

## DFT study of the intermolecular interaction of 3,4-dinitropyrazole (DNP) and H<sub>2</sub>O

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### ABSTRACT

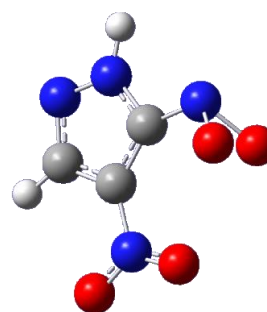
In the present work, the sensitivity to the moisture (hygroscopicity) is studied for 3,4-dinitropyrazole (DNP) as a famous energetic molecule. All of the DNP-H<sub>2</sub>O complex systems (1-3) as well as individual molecules were optimized and bond lengths, bond angles, dihedral angles, charge transfer and stability via NBO analysis, corrected interaction energies with ZPE + BSSE and hydrogen bonds analysis were carried out and related data were gathered and explained with details. According to the NBO analysis, it was observed that the complex 2 was the most stable one among the others. However, on the basis of the interaction energies, complex 3 displayed more strong interactions. So, it proves the existence of the strong hydrogen bonds in complexes 2 and 3 as well as occurrence of the inconsistent manner between interaction energies and charge transfer changes. Furthermore, it shows that charge transfer is not the main and effective parameter of intermolecular interactions in complexes 1-3.

**Keywords:** 3,4-dinitropyrazole (DNP); intermolecular interaction; DFT study

### INTRODUCTION

Recently, many researchers have been focused on the synthesis and computational investigation of nitrogen-rich energetic materials [1-4]. Among the all of the energetic materials, nitrogen-rich ones have attracted more interests, because they have some special features such as numerous C-N and N-N bonds in chemical structure which causes to have high density, fair stability and oxygen balance etc [5]. Pyrazole-based energetic materials are one of the most stable nitrogen-rich ones. Their suitable stability is related to the aromaticity of the pyrazole core. So, study these series of explosives such as 3,4-dinitropyrazole (DNP) (Figure 1) are of great importance and causes to better

understanding of their mechanism of explosion.



**Fig. 1.** The optimized structure of the DNP.

One of the most important topics in the pyrotechnics is the control of the sensitivity of the energetic materials. These

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compounds have different sensitivities to the external shocks such as spark, heat, impact so on, which can lead to the unexpected explosions [6-11]. So, improving the detonation performance as well as controlling the impact and heat resistance is a very challenging problem [12]. Recently, 3,4-dinitropyrazole (DNP) has been presented as one of the stable energetic materials with good detonation properties. DNP belongs to theazole family, which are five-membered nitrogen containing heterocycles. Electrophilic and nucleophilic sites of the DNP have been studied with via computational methods [13]. However, the computational studies on the various pyrotechnic features of DNP are very limited and its decomposition mechanism is still unclear. So, it is necessary to investigate its energy storage properties and the parameters which can affect on its decomposition.

Sensitivity to the moisture which is also named hygroscopicity is one of the most important topics in pyrotechnics. Moisture can be adsorbed by the energetic molecules during the production process or storage period. Hence, the properties such as decomposition, sensitivity and detonation velocity can affect by moisture absorption. Furthermore, it can lead to corrosion of the explosive container which is usually metallic. So, it is very important to study the interaction between energetic molecules (DNP in the present work) and water to evaluate the changes of its structural parameters while encountering to the moisture [14].

In the continuation of our previous work [15] in the present work, the intermolecular interactions of the DNP and water have been studied via computational approach. The DFT calculations at the B3LYP/6-31G\* level carried out to obtain the accurate, qualified and comparable computational results with experimental

observations.

## COMPUTATIONAL METHODS

First, DNP, H<sub>2</sub>O and all of the dimeric complexes were designed and optimized by Gauss view 05 and Gaussian 03 programs, respectively [16]. DFT calculations at the B3LYP/6-31G\* basis set carried out for optimization. Zero point energy (ZPE) correction and basis set superposition error (BSSE) correction were considered for the intermolecular interactions [17]. For detection of the source of the interactions, the natural bond orbital (NBO) analysis was carried out for each of structures.

## RESULTS AND DISCUSSION

The optimized structures of the DNP-H<sub>2</sub>O complexes (1-3) are shown in the figure 2. The optimized structural properties are listed in the Table 1 for all of the three complexes. According to the table 1, the average of the changes in bond lengths in the complexes 2 and 3 are more than complex 1. It can be seen that the changes in bond angles in complexes in comparison with individual DNP molecule are negligible. However, dihedral angles show significant variations, especially at complex 1 implies that there are intermolecular interactions in this type that could affect the clear rotation in the molecule.

The natural bond orbital (NBO) analysis shows the intra and intermolecular interactions between donor and acceptor orbitals. So, NBO analysis is a useful approach which helps to calculate the amount of the charge transfer between donor and acceptor. Second order perturbation energy  $E^{(2)}$  reveals all of the donor(i) and acceptor(j) interactions quantitatively:

$$E^{(2)} = q_i \frac{F2(i,j)}{\epsilon_j - \epsilon_i}$$

**Table 1.** The bond lengths (Å), bond angles and dihedral angles for monomers (DNP and H<sub>2</sub>O) and complexes 1-3. All of the structures were optimized at B3LYP/6-31G\* level.

Bond	Monomer	1	2	3
O <sub>1</sub> -H <sub>2</sub>	0.968	0.970	0.969	0.973
O <sub>1</sub> -H <sub>3</sub>	0.968	0.968	0.973	0.969
C <sub>4</sub> -C <sub>5</sub>	1.395	1.398	1.401	1.402
C <sub>4</sub> -N <sub>11</sub>	1.421	1.422	1.423	1.425
C <sub>1</sub> -N <sub>4</sub>	1.353	1.352	1.353	1.349
C <sub>5</sub> -C <sub>6</sub>	1.402	1.409	1.407	1.407
C <sub>5</sub> -N <sub>12</sub>	1.441	1.434	1.438	1.439
C <sub>6</sub> -H <sub>9</sub>	1.072	1.079	1.079	1.079
C <sub>6</sub> -N <sub>10</sub>	1.331	1.329	1.332	1.331
N <sub>7</sub> -H <sub>8</sub>	1.013	1.012	1.032	1.027
N <sub>10</sub> -N <sub>7</sub>	1.342	1.343	1.340	1.344
N <sub>11</sub> -O <sub>13</sub>	1.433	1.433	1.432	1.431
N <sub>11</sub> -O <sub>14</sub>	1.431	1.429	1.431	1.431
N <sub>12</sub> -O <sub>15</sub>	1.220	1.233	1.228	1.226
N <sub>12</sub> -O <sub>16</sub>	1.231	1.231	1.234	1.234
<b>Bond angle</b>				
4.11.13	112.07	111.68	112.63	111.89
4.11.14	112.11	113.13	112.72	111.82
4.7.10	114.21	114.25	113.63	113.65
4.7.8	125.44	125.40	123.94	129.82
4.5.6	105.17	105.22	104.82	105.08
4.5.12	130.65	130.63	130.85	130.99
5.12.15	118.68	118.90	118.72	118.83
5.12.16	115.77	116.28	115.93	115.77
5.6.9	127.21	127.27	127.20	127.23
5.6.10	111.45	111.39	111.35	111.09
10.6.9	121.33	121.32	121.43	121.66
10.7.8	120.34	120.33	122.42	116.51
7.4.5	104.72	104.70	105.28	105.17
7.4.11	113.45	113.41	113.64	113.58
11.4.5	141.81	141.78	141.07	141.24
13.11.14	61.50	61.55	61.49	61.45
13.11.4	112.07	111.68	112.63	111.89
14.11.4	112.11	113.13	112.72	111.82
15.12.16	125.54	124.81	125.34	125.38
<b>Dihedral angle</b>				
4.5.12.15	-0.05	-10.24	0.11	0.15
4.5.12.16	179.95	170.13	-179.93	-179.83
4.5.6.9	-179.98	179.60	-179.99	179.99
5.4.11.13	-33.63	-29.19	-33.85	-33.64
5.4.11.14	33.36	37.99	33.44	33.16
5.4.7.8	179.96	179.63	-179.87	-179.43
6.10.7.8	-179.98	-179.52	179.87	179.57
6.5.12.15	-179.98	168.41	-179.80	-179.90
6.5.12.16	0.03	-11.20	0.15	0.10
6.5.4.11	-179.94	175.81	179.88	-179.71
10.6.5.12	179.96	-178.74	179.93	-179.90
10.7.4.11	179.95	-177.46	-179.92	179.66
7.4.11.13	146.45	146.30	146.01	146.56
7.4.11.14	-146.55	-146.50	-146.68	-146.62
7.4.5.12	-179.96	178.92	-179.92	-179.96
8.7.10.13	179.98	-179.52	179.87	179.57
8.7.4.11	-0.02	2.51	0.20	0.43
9.6.10.7	179.99	-179.83	179.99	179.88
9.6.5.12	-0.04	0.66	-0.05	0.04

In the above equation,  $q_i$  shows the electron occupancy in the donor orbital,  $F(i,j)$  presents the off diagonal NBO Fock matrix element and  $\epsilon_i$  and  $\epsilon_j$  are diagonal elements in orbital energies. The atomic charges for DNP, H<sub>2</sub>O and complexes 1-3

are listed in the table 2 which are calculated via NBO analysis. In this table,  $\Delta 1$ ,  $\Delta 2$  and  $\Delta 3$  shows the differences of the natural atomic charges of the complexes 1-3 with monomers (DNP and H<sub>2</sub>O) respectively.

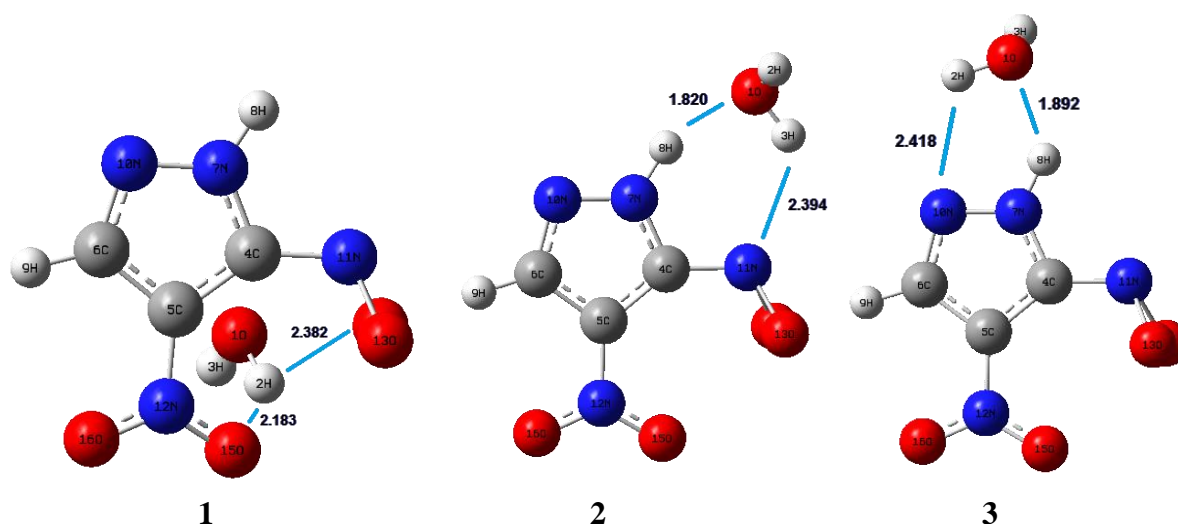


Fig. 2. Optimized structures of complexes 1-3.

Table 2. The resulted natural atomic charges for DNP, H<sub>2</sub>O and complexes 1-3 in B3LYP/6-31G\* level

Atom	Monomer	1	2	3	$\Delta 1$	$\Delta 2$	$\Delta 3$
O <sub>1</sub>	0.939	-0.960	-0.951	-0.953	-0.021	-0.011	-0.013
H <sub>2</sub>	0.469	0.481	0.490	0.498	-0.011	-0.021	-0.028
H <sub>3</sub>	0.469	0.469	0.499	0.487	-0.011	-0.029	-0.017
C <sub>4</sub>	0.298	0.625	0.599	0.612	-0.326	-0.326	-0.313
C <sub>5</sub>	-0.004	0.209	0.194	0.186	-0.213	-0.198	-0.190
C <sub>6</sub>	0.003	0.077	0.066	0.080	-0.073	-0.062	-0.076
N <sub>7</sub>	-0.320	-0.432	-0.462	-0.448	0.111	0.141	0.141
H <sub>8</sub>	0.459	0.378	0.413	0.402	0.081	0.046	0.057
H <sub>9</sub>	0.268	0.200	0.197	0.198	0.068	0.071	0.070
N <sub>10</sub>	-0.249	-0.244	-0.243	-0.298	-0.005	-0.006	0.048
N <sub>11</sub>	0.065	-0.100	-0.148	-0.103	-0.034	-0.082	-0.037
N <sub>12</sub>	0.415	0.341	0.339	0.340	0.074	0.076	0.075
O <sub>13</sub>	-0.105	-0.126	-0.116	-0.118	0.020	0.010	0.012
O <sub>14</sub>	-0.105	-0.113	-0.112	-0.120	0.007	0.006	0.014
O <sub>15</sub>	-0.337	-0.410	-0.392	-0.387	0.072	0.054	0.049
O <sub>16</sub>	-0.386	-0.382	-0.395	-0.396	-0.004	0.008	0.009

The intermolecular interactions between two molecules cause to redistribute the charges of each monomer. The stabilization energies ( $\Delta E$ ) are listed in the table 3 which are obtained via NBO analysis. The bonding-antibonding interactions and the related  $\Delta E$  amounts between monomers were obtained according to the second-order perturbation theory. The  $\Delta E$  amounts are related to the interaction measures. Table 3 demonstrates that in all three complexes 1-3, O<sub>1</sub>-H<sub>2</sub> and O<sub>1</sub>-H<sub>3</sub> bonds act as donor NBO versus the different acceptors. Furthermore, in the complex 1, the oxygen atoms of the nitro group (O<sub>13</sub> and O<sub>14</sub>) donate the lone pairs

to the neighboring O<sub>1</sub>-H<sub>2</sub> antibonds. In the complex 2, there is a very strong donor-acceptor interaction between the oxygen atom of the H<sub>2</sub>O as a lone pair donor and the N<sub>7</sub>-H<sub>8</sub> antibonds as acceptor (20.11 kJ/mol). However, it can be seen that a weaker interaction exists between N<sub>11</sub> as a lone pair donor and the O<sub>1</sub>-H<sub>2</sub> antibonds as an acceptor (2.28 kJ/mol). In the complex 3, the O<sub>1</sub> interaction as the lone pair donor with N<sub>7</sub>-H<sub>8</sub> antibond as an acceptor is lower than that in complex 2 (13.97 kJ/mol). So, it can be concluded that the order of the stabilization energy among the complexes is 2>3>1.

**Table 3.** NBO analysis data for complexes 1-3 at B3LYP/6-31G\* level

Complex	Donor NBO	Acceptor NBO	E(j)-E(i) a.u.	F(i,j) a.u.	$\Delta E$ (kJ/mol)
1	BD(1)O <sub>1</sub> -H <sub>2</sub>	LP(3)O <sub>15</sub>	0.43	0.015	0.18
	BD(1)O <sub>1</sub> -H <sub>2</sub>	RY*(5)O <sub>15</sub>	2.84	0.011	0.05
	BD(1)O <sub>1</sub> -H <sub>2</sub>	BD*(1)O <sub>13</sub> -O <sub>14</sub>	0.70	0.006	0.07
	LP(2)O <sub>1</sub>	RY*(3)C <sub>5</sub>	1.32	0.010	0.10
	LP(2)O <sub>1</sub>	BD*(2)C <sub>4</sub> -C <sub>5</sub>	0.26	0.005	0.09
	LP(2)O <sub>1</sub>	BD*(1)C <sub>5</sub> -N <sub>12</sub>	0.59	0.005	0.06
	LP(2)O <sub>1</sub>	BD*(2)N <sub>12</sub> -O <sub>16</sub>	0.15	0.004	0.08
	LP(2)O <sub>1</sub>	BD*(1)O <sub>13</sub> -O <sub>14</sub>	0.27	0.005	0.13
	LP(1)O <sub>14</sub>	BD*(1)O <sub>1</sub> -H <sub>2</sub>	1.34	0.031	0.92
	LP(2)O <sub>14</sub>	RY*(1)H <sub>2</sub>	1.18	0.007	0.05
	LP(2)O <sub>14</sub>	BD*(1)O <sub>1</sub> -H <sub>2</sub>	0.88	0.015	0.34
	LP(1)O <sub>15</sub>	BD*(1)O <sub>1</sub> -H <sub>2</sub>	1.28	0.037	1.34
	LP(2)O <sub>15</sub>	BD*(1)O <sub>1</sub> -H <sub>2</sub>	0.77	0.028	1.20
	LP(3)O <sub>15</sub>	BD*(1)O <sub>1</sub> -H <sub>2</sub>	0.75	0.040	1.95
	2	BD(1)O <sub>1</sub> -H <sub>2</sub>	BD*(1)N <sub>7</sub> -H <sub>8</sub>	1.17	0.016
BD(1)O <sub>1</sub> -H <sub>3</sub>		RY*(1)H <sub>8</sub>	1.42	0.015	0.19
BD(1)O <sub>1</sub> -H <sub>3</sub>		BD*(1)N <sub>7</sub> -H <sub>8</sub>	1.17	0.030	0.97
BD(1)O <sub>1</sub> -H <sub>3</sub>		BD*(1)N <sub>11</sub> -O <sub>13</sub>	0.84	0.006	0.06
BD(1)O <sub>1</sub> -H <sub>3</sub>		BD*(1)N <sub>11</sub> -O <sub>14</sub>	0.84	0.006	0.05
CR(1)O <sub>1</sub>		BD*(1)N <sub>7</sub> -H <sub>8</sub>	19.45	0.080	0.40
LP(1)O <sub>1</sub>		RY*(1)H <sub>8</sub>	1.17	0.008	0.07
LP(1)O <sub>1</sub>		BD*(1)N <sub>7</sub> -H <sub>8</sub>	0.92	0.019	0.46
LP(2)O <sub>1</sub>		RY*C <sub>4</sub>	1.35	0.009	0.07
LP(2)O <sub>1</sub>		RY*N <sub>7</sub>	2.13	0.019	0.20
LP(2)O <sub>1</sub>		RY*N <sub>7</sub>	2.82	0.013	0.08
LP(2)O <sub>1</sub>		RY*(1)H <sub>8</sub>	1.15	0.011	0.13
LP(2)O <sub>1</sub>		BD*(1)N <sub>7</sub> -H <sub>8</sub>	0.09	0.120	20.11
LP(2)O <sub>1</sub>		BD*(1)N <sub>7</sub> -H <sub>10</sub>	0.86	0.012	0.20
BD(1)N <sub>7</sub> -H <sub>8</sub>		RY*(1)O <sub>1</sub>	1.93	0.017	0.18
BD(1)N <sub>7</sub> -H <sub>8</sub>		BD*(1)O <sub>1</sub> -H <sub>2</sub>	1.13	0.009	0.09
LP(1)N <sub>11</sub>		BD*(1)O <sub>1</sub> -H <sub>2</sub>	0.93	0.041	2.28

Table 3. Continued

3	BD(1)O <sub>1</sub> -H <sub>2</sub>	RY*(2)N <sub>7</sub>	2.04	0.016	0.15
	BD(1)O <sub>1</sub> -H <sub>2</sub>	RY*(1)H <sub>8</sub>	1.38	0.014	0.19
	BD(1)O <sub>1</sub> -H <sub>2</sub>	BD*(1)C <sub>4</sub> -N <sub>7</sub>	1.20	0.008	0.07
	BD(1)O <sub>1</sub> -H <sub>2</sub>	BD*(1)C <sub>6</sub> -N <sub>10</sub>	1.26	0.013	0.16
	BD(1)O <sub>1</sub> -H <sub>2</sub>	BD*(1)N <sub>7</sub> -H <sub>8</sub>	1.16	0.027	0.75
	BD(1)O <sub>1</sub> -H <sub>3</sub>	BD*(1)N <sub>7</sub> -H <sub>8</sub>	1.16	0.013	0.17
	CR(1)O <sub>1</sub>	BD*(1)N <sub>7</sub> -H <sub>8</sub>	19.44	0.063	0.25
	LP(1)O <sub>1</sub>	RY*(1)H <sub>8</sub>	1.15	0.007	0.05
	LP(1)O <sub>1</sub>	RY*(1)N <sub>10</sub>	1.36	0.008	0.06
	LP(1)O <sub>1</sub>	BD*(1)C <sub>6</sub> -N <sub>10</sub>	1.03	0.007	0.06
	LP(1)O <sub>1</sub>	BD*(1)N <sub>7</sub> -H <sub>8</sub>	0.93	0.017	0.38
	LP(2)O <sub>1</sub>	RY*(1)N <sub>7</sub>	1.86	0.010	0.07
	LP(2)O <sub>1</sub>	RY*(1)N <sub>7</sub>	2.14	0.013	0.10
	LP(2)O <sub>1</sub>	RY*(1)H <sub>8</sub>	1.08	0.007	0.06
	LP(2)O <sub>1</sub>	BD*(1)C <sub>4</sub> -N <sub>7</sub>	0.90	0.015	0.31
	LP(2)O <sub>1</sub>	BD*(1)N <sub>7</sub> -H <sub>8</sub>	0.86	0.098	13.97

$\Delta E$ : stabilization energy, **BD**: bonding orbital, **BD\***: antibonding orbital, **LP**: lone pair, **RY\***: empty orbital.

The interaction energies for the DNP-H<sub>2</sub>O complexes are calculated and corrected with zero point energy (ZPE) and basis set superposition error (BSSE) corrections:

$$\Delta E = E(\text{DNP} + \text{H}_2\text{O}) - (E(\text{DNP}) + E(\text{H}_2\text{O}))$$

$$(\Delta E)_{\text{C,ZPE}} = (\Delta E)_{\text{C}} + \text{ZPE}$$

$$(\Delta E)_{\text{C}} = (\Delta E) + \text{BSSE}$$

Table 4 shows that the BSSE amounts are 0.62, 1.06, 1.56 and the corrected ZPEs are 6.13, 6.18 and 6.18 for complexes 1-3, respectively. The corrected interaction energies order among the complexes 1-3 is 3>2>1 with amounts -34.21, -31.59 and -25.80 kJ/mol, respectively. By comparison of table 3 and table 4, it can be seen that the interaction energies occur in an inconsistent fashion with charge transfer changes. It reveals that the charge transfer

is not the main factor of the intermolecular interactions in the complexes 1-3.

The intermolecular hydrogen bond can be assumed as an interaction between H-X as a donor and A-Y as an acceptor (Figure 3). X-H bond length, A-Y bond length, H...A intermolecular distance, X-H...A angle and the X to Y overall length are expressed as  $r$ ,  $\Phi$ ,  $d$ ,  $\alpha_{\text{HB}}$  and  $D$ , respectively. The table 5 demonstrates fair H...A distances which proves the existence of strong hydrogen bonds.

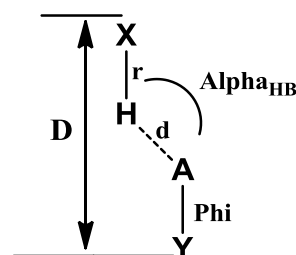


Fig. 3. The hydrogen bond parameters.

Table 4. Uncorrected interaction energy ( $\Delta E$ ), corrected interaction energy with BSSE ( $\Delta E)_{\text{C}}$  and corrected interaction energy with BSSE and ZPE ( $\Delta E)_{\text{C,ZPE}}$

	E	ZPE	$\Delta E$	$\Delta E)_{\text{C}}$	$\Delta E)_{\text{C,ZPE}}$	BSSE	ZPE)_{\text{C}}
DNP	-398500.22	194.91					
H <sub>2</sub> O	-47921.76	55.57					
1	-446454.53	256.69	-32.55	-31.93	-25.80	0.62	6.13
2	-446460.81	258.95	-38.83	-37.77	-31.59	1.06	6.18
3	-446460.81	258.82	-38.83	-40.39	-34.21	1.56	6.18

**Table 5.** The quantitative parameters for hydrogen bonds in complexes 1-3 in B3LYP/6-31G\*

	$r$ Monomer	$r$ Complex	$\Delta r$ (Å)	$d$ (Å)	$\alpha_{HB}$	$D$ (Å)
1	0.962	0.970	0.008	2.183	138.16	3.220
	09.62	0.970	0.008	2.382	110.84	3.506
2	1.012	1.032	0.02	1.820	153.78	2.886
	0.962	0.973	0.011	2.394	125.36	4.241
3	1.012	1.027	0.015	1.892	134.97	2.622
	0.962	0.973	0.011	2.418	115.33	2.968

## CONCLUSION

The sensitivity to moisture, which is called hygroscopicity is a very important case about energetic materials that should be considered carefully. A computational study for structural analysis of the 3,4-dinitropyrazole (DNP) as a famous energetic molecule and its interactions with H<sub>2</sub>O molecule were carried out in B3LYP/6-31G\* level. The corrected interaction energies with ZPE and BSSE are -25.80, -31.59 and -34.21kJ/mol. Therefore, the stability order for three complexes is 3>2>1. Complexes 2 and 3 shows a very strong charge transfer between interacting atoms of the monomers (H<sub>2</sub>O to N<sub>7</sub>-H<sub>8</sub>: 20.11 kJ/mol, N<sub>11</sub> to O<sub>1</sub>-H<sub>2</sub>: 2.28 kJ/mol in the complex 2 and H<sub>2</sub>O to N<sub>7</sub>-H<sub>8</sub>: 13.97 kJ/mol in the complex 3). So, the order of the stabilization energy for the complexes is 2>3>1. Thus, it can be concluded that the interaction energies and charge transfer changes arise in an inconsistent manner. It proves that the charge transfer is not the principal parameter of the intermolecular interactions in the complexes 1-3.

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