

# Ab-initio study of 'N'-hydroxy-pyrimidine-2-carboximidamide by Density Functional Theory

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The present work deals with the quantum mechanical study of the molecular structure of N'-hydroxy-pyrimidine-2-carboximidamide. The equilibrium geometry, harmonic vibrational frequencies and HOMO-LUMO gap have been calculated by the density functional theory (DFT), employing 6-311 G (d, p) as the basis set. A detailed interpretation of the calculated spectra of N'-hydroxy-pyrimidine-2-carboximidamide has been discussed in terms of the normal mode analysis. The thermodynamic calculations related to the title compounds were also performed at B3LYP/6-311 G (d, p) level of theory. The molecular HOMO, LUMO composition, energy gap, and MESP contours have also been drawn to explain the activity of N'-hydroxy-pyrimidine-2-carboximidamide.



## Introduction

An amide also known as an acid amide, is a compound with the functional group  $RnE(O)xNR'2$  (R and R' refer to H or organic groups). Most common are "organic amides" ( $n = 1, E = C, x = 1$ ), but many other important types of amides are known including phosphor amides ( $n = 2, E = P, x = 1$  and many related formulas) and sulfonamides ( $E = S, x = 2$ ) [1-3]. The term amide refers both to classes of compounds and to the functional group  $RnE(O)xNR'2$  within those compounds. Amide can also refer to the conjugate base of ammonia (the anion  $H2N^-$ ) or of an organic amine (an anion  $R2N^-$ ). For discussion of these "anionic amides", see Alkali metal amides. The remainder of this article is about the carbonyl-nitrogen sense of amide. Pain, fever and inflammation have been associated with mankind since beginning. Nonsteroidal antiinflammatory drugs (NSAIDs) are the first choice of drugs in the treatment of pain, degenerative inflammatory joint diseases and rheumatic disorders. In recent years, the dual inhibition of cyclooxygenase and 5-lypoxygenase enzymes for treatment of inflammation and pain has been introduced as a novel therapeutic target, and one of the first examples of dual acting analgesic and anti-inflammatory molecules was tepoxalin, a diarylpyrazole derivative. In addition, many studies also focused on pyridazine derivatives for developing potent and safer NSAIDs without gastric side effects. Among these compounds, 4-ethoxy-2-methyl-5-morpholino-3(2H) - pyridazinone (emorfazone) is currently being marketed in Japan as an analgesic and anti-inflammatory drug. Dogruer et al. subsequently synthesized [6-(4-methoxyphenyl)-3(2H)-pyridazinone-2-yl]acetamide and propanamide derivatives and reported that these compounds showed potential analgesic activity [4].

As a part of our ongoing research [5-12], the main objective of the present study is to investigate in detail the vibrational spectra of important biological molecule N'-hydroxy-pyrimidine-2-

carboximidamide. To the best of our knowledge no detailed DFT calculations have been performed on N'-hydroxy-pyrimidine-2-carboximidamide so far in the literature.

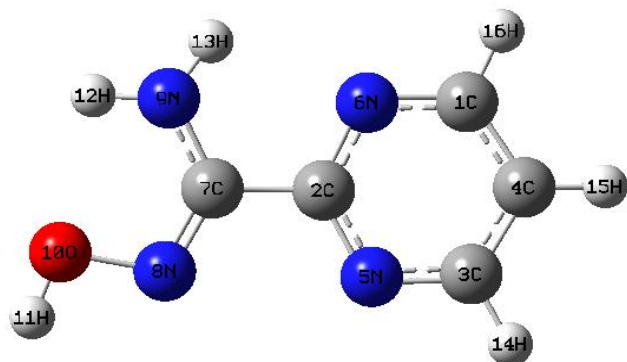
## Computational Methods

Initial geometry was generated from standard geometrical parameters and was minimized without any constraint in the potential energy surface. The gradient corrected Density Functional Theory (DFT) with the three-parameter hybrid functional (B3) [13] for the exchange part and the Lee-Yang-Parr (LYP) correlation function [14] has been employed for the computation of molecular structure, vibrational frequencies, HOMO-LUMO, and energies of the optimized structures, using GAUSSIAN 09 [15]. The calculated vibrational frequencies have also been scaled by a factor of 0.963 [16]. By combining the results of the GAUSSVIEW'S program [17] with symmetry considerations, vibrational frequency assignments were made with a high degree of accuracy. We used this approach for the prediction of IR frequencies of title compound and found it to be very straightforward. Density functional theory calculations are reported to provide excellent vibrational frequencies of organic compound if the calculated frequencies are scaled to compensate for the approximate treatment of electron correlation, for basis set deficiencies and for anharmonicity. A number of studies [18, 19] have been carried out regarding calculations of vibrational spectra by using B3LYP methods with 6-311 G (d, p) basis set. The scaling factor (0.963) was applied successfully for B3LYP method and was found to be easily transferable in a number of molecules. Thus vibrational frequencies calculated by using the B3LYP functional with 6-311G (d, p) as basis set, can be utilized to eliminate the uncertainties in the fundamental assignment in the IR spectra.

## Result and Discussions

### Optimization

Optimized parameters calculated by B3LYP method with 6-31G (d, p) as basis set are listed in Table 1 and are in accordance with the atom numbering scheme as shown in Figure 1. After geometry optimization local minimum energy obtained for structure optimization of N<sup>7</sup>-hydroxy-pyrimidine-2-carboximidamide with 6-311G (d, p) basis set is approximately total energy = -488.32717327 a.u. The (C-C) bond length varies between 1.3906-1.4887 Å, while (C-H) bond length, 1.0841-1.0888 Å. (C-N) bond length varies from 1.2955-1.3686 Å, while (N-O) bond length is at 1.4191 Å. (O-H) bond length is at 0.9654 Å, while (N-H) bond length varies from 1.0083-1.0091 Å. The (C-C-C) bond angle varies from 116.135-121.4148, while (C-C-H) bond angle is at 120.9112-121.9397. (C-C-N) bond angle varies from 115.1974-122.84, while (N-C-N) bond angle varies from 125.4525-125.9776. (N-C-H) bond angle varies from 115.4574-116.4524, while (N-O-H) bond angle is at 101.7627; whereas (C-N-O) bond angle is at 108.5637 degree.



**Fig. 1** Model molecular structure of N<sup>7</sup>-hydroxy-pyrimidine-2-carboximidamide

### Atomic charge, Polarizability, Hyper polarizability and Thermodynamic Properties:

The Mulliken atomic charges for all atoms of the N<sup>7</sup>-hydroxy-pyrimidine-2-carboximidamide compound are calculated by B3LYP, methods with 6-311G (d, p) as basis set in gas phase and are presented in Table (2).

Dipole moment ( $\mu$ ), polarizability  $\langle\alpha\rangle$  and total first static hyper polarizability  $\beta$  [20, 21] are also calculated (In Table 5 and 3) by using density functional theory. They can be expressed in terms of  $x$ ,  $y$ ,  $z$  components and are given by following equations 1, 2 and 3-

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2} \text{----- (1)}$$

$$\langle\alpha\rangle = 1/3 [\alpha_{xx} + \alpha_{yy} + \alpha_{zz}] \text{----- (2)}$$

$$\beta_{\text{Total}} = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2} \\ = [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yxx} + \beta_{yzz})^2 + (\beta_{zzx} + \beta_{zyy})^2]^{1/2} \text{--- (3)}$$

The  $\beta$  components of Gaussian output are reported in atomic units.

Where (1 a.u. = 8.3693X10<sup>-33</sup> e.s.u.).

**Table 1** Bond Lengths (Å) & Bond Angle of N<sup>7</sup>-hydroxypyrimidine-2-carboximidamide

S.No.	Parameters	Experimental Value	Calculated Value
<b>“Bond lengths”</b>			
1.	C <sub>1</sub> -C <sub>4</sub>	1.378	1.3906
2.	C <sub>1</sub> -N <sub>6</sub>	1.343	1.3368
3.	C <sub>1</sub> -H <sub>16</sub>	0.9500	1.0884
4.	C <sub>2</sub> -N <sub>5</sub>	1.336	1.3414
5.	C <sub>2</sub> -N <sub>6</sub>	1.347	1.3446
6.	C <sub>2</sub> -C <sub>7</sub>	1.494	1.4887
7.	C <sub>3</sub> -C <sub>4</sub>	1.376	1.3964
8.	C <sub>3</sub> -N <sub>5</sub>	1.343	1.3327
9.	C <sub>3</sub> -H <sub>14</sub>	0.9500	1.0888
10.	C <sub>4</sub> -H <sub>15</sub>	0.9500	1.0841
11.	C <sub>7</sub> -N <sub>8</sub>	1.295	1.2955
12.	C <sub>7</sub> -N <sub>9</sub>	1.362	1.3686
13.	N <sub>8</sub> -O <sub>10</sub>	1.424	1.4191
14.	N <sub>9</sub> -H <sub>12</sub>	0.92	1.0083
15.	N <sub>9</sub> -H <sub>13</sub>	0.89	1.0091
16.	O <sub>10</sub> -H <sub>11</sub>	0.94	0.9654
<b>“Bond Angles”</b>			
17	C <sub>2</sub> -C <sub>1</sub> -N <sub>6</sub>	116.0	122.2151
18	C <sub>4</sub> -C <sub>1</sub> -H <sub>16</sub>	118.6	121.3325
19	N <sub>6</sub> -C <sub>1</sub> -H <sub>16</sub>	118.6	116.4524
20	N <sub>5</sub> -C <sub>2</sub> -N <sub>6</sub>	125.9	125.9776
21	N <sub>5</sub> -C <sub>2</sub> -C <sub>7</sub>	118.5	118.8242
22	N <sub>6</sub> -C <sub>2</sub> -C <sub>7</sub>	115.6	115.1974
23	C <sub>4</sub> -C <sub>3</sub> -N <sub>5</sub>	122.4	122.84
24	C <sub>4</sub> -C <sub>3</sub> -H <sub>14</sub>	121.6	120.9112
25.	N <sub>5</sub> -C <sub>3</sub> -H <sub>14</sub>	118.8	116.2487
26.	C <sub>1</sub> -C <sub>4</sub> -C <sub>3</sub>	116.7	116.135
27.	C <sub>1</sub> -C <sub>4</sub> -H <sub>15</sub>	121.6	121.9253
28.	C <sub>3</sub> -C <sub>4</sub> -H <sub>15</sub>	121.6	121.9397
29.	C <sub>2</sub> -N <sub>5</sub> -C <sub>3</sub>	116.2	116.1664
30.	C <sub>1</sub> -N <sub>6</sub> -C <sub>2</sub>	116.0	116.6656
31.	C <sub>2</sub> -C <sub>7</sub> -N <sub>8</sub>	117.4	117.9473
32.	C <sub>2</sub> -C <sub>7</sub> -N <sub>9</sub>	117.1	116.592
33.	N <sub>8</sub> -C <sub>7</sub> -N <sub>9</sub>	125.5	125.4525
34	C <sub>7</sub> -N <sub>8</sub> -O <sub>10</sub>	108.7	108.5637
35	C <sub>7</sub> -N <sub>9</sub> -H <sub>12</sub>	118	115.888
36	C <sub>7</sub> -N <sub>9</sub> -H <sub>13</sub>	112	115.4574
37	H <sub>12</sub> -N <sub>9</sub> -H <sub>13</sub>	117	118.8071
38	N <sub>8</sub> -O <sub>10</sub> -H <sub>11</sub>	106.1	101.7627
39	C <sub>7</sub> -N <sub>9</sub> -H <sub>12</sub>	118	115.888
40	C <sub>7</sub> -N <sub>9</sub> -H <sub>13</sub>	112.9	115.4574
41	H <sub>12</sub> -N <sub>9</sub> -H <sub>13</sub>	117	118.8071
42	N <sub>8</sub> -O <sub>10</sub> -H <sub>11</sub>	106.1	101.7627

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For N<sup>7</sup>-hydroxy-pyrimidine-2-carboximidamide, the calculated dipole moment value is 4.2863Debye. Having higher dipole moment than water (2.16 Debye), N<sup>7</sup>-hydroxy-pyrimidine-2-carboximidamide can be used as better solvent. As we see a greater contribution of  $\alpha_{zz}$  in molecule which shows that molecule is elongated more towards Z direction and more contracted to Y direction.  $\beta_{xxx}$ ,  $\beta_{zzz}$  contribute larger part of hyper polarizability in the molecule. This shows that X axis plane and XZ plane are more optical active in these directions.

**Table 2** Mulliken charges for N'-hydroxy-pyrimidine-2-carboximidamide

S.No.	Atom	Atomic charge
1.	C	0.120241
2.	C	0.450841
3.	C	0.118006
4.	C	-0.098526
5.	N	-0.441368
6.	N	-0.502486
7.	C	0.363685
8.	N	-0.218116
9.	N	-0.599099
10.	O	-0.447150
11.	H	0.351010
12.	H	0.277959
13.	H	0.267904
14.	H	0.127183
15.	H	0.102428
16.	H	0.127487

**Table 3** Polarizability and hyperpolarizability of N'-hydroxy-pyrimidine-2-carboximidamide

Polarizability	
$\alpha_{xx}$	-40.5219
$\alpha_{xy}$	-0.1552
$\alpha_{yy}$	-53.3475
$\alpha_{yz}$	-1.0581
$\alpha_{zz}$	-58.5384
$\alpha_{zx}$	1.8430
$\alpha$	50.8026
Hyperpolarizability	
$\beta_{xxx}$	-15.6174
$\beta_{xxv}$	-14.4157
$\beta_{xvv}$	-11.3217
$\beta_{vyy}$	7.1199
$\beta_{zzz}$	-0.8181
$\beta_{xxx}$	-6.0478
$\beta_{xzz}$	-6.4822
$\beta_{vzz}$	-1.0708
$\beta_{vyz}$	-2.9789
$\beta_{xvz}$	0.8903
$\beta_{total}$	35.83159

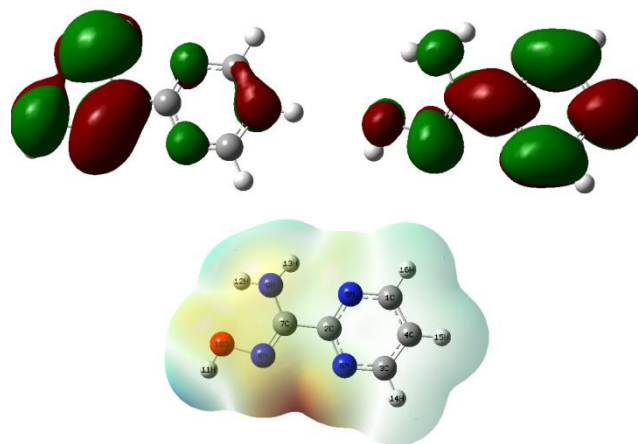
**Table 4** Thermodynamic parameters of N'-hydroxy-pyrimidine-2-carboximidamide

Parameter	E (Thermal) kcal/mol	C <sub>v</sub> (cal/mol- kelvin)	S (cal/mol- kelvin)
Total	80.795	32.462	90.568
Translational	0.889	2.981	40.679
Rotational	0.889	2.981	29.359
Vibrational	79.018	26.500	20.530

Several calculated thermodynamic properties based on the vibration analysis at B3LYP, 6-31G (d, p) level, like internal thermal energy (E), constant volume heat capacity CV, and entropy S, have been calculated and listed in table (4). At the room temperature, conduction band is almost empty so electronic contribution in total energy is negligible. Thermodynamic parameters clearly indicate that vibration motion plays a crucial role in assessing thermo dynamical behavior of title compounds.

### Electronic properties

The interaction with other species in a chemical system is also determined by frontier orbital's, HOMO and LUMO. It can also be determined by experimental data. The frontier orbital gap helps to distinguish the chemical reactivity and kinetic stability of the molecule. A molecule which has a larger orbital gap is more polarized having more reactive part as far as reaction is concerned [22]. The frontier orbital gap is 4.2788 eV for N'-hydroxypyrimidine-2-carboximidamide as given in Table (5). The contour plots of the HOMO, LUMO and MESP structures of the molecule are shown in Figure 2. The importance of MESP lies in the fact that it simultaneously displays molecular size, shape as well as positive, negative, and neutral electrostatic potential region in terms of grading and is very useful in the investigation of molecular structure with its physiochemical property relationship [23, 24].

**Fig. 2** HOMO (Left) - LUMO (Right) and MESP (Below) pictures of N'-hydroxypyrimidine-2-carboximidamide**Table 5** HOMO-LUMO gap and dipole moment of N'-hydroxy-pyrimidine-2-carboximidamide

Parameters	Value
Total energy E(a.u.)	-488.32717327
Dipole moment (Debye)	2.5804
LUMO	-0.04947
HOMO	-0.20678
Frontier Orbital Energy Gap (ev)	0.15731a.u ( 4.278832 eV)

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## Assignment of fundamentals

N<sup>7</sup>-hydroxypyrimidine-2-carboximidamide has 15 atoms with 42 normal modes of vibration. We made a reliable one-to-one correspondence between the fundamentals and the frequencies calculated by DFT (B3LYP) methods. The relative band intensities are also very satisfactory along with their position. Some important modes are discussed hereafter. The harmonic vibrational frequencies, calculated for the title molecule with vibrational assignments are given in Table (6).

**Table 6** Vibrational analysis of N<sup>7</sup>-hydroxypyrimidine-2-carboximidamide

FREQUENCY	IR INTENSITY	VIBRATIONAL ASSIGNMENT <sup>a</sup>
65	0.3875	Molecules bend from joint
118	6.0667	Molecules bend from joint
173	5.2696	$\tau$ (C-C-N-O)
258	1.9765	$\gamma$ (C-C-C)
323	1.9066	$\tau$ (O-N-C-NH <sub>2</sub> )
348	171.0044	Twist (NH <sub>2</sub> )
373	5.9751	$\tau$ (C-C-N-O)
391	2.2473	$\gamma$ (C-C-H)
425	68.6451	Twist (NH <sub>2</sub> )
463	21.8543	Twist (NH <sub>2</sub> )
481	107.6216	Twist (NH <sub>2</sub> )
513	37.626	Twist (NH <sub>2</sub> )
620	9.735	$\tau$ in whole ring
645	24.5887	Twist (NH <sub>2</sub> )
684	38.8079	$\tau$ in whole ring
785	0.6655	$\gamma$ (C-C-H)
795	24.283	$\gamma$ (C-C-H)
815	5.9708	Twist (NH <sub>2</sub> )
931	173.2446	$\nu$ (O <sub>10</sub> -N <sub>8</sub> )
961	0.0428	$\ddot{G}$ (C-H)
962	0.1051	$\ddot{G}$ (C-H)
972	2.7989	Ring deformation
1048	12.3231	Ring breathing
1073	25.1466	Twist (NH <sub>2</sub> )
1083	46.4453	$\beta$ (C-C-H)
1187	31.4516	Twist (NH <sub>2</sub> )
1219	3.5151	Ring deformation
1250	12.6711	$\beta$ (C-C-H)
1304	65.6014	$\beta$ (C-C-H)
1373	28.6933	$\beta$ (C-C-H)
1413	4.732	$\beta$ (C-C-H)
1438	148.5108	$\beta$ (N-C-N)
1531	128.5916	S(H <sub>12</sub> -N <sub>9</sub> -H <sub>13</sub> )
1543	68.6374	$\nu$ (C-C)+ $\nu$ (C-N)
1566	129.6962	$\nu$ (CN in ring)
1648	90.0071	$\nu$ (C <sub>7</sub> -N <sub>8</sub> )
3040	19.948	$\nu$ (C <sub>3</sub> -H <sub>14</sub> )
3044	26.5426	$\nu$ (C <sub>1</sub> -H <sub>16</sub> )+ $\nu$ (C <sub>3</sub> -H <sub>14</sub> )
3095	8.7955	$\nu$ (C <sub>4</sub> -H <sub>15</sub> )
3449	34.0128	$\nu$ (N <sub>9</sub> -H <sub>12</sub> )+ $\nu$ (N <sub>9</sub> -H <sub>13</sub> )
3577	64.6213	$\nu$ (N <sub>9</sub> -H <sub>12</sub> )+ $\nu$ (NH <sub>2</sub> )
3681	106.5581	$\nu$ (O <sub>10</sub> -H <sub>11</sub> )

<sup>a</sup>  $\nu$ : Stretching;  $\beta$ : -in plane bending;  $\gamma$ : out of plane bending,  $\tau$ : torsion,  $\ddot{G}$ : wagging, S: scissoring

## Vibrational modes description

### Spectral region above 2800 cm<sup>-1</sup>

The C-H stretching vibrations are generally observed in the region 2800-3100cm<sup>-1</sup>. Accordingly, in the present study for N<sup>7</sup>-hydroxypyrimidine-2-carboximidamide, the C-H stretching vibrations are calculated at 3044, 3095, 3449, 3577, 3681 cm<sup>-1</sup> respectively.

### Spectral region from 1000 cm<sup>-1</sup> to 2300 cm<sup>-1</sup>

In the present study, in plane bending C-H ( $\beta$ ) vibrations are observed in the regions at 1083, 1250, 1304, 1373, 1413, 1438 cm<sup>-1</sup>. Scissoring C-H vibration is presented at 1531 cm<sup>-1</sup>, while Ring deformation C-C-C at 972, 1219 cm<sup>-1</sup>.

### Spectral region below 1000 cm<sup>-1</sup>

Twisting in while ring is presented at 348, 481, 513, 645, 725, 763, 815, 1073, 1187cm<sup>-1</sup> while out of plane bending  $\gamma$ (C-C-C), at 258, 391, 785, 795cm<sup>-1</sup>. Ring torsion  $\tau$  modes are presented at 173, 323, 373, 620, 684 cm<sup>-1</sup> whereas Ring breathing, at 1048 cm<sup>-1</sup>.

## Conclusion

The frequency assignments for N<sup>7</sup>-hydroxypyrimidine-2-carboximidamide have been made for the first time. The equilibrium geometry and harmonic frequencies of N<sup>7</sup>-hydroxypyrimidine-2-carboximidamide were determined and analyzed at the DFT level of the theory using the 6-311G (d, p) basis set. The vibrational frequency calculations proved that the structure is stable (no imaginary frequencies). We found the geometry obtained by the B3LYP method to be very accurate. Electronic properties show the reactivity of molecule with the help of HOMO-LUMO gap. Hyperpolarizability is mainly controlled by the planarity of the molecules, the donor and acceptor strength, and bond length alteration. The values of hyperpolarizability indicate a possible use of these compounds in electro optical applications. The present work might encourage the need for an extensive study by the experimentalists interested in the vibrational spectra and the structure of this compound.

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## Notes and References

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