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Calculations of bond dissociation energies and dipole moments in energetic materials using density-functional methods

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Abstract

We compare the effectiveness of six exchange/correlation functional combinations (Becke/Lee, Yang and Parr; Becke-3/Lee, Yang and Parr; Becke/Perdew–Wang 91; Becke-3/Perdew–Wang 91; Becke/Perdew 86; Becke-3/Perdew 86) for computing C–N, O–O and N–NO$_2$ dissociation energies and dipole moments of five compounds. The studied compounds are hexabydro-1,3,5-trinitro-1,3,5-triazine (RDX), dimethylnitramine, cyanogen, nitromethane and ozone. The Becke-3/Perdew 86 in conjunction with 6-31G** is found to give the best results, although for the dipole moments of RDX, there is a slightly difference that B3P86/6-31G** is less reliable than B3P86/6-31+G**.
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1. Introduction

It is being demonstrated with increasing frequency that density-functional theory (DFT) [1] can be an effective approach to compute reaction energetics [2,3]. A key advantage over ab initio treatments of comparable accuracy is that density-functional procedures can be applied to much larger systems. Unfortunately, the particular combination of exchange and correlation functionals and basis sets that will give the best results in any given instance can be difficult to predict. In addition, it is well known that many computational chemistry techniques are extremely computer-intensive. Depending on the type of calculation desired, it would take anywhere from minutes to weeks to do a single calculation. There is accordingly a need for extensive evaluation and comparison of various density-functional procedures for computing reaction energetics, and such studies are very important while developing the molecular design technique for explosives. Branko [4] evaluated the accuracy of high level ab initio, gradient-corrected density functional, and hybrid DFT methods for computing bond dissociation energies

(BDE) and enthalpies of formation in the gas phase of small polar molecular systems. Politzer and Lane [5] compared the effectiveness of three exchange/correlation functional combinations for computing C–NO$_2$, N–NO$_2$ and C–NF$_2$ bond lengths and dissociation energies, but there was no information about the O–O bond rupture.

In the present work, we focus on not only bond dissociation energy but also dipole moment that is an important physical property for studying the shock sensitivity of energetic materials [6]. Some useful information of molecular performance can be obtained by analyzing the impact of molecular structure on the electrical dipole moments [7]. We test the effectiveness of six exchange/correlation combinations and five basis sets for computing the bond dissociation energies and dipole moments of a system including ozone, nitromethane, cyanogen, dimethylnitramine and hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX). The nitromethane and RDX are chosen for the current studies because they are widely used energetic materials. Ozone is chosen because, although not an explosive in practical use, its solid state is a simple model for studying energetic materials and promising high power energetic materials [8], and the O–O dissociation energies are also useful for studying energetic materials. Our objective is to examine which approach is likely to be most reliable in applications to systems of energetic

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materials. Such studies can contribute to designing and synthesizing new and proposed energetic compounds, i.e. explosives and propellants, which can promote the development of materials that combine improved performance with diminished vulnerability (sensitivity) to unintended external stimuli, such as impact and shock.

2. Computational methodologies

DFT methods provide an accurate solution to the Schrodinger equation by postulating an approximate functional relating charge density to energy. Modern functionals depends on the value of the charge density and its gradient. These "gradient corrected" functionals are found to yield enhanced accuracy in the prediction of many molecular properties over "local" functionals that depend only on the value of the charge density.

All calculations are carried out with the Gaussian '98 [9] implementation of the DFT methods. All of the geometries for the studied compounds are fully optimized without using the symmetry or structural constraints. This is accomplished by using the default Gaussian convergence criteria. Some density-functional procedures, differing in their combinations of exchange and correlation functionals and basis sets, are tested for accuracy in computing the bond dissociation energies and dipole moments of ozone, nitromethane, dimethylnitramine, cyanogen, and RDX. Among the procedures, the exchange functionals are B and B3. B refers to the Becke's 1988 gradient-corrected exchange functional [10] which reproduces the exact asymptotic behavior of exchange-energy density in finite system, and B3 is denoted for the Becke's hybrid method [11] of mixing Hartree–Fock exchange energy into the exchange functional. The correlation functionals are the Lee, Yang and Parr (LYP) [12], the Perdew–Wang 91 (PW91) [13] and the Perdew 86 (P86) [14]. We use the 6-31G*, 6-31G**, 6-311G(3df,3pd), 6-311G** basis sets [15] and Dunning's most recent correlation consistent polarized valence double zeta basis set (cc-pVDZ) [16]. Molecular and fragment geometries are re-optimized for each computational approach.

Zero-point energy corrections are included, since it may be necessary and advantageous to use these small energy corrections from density-functional calculations in the calculation of thermochemical data. We have converted the computed BDE to 298 K, using the following expression, as implemented in Gaussian '98, with the temperature correction calculated at this level of theory:

$$BDE_{298} = \Delta_f H_{298}(R_1) + \Delta_f H_{298}(R_2) - \Delta_f H_{298}(R_1 - R_2)$$

where

$$R_1 - R_2 \rightarrow R_1 + R_2$$
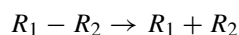
3. Results and discussion

3.1. Bond dissociation energies

The stabilities and impact/shock sensitivities of energetic materials have frequently been related to the strengths of C–NO$_2$

and/or N–NO$_2$ bonds. For designing and evaluating new compounds, it is accordingly important to be able to determine computationally the dissociation energies of these bonds. We investigate the effectiveness of different exchange/correlation functional combinations in reproducing the C–N bond dissociation energies in nitromethane and cyanogen, the N–NO$_2$ bond dissociation energies in RDX and dimethylnitramine, and the O–O dissociation energies in ozone.

As demonstrated by Politzer and Lane, the weakest bond of nitromethane was the C–NO$_2$ [5]. Therefore, the initial step of decomposition is the C–NO$_2$ bond breaking to form two radicals, CH$_3$ and NO$_2$. Bond dissociation energies for nitromethane computed with density-functional theory are presented in Table 1. It is believed that the H$_3$C–NO$_2$ dissociation energy should be approximately 58.9 kcal mol^{-1} [17]. The numbers in parentheses correspond to the absolute deviations between computational results and experimental data (Table 1). We can confirm that the B3P86/6-31G** is overall the best method, followed by the B3P86/6-31+G** and the B3P86/6-311G**. All three can be expected to give results that are accurate, on the average, to within 1.0–1.5 kcal mol^{-1}. In addition, the basis sets have little effect on the results of C–NO$_2$ dissociation energies, that is, there is a lower basis set sensitivity. For example, starting from a small basis set like 6-31G*, to the extended basis set like 6-311G(3df,3pd), the predicted C–NO$_2$ bond dissociation energies changes only 1.5 kcal for the B3LYP. In contrast, different exchange/correlation combinations with the same basis set have great impact on the calculated results.

As for ozone, photodissociation by ultraviolet radiation played a key role in atmospheric chemistry. Considerable experimental effort for the purpose of investigating the photodissociation processes of ozone in the ultraviolet region turned out that channel O$_3$ + $\hbar\nu$(<1180 nm) → O(^{3}P)+O$_2$(X$^3\Sigma_g^-$) was predominant in the Hartley band photodissociation at λ < 305 nm [18].

In the case of O–O bond dissociation energies of ozone, comparing to the experimental value previously reported by Tsuneda et al. [19], the results computed by B3LYP, B3PW91 and B3P86 DFT methods are slightly lower than the experimental value, and the most excellent data comes from B3P86/6-31G**, which is the same method as the optimal method for computing the C–NO$_2$ bond dissociation energies of nitromethane. In contrast, the values given by BLYP are poor and usually overestimate the bond dissociation energies. A similar behavior is observed when evaluating the bond dissociation energies for nitromethane.

Numerous experimental studies showed that N–NO$_2$ bond homolysis was the initial step in the thermal decomposition of RDX. For instance, a supporting evidence for this path was given by the transient IR laser pyrolysis experiments of Wight and Botcher [20]. Using a solid RDX thin film, they found that the initial decomposition products related mostly to the N–NO$_2$ bond rupture [20]. In addition, their experiments on samples with isotopically labeled nitrogen also showed that decomposition of RDX was mostly unimolecular and involved the removal of only one NO$_2$ [21].

Table 1
Calculated bond dissociation energies (zero-point energy corrections included) and dipole moments[a]

Theory level	Nitromethane		Cyanogen	Ozone	
	BDE (kcal mol^{-1})	Dipole moments (D)	BDE (kcal mol^{-1})	BDE (eV)	Dipole moments (D)
B3LYP/6-31G*	54.8 (−4.1)	3.48 (0.02)	173.2 (−4.8)	0.584 (−0.250)	0.61 (0.08)
B3LYP/6-31+G*	54.5 (−4.4)	3.80 (0.34)	171.4 (−6.6)	0.543 (−0.291)	0.69 (0.16)
BLYP/6-31G*	52.1 (−6.8)	3.30 (−0.16)	186.0 (8.0)	1.490 (0.656)	0.55 (0.02)
B3PW91/6-31G*	55.6 (−3.3)	3.48 (0.02)	172.8 (−5.2)	0.570 (−0.264)	0.62 (0.09)
B3PW91/6-31+G*	55.6 (−3.3)	3.75 (0.29)	171.2 (−6.8)	0.544 (−0.290)	0.69 (0.16)
B3LYP/6-31G**	54.5 (−4.4)	3.49 (0.03)	173.2 (−4.8)	0.584 (−0.250)	0.61 (0.08)
BLYP/6-31G**	51.9 (−7.0)	3.31 (−0.15)	186.0 (8.0)	1.490 (0.656)	0.55 (0.02)
BPW91/6-31G**	53.3 (−5.6)	3.32 (−0.14)	186.2 (8.2)	1.482 (0.648)	0.56 (0.03)
B3PW91/6-31G**	55.4 (−3.5)	3.49 (0.03)	172.8 (−5.2)	0.570 (−0.264)	0.62 (0.09)
BP86/6-31G**	55.4 (−3.5)	3.32 (−0.14)	191.0 (13.0)	1.666 (0.832)	0.56 (0.03)
B3P86/6-31G**	58.3 (−0.6)	3.50 (0.04)	178.5 (0.5)	0.774 (−0.060)	0.62 (0.09)
B3P86/6-31+G**	58.2 (−0.7)	3.77 (0.31)	177.0 (−1.0)	0.753 (−0.081)	0.69 (0.16)
B3LYP/6-311G**	52.7 (−6.2)	3.52 (0.06)	174.1 (−3.9)	0.425 (−0.409)	0.62 (0.09)
B3P86/6-311G**	56.9 (−2.0)	3.54 (0.08)	179.1 (1.1)	0.617 (−0.217)	0.63 (0.10)
BLYP/6-311G**	50.0 (−8.9)	3.33 (−0.13)	186.9 (8.9)	1.330 (0.496)	0.55 (0.02)
BLYP/cc-pVDZ	50.4 (−8.5)	3.16 (−0.30)	184.5 (6.5)	1.434 (0.600)	0.62 (0.09)
B3P86/cc-pVDZ	56.8 (−2.1)	3.41 (−0.05)	176.8 (−1.2)	0.682 (−0.152)	0.58 (0.05)
B3LYP/6-311G(3df,3pd)	53.3 (−5.6)	3.31 (−0.15)	177.6 (−0.4)	0.618 (−0.216)	0.57 (0.04)
Experimental	58.9[b]	3.46[c]	178.0[d]	0.834[e]	0.53[f]

[a] Values in parentheses are the absolute deviations between computational results and experimental data.
[b] Ref. [17].
[c] Ref. [28].
[d] Ref. [30].
[e] Ref. [19].
[f] Ref. [28].

The computed dissociation energies of RDX follow the same qualitative patterns as observed for nitromethane and ozone, and the B3P86/6-31G** is still in good agreement with the relatively precise theoretical data deduced from Ref. [17]. As usual, BLYP is still inferior to the other density-functional procedures. Unfortunately, all our DFT values of the N–NO$_2$ bond dissociation energies in RDX are significantly smaller than 45.0 kcal mol^{-1} [17]. For example, Ref. [22] gave an N–NO$_2$ bond dissociation energy for RDX of 42 kcal mol^{-1} using B3LYP/6-311G**, while we present a value of 8 kcal mol^{-1} less for this quantity with the same DFT method/basis set. After carefully checking, we find that the former includes a correction for the tendency for B3LYP/6-311G** theory to underestimate N–NO$_2$ bond strengths by 6 kcal mol^{-1} compared with high level G2 theory [22], which can throw lights on our future work.

Dimethylnitramine exhibits many of the properties of the larger nitramines such as 1,3,3-trinitroazetidine (TNAZ) and 1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane (HMX) that are used as propellants and explosives, and thus it has often been used as a prototype because it is more amenable to experimental and theoretical studies. Most experimental and theoretical studies indicate that the N–NO$_2$ bond fission has the lowest energy barriers [23,24]. The dissociation energies of dimethylnitramine calculated by the 14 procedures are also listed in Table 2. Overall, they cover a range of about 10 kcal mol^{-1}, approximately centered on the experimental value of 46.5 kcal mol^{-1} [23]. As expected, an excellent agreement for the N–NO$_2$ bond dissociation energy of dimethylnitramine is obtained using

B3P86/6-31G**. For any given exchange/correlation combination, the calculated dissociation energies are essentially the same for the 6-31G* and 6-31G** basis sets. However, they decrease by roughly 1 kcal mol^{-1} in proceeding to the 6-31+G**. This

Table 2
Calculated bond dissociation energies (zero-point energy corrections included) and dipole moments[a]

Theory level	RDX		Dimethylnitramine
	BDE (kcal mol^{-1})	Dipole moments (D)	BDE (kcal mol^{-1})
B3LYP/6-31G*	34.8 (−10.2)	4.22 (−1.57)	41.0 (−5.5)
B3LYP/6-31+G*	32.9 (−12.1)	4.57 (−1.22)	39.5 (−7.0)
BLYP/6-31G*	32.0 (−13.0)	3.86 (−1.93)	38.2 (−8.3)
B3PW91/6-31G*	36.6 (−8.4)	4.37 (−1.42)	43.2 (−3.3)
B3PW91/6-31+G*	35.4 (−9.6)	4.60 (−1.19)	42.1 (−4.4)
B3LYP/6-31G**	34.9 (−10.1)	4.27 (−1.52)	41.1 (−5.4)
BLYP/6-31G**	32.1 (−12.9)	3.89 (−1.90)	38.3 (−8.2)
B3PW91/6-31G**	36.7 (−8.3)	4.43 (−1.36)	43.3 (−3.2)
B3P86/6-31G**	40.2 (−4.8)	4.41 (−1.38)	46.8 (0.3)
B3P86/6-31+G**	39.0 (−6.0)	4.66 (−1.13)	45.7 (−0.8)
B3LYP/6-311G**	34.1 (−10.9)	4.46 (−1.33)	40.0 (−6.5)
B3P86/6-311G**	39.6 (−5.4)	4.61 (−1.18)	45.8 (−0.7)
BLYP/6-311G**	31.4 (−13.6)	4.06 (−1.73)	37.2 (−9.3)
BPW91/cc-pVDZ	34.2 (−10.8)	4.48 (−1.31)	40.7 (−5.8)
Experimental	45.0[b]	5.79[c]	46.5[d]

[a] Values in parentheses are the absolute deviations between computational results and experimental data.
[b] Deduced from Ref. [17].
[c] Deduced from Ref. [28].
[d] Deduced from Ref. [23].

may reflect the diminishing effect of basis set superposition error (BSSE).

BSSE is a consequence of set incompleteness and reflects the error in the interaction of a molecular fragment when bonded to other relative to when it is not bonded, a "counterpoise" technique was proposed as a correction for this problem [25], but there has been a great deal of disagreement concerning its effectiveness, and it has been shown to sometimes actually worsen the accuracy of the results (see the numerous references cited by Szalewicz et al. [26]). Politzer et al. [27] carried out a series of DFT calculations (B3PW91 in conjunction with four different basis sets) of interaction of two dimethylnitramine molecules to assess the possible role of BSSE, and concluded that BSSE was very small. Therefore, BSSE is not taken into account in the present work.

3.2. Dipole moments

For ozone, we note that all density-functional methods yield accurate dipole moments, and the largest deviation between the dipole moment produced by B3LYP/6-31+G* and experimental value [28] is only 0.16 D (Table 1). Obviously, BLYP approaches obtain the most accurate dipole moment (only 0.02 D larger than the experimentally determined value). It seems that increasing the size of the basis sets can improve the accuracy, however, the larger basis sets calculations require more computer resources and time, especially dealing with the more complicated systems. Lei calculated the energetics of the OH-isoprene reaction system, and found that the method of gradient corrected density functionals in conjunction with moderate basis sets gave satisfactory molecular geometries and vibrational frequencies [29]. To our delight, B3P86, B3PW91 and B3LYP in combination with moderate basis sets, such as 6-31G* and 6-31G**, also yield relatively close dipole moments to the experimental value in our work. Being the best method computing the O–O bond dissociation energies, B3P86/6-31G** should be top-priority. In addition, adding diffuse functions to the 6-31G** basis set considerably degrades the accuracy of at the B3P86 level.

For nitromethane, all calculated dipole moments were almost identical to the experiment value [28]. Surprisingly, better results are obtained with a modest size basis set, such as 6-31G*, rather than with a larger basis set, such as 6-311G(3df,3pd). Both B3PW91/6-31G* and B3LYP/6-31G* yield the best value (3.48 D), which is 0.02 D higher than the experimental value (Table 1), followed by B3PW91/6-31G* and B3LYP/6-31G**. Overall speaking, B3PW91 methods give closer estimations than B3LYP. Like ozone, using the DFT methods adding diffuse functions cause the larger deviation, ranging from 0.29 D (B3PW91/6-31+G*) to 0.34 D (B3LYP/6-31+G*). Finally, the results obtained by all BLYP methods underestimate the dipole moment of nitromethane.

On the RDX molecule, there is a pretty large dipole moment of about 5.79 D [28]. This is because in the RDX molecule, the more electro negative oxygen atoms exert a greater pull on the electrons than the Hydrogen and Carbon atoms do. Because the RDX molecule is lopsided with high density of electrons all

in one region, it creates a dipole moment pointing towards the oxygen atoms.

From Table 2, the computed dipole moments of RDX show slightly different trends comparing with the nitromethane and ozone. First of all, B3P86 in combination with the 6-31+G**, instead of 6-31G**, gives the highest accuracy. Secondly, to our surprise, contrary to the above two molecules, the results obtained by the DFT methods adding diffuse functions are superior to those adding polarization functions. Overall speaking, the accuracy ranking for the five available methods are: BLYP < BPW91 < B3LYP < B3PW91 < B3P86.

To sum up, that B3P86 is obviously superior to other three DFT methods is not occasional, therefore, it is necessary to discuss the underlying physical mechanisms. Above all, despite the well-intentioned efforts of density-functional researchers to circumvent the calculation of exact-exchange energies, we shall see that a small exact-exchange component is a natural and necessary constituent of any exchange-correlation approximation aiming for accurate molecular energetics. In the B3 exchange functional, a better semiempirical combination of exact exchange, the local-spin-density exchange correlation approximation (LSDA), and gradient correction is used. It performs significantly better than B exchange functional.

Secondly, it is known that the major obstacle towards an accurate self-consistent-field theory for atoms, molecules, and solids is the electron correlation problem, since everything else may be treated more or less exactly (as in the spin-unrestricted Hartree–Fock approximation). Ground-state density-functional approximations, starting from the limit of the electron gas of slowly varying density, have traditionally made serious errors in the correlation energy E_c for the realistically inhomogeneous systems. However, comparing with the other two correlation functionals (LYP and PW91), P86 functional is improved in two ways: (1) the natural separation between exchange and correlation is made, so that the density-gradient expansion of each is recovered in the slowly varying limit. (2) Uniform-gas and inhomogeneity effects beyond the random-phase approximation are built in.

4. Conclusions

First of all, when comes to computing the C–N, O–O and N–NO$_2$ dissociation energies, the B3P86 hybrid functional in combination with the 6-31G** basis set gives quite reliable bond dissociation energies. In addition, it seems that we should avoid making use of the BLYP with the purpose of improving the accuracy and save the computer resources.

Secondly, B3P86, B3PW91 and B3LYP yield relatively similar dipole moments for all the studies compounds. In other words, comparing with the calculated bond dissociation energies, the accuracy of computed dipole moments rely little on the chosen three methods. We note that the absolute errors of dipole moments carried out by B3P86/6-31G** (for ozone and nitromethane) and B3P86/6-31+G** (for RDX) are very small, therefore, as a whole, B3P86 should be the best option.

In a word, for the studied system including ozone, nitromethane, dimethylnitramine, cyanogen and RDX, the best

is found to be B3P86/6-31G** for computing both bond dissociation energies and dipole moments, although for the dipole moments of RDX, there is a slightly difference that B3P86/6-31G** is less reliable than B3P86/6-31+G**. As a result, the B3P86/6-31G** method can be considered as a successful step towards the ultimate goal of chemical accuracy for the evaluation of both bond dissociation energies and dipole moments.

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