

Density Functional Calculations on a Double Hydrogen Bonded Dimer of 1-(2-Furylmethylene)-4-phenyl Thiosemicarbazide

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Density functional theory (DFT) calculations on a double hydrogen-bonded dimer of 1-(2-furylmethylene)-4-phenyl thiosemicarbazide were carried out at B3LYP/6-311G** level. The optimized geometry of the dimer closely resembles that in the crystal. The calculated results show that the total energy of the dimer is much lower than the sum of energies of the two monomers and the average strength of the double hydrogen bond is about 21.660 kJ/mol. In order to probe the origin of the interactions in the dimer, natural bond orbital (NBO) analyses have been performed. The thermodynamic properties of the title compound at different temperatures have also been calculated on the basis of vibrational analyses and the change of Gibbs free energy for dimerization of the two monomers $\Delta G_T = -17.365$ kJ/mol at 298.15 K and 0.1 MPa, which implies the spontaneous process of the dimer formation.

Key Words: Dimer, Density functional theory, Natural bond orbital, Thermodynamic properties.

INTRODUCTION

The importance of hydrogen-bonded dimers has become apparent in the last decade. Hydrogen bond interactions are known to play important roles in determining the structure of molecular crystals and biological systems¹⁻³. This has prompted experimentalists^{4,5} as well as theoreticians^{6,7} to focus their attention on these small systems. Density functional theory (DFT) has long been recognized as a better alternative tool in the study of organic chemical systems than the *ab initio* methods used in the past⁸ due to the fact that it is computationally less demanding for inclusion of electron correlation. Detailed analyses^{9,10} on the performance of different DFT methods had been carried out particularly for equilibrium structure properties of molecular systems. The general conclusion from these studies was that DFT methods, particularly with the use of nonlocal exchange-correlation functionals, can predict accurate equilibrium structure properties. The suitability of DFT to reliably describe hydrogen-bonded systems has been the subject of many investigations¹¹⁻¹⁴ and has proved quite useful for the study of hydrogen-bonded complexes⁷.

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With these in mind, when we synthesized 1-(2-furylmethylene)-4-phenyl thiosemicarbazide and found 1-(2-furylmethylene)-4-phenyl thiosemicarbazide to exist as a dimeric form in the crystal structure linking by hydrogen bonds of N–H...S¹⁵, we carried out DFT calculations on this dimer and made comparison between the experimental structure and the optimized geometry. In order to probe the origin of the interactions in the dimer, we performed natural bond orbital (NBO) analyses. The thermodynamic properties of the title compound at different temperatures have also been calculated on the basis of vibrational analyses and the change of Gibbs free energy for the aggregation from the two monomers to the dimer $\Delta G_T = -17.365$ kJ/mol at 298.15 K and 0.1 MPa, which implies the spontaneous formation of the dimer. In fact, in our previous reports, we ever reported dimers joined by hydrogen bonds of O–H...O^{12,13}, O–H...N¹² and N–H...O^{13,16}, however, dimers joined by N–H...S hydrogen bond were not investigated. Herein, we wish to report the calculated results, using DFT at B3LYP/6-311G** level on the 1-(2-furylmethylene)-4-phenyl thiosemicarbazide dimer. The present research will be helpful to the study of self-assembling supramolecular structure systems.

COMPUTATIONAL METHOD

The crystal structure of 1-(2-furylmethylene)-4-phenyl thiosemicarbazide was used as initial molecular geometry¹⁵, then it was optimized by using MM+ molecular modeling and semi-empirical AM1 methods¹⁷ (HYPERCHEM 6.0, Hypercube, Ont., Canada). In the next step, *ab initio* calculations with B3LYP/6-311G** level of theory by the Berny method¹⁸ were performed with Gaussian 03 software package¹⁹. The vibrational frequencies calculation prove that the structure is stable (no imaginary frequencies). Natural bond orbital analyses²⁰ were performed on the optimized structure. Thermodynamic properties and their changes in the aggregation were derived from statistical thermodynamics based on the frequencies.

The interaction energy of the complex is evaluated as the sum of the self-consistent field (SCF) interaction energy and the correlation interaction energy.

For the following progress:



The interaction energy (ΔE) of the complex is determined as:

$$\Delta E = E_{A-A} - 2E_A$$

where E_{A-A} and E_A are the total energies of the dimer and isolated molecule A, respectively.

The energies obtained at the equilibrium geometry of the complex for each subsystem are lower than those calculated at the same geometry with the basis functions of the respective subsystem alone. This energy difference is the so-called BSSE that can be checked by Boys and Bernardi's counterpoise procedure (CP)²¹⁻²³. For a dimer of two submolecules, the BSSE is:

$$\begin{aligned} \text{BSSE} &= \text{BSSE}(A) + \text{BSSE}(B) \\ &= \{E(A) - E(A[B])\} + \{E(B) - E(B[A])\} \end{aligned}$$

where the $E(A[B])$ and $E(B[A])$ are the energies of A and B respectively when the other subsystem's basis sets are added. After being corrected for BSSE and for zero-point energy (ZPE), the interaction energies is:

$$\Delta E_{C,ZPEc} = \Delta E_C + ZPE_C = \Delta E + BSSE + ZPE_C$$

All calculations were performed on a Pentium IV computer using the default convergence criteria.

RESULTS AND DISCUSSION

Total energies and interaction energies: The total energies and interaction energy calculated at B3LYP/6-311G** are given in Table-1, along with the zero-point energies (ZPEs) and the BSSE value. The scaling factor for the calculated harmonic vibrational frequencies is 0.96, which is a typical value for B3LYP calculations.

TABLE-1
ENERGIES (kJ/mol) OF THE MONOMERS AND
THE DIMER AT B3LYP/6-311G**LEVEL^a

	<i>E</i>	ZPE	BSSE	ΔE	$\Delta E_{C,ZPEc}$
Monomer	-2892588.177	561.477	–	–	–
Dimer	-5785219.674	1126.086	3.524	-43.320	-36.664

^a*E* is the total energy; ΔE is the uncorrected interaction energy; $\Delta E_{C,ZPEc}$ is the interaction energy corrected for BSSE and ZPE.

It can be seen from Table-1 that, without BSSE and ZPE corrections, the total energy of the dimer is lower than the sum of energies of two monomers by 43.320 kJ/mol. After being corrected for BSSE and ZPE, the energy of the dimer is still very low, which suggests that the dimer of 1-(2-furylmethylene)-4-phenyl thiosemicarbazide can be subsistent and is very stable. In addition, because the dimer is connected only by two hydrogen bonds of N–H...S, whole interaction can be attributed (approximately) to these hydrogen bonds. Hence, the average energy per hydrogen bond can be deduced, which is about 21.660 kJ/mol before being corrected and 18.332 kJ/mol after being corrected. These two values are of medium grade, in comparison with those reported previously (8-54 kJ/mol)²⁴. The proportion of BSSE to the corrected interaction $\Delta E_{C,ZPEc}$ is more than 5 % and less than 10 %, which indicates that the BSSE correction for the interaction is necessary.

Optimized geometry: The molecular structures of the dimer and monomer are both optimized at the B3LYP/6-311G** level of theory and the optimized molecular structure of the dimer with the atomic numbering scheme is shown in Fig. 1. The atomic numbering scheme of the monomer is the same as the top one in the dimer. Some selected X-ray diffraction data¹⁵ together with some optimized geometrical parameters for the monomer and the dimer are listed in Table-2. (In view of the symmetry of the dimer, only one molecule's geometrical parameters are listed).

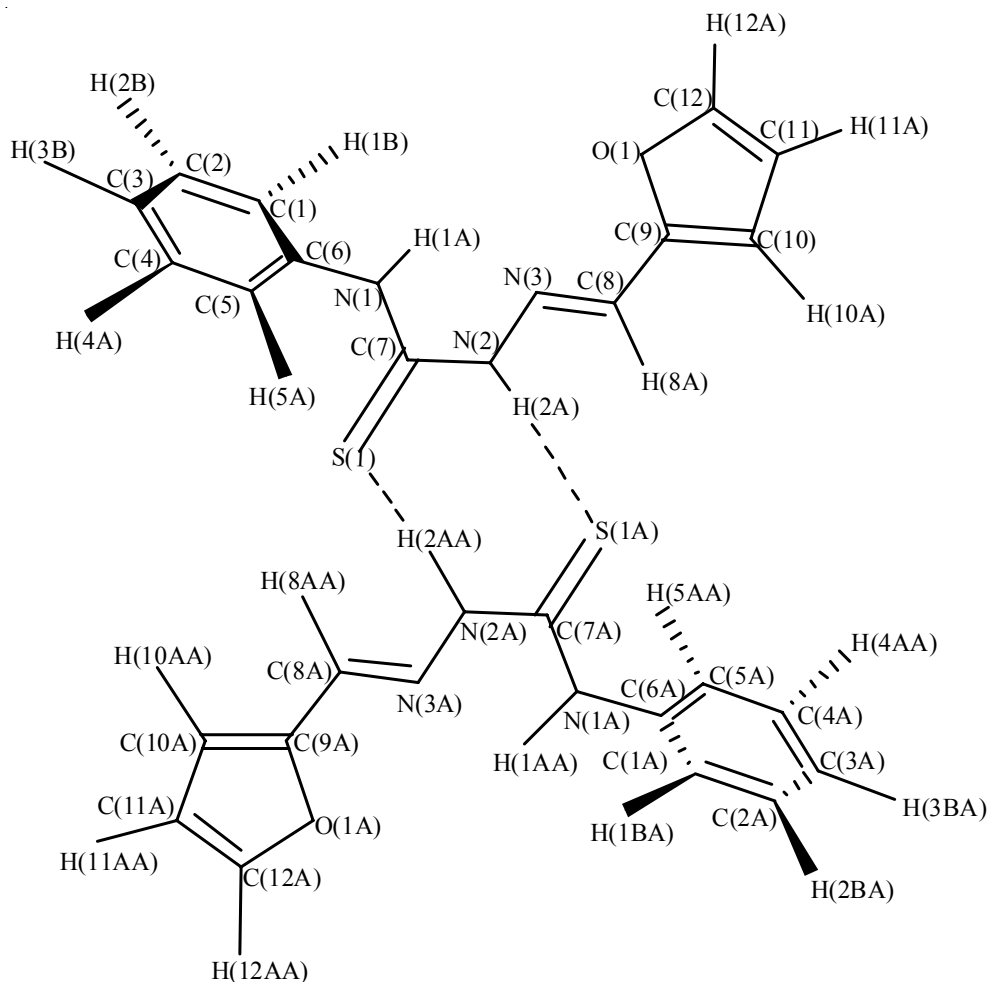


Fig. 1. Optimized molecular structure of the dimer with atomic numbering scheme

According to the data in Table-2, one can draw two conclusions: (1) most of the optimized bond lengths are slightly larger than the experimental values. This is due to the fact that the theoretical calculations belong to isolated molecules in the gaseous phase at 0 K while the experimental results belong to molecules in the solid phase; (2) in both of the monomer and dimer, all the values of bond lengths and bond angles in phenyl ring and furan nucleus are almost the same, while the geometric parameters related to the atoms involved in hydrogen bonds of N(2)-H(2A)···S(1A) [N(2A)-H(2AA)···S(1)] are different, with their values in the dimer being much more nearer to the experimental values than those in the monomer. For instance, S(1)-C(7) bond length in the dimer is 1.6922 Å, which is almost equal to that in the experiment [1.692(2) Å], while in the monomer, the bond length of S(1)-C(7) is only 1.6707 Å. The other bonds lengths of N(1)-C(7), N(2)-C(7) and N(2)-N(3)

TABLE-2
SELECTED MOLECULAR STRUCTURE PARAMETERS

Bond lengths (Å)	Exp.	B3LYP/6-311G** (monomer)		B3LYP/6-311G** (dimer)	
		Calc.	Calc.-Exp.	Calc.	Calc.-Exp.
S(1)-C(7)	1.692(2)	1.6707	-0.0213	1.6922	0.0002
O(1)-C(9)	1.356(4)	1.3660	0.0100	1.3670	0.0110
O(1)-C(12)	1.407(5)	1.3593	-0.0477	1.3587	-0.0483
N(1)-C(7)	1.345(3)	1.3522	0.0072	1.3514	0.0064
N(1)-C(6)	1.432(3)	1.4099	-0.0221	1.4100	-0.0220
N(2)-C(7)	1.347(3)	1.3858	0.0388	1.3707	0.0237
N(2)-N(3)	1.381(3)	1.3473	-0.0337	1.3553	-0.0257
N(3)-C(8)	1.280(3)	1.2858	0.0058	1.2863	0.0063
C(1)-C(6)	1.379(4)	1.4041	0.0251	1.4042	0.0252
C(1)-C(2)	1.395(4)	1.3877	-0.0073	1.3878	-0.0072
C(3)-C(4)	1.380(4)	1.3914	0.0114	1.3914	0.0114
C(5)-C(6)	1.392(4)	1.3991	0.0071	1.3991	0.0071
C(8)-C(9)	1.433(4)	1.4367	0.0037	1.4366	0.0036
C(9)-C(10)	1.349(3)	1.3720	0.0230	1.3718	0.0228
C(10)-C(11)	1.428(6)	1.4258	-0.0022	1.4256	-0.0024
C(11)-C(12)	1.301(6)	1.3606	0.0596	1.3609	0.0599
Bond angles (°)					
C(9)-O(1)-C(12)	104.8(3)	106.987	2.1870	106.968	2.1680
C(7)-N(1)-C(6)	127.21(19)	133.034	5.8240	133.705	6.4950
C(7)-N(2)-N(3)	120.0(2)	122.100	2.1000	120.343	0.3430
C(8)-N(3)-N(2)	116.5(2)	118.513	2.0130	118.068	1.5680
N(1)-C(7)-N(2)	114.9(2)	112.430	-2.4700	113.276	-1.6240
N(3)-C(8)-C(9)	120.8(2)	122.341	1.5410	121.830	1.0300
N(1)-C(7)-S(1)	125.35(17)	130.091	4.7410	128.018	2.6680
N(2)-C(7)-S(1)	119.72(18)	117.478	-2.2420	118.705	-1.0150
C(6)-C(1)-C(2)	119.3(3)	120.631	1.3310	120.662	1.3620
C(4)-C(3)-C(2)	120.0(2)	119.095	-0.9050	119.078	-0.9220
C(4)-C(5)-C(6)	119.4(2)	119.428	0.0280	119.497	0.0970
C(10)-C(9)-O(1)	111.9(3)	109.718	-2.1820	109.692	-2.2080
C(12)-C(11)-C(10)	108.9(3)	106.025	-2.8750	106.007	-2.8930

corresponding with the hydrogen bond in the dimer are also more adjacent to the experimental values than those in the monomer. As for the bond angles related to atoms in the hydrogen bond of N-H...S, such as the bond angles of N(1)-C(7)-N(2), N(1)-C(7)-S(1) and N(2)-C(7)-S(1), their values in the dimer are also close to the values in the crystal structure than those in the monomer. Namely, the optimized geometric parameters in the dimer show more remarkable agreement with the experiment than the monomer, which support the fact that the 1-(2-furylmethylene)-4-phenyl thiosemicarbazide exists as a hydrogen-bonded dimer in the solid state as shown in Fig. 1.

The experimental and calculated hydrogen bond distances and angles are listed in Table-3. Since in the crystal structure, the hydrogen atom positions were fixed geometrically at calculated distances and allowed to ride on the parent C and N atoms, it can not be acceptable to compare the experimental distances of D-H (hydrogen donor-hydrogen) and A-H (hydrogen acceptor-hydrogen) with the calculated values. So, we can draw a comparison between the distance of D-A (hydrogen donor- hydrogen acceptor) in the predicted structure with the experimental value. As seen from Table-3, the calculated distance of D-A is close to that in the crystal structure and the deviation is 0.087 Å. The deviation of the hydrogen-bond angle between the theoretical value and the experimental value is only 1.15°, which prove the point that 1-(2-furylmethylene)-4-phenyl thiosemicarbazide exists as a hydrogen-bonded dimer in the solid state once again.

TABLE-3
HYDROGEN BOND DISTANCES (Å) AND \angle D-H...A (°) FOR THE DIMER^a

D-H...A	D-H		H-A		D...A		\angle D-H...A	
	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.
Dimer N(2)-H(2A) ...S(1A)	0.860	1.027	2.541	2.461	3.382	3.469	165.96	167.14

^aD means hydrogen donor; A means hydrogen acceptor.

In conclusion, all of aforementioned results reveal that the optimized dimer closely resembles to the crystal structure and B3LYP/6-311G** level is suitable for the system studied here. So the discussion above and thereafter is derived from the optimized structure by using this level.

Natural bond orbital analysis: In order to probe the origin of the interaction in the dimer, natural bond orbital (NBO) analyses at B3LYP/6-311G** level were performed. The donor and acceptor (here, donor = electron donor and acceptor = electron acceptor) of NBO in the dimer and their interacting stable energies are collected in Table-4. The stable energies are proportional to the NBO interacting intensities. In the symmetric dimer, the atoms S(1) and S(1A) offer their first and second lone pair electrons to the N(2A)-H(2AA) and N(2)-H(2A) antibonds, respectively. Each of them gives total stable energy of 51.714 kJ/mol, which corresponds to intermolecular hydrogen bond.

TABLE-4
NATURAL BOND ORBITAL INTERACTING AND THE
CORRESPONDING STABLE ENERGY (kJ/mol)^a

Donor	Acceptor	E
LP(1) S(1)	BD* N(2A)-H (2AA)	6.987
LP(2) S (1)	BD* N(2A)-H (2AA)	44.727
LP(1) S (1A)	BD* N(2)-H (2A)	6.987
LP(2) S (1A)	BD* N(2)-H (2A)	44.727

^aLP means lone pair; BD* represents antibond.

Thermodynamic properties: On the basis of vibrational analysis and statistical thermodynamics, the standard thermodynamic functions, heat capacities ($C_{p,m}^0$), entropies (S_m^0) and enthalpies (H_m^0), were obtained and listed in Table-5.

TABLE-5
THERMODYNAMIC PROPERTIES OF 1-(2-FURYL METHYLENE)-
4-PHENYL THIOSEMICARBAZIDE MONOMER AND THE
DIMER AT DIFFERENT TEMPERATURES^a

Structure	T (K)	$C_{p,m}^0$ (J mol ⁻¹ K ⁻¹)	S_m^0 (J mol ⁻¹ K ⁻¹)	H_m^0 (kJ mol ⁻¹)	ΔS_T (J mol ⁻¹ K ⁻¹)	ΔH_T (kJ mol ⁻¹)	ΔG_T (kJ mol ⁻¹)
Monomer	200.00	175.16	466.77	21.51	–	–	–
	298.15	251.16	550.83	42.42	–	–	–
	400.00	323.85	635.09	71.80	–	–	–
	500.00	382.01	713.85	107.21	–	–	–
	600.00	427.78	787.71	147.79	–	–	–
	700.00	463.99	856.47	192.45	–	–	–
	800.00	493.18	920.40	240.35	–	–	–
Dimer	200.00	361.66	861.20	44.38	-72.34	-38.828	-24.36
	298.10	513.90	1033.85	87.32	-67.81	-37.708	-17.365
	400.00	660.11	1205.88	147.31	-64.30	-36.478	-10.758
	500.00	777.24	1366.26	219.40	-61.44	-35.208	-4.488
	600.00	869.50	1516.46	301.92	-58.96	-33.848	1.528
	700.00	942.54	1656.19	392.66	-56.75	-32.428	7.297
	800.00	1001.44	1786.02	489.96	-54.78	-30.928	12.896

^a $\Delta S_T = (S_m^0)_{dimer} - 2 \times (S_m^0)_{monomer}$; $\Delta H_T = (H_m^0 + E + ZPE)_{dimer} - 2 \times (H_m^0 + E + ZPE)_{monomer}$; $\Delta G_T = \Delta H_T - T\Delta S_T$ and the scale factor for frequencies is 0.96.

It can be observed from the Table-5 that the heat capacities, entropies and enthalpies increase with the increase of temperature from 200 to 800 K. It is because that the intensities of molecular vibrations increase when the temperature increases. The value of $C_{p,m}^0$ for the dimer is slightly larger than the sum of the corresponding values of $C_{p,m}^0$ of two monomers at each temperature.

During the process from the two monomers to the dimer, both the entropy and enthalpy decrease with the increase of temperature from 200 to 800 K ($\Delta S_T < 0$, $\Delta H_T < 0$) and the changes of ΔS_T and ΔH_T decrease as temperature increases. Therefore, the intermolecular interaction is an exothermic process that is accompanied by the decrease of confusion degree. According to the equation of $\Delta G_T = \Delta H_T - T\Delta S_T$, the values of change of Gibbs free energy (ΔG_T) in the processes are from negative to positive. From T = 200 to 500 K, $\Delta G_T < 0$, which implies that the dimer forms *via* spontaneous process. At 298.15 K on the calculation model of ideal-gas, the calculated equilibrium constant, based on the equation $\Delta G_T = -RT \ln K_p$, is 1.102×10^3 . It reveals that the dimer is the main component at this temperature. From 600 to 800 K and thereafter, the $\Delta G_T > 0$, indicates that the formation of the dimer is not spontaneous. Based on the values of ΔS_T , ΔH_T at 298.15 K and 0.1 MPa, the transition

temperature of this spontaneous reaction is about 556.08 K. Although above conclusions are drawn based on the gaseous-phase state structure, they provide useful information for the synthesis of the dimer under experimental conditions.

Conclusion

Dimer of 1-(2-furylmethylene)-4-phenyl thiosemicarbazide connected through N–H...S hydrogen bonds has been investigated by DFT method at B3LYP/6-311G** level of theory. The calculated results reveal that the dimer is more stable than the monomer, with the total energy of the dimer being lower than that of the sum of the two monomers. Comparisons of optimized geometric parameters with the experimental data indicate that 1-(2-furylmethylene)-4-phenyl thiosemicarbazide exists as a dimeric form in the crystal. Natural bond orbital analysis shows that in the dimer, the atoms S(1) and S(1A) offer their first and second lone pair electrons to the N(2A)-H(2AA) and N(2)-H(2A) antibond and each of them gives total stable energy of 51.714 kJ/mol. The calculations of thermodynamic property suggest that at 298.15K and 0.1MPa, in the process of forming the dimer, the values of ΔG_T is -17.365 kJ/mol, which implies that the dimer forms *via* spontaneous process and the equilibrium constant K_p , is 1.102×10^3 .

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