Research Article

Synthesis and Theoretical Study of the Novel 2-Oxopyrimidin-1(2H)-yl-Amides Derivative

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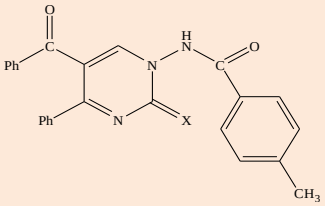
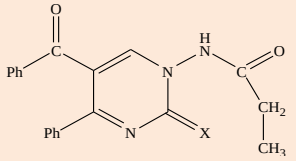
Abstract

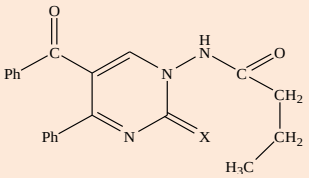
The 1-amino-5-benzoyl-4-phenyl-1*H*-pyrimidine-2-one/-thione (1a-b) were synthesized with the reaction of 4-benzoyl-5-phenyl-2,3-furandione and acetophenonsemicarbazone/-thiosemicarbazone. The study was extended to reactions of the compounds (1a-b) with acide chlorides (2a-d). Thus, some new pyrimidine derivatives (3a-h) were synthesized. The novel 2-oxopyrimidin-1(2*H*)-yl-amides derivatives were characterized by elemental analysis, IR, ^{1}H and ^{13}C NMR spectral data. All of them were evaluated according to their previous analogues. In addition to experimental analysis, quantum-mechanical calculations for derivatives of 2-oxopyrimidin-1(2*H*)-yl-amides were performed by using B3LYP method with the 6-311G(d,p), 6-311++G(2d,2p) basis sets in order to find molecular properties. As a result, both frontier orbital energies for the containing-sulphur molecules were found low while these energies were high for the containing-oxygen molecules.



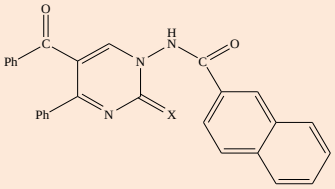
3a, 3b



3c, 3d



3e, 3f



3g, 3h

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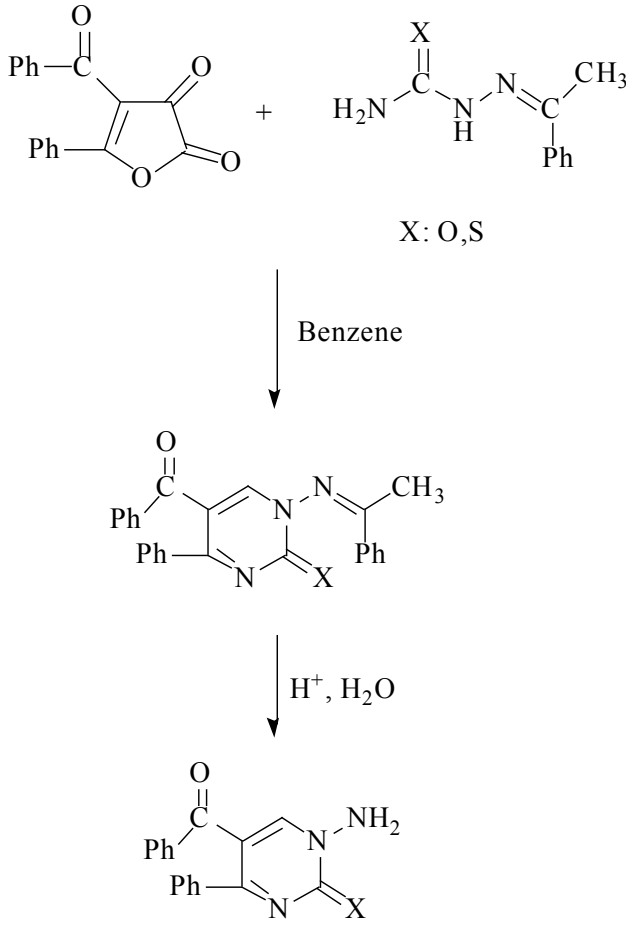
Introduction

Pyrimidines bases are an integral part of nucleic acids and natural products. They show various interesting pharmacological properties including antiviral, antiparasitic, antibacterial and antitumor [1-4]. Some of pyrimidines are used in many drugs for the treatment of some diseases such as cancer chemotherapy, hypertension, HIV infection, hypothyroidy [5].

For these reasons, the aim of this study is to synthesize various pyrimidine derivatives to make notable contributions to this class of heterocyclic compounds. There were reports published about synthesis of some 1-aminopyrimidine-2(1*H*)-one/-thione derivatives 1a-b from 2,3-furandiones. It was reported that the 1-amino-5-benzoyl-4-phenyl-1*H*-pyrimidine-2-one/-thione 1a-b were obtained from acetophenonsemicarbazone and acetophenonthiosemicarbazone with 4-benzoyl-5-phenyl-furan-2,3-dione **Scheme 1** [6-8].



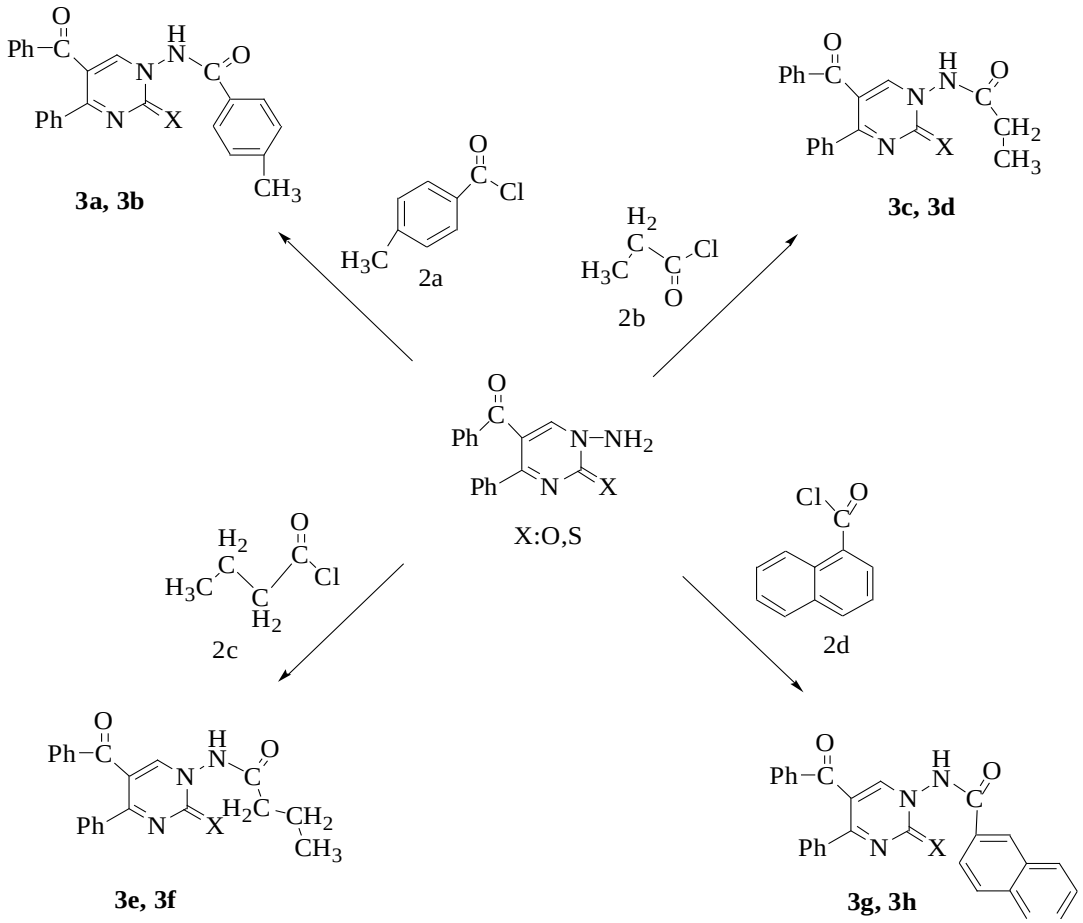
Scheme 1 Synthesis of the compounds 1a, 1b

The 1-amino-pyrimidine derivatives exhibiting a free N-NH_2 moiety was applied to several subsequent reactions. Recently, the reactions of 1-amino-pyrimidine derivatives with several anhydrides, isocyanates, isothioyanatesand 1,3-dicarbonyl compounds have been performed at various temperatures and in different solvents [9-14]. Nucleophilic attack at the 1-amino-pyrimidine derivatives nitrogen caused to begin the reactions.

In this study, the reactions of compounds 1a-b with some acide chlorides 2a-d, yielding the new series of 2-oxopyrimidin-1(2*H*)-yl-amides 3a-h, have been examined in **Scheme 2**. Also the present work deals with DFT computations with B3LYP in Gaussian 03 (revision D.01) package [15] to calculate dipole moments (DM), lowest unoccupied molecular orbital energy (E_{LUMO}), the highest occupied molecular orbital energy (E_{HOMO}), the energy gap (ΔE), molecular volume (MV), sum of the total negative charge (TNC), chemical potential (μ), softness (σ), chemical hardness (η), global electrophilicity (ω), electronegativity (χ), sum of electronic and zero-point energies (SEZPE). The scheme of the reactions studied is presented in Scheme 1. Lately, there have been several researches to understand the relationship between synthesis of new compounds and quantum-mechanical calculations by using B3LYP [16-19].

Computational detail

The DFT calculations with basis sets of the B3LYP/6-311G(d,p) and the B3LYP/6-311++G(2d,2p) were used to compute E_{HOMO}, E_{LUMO}, ΔE, DM, MV, TNC, η, σ, π,μ, χ, ω and SEZPE.



Scheme 2 Synthesis of the 2-Oxopyrimidin-1(2*H*)-yl-amides (3a-h)

Results and discussion

N-aminopyrimidine derivatives 1a-b were synthesized based on the procedures available in the literature (Scheme 1) [9-14]. 2-oxopyrimidin-1(2*H*)-yl]-amides derivatives 3a-h in moderate yielding (51-67%) as shown in Scheme 2 were obtained with the reactions of the compounds 1a-b with some acide chlorides 2a. All the reactions were performed by stirring in acetonitrile at room temperature, (for details see Experimental Section).

The reactions are generally initiated with the nucleophilic attack of the nitrogen atom of 1 to the carbonyl group of the acide chlorides 2a-d. In compounds 2, carbonyls' carbons have electrophilic sites and react with nucleophiles in the reaction. In compounds 2, carbonyls' carbons represent electrophilic sites and could be used for the construction reaction with nucleophiles. Reaction might be initiated with the lone pair electrons belonging to nitrogen atom of 1a-b to the carbonyls' carbons of 2a-d. We represented in detail the reaction pathway of 1 with 2 as outlined in Scheme 2. The novel synthesized compounds 3a-h were purified by recrystallization and their structures were confirmed by ^{1}H NMR, IR spectroscopic techniques and elemental analysis which supported the assignment.

In the first experiment, the product N-5-benzoyl-4-phenyl-2-oxopyrimidin-1(2*H*)-yl-4-methylbenzamide (3a) was obtained with a 54% yield by treating (1a) with benzoyl chloride (2a) and by stirring them in 3 mL acetonitrile at room temperature for 24 h. In the IR spectra of compound 3a, the absorption band of -N-H is observed at about 3203.5 cm^{-1}. The C=O absorption bands are found to be 1693.4, 1647.1 cm^{-1}.

The multiple peaks between 7.30-7.91 ppm belong to the aromatic protons for 3a. The peak at 12.11 ppm represents the -NH. In the ^{13}C NMR spectrum of 3a, the peaks corresponding to 191.59 ppm and 166.57 ppm indicate

the presence of (Ph-C=O, benzoyl) and (Ph-C=O, amide) groups. The results of measurements of 3b-h were given in the experimental part.

Molecular structure

E_{HOMO}, E_{LUMO}, ΔE, DM, MV, TNC, η, σ, μ, χ, ω, SEZPE were calculated for the 2-oxopyrimidin-1(2*H*)-yl-amides 3a-h molecule by using the B3LYP/6-311G(d,p) and B3LYP/6-311++G(2d,2p) for gas phase and B3LYP/6-311G(d,p) for solvent phase, as shown in **Figures 1** and **2**. HOMO-LUMO gap is smaller when the basis set of atomic orbitals are magnified due to the changing of HOMO, usually to a more negative energy, and decreasing in energy of LUMO [20].

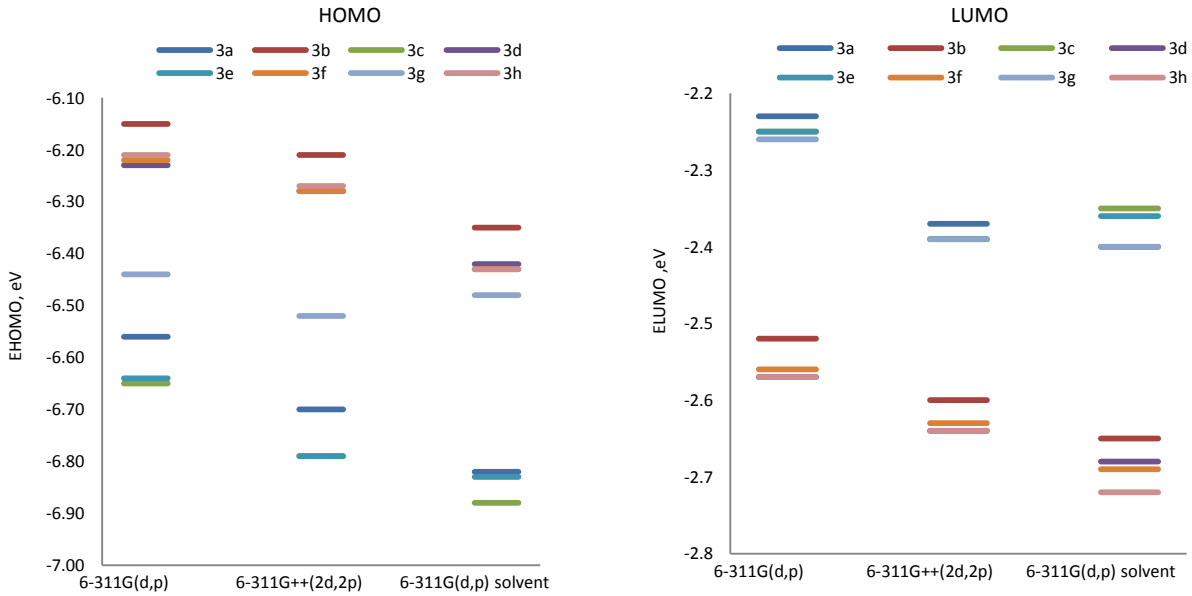


Figure 1 The calculated HOMO and LUMO parameters for the non-protonated for gas and solvent phase compounds using B3LYP/6-311G(d,p), B3LYP/6-311++G(2d,2p) methods

The calculated E_{HOMO} increases in the sulfur-containing molecules while E_{LUMO} will decrease. E_{HOMO} values for 3a, 3c, 3e and 3g molecules containing oxygen atom are -6.56, -6.65, -6.64, -6.44 eV, respectively. For ones including sulphur atom (3b, 3d, 3f and 3h molecules) the values are -6.15, -6.23, -6.22, and -6.21 eV, respectively. There is no significant change in the E_{HOMO} values according to length of the chain. Higher E_{HOMO} is essential for molecular reaction with nucleophiles while lower E_{LUMO} reacts easily with electrophiles [21].

ΔE of 3a, 3c, 3e and 3g molecules is 4.33, 4.40, 4.39, 4.18 eV, respectively. Similar situation is observed for 3b, 3d, 3f and 3h molecules their values are 3.63, 3.66, 3.66, and 3.64 eV, respectively. ΔE for sulfur containing molecules is less than containing oxygen molecules. 3a, 3c, 3e and 3g molecules are found more stable than 3b, 3d, 3f and 3h molecules due to the fact that a large HOMO-LUMO gap is observed.

The average values of the HOMO and LUMO energies have been defined as the electronegativity (χ). The chemical potential (μ) was defined as the first derivative of the total energy with respect to the number of electrons. The negative of the electronegativity was known as chemical potential. Chemical potential, electronegativity, and hardness are descriptors for the predictions about chemical properties of molecules. Chemical potential sulfur containing molecules are generally lower than the oxygen containing molecules, except the molecules containing 1-naphthamide (3g and 3h).

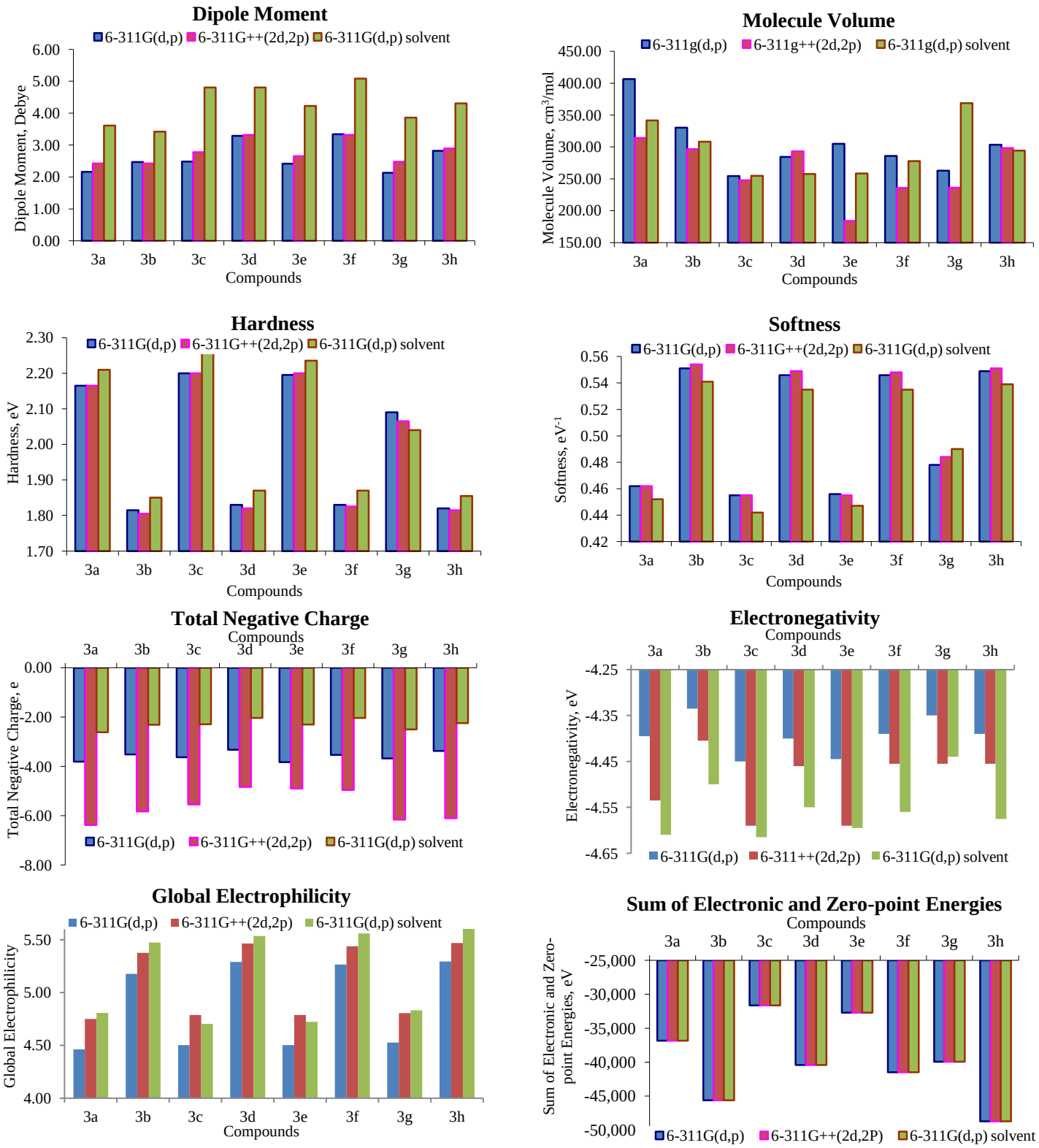


Figure 2 The calculated quantum chemical parameters for the non-protonated for gas and solvent phase compounds using B3LYP/6-311G(d,p), B3LYP/6-311++G(2d,2p) methods

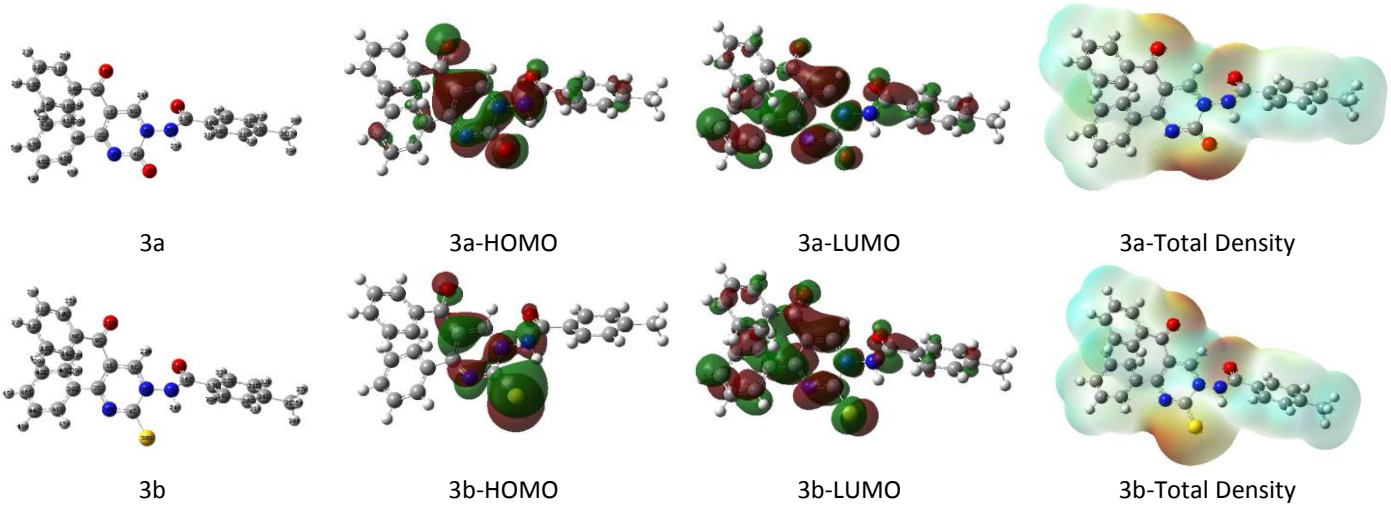
Total electronic charge values calculated with the 6-311++G(2d,2p) basis sets are higher than calculated with 6-311G(d,p) basis set. Total electronic charge values are lower in solvent phase than in gas phase. As can be seen from **Figure 3** negative charge densities are concentrated around oxygen atoms for 3a, 3c, 3e, 3g molecules and concentrated around oxygen atoms and sulphur atoms for 3b, 3d, 3f, 3h molecules.

The hardness and softness is widely used in chemistry for explaining stability of compounds. The hardness is just half the energy gap between the E_{HOMO} and E_{LUMO}. If a molecule has a large energy gap, it is called hard and, otherwise is called soft [22].

Chemical hardness was initially introduced as a global electrophilicity (ω) of molecules which is simply defined as $\omega=\mu^2/2\eta$ for measuring of the stabilization in energy when additional electronic charge ΔN from the environment is acquired from the environment. Analysis of the calculated electrophilicity values shows that the presence of sulphur atom in the molecule increases the electrophilicities of the molecules. In fact, the sulphur containing molecules have low both frontier orbital energies, while these energies are high for oxygen containing molecules. So, the presence of oxygen atom has the least electrophilicity in the under study molecule series. The calculated electrophilicities is affected by the change in basis set, and also according to calculations conducted in liquid or gas phase.

A typical electron density distribution of HOMO and LUMO 3a, 3b, 3c, 3d, 3e, 3f, 3g are shown in Figure 3. HOMO and LUMO were calculated with AOmix program [23-24] after optimization of molecules. HOMO orbitals for 3a, 3c, 3e, 3g consist of + 10.8% 3pz(C1) + 7.4% 4pz(C1) + 4.8% 2pz(C1) + 4.7% 3pz(O7) - 4.6% 3pz(N5) + 4.1% 4pz(O7); + 11.0% 3pz(C1) + 7.6% 4pz(C1) + 4.9% 2pz(C1) + 4.8% 3pz(O43) - 4.3% 3pz(N5) + 4.1% 4pz(O43); + 10.9% 3pz(C1) + 7.5% 4pz(C1) + 4.9% 2pz(C1) + 4.5% 3pz(O42) - 4.2% 3pz(N5) - 3.9% 3py(O15); + 7.2% 3pz(C46) - 7.2% 3pz(C40) - 6.2% 4pz(C40) + 6.0% 4pz(C46) + 5.8% 3pz(C37) - 5.1% 3pz(C47) and their LUMO consist of 8.9% 3pz(C2) + 5.9% 4pz(C2) - 5.3% 4pz(C6) - 4.6% 3pz(C6) + 4.4% 2pz(C2) - 4.2% 3pz(N3); + 9.4% 3pz(C2) + 6.2% 4pz(C2) - 5.2% 4pz(C6) + 4.7% 2pz(C2) - 4.5% 3pz(N3) - 4.2% 3pz(C6); + 9.1% 3pz(C2) + 6.0% 4pz(C2) - 5.2% 4pz(C6) + 4.5% 2pz(C2) - 4.4% 3pz(N3) - 4.3% 3pz(C6). As seen from Figure 3 and given above HOMO of 3a, 3c, 3e, 3g molecules consist of mainly C1, O7 and N5 atoms. HOMO orbitals for 3b, 3d, 3f, 3h consist of mainly S50 and C1 atoms.

Sum of electronic and zero-point Energies (SEZPE) for molecules containing sulphur atom (3b, 3d, 3f, 3h) is higher than those containing oxygen atom (3a, 3c, 3e, 3g). In Figure 2 total electron density is also given. This figure shows that there is much more electron density in the vicinity of oxygen atoms for 3a, 3c, 3e, 3g molecules, oxygen and sulphur atom for 3b, 3d, 3f, 3h molecules.



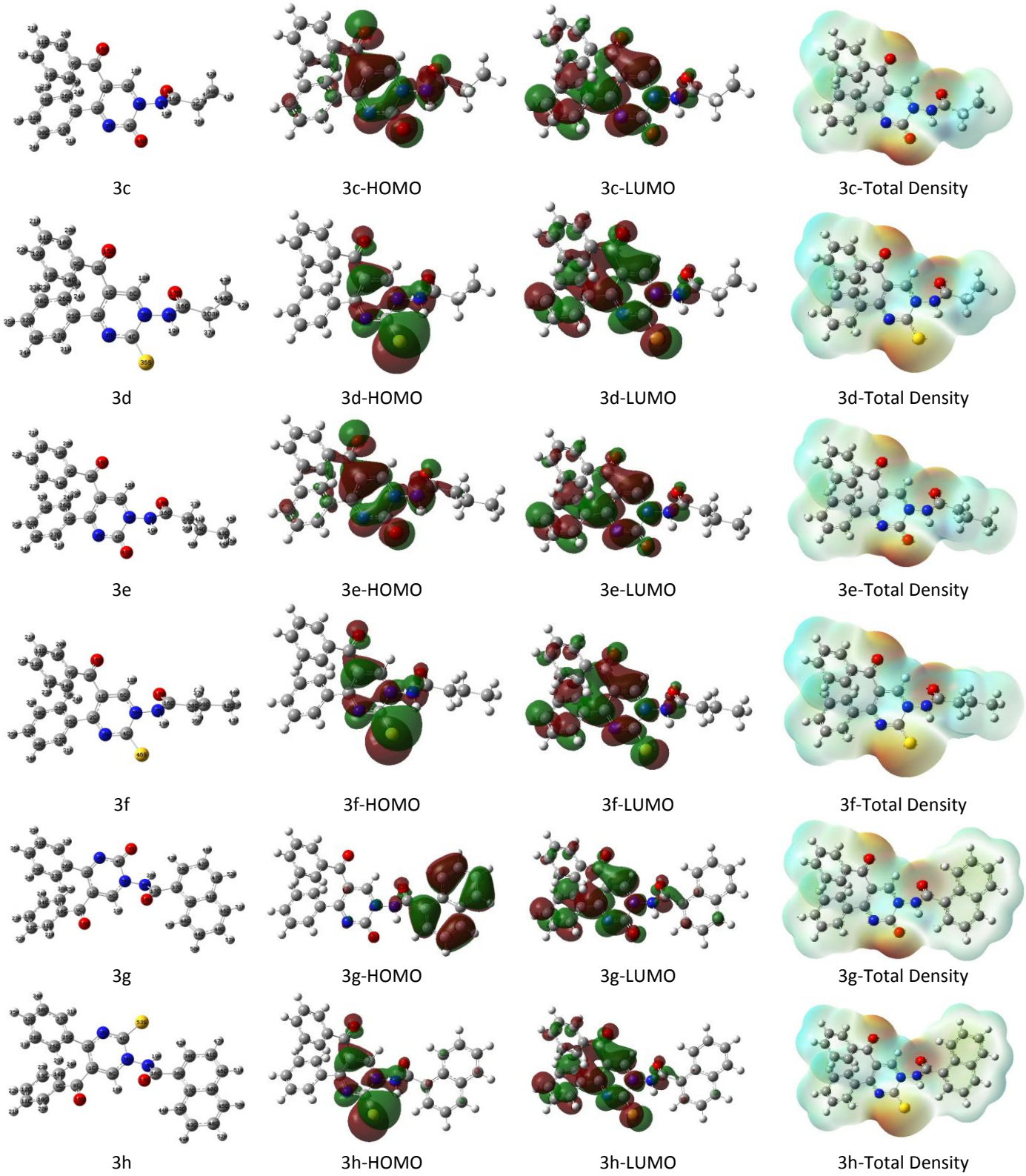


Figure 3 The optimized molecular structures, HOMO, LUMO and total density of the non-protonated inhibitor molecules using DFT/B3LYP/6-311++G(2d,2p)

Experimental

Solvents were refluxed with the appropriate drying agent and distilled before use. Microanalyses were performed using Carlo Erba elemental analyser, model 1108. The IR spectra were recorded on a Shimadzu Model 8400 FT IR spectrophotometer. Melting points were performed on an Electrothermal 9200 apparatus and are uncorrected. The ^{1}H and ^{13}C NMR spectra were recorded on Bruker-400 MHz Ultra Shield instrument. The chemical shifts reported in ppm from tetramethylsilane as an internal standard were given in δ (ppm). TLC using DC Alufolien Kieselgel 60 F_{254} Merck and Camag TLC lamp (254/366 nm) were used to follow experiments.

General Procedure for the Preparation of Compounds (3a-h)

0.2 g 1-amino-5-benzoyl-4-phenyl-1*H*-pyrimidine-2-one/-thione (**1a-b**) and acide chlorides (**2a-d**) (1:4 mol) were dissolved in 3 mL acetonitrile at room temperature. The reaction mixture was stirred by a magnetic stirrer at room temperature for 24 h. The solvent was evaporated. Then, the residue was treated with dry diethyl ether. The solid products **3a-h** were collected by filtration and thoroughly with water and crystallization from n-butanol and allowed to dry on P_2O_5.

N-(5-benzoyl-2-oxo-4-phenylpyrimidin-1(2H)-yl)-4-methylbenzamide (3a)

Yield 57%; m.p.: 268 ^{o}C; IR (KBr, cm^{-1}): 3203.5 ν (-N-H), 3058.9 ν (aromatic C-H), 2950 ν (-CH_3), 1693.4-1647.1 ν (C=O), 800-670 ν (pyrimidine ring); ^{1}H NMR ($CDCl_3$, δ): 12.11 (s, 1H, N-H), 7.30-7.91 (m, 15H, ArH), 2.42 ppm (s, 3H, -CH_3); ^{13}C NMR ($CDCl_3$): δ=191.59 (C=O, benzoyl), 166.57 (C=O, amide), 152.80 (C=O, pyrimidine ring), 154.87-116.60 (aromatic C), 21.59 ppm (-CH_3). Anal. calc. for $C_{25}H_{19}N_3O_3$: C, 73.34; H, 4.67; N, 10.26%; Found: C, 73.05; H, 4.51; N, 10.08%.

N-(5-benzoyl-2-thioxo-4-phenylpyrimidin-1(2H)-yl)-4-methylbenzamide (3b)

Yield 65%; m.p.: 260 ^{o}C; IR (KBr, cm^{-1}): 3203.5 ν (-N-H), 3066.6 ν (aromatic C-H), 2964.4 ν (-CH_3), 1693.4-1647.1 ν (C=O), 1200.1 ν (C=S), 800-670 ν (pyrimidine ring); ^{1}H NMR ($CDCl_3$, δ): 11.15 (s, 1H, N-H), 7.96-7.11 (m, 15H, ArH), 2.50 ppm (s, 3H, -CH_3); ^{13}C NMR ($CDCl_3$): δ=190.85 (C=O, benzoyl), 166.72 (C=O, amide), 158.80 (C=S, pyrimidine ring), 143.91-117.26 (aromatic C), 21.61 ppm (-CH_3). Anal. calc. for $C_{25}H_{19}N_3O_2S$: C, 70.58; H, 4.47; N, 9.88; S, 7.53%; Found: C, 70.35; H, 4.51; N, 10.08; S, 7.33%.

N-(5-benzoyl-2-oxo-4-phenylpyrimidin-1(2H)-yl)propanamide (3c)

Yield 63%; m.p.: 260 ^{o}C; IR (KBr, cm^{-1}): 3219.0 ν (-N-H), 3058.9 ν (aromatic C-H), 2970.2 ν (-CH_3), 1726.2-1664.4 ν (C=O), 800-670 ν (pyrimidine ring); ^{1}H NMR ($CDCl_3$, δ): 11.52 (s, 1H, N-H), 7.91-7.13 (m, 11H, ArH), 2.35 (s, 2H, -CH_2-), 1.0 ppm (s, 3H, -CH_3); ^{13}C NMR ($CDCl_3$): δ=189.52 (C=O, benzoyl), 168.81 (C=O, amide), 157.57 (C=S, pyrimidine ring), 150.41-111.10 (aromatic C), 27.10 ppm (-CH_2-), 11.25 ppm (-CH_3). Anal. calc. for $C_{20}H_{17}N_3O_2$: C, 69.16; H, 4.89; N, 12.10%; Found: C, 68.91; H, 4.96; N, 11.98%.

N-(5-Benzoyl-2-thioxo-4-phenylpyrimidin-1(2H)-yl)propanamide (3d)

Yield 67%; m.p.: 280 ^{o}C; IR (KBr, cm^{-1}): 3215.0 ν (-N-H), 3050.9 ν (aromatic C-H), 2975.2 ν (-CH_3), 1720.2-1654.4 ν (C=O), 800-670 ν (pyrimidine ring); ^{1}H NMR ($CDCl_3$, δ): 11.45 (s, 1H, N-H), 7.91-7.03 (m, 11H, ArH), 2.45 (s, 2H, -CH_2-), 1.01 ppm (s, 3H, -CH_3); ^{13}C NMR ($CDCl_3$): δ=188.82 (C=O, benzoyl), 171.38 (C=O, amide), 158.57 (C=O, pyrimidine ring), 147.41-116.18 (aromatic C), 27.19 ppm (-CH_2-), 11.10 ppm (-CH_3). Anal. calc. for $C_{20}H_{17}N_3O_2S$: C, 66.10; H, 4.71; N, 15.56; S, 8.82%; Found: C, 65.92; H, 4.51; N, 15.30; S, 8.68%.

N-(5-Benzoyl-2-oxo-4-phenylpyrimidin-1(2H)-yl)butanamide (3e)

Yield 60%; m.p.: 248 ^{o}C; IR (KBr, cm^{-1}): 3200.0 ν (-N-H), 3058.9 ν (aromatic C-H), 2802.4-2729.1 ν (-CH_3), 1652.9

ν (C=O), 800-770 ν (pyrimidine ring); ^{1}H NMR ($CDCl_3$, δ): 11.54 (s, 1H, N-H), 7.97-7.12 (m, 11H, ArH), 2.49 (t, 2H, -CH_2-C=O), 1.65 (h, 2H, -CH_2-CH_3), 0.95 ppm (t, 3H, -CH_3); ^{13}C NMR ($CDCl_3$): δ=191.60(C=O, benzoyl), 173.05 (C=O, amide), 152.61(C=O, pyrimidine ring), 154.57-116.30 (aromatic C), 35.43 (-CH_2-C=O) 18.57 (-CH_2-CH_3), 13.96 ppm (-CH_3). Anal. calc. for $C_{21}H_{19}N_3O_3$: C, 68.76; H, 5.44; N, 12.03%; Found: C, 69.04; H, 5.26; N, 11.98%.

N-(5-Benzoyl-2-thioxo-4-phenylpyrimidin-1(2H)-yl)butanamide (3f)

Yield 65%; m.p.: 258 ^{o}C; IR (KBr, cm^{-1}): 3205.0 ν (-N-H), 3048.9 ν (aromatic C-H), 2752.4-2729.1 ν (-CH_3), 1652.9 ν (C=O), 800-770 ν (pyrimidine ring); ^{1}H NMR ($CDCl_3$, δ): 11.57 (s, 1H, N-H), 8.07-7.15 (m, 11H, ArH), 2.39 (t, 2H, -CH_2-C=O), 1.55 (h, 2H, -CH_2-CH_3), 0.99 ppm (t, 3H, -CH_3); ^{13}C NMR ($CDCl_3$): δ=190.60(C=O, benzoyl), 166.05 (C=O, amide), 155.61(C=S, pyrimidine ring), 154.57-115.30 (aromatic C), 35.03 (-CH_2-C=O) 18.17 (-CH_2-CH_3), 13.66 ppm (-CH_3). Anal. calc. for $C_{21}H_{19}N_3O_2S$: C, 66.82; H, 5.06; N, 11.13; S,8.49%; Found: C, 66.82; H, 5.06; N, 11.13; S, 8.29%.

N-(5-Benzoyl-2-oxo-4-phenylpyrimidin-1(2H)-yl)-1-naphthamide (3g)

Yield 53%; m.p.: 289 ^{o}C; IR (KBr, cm^{-1}): 3292.3 ν (-N-H), 3051.2 ν (aromatic C-H), 1708.8-1639.4 ν (C=O), 800-770 ν (pyrimidine ring); ^{1}H NMR ($CDCl_3$, δ): 12.33 (s, 1H, N-H), 8.62-7.17 ppm (m, 18H, ArH); ^{13}C NMR ($CDCl_3$): δ=191.60(C=O, benzoyl), 173.44(C=O, amide), 152.76(C=O, pyrimidine ring), 154.84-116.67 ppm (aromatic C). Anal. calc. for $C_{28}H_{19}N_3O_3$: C, 75.50; H, 4.30; N, 9.40%; Found: C, 75.32; H, 4.46; N, 9.20%.

N-(5-Benzoyl-2-thioxo-4-phenylpyrimidin-1(2H)-yl)-1-naphthamide (3h)

Yield 51%; m.p.: 292 ^{o}C; IR (KBr, cm^{-1}): 3292.3 ν (-N-H), 3043.5 ν (aromatic C-H), 1683.7-1643.2 ν (C=O), 1683.7-1643.2 ν (C=O), 1240.1 ν (C=S) 800-770 ν (pyrimidine ring); ^{1}H NMR ($CDCl_3$, δ): 12.33 (s, 1H, N-H), 8.62-7.34 ppm (m, 18H, ArH); ^{13}C NMR ($CDCl_3$): δ=191.60 (C=O, benzoyl), 173.44 (C=O, amide), 166.74 (C=S, pyrimidine ring), 154.84-116.66 ppm (aromatic C). Anal. calc. for $C_{28}H_{19}N_3O_2S_1$: C, 72.88; H, 4.12; N, 9.11; S, 6.94%; Found: C, 72.68; H, 4.26; N, 9.20; S, 6.84%.

Conclusions

This research examined the synthesis 2-oxopyrimidin-1(2*H*)-yl]-amides derivatives. The results show that both frontier orbital energies for the containing-sulphur molecules were found low while these energies were high for the containing-oxygen molecules. So, the presence of oxygen atom has the least electrophilicity in the under study molecule series.

Acknowledgements

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