Theoretical Study of the Molecular Complexes between Pyridyne and Acid Sites of Zeolites

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ABSTRACT *The main interaction between pyridine and zeolites leads to form a hydrogen bond between the N atom of pyridine and OH groups of zeolites. The present work reports a theoretical study about the structural, vibrational and topological properties of the charge distribution of the molecular complexes between pyridine and a series of acids sites of zeolites. The calculated structural parameters are the highest occupied molecular orbital energy (E_{HOMO}), lowest unoccupied molecular orbital energy (E_{LUMO}), energy gap (ΔE), hardness (η), softness (S), the absolute electronegativity (χ), the electrophilicity index (ω) and the fractions of electrons transferred (ΔN) from zeolites molecules to pyridine. We show N atom of pyridine attacks to the H atom of the OH bridged group of zeolite clusters.*

KEYWORDS: *Pyridine; Zeolites, MP2; Fukui function.*

INTRODUCTION

The pyridine ring system occurs in the structures of many natural products, pharmaceutical and agrochemical compounds, and other commercial substances [1]. These compounds serve as initial substances for many important syntheses, form the structural units of various products, and represent the building blocks for promising novel materials [2, 3]. Hence, the physical chemistry, spectroscopy and electronic structure of these molecules have attracted high attention. In particular, it has been used as an electron acceptor in studies involving hydrogen bonding complexes [4].

Zeolites are crystalline aluminosilicate compounds which have used as acid catalysts in many important industrial processes [5-10]. The acidic properties of these materials arise from the presence of hydroxyl groups named acid sites of zeolites. These zeolite acids were represented as $H_3Si(OH)AlH_3$ (B_1), $(OH)_3Si(OH)Al(OH)_3$ (B_1OH) and the $H_3Si(OH)Al(OH)_2OSiH_3$ (B_2). The optimized electronic structure, vibrational frequencies, topological properties and relationship between the Mulliken populations of the H atom of the OH of these compounds have been reported at the DFT and MP2/6-31G (d, p) theories level [11,12].

Understanding of the interaction mechanism between pheylalanine and its palladium(II) complexes [13], vanillin with alpha, beta and gamma cyclodextrin as drug delivery carriers [14], paracetamol and water [15], zeolites and furan [16], Li-graphene and Li-Born Nitride[17] was recently provided by our group. In the present work, we consider the interaction between the N atom of pyridine and the H atoms of the OH bridge groups of the zeolite clusters, giving a series of pyridine–zeolite
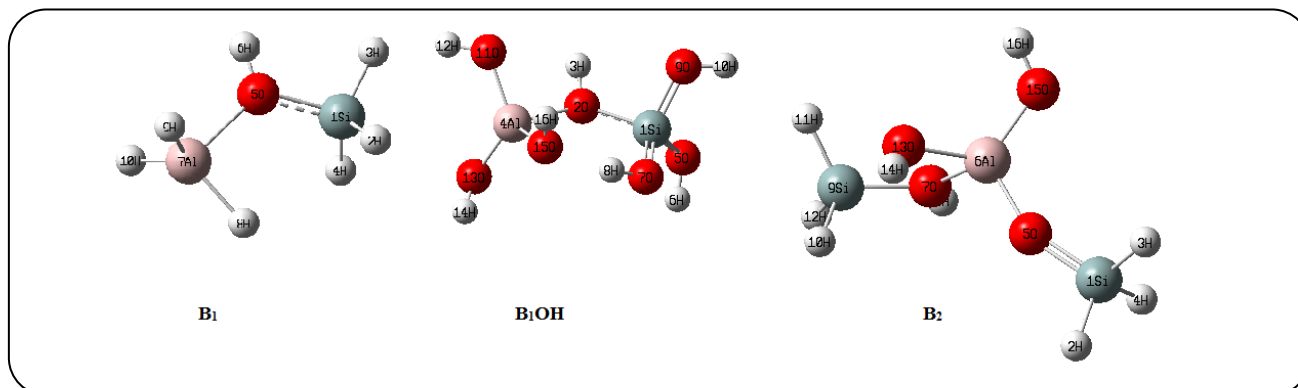
Fig. 1: Structures of B₁, B₁OH, and B₂ clusters.

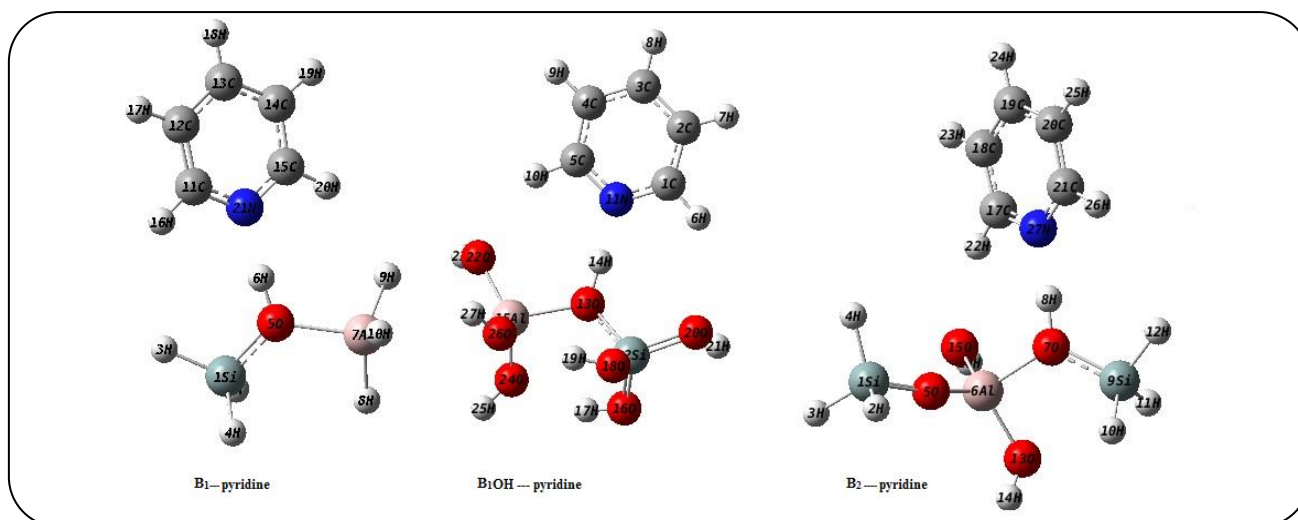*Fig. 2. Structures of B₁ – pyridine, B₁OH – pyridine, and B₂ – pyridine clusters.*

molecular complexes. interaction We report a theoretical study of the topological properties of the charge distribution of these molecular complexes. The structures of zeolites and complexes are shown in Figs. 1 and 2, respectively. For the isolated species and complexes, we have used *ab initio* calculations [18, 19] to study the geometric, electronic and vibrational properties. The topological properties of the pyridine-zeolite complexes have been calculated by the theory of Bader of Atoms in Molecules (AIM) [20] as developed by *Cioslowski* and *Coworkers* [21] in the Gaussian 03 set of programs [22]. These results show that the pyridine zeolites molecular complexes are energetically and structurally stable. The theory of AIM gives a particular quantum mechanical description for the charge distribution of this interaction. These results are analyzed using the vibrational features of the OH groups, the

structural properties of the complexes, and the energetic properties.

COMPUTATIONAL SECTION

All calculations were performed using Guassian 03 package [22]. The ground state geometry of the investigated various structures was optimized at the second order Møller–Plesset theory MP2 method with employing cc-PVTZ basis set. Then corresponding frequency calculations were carried out at the same level to ensure that the optimized structures are true minima.

The theory of atoms in molecules (QTAIM) gives a description for the charge distribution, so analysis of the molecular electron density distribution provides valuable information about chemical systems. QTAIM is based on the Critical Point (CP) of the molecular electronic charge density. In this theory, properties of Line Critical Points (LCPs),

have been used to analyze the bonding properties [23]. The resulting formatted wave function files were used as inputs to Multiwfn program [24].

In the present study, we have applied the theory of *Bader* [20] as implemented by *Cioslowsky et al.* [21] to characterize the topological properties of the electronic charge density of the interaction between pyridine and acid sites of zeolites. Molecular geometries and vibrational properties of pyridine and the B_1, B_1OH, B_2 clusters and the corresponding pyridine–zeolite complexes were calculated at the MP2/cc-PVTZ level theory.

RESULTS AND DISCUSSION
Geometric structure of complexes

The consideration of electronic and structural nature of the pyridine–zeolite interaction is the main goal of this work. We are concerned on geometrical, vibrational and electronic features of pyridine and its complexes.

Pyridine is a planar molecule and belongs to the C_{2v} symmetry group. Results for the C_{2v} optimized structure of the pyridine with MP2/cc-PVTZ and B3LYP/cc-PVTZ levels of theory were reported previously [25,26].

We start the calculations with the $H_3Si(OH)AlH_3$, $(OH)_3Si(OH)Al(OH)_3$ and the $H_3Si(OH)Al(OH)_2OSiH_3$ clusters referred as B_1, B_1OH and B_2, respectively whose structural, electronic and conformational properties have been reported [9]. The B_1OH structure is similar to the B_1 cluster, except OH groups substitute the terminal H atoms of Si and Al ones. The B_2 structure is a well-known cluster [11,12]. Fig. 1 shows the structures of zeolites clusters. The optimized geometric parameters of the isolated zeolite clusters (B_1, B_1OH, and B_2) are reported in Table 1. The MP2 results for the main bond of these clusters are around the values of 1.68353 Å for the Si—O bond, 1.8289 Å for the Al—O bond, and 0.9565 Å for the O—H bond.

We have started a research program to establish systematically the theoretical aspects of the adsorption of pyridine over zeolites. In this work, we have considered a perpendicular interaction of the pyridine molecules with the OH bridged groups of zeolite clusters. When each of the B_1, B_1OH, and B_2 clusters approaches to a pyridine molecule, a bond is formed between the N atom of pyridine and the OH group of each cluster, then the B_1–pyridine, B_1OH–pyridine, and B_2–pyridine stable complexes are created (Fig. 2). The corresponding optimized geometries for the B_1, pyridine B_1OH–pyridine and B_2—pyridine complexes are reported in Table 2.

Electronic properties and interaction energies

The total energies ($-E_t$/hartrees), (μ/debyes), and Mulliken atomic charges for Al, Si, O, N, and H atoms of pyridine, clusters and complexes are reported in Table 3. The interaction energy (E_i) is an important theoretical measure for the strength of the formation of the studied complexes. It is calculated from the difference of the total energies between the zeolite—pyridine ($E_{z-pyridine}$) complex and the isolated species ($E_z+E_{pyridine}$) at MP2/cc-PVTZ level theory and is reported in Table 3. The values of the E_i quantity are negative, indicating that the pyridine–zeolite interaction is attractive. The charge distribution taken in terms of the Mulliken populations is displayed in Table 3. From these results, it seems that there exists a significant variation into the N atom populations of the pyridine moiety. There exists an electronic charge migration from the zeolite structure to the N atom of pyridine and it behaves as an electron acceptor so that charge on the N atom increases.

Vibrational properties

The harmonic vibrational OH frequency of zeolite clusters and the corresponding pyridine complexes were calculated at the MP2/cc-PVTZ level theory. The vibrational frequencies of the OH-bridged stretching mode (cm^{-1}) of B_1, B_1—pyridine, B_1OH, B_1OH—Pyridine, B_2, and B_2—pyridine are 3849.06, 2438.75, 3803.89, 2159.03, 3855.96 and 3461.42 cm^{-1}, respectively. The experimental vibrational frequency of the OH-bridged of B_2 is 3610 cm^{-1} [22]. The difference of frequency of stretching between OH groups and OH bridged of pyridine complexes are named frequency shifts, Δv. The Δv for B_1, B_1OH, and B_2 are 1410.31, 1644.86 and 394.45 cm^{-1}, respectively. The obtained results show that vibrational OH frequencies of isolated zeolites are more than one of the pyridine complexes. So the interaction of pyridine with OH groups produces a contraction in the OH frequency.

Quantum theory of atoms in molecules

The topologic properties of the charge distribution of the pyridine molecule and the B_1, B_1OH and B_2 zeolite

Table. 1: Selected ground-state geometry parameters of B_1, B_1OH and B_2.

B₁				B₁OH				B₂			
Bond lengths (Å)		Bond angles (deg)		Bond lengths (Å)		Bond angles (deg)		Bond lengths (Å)		Bond angles (deg)	
R(1,2)	1.475	A(2,1,5)	104.2	R(2,3)	0.9647	A(1,5,6)	117.2	R(7,8)	0.959	A(2,1,3)	107.9
R(1,2)	1.466	A(3,1,5)	108.5	R(2,4)	1.938	A(1,7,8)	115.3	R(7,9)	1.756	A(1,5,6)	162.7
R(1,4)	1.466	A(4,1,5)	108.5	R(2,1)	1.704	A(1,9,10)	118.1	R(9,10)	1.497	A(5,6,7)	105.0
R(1,5)	1.712	A(8,7,5)	90.5	R(4,11)	1.728	A(5,1,2)	112.3	R(9,11)	1.468	A(5,6,15)	114.7
R(5,6)	0.961	A(9,7,5)	102.2	R(4,13)	1.723	A(7,1,2)	104.5	R(9,12)	1.471	A(5,6,13)	117.8
R(5,7)	1.999	A(10,7,5)	102.2	R(4,15)	1.764	A(1,2,3)	117.05	R(7,6)	1.893	A(6,15,16)	121.9
R(7,8)	1.603	A(1,5,6)	117.3	R(11,12)	0.955	A(4,2,3)	109.5	R(6,13)	1.785	A(6,13,14)	123.5
R(4,9)	1.591	A(7,5,6)	121.1	R(13,14)	0.956	A(2,4,11)	94.94	R(6,15)	1.714	A(6,7,8)	121.3
R(7,10)	1.591			R(15,16)	0.957	A(2,4,13)	105.1	R(13,14)	0.955	A(7,9,11)	110.9
				R(1,5)	1.633	A(2,4,15)	99.03	R(15,16)	0.957	A(8,7,9)	117.6
				R(1,7)	1.632	A(4,11,12)	121.9	R(5,6)	1.708	A(7,9,10)	109.6
				R(1,9)	1.612	A(4,13,14)	121.3	R(1,5)	1.630	A(7,9,11)	110.9
				R(5,6)	0.958	A(4,15,16)	119.9	R(1,2)	1.482		
				R(7,8)	0.9599			R(1,3)	1.481		
				R(9,10)	0.9908			R(1,4)	1.481		

clusters are reported in Table 4. The LCP of our complexes were obtained and the selected quantities (electron density, Laplacian of the electron density, and the energy density and delocalization indices) for these LCPs of all complexes and their basin paths are reported in Table 5. In the structure of Table 4, one LCP were found between the N atom of pyridine and the H atom of B_1, B_1OH, and B_2. The values of the Laplacian of the electron density ($\nabla^2\rho(r)$) at LCPs are positive for B_1—pyridine and B_2—pyridine but it is negative for B_1OH—pyridine that show strong hydrogen bond between pyridine and B_1OH.

In Table 5, the energy density of $N_{Pyridine} \dots H_{Zeolite}$ interactions are -0.046, -0.29 and -0.037 for B_1—pyridine, B_1OH—Pyridine, and B_2—pyridine, respectively.

Delocalization index (δ) is a useful property for characterizing the chemical bonds. Delocalization index can be defined between two atoms that consider the existence of LCP between them. In fact, the delocalization index quantifies the extent of the electron exchange between two atoms that can be used as a direct measure of covalence nature of interaction [24].

Delocalization index for B_1—pyridine, B_1OH—pyridine and B_2—pyridine interactions are 0.22, 0.38 and 0.21, respectively. The results show more electron exchange between the N atom of pyridine and the H atom of B_1OH that is concordant with energy density results.

Chemical reactivity
Global reactivity descriptors

We should find the energy of the molecules to understand the quantum chemical properties of molecules. The vibrations and rotations of molecules are sources of chemical energy in the chemical reaction which is a rearrangement of atoms. Theoretical methods have been successful in providing an appropriate view to the chemical reactivity and selectivity, regarding global parameters such as chemical potential (μ), electronegativity (χ), global softness (S), global hardness (η) and electrophilicity index (ω). On the basis of Koopman's theorem [19], global reactivity descriptors are calculated using the energies of frontier molecular orbitals ε_{HOMU} and ε_{LUMO}, these corresponding equations are given in Eqs. (1) – (5) [28,29].

Table 2: Selected ground-state geometry parameters of B₁—pyridine, B₁OH—pyridine and B₂—pyridine.
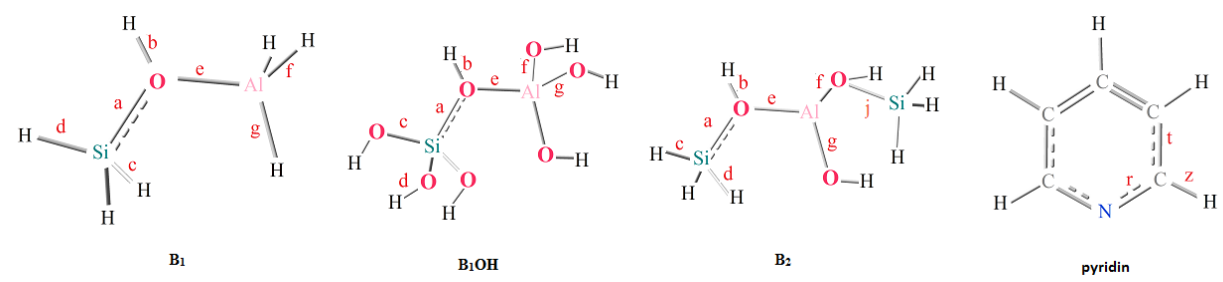
B₁—pyridine				B₁OH--pyridine				B₂--pyridine			
Bond lengths (Å)		Bond angles (deg)		Bond lengths (Å)		Bond angles (deg)		Bond lengths (Å)		Bond angles (deg)	
R(1,3)	1.484	A(2,1,3)	109.7	R(1,2)	1.386	A(1,11,5)	119.5	R(1,2)	1.489	A(2,1,3)	107.5
R(1,2)	1.477	A(2,1,4)	111.1	R(1,6)	1.082	A(6,1,11)	115.9	R(1,3)	1.489	A(2,1,5)	110.5
R(1,5)	1.685	A(3,1,5)	106.1	R(5,11)	1.337	A(10,5,11)	115.5	R(1,4)	1.491	A(3,1,5)	11193
R(1,4)	1.475	A(1,5,7)	124.6	R(5,10)	1.084	A(1,11,14)	121.4	R(1,5)	1.619	A(4,1,5)	111.6
R(5,6)	1.035	A(1,5,6)	118.8	R(2,3)	1.389	A(5,11,14)	119.0	R(5,6)	1.720	A(1,5,6)	162.4
R(5,7)	1.955	A(6,5,7)	115.1	R(3,4)	1.388	A(11,14,13)	178.0	R(6,13)	1.737	A(5,6,13)	117.7
R(7,8)	1.603	A(5,7,9)	100.7	R(4,5)	1.387	A(12,13,14)	118.6	R(6,15)	1.741	A(5,6,15)	113.2
R(7,9)	1.607	A(5,7,10)	104.4	R(5,11)	1.337	A(15,13,14)	116.9	R(13,14)	0.955	A(5,6,7)	105.9
R(7,10)	1.597	A(5,6,21)	174.8	R(5,10)	1.084	A(16,12,13)	105.5	R(15,16)	0.957	A(7,6,13)	95.2
R(11,12)	1.385	A(6,21,11)	123.8	R(11,14)	1.526	A(13,12,18)	106.2	R(6,7)	1.893	A(7,6,8)	116.5
R(11,16)	1.082	A(6,21,15)	117.1	R(14,13)	1.052	A(13,12,20)	109.3	R(7,8)	1.047	A(8,7,9)	119.4
R(11,21)	1.336	A(11,12,21)	122.5	R(13,12)	1.699	A(12,16,17)	111.5	R(7,9)	1.691	A(7,9,11)	111.5
R(12,13)	1.389	A(16,11,21)	116.3	R(13,15)	1.874	A(13,15,22)	106.5	R(9,10)	1.473	A(7,9,10)	109.8
R(12,17)	1.080	A(11,12,13)	118.5	R(12,16)	1.629	A(13,15,24)	97.46	R(9,11)	1.475	A(7,8,27)	174.2
R(13,14)	1.387	A(12,13,14)	118.9	R(12,18)	1.625	A(15,26,27)	122.2	R(9,12)	1.486	A(8,27,17)	116.7
R(13,18)	1.081	A(12,13,18)	120.4	R(12,20)	1.641	A(15,22,23)	119.6	R(8,27)	1.545	A(8,27,21)	124.0
R(14,15)	1.387	A(14,15,21)	122.2	R(15,22)	1.735			R(17,27)	1.339	A(22,17,27)	115.6
R(15,20)	1.083			R(15,24)	1.755			R(17,22)	1.084		
R(15,21)	1.337			R(15,26)	1.751			R(21,26)	1.082		
R(21,6)	1.581			R(22,23)	0.9570			R(17,18)	1.387		
				R(20,21)	0.9599			R(20,21)	1.385		
								R(18,19)	1.387		
								R(19,20)	1.389		

Table. 3: Total energies (−Eₜ/hartrees), interaction energies (Eᵢ/hartrees) and Mulliken atomic charges of q(Al), q(Si), q(Si'),
q(O), q(H), and q(S) atoms, of pyridine, cluster and complexes.

	−Eₜ	Eᵢ	q(Al)	q(Si)	q(Si')	q(O)ᵃ	q(H)ᵃ	q(N_Pyridine)
Pyridine	248.4							-0.4224
B₁	611.4		1.050	1.197		-1.087	0.527	
B₁OH	1063		2.020	2.397		-2.226	0.539	
B₂	1128		2.066	1.207	1.274	-1.093	0.528	
B₁—Pyridine	859.8	-0.0131	1.054	1.211		-1.149	0.528	-0.4810
B₁OH—Pyridine	1311.4	-0.0164	2.011	2.407		-1.184	0.513	-0.4791
B₂—Pyridine	1376.4	-0.0182	2.063	1.279	1.217	-1.164	0.523	-0.4840

ᵃ *O and H atoms are the atoms of the OH bridge group of zeolite.*

Table 4: Topological properties of the charge density at the line critical point of pyridine, B₁, B₁OH, and B₂:
total density ρ(r), Laplacian density ∇²ρ(r), and ellipticity ε.

	Molecule	a	b	c	d	e	f	g	j	r	t	z
ρ(r)	Pyridine									0.3506	0.3201	0.2976
	B₁	0.0044	0.3640	0.1275	0.1239	0.1165	0.0773	0.0793				
	B₁OH	0.1187	0.3589	0.1454	0.1451	0.0535	0.1013	0.1032				
	B₂	0.1129	0.3642	0.1282	0.1227	0.0532	0.1002	0.3707	0.1417			
∇²ρ(r)	Pyridine											
	B₁	-0.0703	0.6748	-0.046	-0.436	-0.166	-0.060	-0.014		0.2603	0.2722	0.3018
	B₁OH	-0.1639	0.6715	-0.227	-0.227	-0.089	-0.193	-0.197				
	B₂	-0.1521	0.6779	-0.041	-0.046	-0.092	-0.201	0.6619	-0.2389			
ε	Pyridine									0.1300	0.2064	0.2973
	B₁	0.0023	0.0088	0.0367	0.0309	0.0799	0.0007	0.0103			0.2722	
	B₁OH	0.0748	0.0092	0.0938	0.0894	0.0362	0.0779	0.0836				
	B₂	0.0722	0.0096	0.0289	0.0310	0.0178	0.0190	0.0015	0.0017			

Table 5: Topological properties of the charge density at the line critical point of B₁-pyridine, B₁OH-pyridine, and B₂-pyridine
complexes: total density ρ(r), Laplacian of the density ∇²ρ(r), energy density and electron delocalization index (δ).

q (N…H)	ρ (r)	∇²ρ(r)	Energy Density	δ
B₁—Pyridine	0.098	0.033	- 0.046	0.22
B₁OH—Pyridine	0.21	-0.92	- 0.29	0.38
B₂—Pyridine	0.091	0.054	- 0.037	0.21

$$\chi = -\frac{1}{2}\left(\varepsilon_{HOMO} + \varepsilon_{LUMO}\right) \tag{1}$$

$$\mu = -\chi = \frac{1}{2}\left(\varepsilon_{HOMO} + \varepsilon_{LUMO}\right) \tag{2}$$

$$\eta = \frac{1}{2}\left(\varepsilon_{LUMO} - \varepsilon_{HOMO}\right) \tag{3}$$

$$S = \frac{\eta}{2} \tag{4}$$

$$\omega = \frac{\mu^2}{2\eta} \tag{5}$$

According to *Parr et al.,* electrophilicity index (ω) [30] is a global reactivity index similar to the chemical hardness and chemical potential. This is a positive and conclusive quantity. This new reactivity index measures the stabilization in energy when the system reserves additional electronic charge (ΔN). The direction of the charge transfer is determined by the electronic chemical

Table 6: Topological parameters of the pyridine, B_1OH, B_1 and B_2 compounds.

Sample	ε_{HOMU} (eV)	ε_{LUMO} (eV)	χ (eV)	μ (eV)	η (eV)	S (eV)	ω (eV)
Pyridine	-0.2617	-0.0356	0.1487	-0.1087	0.1130	0.0565	0.0978
B_1OH	-0.4637	0.1102	0.1768	-0.1768	0.2869	0.1435	0.0544
B_2	-0.4355	0.0981	0.1687	-0.1687	0.2668	0.1334	0.0533
B_1	-0.3910	0.0780	0.1565	-0.1565	0.2345	0.1173	0.0522

the potential of the molecule because an electrophile is a chemical species capable of accepting electrons from the environment; its energy must decrease upon accepting an electronic charge. So its electronic chemical potential must be negative. The energies of frontier molecular orbitals (ε_{HOMU}, ε_{LUMO}), for pyridine and zeolites molecules, are listed in Table 6.

In the reaction between two molecules, the molecule with a lower value of electrophilicity index can act as a nucleophile. The values of μ are listed in Table 6 that show pyridine is good nucleophile, so that nucleophile can attack to B_1, B_1OH, and B_2. Electrophilic charge transfer (ECT) [28] is explained as the difference between the ΔN_{max} values of interacting molecules. We consider two molecules A(pyridine) and B(B_1, B_1OH and B_2) approach to each other, where two cases exits, (i) ECT > 0, charge flow from B to A, (ii) ECT < 0, charge flow from A to B. ECT is calculated as the following equation:

$$ECT = \left(\Delta N_{max}\right)_A - \left(\Delta N_{max}\right)_B \qquad (6)$$

Where $(\Delta N_{max})_A = \mu_A / \eta_A$ and $(\Delta N_{max})_B = \mu_B / \eta_B$.

We have obtained ECT as 0.306421, 0.255238 and 0.271601 for B_1—pyridine, B_1OH—pyridine and B_2—pyridine complexes, respectively. These results show that electrons are transferred from the pyridine to zeolites. Therefore, all zeolites treat as an electron acceptor and pyridine so treats as an electron donor. As shown in Table 6, the high value of μ for pyridine favor its nucleophilic behavior.

Local reactivity descriptors

The Fukui Function (FF) [32,33] or frontier function (f_k^+, f_k^-) measures changes in electron number (removing electrons from the HOMO or adding electrons to the LUMO, respectively) in chemical reactions and has been used to predict the reactivity of sites in a molecule.

This function is a local density functional descriptor which is calculated using the procedure proposed that based on a finite difference method by Yang and Mortier [34].

In this work, the two functions f^+ and f^- were used to determine electrophilic and nucleophilic attack, respectively. These functions can be given by

$$f_k^+ = q_k^{(N+1)} - q_k^{(N)} \qquad \text{For atom k as an electrophile} \qquad (7)$$

$$f_k^- = q_k^{(N)} - q_k^{(N-1)} \qquad \text{For atom k as a nucleophile} \qquad (8)$$

Where the parameter $q_k^{(N)}$ is the electron population on atom k which equals to the difference between an atomic number of atom k and charge obtained from NBO calculations for the molecule. These functions are calculated at MP2/cc-PVTZ level theory. Electrophilic reactivity descriptors (f_k^+) and nucleophilic reactivity descriptors (f_k^-) for all molecules are listed in Table 7. The maximum values of the nucleophilic reactivity descriptors at H_6, H_{14}, and H_8 indicate that these sites are more prone to electrophilic attack in B_1, B_1OH, and B_2 molecules, respectively. So that, we can say the N atom of pyridine attacks to H atom of the OH bridged group of zeolite clusters, in zeolite complexes.

CONCLUSIONS

The structural, vibrational, and topological properties of the molecular complexes between pyridine and a series of B_1, B_1OH, and B_2 clusters have been studied at MP2/cc-PVTZ levels theory. The hydrogen bonding between the N atom of the pyridine molecule and the OH zeolite groups has been assigned as the dominant interaction. We have shown that the OH frequencies of the bridged groups are decreased by the effect of the complex formation in the adsorption of pyridine into zeolites. Electrophilic Charge Transfer (ECT) confirms

Table 7: Selected reactivity descriptors indexes of the pyridine, B₁, B₂, and B₁OH compounds.

		q(N)	q(N-1)	q(N+1)	f_k^+	f_k^-
Pyridine N		-0.4224	-0.3851	-0.6285	0.2060	0.0372
B_1	H_6	0.5276	0.5466	0.4160	0.1116	0.0189
B_2	H_8	0.5310	0.5464	0.3888	0.1421	0.0226
	H_{14}	0.4963	0.5136	0.4426	0.0537	0.0173
	H_{16}	0.4792	0.5019	0.4472	0.0320	0.0154
B_1OH	H_3	0.5499	0.5652	0.4401	0.1098	0.0142
	H_6	0.5068	0.5217	0.4068	0.0999	0.0148
	H_8	0.5322	0.5309	0.4981	0.0340	0.0032
	H_{10}	0.5059	0.5316	0.3807	0.1251	0.0257
	H_{12}	0.4831	0.51558	0.4244	0.0587	0.0323
	H_{14}	0.4820	0.5163	0.4361	0.0458	0.0343
	H_{16}	0.4906	0.5217	0.4298	0.0607	0.0310

electrons are transferred from the zeolites to pyridine. So that, the pyridine treats as an electron acceptor and so all zeolites treat as an electron donor.

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