x. In general, the asynchronicity shown by

Table 1

Relative Gibbs free energies (ΔG , in kcal mol⁻¹), enthalpies (ΔH , in kcal mol⁻¹) computed at 298.15 K and 1 atm in gas phase and toluene for the transition states (TSs) and cycloadducts (CAs) involved in the 1,3-DC reactions of **1** with **2E**, **2Z** and **3E**, **3Z**.

	Gas phase		Solvent phase	
	ΔG	ΔH	ΔG	ΔH
TS-5-2n (5-regio, endo) ^a	24.25	9.57	25.81	11.13
TS-5-2x (5-regio, exo) ^a	26.68	13.10	28.29	14.52
TS-4-2n (4-regio, endo) ^a	27.78	12.79	29.06	14.08
TS-4-2x (4-regio, exo) ^a	31.12	17.98	32.39	19.26
TS-5-3n (5-regio, endo) ^b	25.10	9.87	27.06	11.15
TS-5-3x (5-regio, exo) ^b	25.42	11.97	26.72	13.24
TS-4-3n (4-regio, endo) ^b	27.70	12.09	29.52	13.35
TS-4-3x (4-regio, exo) ^b	28.80	15.19	30.19	16.53
CA-5-2n (5-regio, endo) ^a	-43.95	-45.57	-43.60	-45.18
CA-5-2x (5-regio, exo) ^a	-45.48	-47.04	-45.16	-46.64
CA-4-2n (4-regio, endo) ^a	-46.34	-47.43	-45.78	-46.83
CA-4-2x (4-regio, exo) ^a	-47.93	-49.68	-47.17	-49.01
CA-5-3n (5-regio, endo) ^b	-44.14	-45.72	-43.55	-45.12
CA-5-3x (5-regio, exo) ^b	-45.93	-47.93	-45.33	-47.30
CA-4-3n (4-regio, endo) ^b	-44.82	-45.80	-44.32	-45.41
CA-4-3x (4-regio, exo) ^b	-46.48	-47.91	-46.28	-47.51

^a Relative to **1** + (**2E**, **2Z**).

^b Relative to **1** + (**3E**, **3Z**).

the geometrical data is accounted for by the BO values. All the reactions progressed exothermically with large ΔH values (Table 1). According to Hammond's postulate, the TSs should then be closer to the reactants.

As shown in Table 1 and Scheme 1, the relative Gibbs free energy values, ΔG , for the TSs corresponding to the four competitive reactive channels are: 24.25 (**TS-5-2n**), 26.68 (**TS-5-2x**), 27.28 (**TS-4-2n**) and 31.12 (**TS-4-2x**) kcal mol⁻¹ for the 1,3-DC reaction of nitrene **1** with **2** (**E**, **Z**) and 25.10 (**TS-5-3n**), 25.42 (**TS-5-3x**), 27.70 (**TS-4-3n**) and 28.80 (**TS-4-3x**) kcal mol⁻¹ for the 1,3-DC reaction of nitrene **1** with **3** (**E**, **Z**). For these substituted ethenes, the 5-regio cycloaddition modes are more favorable than the 4-regio ones by about 3 kcal mol⁻¹ and 3.7 kcal mol⁻¹, respectively, leading to the formation of the 5-regio cycloadducts **CA-5-yx** and **CA-5-yn**. In addition, the endo approach modes giving **CA-5-2n** and **CA-5-3n** are more favorable, by ca. 2 kcal mol⁻¹, than the exo ones. Therefore, the presence of the trifluoromethyl group at position 2 of these substituted fluoroethenes neither changes the complete 5-regioselectivity, nor the high endo selectivity. These results are in agreement with the experimental data [10].

As the 1,3-DC reactions between nitrene **1** and dipolarophiles **2** (**E**, **Z**) and **3** (**E**, **Z**) were carried out in toluene, which can have some prevalence on the energies and geometries, solvent effects in these 1,3-DC reactions were considered by full optimization of the gas

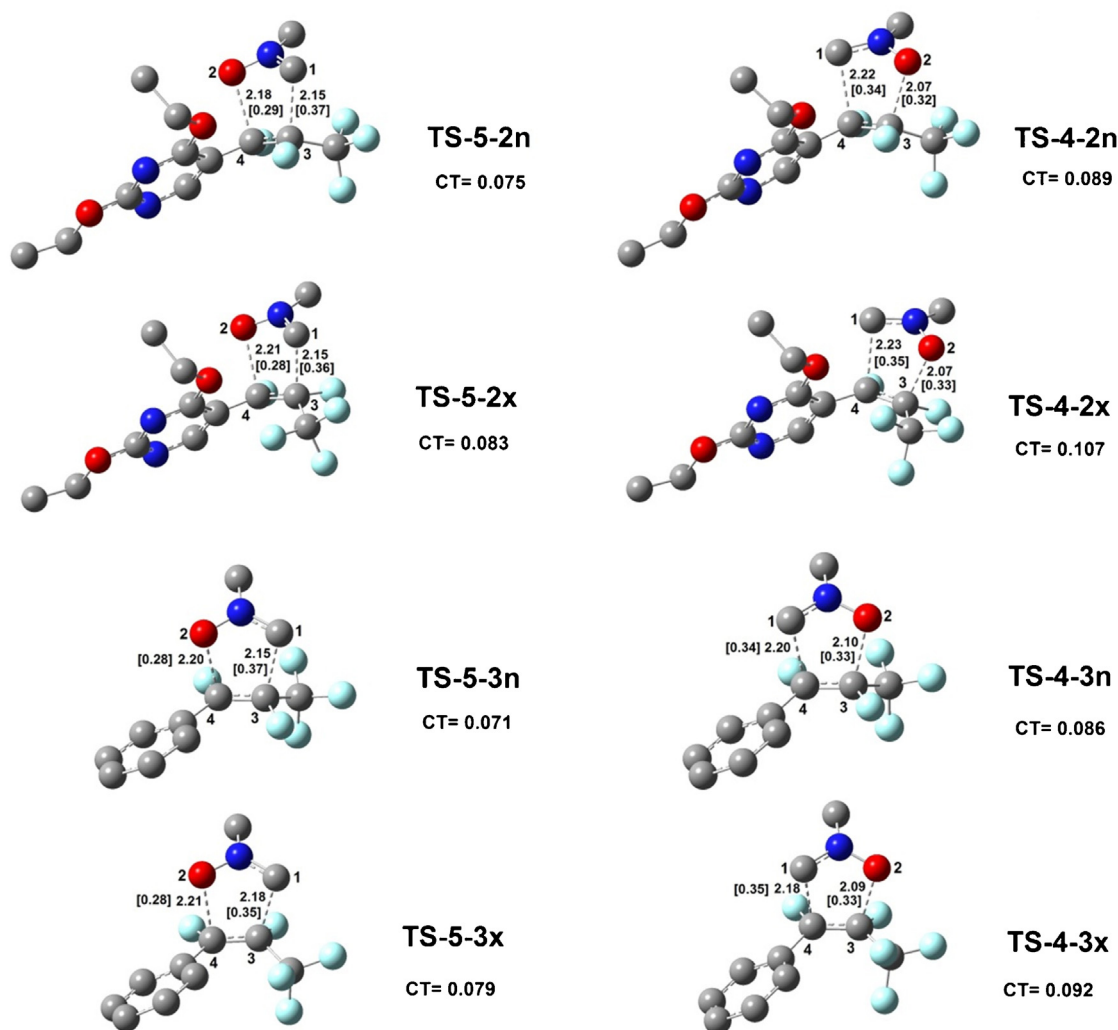


Fig. 1. Optimized geometries for transition state structures at the B3LYP/6-31G (d) level of theory. Hydrogen atoms have been omitted for clarity. Distances of forming bonds are given in angstroms. The bond orders are given in brackets.

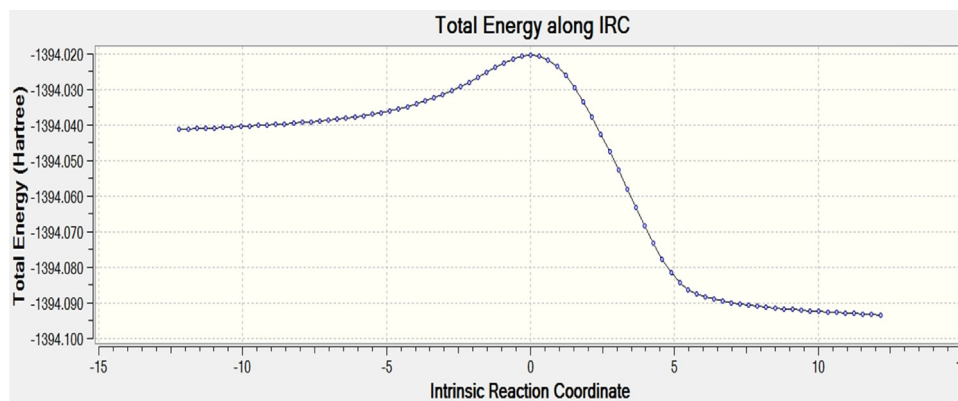


Fig. 2. B3LYP/6-31G (d) IRC plot for the reaction pathway leading to **CA-5-2n**.

phase geometries using the PCM model of Tomasi's group [25]. The relative energy results are summarized in Table 1. With the incorporation of solvent effects, reactants are more stabilized than TSs and CAs [35]. As a result, in toluene, the relative Gibbs free energies associated with 5-regio TSs are moderately increased between 1.6 and 2.0 kcal mol⁻¹, while for the 4-regio TSs they are increased between 1.3 and 1.8 kcal mol⁻¹. Furthermore, in toluene, **TS-5-3x** (5-regio, *exo*) is more stabilized than **TS-5-3n** (5-regio, *endo*), (see Table 1).

The polar nature of the two cyclization modes can be estimated by a charge transfer (CT) analysis at the TSs. The CT from dipole **1** to dipolarophiles **2E**, **2Z** is 0.075 e at **TS-5-2n**, 0.083e at **TS-5-2x**, 0.089e at **TS-4-2n** and 0.107 e at **TS-4-2x**. Therefore, the CT calculations show an NED (normal electron demand) character for this reaction. For **1** + **3** (**E**, **Z**), the CT from dipole **1** to dipolarophile **3** (**E**, **Z**) is 0.071 e at **TS-5-3n**, 0.079e at **TS-5-3x**, 0.086e at **TS-4-3n** and 0.092e at **TS-4-3x**. Thus, the CT calculations show an NED character for this process.

IRC calculations were carried out for all studied reactions, and presented only for the reaction pathway leading to **CA-5-2n** (Fig. 2). This figure shows saddle point clearly, and demonstrates that the TS connect to the associated minima of the concerted mechanism.

3.2. DFT-based reactivity indices

The HOMO and LUMO energies, electronic chemical potential μ , chemical hardness η , global electrophilicity ω and global

nucleophilicity N of the nitrone **1** and dipolarophiles **2E**, **2Z**, **3E** and **3Z** are given in Table 2.

As it can be seen in Table 2, the electronic chemical potential (μ) of dipole **1** (−0.1211) is greater than those of dipolarophiles **2E** (−0.1448), **2Z** (−0.1447), **3E** (−0.1514) and **3Z** (−0.1506) which shows the charge transfer is taking place from dipole **1** to dipolarophiles **2E**, **2Z**, **3E** and **3Z**. Consequently, the dipolarophiles **2E**, **2Z**, **3E** and **3Z** can act as electrophile in these 1,3-DC reactions. These results are in agreement with CT calculations at the TSs.

The stabilization of the promoted complex for the pathway leading to (4*R*, 5*S*)-4,5-difluoro-2-methyl-5-(2,4-diethoxypyrimidine)-4-(trifluoromethyl)isoxazolidine **CA-5-2n** is [8]

$$\Delta \Omega_{\text{CA-5-an}} = -\frac{1}{2}(\mu_1 - \mu_{2E})^2 \left\{ \frac{S_{C3}S_{C4}}{S_{C3} + S_{C4}} + \frac{S_{O1}S_{C5}}{S_{O1} + S_{C5}} \right\} \quad (10)$$

where the atoms are numbered in Scheme 1. The grand potential change ($\Delta\Omega$) for adducts **CA-5-3n**, **CA-5-2x**, **CA-5-3x**, **CA-4-2n**, **CA-4-3n**, **CA-4-2x** and **CA-4-3x** can be similarly obtained.

From the $\Delta\Omega$ values presented in Table 3, we can conclude that there is a specific site-selectivity in the reactions leading to **CA-5-2n**, **CA-5-2x**, **CA-5-3n** and **CA-5-3x**. Furthermore, it is obvious that the difference $\delta\Delta\Omega$ between **CA-5-2n**, **CA-5-2x** and **CA-5-3n**, **CA-5-3x** is about −2.82 and −13.65 kcal mol⁻¹, respectively. The negative sign of $\delta\Delta\Omega$ indicates that the products **CA-5-2n** and **CA-5-3n** are always the major one, in accordance with the experimental results [10].

The difference in electrophilicity for the dipole/dipolarophile pair, $\Delta\omega$, was found to be a measure of the high- or low-polar

Table 2

HOMO energies in a.u., ionization potential (IP in a.u.), electron affinity (EA in a.u.), electronic chemical potential (μ in a.u.), chemical hardness (η in a.u.), global electrophilicity (ω , in eV) and global nucleophilicity (N , in eV) for reactants **1**, **2E**, **2Z**, **3E** and **3Z**.

Reactants	ϵ_{HOMO}	IP	EA	μ	η	ω	N^a
1	−0.2199	0.3213	−0.0791	−0.1211	0.4004	0.498	3.14
2E	−0.2381	0.3027	−0.0131	−0.1448	0.3158	0.904	2.64
2Z	−0.2387	0.3035	−0.0141	−0.1447	0.3176	0.897	2.63
3E	−0.2433	0.3140	−0.0113	−0.1514	0.3254	0.958	2.50
3Z	−0.2450	0.3166	−0.0155	−0.1505	0.3320	0.929	2.45

^a The HOMO energy of tetracyanoethylene is −0.3351 a.u. at the same level of theory.

Table 3

Grand potential stabilization $\Delta\Omega$ values of the eight possible cycloadducts. See Scheme 1 for products notation.

$\Delta\Omega$ (kcal mol ⁻¹)							
CA-5-2n	CA-5-2x	CA-4-2n	CA-4-2x	CA-5-3n	CA-5-3x	CA-4-3n	CA-4-3x
−178.74	−175.92	−60.86	−63.97	−417.94	−404.29	−153.66	−189.68

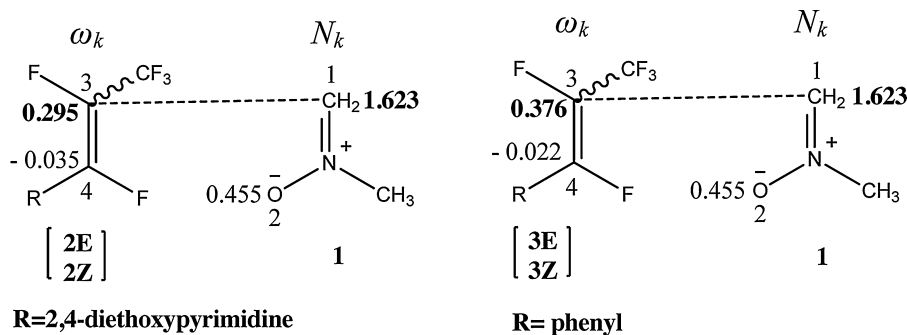


Fig. 3. Illustration of the favorable interactions using Local nucleophilicities, N_k and local electrophilicities, ω_k .

Table 4

Parr indices (P_k^\pm), local electrophilicity indices (ω_k in eV) and local nucleophilicity indices (N_k in eV) for the C1 and O2 atoms of the dipole **1** and for atoms C3 and C4 of the dipolarophiles **2E**, **2Z**, **3E** and **3Z**.

Reactants	Atom number	P_k^-	P_k^+	ω_k	N_k
1	C1	0.517			1.623
	O2	0.145			0.455
2E	C3		0.326	0.295	
	C4		-0.039	-0.035	
2Z	C3		0.303	0.272	
	C4		-0.036	-0.032	
3E	C3		0.393	0.376	
	C4		-0.023	-0.022	
3Z	C3		0.363	0.337	
	C4		-0.002	-0.002	

character of the cycloaddition [36]. The small $\Delta\omega$ between **1** and **2E**, 0.406 eV, 0.399 eV for **1** + **2Z**, 0.460 eV for **1** + **3E** and 0.431 eV for **1** + **3Z** shows a low-polar character for these 1,3-DC reactions.

The Parr indices, local electrophilicity indices and local nucleophilicity indices for the atoms C1 and O2 of the dipole **1** and for the atoms C3 and C4 of the dipolarophiles (**2E**, **2Z**, **3E** and **3Z**) are given in Table 3 (see Fig. 1 for atom numbering). Parr functions computed based on the Mulliken atomic spin density analysis (Table 4).

In Fig. 3, we have reported the values of local nucleophilicities N_k for atoms C1 and O2 of the dipole **1** and the local electrophilicities ω_k for atoms C3 and C4 of the dipolarophiles **2** (**E**, **Z**) and **3** (**E**, **Z**). According to the Domingo's model [29,31], in a polar cycloaddition reaction between unsymmetrical reagents, the more favorable two-center interaction will take place between the more electrophile center characterized by the highest value of the local electrophilicity index ω_k at the electrophile, and the more nucleophile center characterized by the highest value of the local nucleophilicity index N_k at the nucleophile. According to this model, in the reaction between **1** and **2** (**E**, **Z**), the most favorable two-center interaction takes place between C1 of the dipole **1** and C3 of the dipolarophiles **2** (**E**, **Z**) leading to the formation of the **CA-5-2** (**n** or **x**) regioisomer which is in agreement with experimental observations [10]. In the reaction between **1** and **3** (**E**, **Z**) the most favorable two-center interaction takes place between C1 of the dipole **1** and C3 of the dipolarophiles **3** (**E**, **Z**) leading to the formation of the **CA-5-3** (**n** or **x**) regioisomer which is in agreement with experimental findings [10].

4. Conclusion

Mechanism and regiochemistry for the 1,3-dipolar cycloaddition reactions of the dipole **1** with dipolarophile **2** (**E**, **Z**) and **3** (**E**, **Z**) has been investigated using activation energy calculations and DFT-based reactivity indices at the B3LYP/6-31G (d) level of theory. The results obtained in this work allow us to conclude that

activation energy calculations and DFT-based reactivity indices clearly predict the regiochemistry of the isolated cycloadducts.

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