

# Optical and vibrational properties of 1,2-benzenedicarboxylic anhydride

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Received: 10 October 2008 / Accepted: 9 January 2009 / Published online: 21 February 2009  
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**Abstract** The solvent-induced changes in the optical and spectroscopic properties of 1,2-benzenedicarboxylic anhydride are studied using time dependent Hartree-Fock and density functional theory calculations within the framework of two reaction field procedures. To investigate the influence of the cavity shape, the Onsager reaction field is compared with the polarized continuum model (PCM). It is observed that solvent polarity has noticeable effects on the vibrational properties as well as the linear and nonlinear optical characteristics of the molecule. Furthermore, the Onsager and PCM procedures may lead to contradicted harmonic vibrational frequencies; in the case of the studied molecule the Onsager model predicts the blue-shifted CH stretching band while PCM leads to red-shifted CH stretching mode.

**Keywords** First hyperpolarizability, 1,2-benzenedicarboxylic anhydride · Polarizability

## Introduction

Nonlinear optical materials have great impact on information technology; these materials can be used for data storage, optical information processing, and telecommunication. Determination of polarizability and hyperpolarizability of molecules can provide valuable information regarding the linear and nonlinear optical properties of materials [1–12]. The molecular polarizability and hyperpolarizability of some new chromophores were recently

determined by Avcı et al. [4] using ab initio Hartree-Fock method; the result of this study showed significant second order nonlinearity for the studied molecules. Guthmuller and Simon [13] investigated the optical responses of three aromatic amino acids, tryptophan, tyrosine, and phenylalanine by time dependent density functional theory (TDDFT), and suggested that these amino acids have large contribution to the nonlinear optical response of proteins.

It is known that the electric properties of molecules can be influenced by solvents [14–16]. For instance, using time dependent Hartree-Fock (TDHF) method, Balakina and Nefediev [14] showed that chloroform and acetone enhanced the calculated first hyperpolarizability  $\beta$  of several chromophores by a factor of 2.9–2.3 and 3.9–2.8, respectively. Moreover, Ray and coworkers [15] studied the first hyperpolarizabilities of a series of benzoic and cinnamic acids in water and found that solvent effects must be considered for accurate calculation of the first hyperpolarizability of these acids. Self-consistent reaction field (SCRF) approach is an appropriate method for including the solvent effects and hitherto, different reaction field models such as polarized continuum model (PCM) and Onsager reaction field have been successfully used to study the effects of solvent on solute [17–19]; in the Onsager model, solute is considered in a fixed spherical cavity while PCM defines a more realistic shape for the solute cavity.

To the best of our knowledge, the optical and vibrational properties of 1,2-benzenedicarboxylic anhydride (phthalic anhydride) in the reaction field has not yet been investigated. Phthalic anhydride is chosen for this study due to several reasons: (a) it has been observed that the PCM and Onsager models may lead to inconsistent geometrical and vibrational results for aromatic compounds [20]. Here we intend to examine the compatibility between these two models in predicting solvent effects on vibrational and

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electric properties of an aromatic molecule with low flexibility; (b) the Onsager SCRF method does not show solvent effects for compounds having dipole moment of zero. According to the experimental data, phthalic anhydride has a dipole moment of  $5.29 \pm 0.03$  Debye in benzene [21, 22]; thus, both the Onsager and PCM procedures can be used to study this molecule; (c) phthalic anhydride can be used as a precursor to many nonlinear optical polymers [23–25] therefore investigating its polarizability and hyperpolarizability can provide useful information.

In this paper, solvent effects on energy, dipole moment, polarizability, first hyperpolarizability, and vibrational frequencies of phthalic anhydride are studied using density functional theory and time dependent Hartree-Fock methods including SCRF approach.

## Theory

According to the Onsager model, the final reaction field  $V_i$  can be written as

$$V_i = -F_i = -g\mu_i = -\frac{2(\varepsilon - 1)}{(2\varepsilon + 1)a_0^3}\mu_i \quad (1)$$

where  $F_i$  is the electric field,  $g$  is a constant,  $\mu_i$  is the dipole moment of the molecule in the reaction field,  $\varepsilon$  is the dielectric constant of the medium, and  $a_0$  is the radius of the spherical cavity (the subscript  $i$  denotes Cartesian coordinate component).

The linear and nonlinear optical properties can be determined as follows:

The mean polarizability  $\bar{\alpha}$  and the anisotropy of the polarizability  $\Delta\alpha$  are given by [2]

$$\bar{\alpha} = \frac{1}{3}(\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \quad (2)$$

$$\Delta\alpha = \left[ \left( (\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 \right) / 2 \right]^{1/2} \quad (3)$$

For the first hyperpolarizability, the vector component along the dipole moment direction is

$$\beta_\mu = \frac{3}{5} \frac{\sum_i \mu_i \beta_i}{|\mu|} \quad i = x, y, z \quad (4)$$

where

$$\beta_i = \beta_{iii} + \frac{1}{3} \sum_{j \neq i} (\beta_{ijj} + \beta_{jij} + \beta_{jji}) \quad i, j = x, y, z.$$

The total intrinsic quadratic hyperpolarizability  $\beta_{tot}$  is another quantity of interest which has the form

$$\beta_{tot} = \left( \beta_x^2 + \beta_y^2 + \beta_z^2 \right)^{1/2} \quad (5)$$

## Methodology

Phthalic anhydride is considered as a solute and the reaction field effects on the energy, dipole moment, polarizability, first hyperpolarizability, and vibrational frequencies of the molecule are investigated including SCRF approach. Using Gaussian 03 program package [26] several density functional methods (SVWN, HCTH, and B3LYP) are employed along with a couple of Dunning's correlation consistent basis sets (cc-pVTZ and cc-pVDZ) which are appropriate for the calculation of the electric properties. Solvation effects are taken into consideration in the context of the Onsager reaction field and PCM procedures for several dielectric media ( $\varepsilon=1.43$ ,  $\varepsilon=2.247$ ,  $\varepsilon=4.335$ , and  $\varepsilon=78.39$ ). In the case of the Onsager model, the initial electric fields applied on the system are produced by changing the dielectric constant of the medium while the radius of the spherical cavity is constant. We also performed TDHF calculations available through GAMESS software [27, 28] to determine nonlinear optical properties of phthalic anhydride.

Here, some of the quantities are represented in atomic units (a.u.). The conversion factors from atomic units to other units are:

- 1 a.u. of energy = 27.2114 eV
- 1 a.u. of dipole moment = 2.541746 Debye
- 1 a.u. of polarizability =  $0.148185 \text{ \AA}^3$
- 1 a.u. of first hyperpolarizability =  $8.65710 \times 10^{-33}$  esu.

## Results and discussion

### Electric properties

To investigate the effect of solvent on the electric properties of the molecule two SCRF models, i.e., the Onsager dielectric continuum model (denoted by 'dipole') and the PCM were employed. The molecular dipole moments determined by the DFT and TDHF calculations are given in Table 1. As expected the dipole moment increases uniformly with increasing solvent polarity. In the case of SVWN/cc-pVTZ/dipole, for instance, the dipole moment of the molecule increases from 5.60 Debye in vacuum to 7.47 Debye in dielectric medium  $\varepsilon=78.39$ . The experimental molecular dipole moment of phthalic anhydride in benzene

**Table 1** Energy (a.u.), dipole moment (Debye), polarizability (a.u.), and first hyperpolarizability ( $10^{-33}$  esu) of phthalic anhydride

method	medium	$\mu$	$\bar{\alpha}$	$\Delta\alpha$	$\beta_{\mu}$	$\beta_{tot}$	energy
SVWN/cc-pVTZ/dipole	vacuum	5.60	94.10	74.57	236.57	394.28	-530.294
	$\epsilon=1.43$	5.93	98.68	80.20	126.19	210.32	-530.295
	$\epsilon=2.247$	6.32	103.99	86.86	-56.26	93.77	-530.296
	$\epsilon=4.335$	6.79	110.18	94.79	-348.54	580.90	-530.297
	$\epsilon=78.39$	7.47	119.03	106.37	-968.09	1613.48	-530.300
SVWN/cc-pVDZ/dipole	vacuum	5.32	86.72	78.98	354.60	591.00	-530.111
	$\epsilon=1.43$	5.61	90.65	84.17	290.80	484.66	-530.112
	$\epsilon=2.247$	5.95	95.19	90.22	180.57	300.95	-530.113
	$\epsilon=4.335$	6.36	100.41	97.29	1.54	2.56	-530.115
	$\epsilon=78.39$	6.93	107.79	107.39	-380.65	634.41	-530.116
B3LYP/cc-pVDZ/dipole	vacuum	5.50	85.05	76.85	182.47	304.12	-532.99
	$\epsilon=1.43$	5.79	88.83	81.81	99.24	165.40	-532.991
	$\epsilon=2.247$	6.13	93.18	87.60	-34.68	57.81	-532.992
	$\epsilon=4.335$	6.54	98.20	94.34	-246.38	410.63	-532.994
	$\epsilon=78.39$	7.12	105.26	103.97	-676.04	1126.74	-532.996
SVWN/cc-pVDZ/PCM	vacuum	5.32	86.72	78.98	354.60	591.00	-530.111
	$\epsilon=1.43$	5.73	93.12	86.81	165.07	275.11	-530.114
	$\epsilon=2.247$	6.18	100.52	95.65	-129.27	215.44	-530.117
	$\epsilon=4.335$	6.68	109.10	105.54	-590.51	984.19	-530.121
	$\epsilon=78.39$	7.34	122.05	119.55	-1539.85	2566.42	-530.125
TDHF/cc-pVDZ/PCM	vacuum	6.04	78.53			384.49	
	$\epsilon=2.247$	6.82	89.79			90.02	
	$\epsilon=4.9$	7.31	97.58			593.39	
	$\epsilon=78.39$	7.80	106.22			1322.70	

is  $5.29 \pm 0.03$  Debye [21]. Applying HCTH density functional along with different basis sets (Pople's, Dunning/Huzinaga, Dunning's correlation consistent, and so on) we found that Dunning's correlation consistent basis sets and MidiX of Truhlar and coworkers provide dipole moment values in better agreement with the experimental data. The DFT- and TDHF-calculated dipole moment values in benzene ( $\epsilon=2.247$ ) are shown in Table 2. These results demonstrate the influence of the selected method and basis set in the calculated dipole moment. It should also be noted

**Table 2** DFT- and TDHF-calculated dipole moment (Debye) of phthalic anhydride in benzene

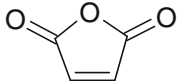
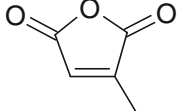
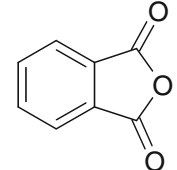
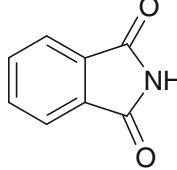
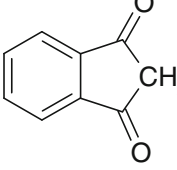
Method	Dipole moment
SVWN/cc-pVTZ/dipole	6.32
SVWN/cc-pVDZ/dipole	5.95
HCTH/cc-pVDZ/dipole	5.88
HCTH/MidiX/dipole	5.32
B3LYP/cc-pVDZ/dipole	6.13
B3LYP/MidiX/dipole	5.45
SVWN/cc-pVDZ/PCM	6.18
TDHF/cc-pVDZ/PCM	6.82

that for the same level of theory, polarized continuum model results in higher dipole moment values in comparison with Onsager reaction field (Table 1).

Table 3 shows the dipole moments of several diketones in benzene; a reasonable agreement is found between the experimental and calculated (SVWN/cc-pVDZ/dipole) values indicating the efficiency of Dunning's correlation consistent basis set in predicting electric properties.

The DFT-calculated mean polarizability  $\bar{\alpha}$  and anisotropy of the polarizability  $\Delta\alpha$  for phthalic anhydride are included in Table 1. Increasing the dielectric constant of the medium results in higher  $\bar{\alpha}$  and  $\Delta\alpha$ . For the SVWN/cc-pVTZ method, the mean polarizability is found to be 94.10 a.u. in vacuum and 119.03 a.u. in a medium of dielectric constant  $\epsilon=78.39$  (considering SCRF=dipole). The anisotropy of the polarizability using the same procedure is 74.57 a.u. in vacuum and 106.37 a.u. in a medium with  $\epsilon=78.39$ . As can be seen from the Table, there is a close agreement between the results of the two self-consistent reaction field procedures exhibiting similar trends although both quantities  $\bar{\alpha}$  and  $\Delta\alpha$  have larger values in the case of the polarized continuum model (see the SVWN/cc-pVDZ calculated values within the framework of the PCM and Onsager reaction field in Table 1).

**Table 3** Dipole moments (Debye) of several diketones in benzene: maleic anhydride (1), citraconic anhydride (2), phthalic anhydride (3), phthalimide (4), and indane-1,3-dione (5)

no.	structure	$\mu$ calc.	$\mu$ obs.
1		4.05	3.95 <sup>a</sup>
2		4.73	4.26 <sup>a</sup>
3		5.95	5.29 <sup>b</sup>
4		2.69	2.12 <sup>c</sup>
5		3.13	2.73 <sup>c</sup>

<sup>a</sup> Ref. 22 <sup>b</sup> Ref 21 <sup>c</sup> Ref 29

The polarizability components ( $\alpha_{xx}$ ,  $\alpha_{yy}$ , and  $\alpha_{zz}$ ) of the isolated molecule based on the time dependent HF method are, respectively, 100.22, 34.80, and 100.59 a.u. These values are, respectively, ca. 1.4, 1.3, and 1.3 times higher in water ( $\epsilon=78.39$ ) compared with the corresponding values in the gas phase demonstrating a considerable dependency on the solvent polarity.

According to SVWN/cc-pVDZ procedure (Table 1) the first hyperpolarizability  $\beta_{\mu}$  of phthalic anhydride in vacuum is  $354.60 \times 10^{-33}$  esu. In a medium of dielectric constant  $\epsilon=78.39$  the quantity  $\beta_{\mu}$  decreases to  $-380.65 \times 10^{-33}$  esu (for the Onsager model), and  $-1539.85 \times 10^{-33}$  esu (for PCM). The influence of the basis set and the reaction field model is obvious in the values of the first hyperpolarizability (see Table 1). Another quantity of interest is the total intrinsic quadratic hyperpolarizability  $\beta_{\text{tot}}$  which based on SVWN/cc-pVDZ level of theory is evaluated to be  $591.00 \times 10^{-33}$  esu for the isolated molecule and  $634.41 \times 10^{-33}$  esu (Onsager model) and  $2566.42 \times 10^{-33}$  esu (PCM) in a medium with  $\epsilon=78.39$ . The data in Table 1 indicate that the values of the hyperpolarizabilities calculated

by the two reaction field models are generally in good agreement.

The above results demonstrate the influence of the solvent on the linear and nonlinear optical properties of phthalic anhydride. In the case of SVWN/cc-pVDZ/dipole calculations, the dipole moment  $\mu$ , mean polarizability  $\alpha$ , anisotropy of the polarizability  $\Delta\alpha$ , and the total hyperpolarizability  $\beta_{\text{tot}}$  are, respectively,  $\sim 1.3$ , 1.2, 1.4, and 1.1 times greater in water ( $\epsilon=78.39$ ) in comparison with the corresponding values in the vacuum.

For the SVWN/cc-pVDZ/PCM, the dipole moment, mean polarizability, anisotropy of the polarizability, and total hyperpolarizability are, respectively, ca. 1.4, 1.4, 1.5, and 4.3 times higher in water compared with the related values in the gas phase. It is observed that the quantity  $\beta_{\text{tot}}$  is maximally affected by the choice of the reaction field model.

The energy of the molecule can be expressed as a Taylor series in the electric field strength, thus in the case of the Onsager model, we have

$$W = W^0 + \mu_i^0 V_i - \frac{1}{2} \alpha_{ij}^0 V_i V_j + \frac{1}{6} \beta_{ijk}^0 V_i V_j V_k - \frac{1}{2} \mu_i V_i$$

in which  $W^0$ ,  $\mu_i^0$ ,  $\alpha_{ij}^0$ , and  $\beta_{ijk}^0$  are the energy, dipole moment, polarizability, and hyperpolarizability, respectively, of the molecule in the absence of field. The above equation indicates the contribution of electric properties in the total energy of the molecule. It is possible to show that the hyperpolarizability term has negligible contribution in comparison with the other terms [19]. The energy of the molecule in reaction field obtained by SVWN and B3LYP density functional methods is represented in Table 1. It is found that SVWN/cc-pVTZ and SVWN/cc-pVDZ lead to more positive energies ( $\sim -530$  a.u.) compared to B3LYP/cc-pVDZ ( $\sim -532$  a.u.). Furthermore, due to the polarization of the molecule, it is expected that dipole moment increases and energy decreases with the applied electric field. For example, according to the SVWN/cc-pVTZ/dipole method, the calculated energy of the molecule decreases from  $-530.294$  a.u. for the isolated molecule to  $-530.300$  a.u. in a medium of dielectric constant  $\epsilon=78.39$ . It is also observed that there is good consistency between the results of the two reaction field models, both decreasing with dielectric constant.

#### Frontier orbitals

The energies of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) are given in Table 4. As can be seen, in both SCRF models the HOMO energy decreases while the LUMO energy changes to more positive values. In the

**Table 4** HOMO and LUMO energies (a.u.) of phthalic anhydride in several dielectric media

Method	Medium	HOMO	LUMO
SVWN/cc-pVDZ/dipole	Vacuum	-0.2643	-0.1506
	$\epsilon=1.43$	-0.2650	-0.1503
	$\epsilon=2.247$	-0.2657	-0.1500
	$\epsilon=4.335$	-0.2666	-0.1500
	$\epsilon=78.39$	-0.2679	-0.1497
SVWN/cc-pVDZ/PCM	vacuum	-0.2643	-0.1506
	$\epsilon=1.43$	-0.2651	-0.1495
	$\epsilon=2.247$	-0.2662	-0.1489
	$\epsilon=4.335$	-0.2676	-0.1484
	$\epsilon=78.39$	-0.2695	-0.1476

case of the Onsager model (PCM), the HOMO energy decreases from -0.2643 in vacuum to -0.2679 (-0.2695) a.u. in a solvent with  $\epsilon=78.39$  while the LUMO energy increases from -0.1506 in vacuum to -0.1497 (-0.1476) a.u. in a medium of dielectric constant  $\epsilon=78.39$ .

#### Harmonic vibrational frequencies

As we mentioned earlier, the PCM and Onsager models may lead to inconsistent geometrical and vibrational results for aromatic compounds. Thus, it is instructive to study the vibrational properties of phthalic anhydride using the aforementioned models. Table 5 represents the harmonic vibrational frequencies of some normal modes of phthalic anhydride, including  $\nu_{34}$ ,  $\nu_{35}$  (C=O stretching) and  $\nu_{36}$ ,  $\nu_{37}$ ,  $\nu_{38}$ ,  $\nu_{39}$  (C–H stretching) for SVWN/cc-pVDZ/dipole and SVWN/cc-pVDZ/PCM. According to the Onsager model, the C=O stretching frequency is red-shifted while in the

case of C–H bond blue-shifted CH stretching frequency results; for example, in the range of the dielectric constants studied  $\nu_{34}$  decreases from 1853.8 to 1838.8  $\text{cm}^{-1}$  and  $\nu_{39}$  increases from 3147.9 to 3150.6  $\text{cm}^{-1}$ . PCM results, on the other hand, show red-shifted stretching frequencies for both C=O and C–H bonds;  $\nu_{34}$  decreases from 1853.8 to 1809.1  $\text{cm}^{-1}$  and  $\nu_{39}$  is reduced from 3147.9 to 3061.4  $\text{cm}^{-1}$ .

This discrepancy can be attributed to the fact that in the case of the Onsager model only the dipole moment contribution is taken into account but it should be noted that the higher order multipoles are not negligible for aromatic compounds. Moreover, if we consider the interaction of the C=O (or C–H) bond of the solute with solvent molecules, it is expected that increasing the interactions results in bond lengthening and red-shifted stretching modes.

#### Conclusions

A comparative study is made between two reaction field models, the PCM and the Onsager model. Accordingly, the vibrational frequencies as well as the linear and nonlinear optical properties of 1,2-benzenedicarboxylic anhydride (phthalic anhydride) molecule are investigated through density functional theory and time dependent Hartree-Fock methods. It is found that the calculated electric properties (dipole moment, polarizability, and first hyperpolarizability) from the two reaction field models are in reasonable agreement although the polarized continuum model shows larger solvent effects. Studying harmonic vibrational frequencies by the Onsager and PCM procedures, on the other hand, may lead to contradicted

**Table 5** Unscaled vibrational frequencies ( $\text{cm}^{-1}$ ) of the C=O ( $\nu_{34}$ ,  $\nu_{35}$ ) and C–H ( $\nu_{36}$ ,  $\nu_{37}$ ,  $\nu_{38}$ ,  $\nu_{39}$ ) stretching modes of phthalic anhydride

SVWN/cc-pVDZ/dipole						
Medium	$\nu_{34}$	$\nu_{35}$	$\nu_{36}$	$\nu_{37}$	$\nu_{38}$	$\nu_{39}$
Vacuum	1853.79	1906.60	3124.09	3135.00	3143.64	3147.89
$\epsilon=1.43$	1851.69	1905.40	3125.46	3135.83	3144.08	3148.52
$\epsilon=2.247$	1849.14	1903.87	3126.81	3136.62	3144.53	3149.14
$\epsilon=4.335$	1844.38	1899.93	3128.27	3137.59	3145.28	3149.94
$\epsilon=78.39$	1838.81	1895.74	3129.75	3138.49	3145.93	3150.60
SVWN/cc-pVDZ/PCM						
medium	$\nu_{34}$	$\nu_{35}$	$\nu_{36}$	$\nu_{37}$	$\nu_{38}$	$\nu_{39}$
vacuum	1853.79	1906.60	3124.09	3135.00	3143.64	3147.89
$\epsilon=1.43$	1846.47	1901.52	3111.20	3120.63	3127.93	3132.75
$\epsilon=2.247$	1835.70	1893.26	3095.00	3103.20	3109.76	3114.92
$\epsilon=4.335$	1824.84	1885.50	3075.20	3081.89	3087.92	3093.73
$\epsilon=78.39$	1809.08	1874.33	3043.77	3048.30	3054.48	3061.44

outcomes. In the case of the studied molecule, the Onsager model predicts the blue-shifted CH stretching band while PCM leads to red-shifted CH stretching mode.

Furthermore, it is shown that the choice of the basis set and/or the theoretical method (DFT, TDHF) may have a noticeable effect on the calculated values of the dipole moment, polarizability, and first hyperpolarizability of the molecule.

**Acknowledgement** M. Asghari-Khiavi acknowledges the support from Monash University scholarships (MGS and MFRS).

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