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Chemical Physics xxx (2004) xxx–xxx

Chemical Physics

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Vibrational contributions to the dynamic electric properties of the NaF molecule

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Received 7 July 2004; accepted 29 July 2004

Abstract

In this work, we report calculations of the vibrational corrections to the dynamic polarizability and first hyperpolarizability of the NaF molecule performed through the CPHF method. We have considered frequencies varying from 0 to 0.12 hartree. Results obtained show that the zpva contributions are small in comparison with the corresponding electronic contributions. It is shown that both contributions can be well described by quartic polynomial fits. The pv contributions are important on the vibrational range of frequencies but negligible on the visible region, except for $\beta_{xxz}(-\omega;\omega,0)$ and $\beta_{zzz}(-\omega;\omega,0)$. A detailed study of the pv contributions over the range of vibrational frequencies, including an electron correlation treatment at the CCSD(T) level, is presented.
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Keywords: Hyperpolarizability; Vibrational corrections; NaF

1. Introduction

The important role played by dynamic electric properties in technological applications has been reviewed in a number of previous papers [1–5]. Alkali metal halides molecules attract especial interest because of their strong ionic character, which is responsible for large values for the dipole moment and first hyperpolarizability [6]. Recent studies [7,8] have also shown that, as consequence of their ionic character, these systems present remarkably large vibrational corrections to the static polarizability and hyperpolarizability. In this work, we investigate the importance of the vibrational corrections on calculations of frequency-dependent electric properties for alkali metal halides. We have chosen the NaF molecule as a representative case because the existence of previous calculations [8] on vibrational corrections for the polarizability and hyperpolarizability of this system in the static limit.

We have calculated the dynamic polarizability and hyperpolarizability of the NaF molecule for frequencies varying from 0 to 0.12 hartree. This interval includes frequencies which are in the range of the vibrational transition frequencies and also in the range of the visible spectrum (between 0.06 and 0.12 hartree). Although vibrational corrections tend to be smaller for higher frequencies, previously reported results for other systems [9,10] have shown that these corrections are not always negligible on the visible range. Dipole hyperpolarizabilities calculated in this work are $\beta(-\omega;\omega,0)$, which is related to the electro-optic Pockels effect, and $\beta(-2\omega;\omega,\omega)$, which corresponds to the second harmonic generation.

2. Computational details

The great majority of the ab initio molecular calculations is based on the Born–Oppenheimer approximation which treat separately the electronic and nuclear motions. In the context of this approximation, the calculated

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doi:10.1016/j.chemphys.2004.07.040

molecular electric properties are also separated into electronic and nuclear contributions. Besides, the nuclear contribution can be further divided into vibrational and rotational contributions. Since the rotational contribution is usually negligible, as compared with its electronic and vibrational counterparts [11], it has not been included in this work.

Electronic contribution calculations for the dynamic electric properties presented in this work were performed by means of the coupled perturbed Hartree–Fock (CPHF) method [12–14], using the Gaussian 03 program [15]. We have employed the same basis set of even-tempered Cartesian Gaussian-type functions previously used on the calculations of the static electric properties of the NaF molecule [8]. This basis set comprises a total of 119 uncontracted Gaussian-type functions and can be denoted as 14s10p6d for Na and 13s9p5d for F. It was carefully prepared aiming at giving static values for both components of the hyperpolarizability with errors smaller than 1%.

Two well known formulations have been put forward to compute the vibrational contributions for the electric properties: the finite field and sum-over-states methods. In the framework of the finite field method [4,5,16,17] the vibrational corrections are divided into nuclear relaxation and curvature contributions. The former arises from the changes on the equilibrium positions of the nuclei in the presence of the external electric fields while the latter contribution is associated with the changes on the form of the potential surface on which the nuclei vibrate. Unfortunately, this methodology is not applicable in the case of frequency-dependent electric fields.

In this work, we have employed the sum-over-states formulation [4,5,18,19] to compute the vibrational contributions to the dynamic electric properties of the NaF molecule. According to this methodology, the vibrational corrections are divided into zero-point vibrational averaging (zpva) and pure vibrational (pv) contributions. Thus, the total (tot) values of the hyperpolarizability can be written as

$$\beta^{\mathrm{tot}} = \beta^{\mathrm{el}} + \beta^{\mathrm{zpva}} + \beta^{\mathrm{pv}}, \tag{1}$$

where the el superscript indicates the electronic contribution calculated at the equilibrium geometry. A similar expression can be written for α^{tot}.

The zpva contribution is given by the difference between the average of the corresponding electronic contribution, calculated using the vibrational wave function, and the equilibrium electronic value.

General formulas to compute the pure vibrational contributions for dynamic electric properties have been derived by Bishop [18,19]. Formulas for diatomic molecules, used in this work, are shown below. For the dipole polarizability only the α_{zz} component possess pv contribution which is given by

$$\alpha^{\mathrm{pv}}_{zz}(-\omega;\omega) = \sum_v |\langle 0|\mu_z|v\rangle|^2 \left(\frac{1}{\epsilon_{v0}-\omega} + \frac{1}{\epsilon_{v0}+\omega}\right), \tag{2}$$

where $|0\rangle$ denotes the vibrational ground state while $|v\rangle$ symbolizes the excited states. The ϵ_0 and ϵ_v are the corresponding vibrational energies, and $\epsilon_{v0}(=\epsilon_v-\epsilon_0)$ represents the energy difference between the $|0\rangle$ and $|v\rangle$ states. Following the usual notation, ω is expressed in units of energy, where the $\hbar$ factor is omitted.

The zzz component of the hyperpolarizability is given by

$$\begin{aligned}\beta^{\mathrm{pv}}_{zzz}(-\omega_\sigma;\omega_1,\omega_2) = {} & \sum P_{-\sigma,1,2} \sum_v \langle 0|\mu_z|v\rangle\langle 0|\alpha_{zz}|v\rangle \\ & \times \left(\frac{1}{\epsilon_{v0}-\omega_\sigma} + \frac{1}{\epsilon_{v0}+\omega_\sigma}\right) + \sum P_{-\sigma,1,2} \\ & \times \left\{ \sum_v \sum_u \frac{\langle 0|\mu_z|v\rangle\langle 0|\mu_z|u\rangle\langle v|\mu_z|u\rangle}{(\epsilon_{v0}-\omega_\sigma)(\epsilon_{u0}-\omega_1)} \right. \\ & \left. - \sum_v \frac{|\langle 0|\mu_z|v\rangle|^2\langle 0|\mu_z|0\rangle}{(\epsilon_{v0}-\omega_\sigma)(\epsilon_{v0}-\omega_1)} \right\},\end{aligned} \tag{3}$$

where the symbol $\sum P_{-\sigma,1,2}$ indicates the summation over all distinct terms obtained by permuting the frequencies $-\omega_\sigma$, ω_1 and ω_2.

Formulas for the others independent components of the β tensor are simpler and can be written as:

$$\beta^{\mathrm{pv}}_{zxx}(-\omega_\sigma;\omega_1,\omega_2) = \sum_v \langle 0|\mu_z|v\rangle\langle 0|\alpha_{xx}|v\rangle \left(\frac{1}{\epsilon_{v0}-\omega_\sigma} + \frac{1}{\epsilon_{v0}+\omega_\sigma}\right), \tag{4}$$

$$\beta^{\mathrm{pv}}_{xzx}(-\omega_\sigma;\omega_1,\omega_2) = \sum_v \langle 0|\mu_z|v\rangle\langle 0|\alpha_{xx}|v\rangle \left(\frac{1}{\epsilon_{v0}-\omega_1} + \frac{1}{\epsilon_{v0}+\omega_1}\right), \tag{5}$$

$$\beta^{\mathrm{pv}}_{xxz}(-\omega_\sigma;\omega_1,\omega_2) = \sum_v \langle 0|\mu_z|v\rangle\langle 0|\alpha_{xx}|v\rangle \left(\frac{1}{\epsilon_{v0}-\omega_2} + \frac{1}{\epsilon_{v0}+\omega_2}\right). \tag{6}$$

The above formulas do not consider damping effects [20] which are negligibly small for the electronic and vibrational transitions considered here. As $\beta^{\mathrm{pv}}_{xzx}(-\omega;\omega,0) = \beta^{\mathrm{pv}}_{zxx}(-\omega;\omega,0)$ and $\beta^{\mathrm{pv}}_{xzx}(-2\omega;\omega,\omega) = \beta^{\mathrm{pv}}_{xxz}(-2\omega;\omega,\omega)$, only the $\beta^{\mathrm{pv}}_{zxx}$ and $\beta^{\mathrm{pv}}_{xxz}$ components are quoted in the text.

In order to compute the pv contributions, we have taken into account the four lowest excited vibrational states. In a previous work [8] on NaF, it has been shown that the inclusion of the three lowest excited states is sufficient to find static pv contributions for α and β with precisions of 0.001 and 0.1 a.u., respectively. Here being more cautious, we have included one more excited state on the summations which leads to the pv contributions to dynamic electric properties. As regards the computation of the vibrational energies and wave functions we have made use of the potential energy curves obtained

as polynomial fits of seven points (separated by 0.06 Å) and employed the Numerov–Cooley procedure [21]. We have adopted the more abundant isotopes ^{19}F and ^{23}Na which gives a reduced mass of 10.40546 a.u. for the NaF molecule.

According to Bishop [5], the electronic properties appearing in the numerators of formulas (2)–(6) take their static values implying that the frequency dependence of the pure vibrational contributions is restricted to the terms in the denominators of these equations. Thus, electron correlation effects for the dynamic pv contributions can be obtained by the use of correlated vibrational energies, correlated vibrational wave functions and correlated static electronic properties. In this work, we have introduced the electron correlation corrections on the calculations of the pv contributions through the CCSD(T) [22] method. We have included in the electron correlation process the orbitals ranging from 4 to 104. As already stressed in [8], the excluded orbitals have no appreciable effect on the calculations of the electron correlation effects for the properties studied here.

3. Results and discussions

In this section, we report results for the dynamic electric properties of the NaF molecule. Results obtained for the electronic, zpva and pv contributions are displayed in Tables 1–3. We have chosen the positive z-axis pointing from the F to Na, which leads to a positive dipole moment.

Results presented in Tables 1 and 2 show that the zpva contributions are very small as compared with the corresponding electronic contributions. One can also see that the relative importance of the zpva contribution is practically independent of the frequency for all properties studied. The zpva contribution represents less than 0.5% of the corresponding electronic contribution for both components of α. Excluding the two highest frequencies at the columns corresponding to the components of the $\beta(-2\omega;\omega,\omega)$ tensor, one can note that the ratio between zpva and electronic contributions vary from 1% to 1.6% for the β_{xxz} components and from 2.5% to 3% for the β_{zzz} components.

From Tables 1 and 2, one can see that the values obtained for the electronic and zpva contributions are practically the same for the frequencies of 0.0 and 0.0045 hartree. In fact we have performed a series of calculations for a number of other frequencies in this range, and obtained for all of them very similar results. An overall look at these tables show that, in general, such contributions change smoothly with the frequency. It is possible to represent the frequency dependence of the electronic and zpva contributions by means of quartic polynomials. Taking α_{zz} as an example, we can write

$$\alpha_{zz}(-\omega;\omega) = \alpha_{zz}(-0;0)(1 + a\omega^2 + b\omega^4). \quad (7)$$

Similar expressions can be written for the other properties. Values of a and b obtained through the least-square method are displayed in Table 4. An estimate of the fitting accuracy is given by the relative root-mean-square deviation (δ), which is defined as the root-mean-square deviation divided by the static value

Table 1
Electronic contributions to the dynamic polarizability and hyperpolarizability of the NaF molecule (in atomic units)

ω	$\alpha_{xx}^{el}(\omega;\omega)$	$\alpha_{zz}^{el}(\omega;\omega)$	$\beta_{xxz}^{el}(-\omega;\omega,0)$	$\beta_{zxx}^{el}(-\omega;\omega,0)$	$\beta_{zzz}^{el}(-\omega;\omega,0)$	$\beta_{xxz}^{el}(-2\omega;\omega,\omega)$	$\beta_{zxx}^{el}(-2\omega;\omega,\omega)$	$\beta_{zzz}^{el}(-2\omega;\omega,\omega)$
0.00	8.9988	9.1476	−15.553	−15.553	−32.722	−15.553	−15.553	−32.722
0.0045	8.9997	9.1485	−15.563	−15.561	−32.742	−15.576	−15.581	−32.782
0.02	9.0151	9.1634	−15.724	−15.697	−33.072	−15.963	−16.048	−33.790
0.04	9.0648	9.2114	−16.258	−16.141	−34.158	−17.293	−17.691	−37.327
0.06	9.1500	9.2938	−17.214	−16.923	−36.088	−19.903	−21.100	−44.597
0.08	9.2749	9.4145	−18.716	−18.116	−39.076	−24.692	−28.052	−59.066
0.10	9.4461	9.5797	−20.986	−19.843	−43.491	−34.096	−45.012	−91.893
0.12	9.6741	9.7993	−24.430	−22.308	−49.973	−57.864	−123.409	−202.408

Table 2
Zero-point vibrational averaging contributions to the dynamic polarizability and hyperpolarizability of the NaF molecule (in atomic units)

ω	$\alpha_{xx}^{zpva}(\omega;\omega)$	$\alpha_{zz}^{zpva}(\omega;\omega)$	$\beta_{xxz}^{zpva}(-\omega;\omega,0)$	$\beta_{zxx}^{zpva}(-\omega;\omega,0)$	$\beta_{zzz}^{zpva}(-\omega;\omega,0)$	$\beta_{xxz}^{zpva}(-2\omega;\omega,\omega)$	$\beta_{zxx}^{zpva}(-2\omega;\omega,\omega)$	$\beta_{zzz}^{zpva}(-2\omega;\omega,\omega)$
0.00	0.0136	0.0367	−0.177	−0.177	−0.814	−0.177	−0.177	−0.814
0.0045	0.0136	0.0367	−0.177	−0.177	−0.814	−0.177	−0.177	−0.816
0.02	0.0137	0.0368	−0.180	−0.179	−0.825	−0.184	−0.185	−0.847
0.04	0.0139	0.0375	−0.188	−0.187	−0.858	−0.208	−0.214	−0.931
0.06	0.0144	0.0387	−0.205	−0.201	−0.920	−0.260	−0.279	−1.212
0.08	0.0151	0.0405	−0.233	−0.223	−1.019	−0.369	−0.439	−1.783
0.10	0.0162	0.0431	−0.276	−0.256	−1.172	−0.652	−1.012	−3.459
0.12	0.0177	0.0466	−0.350	−0.307	−1.411	−2.051	−10.067	−14.071

Table 3
Pure vibrational contributions to the dynamic polarizability and hyperpolarizabilitiy of the NaF molecule (in atomic units)

ω	$\alpha_{zz}^{pv}(\omega;\omega)$	$\beta_{zzz}^{pv}(-\omega;\omega,0)$	$\beta_{xxz}^{pv}(-2\omega;\omega,\omega)$	$\beta_{zxx}^{pv}(-2\omega;\omega,\omega)$	$\beta_{zzz}^{pv}(-2\omega;\omega,\omega)$
0.00	7.2989	230.171	8.288	8.288	230.171
0.0045	−2.3010	212.592	−2.486	−1.090	−14.615
0.02	−0.1126	17.777	−0.128	−0.032	−0.639
0.04	−0.0278	18.358	−0.032	−0.008	−0.159
0.06	−0.0123	18.468	−0.014	−0.003	−0.070
0.08	−0.0069	18.507	−0.008	−0.002	−0.040
0.10	−0.0044	18.526	−0.005	−0.001	−0.025
0.12	−0.0031	18.535	−0.003	−0.001	−0.018

of the property. The small values of δ displayed in Table 4 certificate the good quality of the fits. It is worthwhile mentioning that if all values of frequency displayed in Tables 1 and 2 were included on the fits of the $\beta(-2\omega;\omega,\omega)$ tensor components, the results would not be good. This disagreement occurs because the quartic expansion fails for high frequencies. In face of this situation, the values of δ displayed in Table 4 for the $\beta(-2\omega;\omega,\omega)$ components were obtained excluding the two higher frequencies.

Previous results for the electronic contributions computed through the TDHF method have been reported by Pluta [6] for frequencies of 0.0345, 0.0428, 0.0656 and 0.0886 hartree. We have obtained results for these frequencies employing Eq. (7) with the values of a and b taken from Table 4. Comparison of our results with those obtained by Pluta shows a very good agreement.

Values for the pv contributions are displayed in Table 3. It is evident from Eq. (6) that $\beta_{xxz}^{pv}(-\omega;\omega,0)$ is independent of the frequency. It is also easily seen, from Eqs. (4) and (6), that $\beta_{zxx}^{pv}(-\omega;\omega,0)=\beta_{xxz}^{pv}(-2\omega;\omega,\omega)$. Thus, columns corresponding to $\beta_{xxz}^{pv}(-\omega;\omega,0)$ and $\beta_{zxx}^{pv}(-\omega;\omega,0)$ are not included in Table 3. One can observe that pv contributions are negligible for frequencies on the visible region (above 0.06 hartree), except for $\beta_{xxz}^{pv}(-\omega;\omega,0)$ and $\beta_{zzz}^{pv}(-\omega;\omega,0)$. The former is independent of the frequency and its magnitude is given by the static value of 8.288 a.u. while the latter converges to 18.53 a.u.; these values are not negligible in comparison with their electronic counterparts. The behavior of $\beta_{zzz}^{pv}(-\omega;\omega,0)$ for high frequencies can be found from Eq. (3) which shows that $\beta_{zzz}^{pv}(-\omega;\omega,0)$ tends to $2\sum_v(\langle 0|\mu_z|v\rangle\langle 0|\alpha_{zz}|v\rangle/\epsilon_{v0})$ when ω approaches infinity.

It comes out from Table 3 that the pure vibrational contributions are very important on the range of vibrational frequencies. A detailed analysis of the frequency dependence of the pv contributions over this range of frequencies is shown in Figs. 1–5. In these figures, ω varies from 0 to 0.0045 hartree which corresponds to approximately $2\epsilon_{10}$. Resonances are observed wherever the pv contributions present divergent behaviors. We have performed test calculations in which the damping effects were simulated by the inverse radiative lifetime of the state $|v\rangle$ and the results obtained have shown that the extreme values of α and β are incomparably larger than the corresponding static values. Thus, in order to keep a reasonable scale to visualize the pv contribution away from the resonances we have omitted those pieces of the curves close to the poles.

Resonance frequencies can be readily obtained from formulas (2)–(6). Properties shown in Figs. 1–3 present resonances for $\omega=\epsilon_{10}$ which corresponds to frequencies of 0.002459 hartree at the SCF level and 0.002371 hartree at the CCSD(T) level. Figs. 4 and 5 present three resonances which occur for $\omega=\frac{1}{2}\epsilon_{10}$, $\frac{1}{2}\epsilon_{20}$ and $\frac{1}{2}\epsilon_{30}$, corresponding to frequencies of 0.001230, 0.002443 and 0.003640 hartree at the SCF level, and 0.001185, 0.002355 and 0.003509 hartree at the CCSD(T) level. Other resonances, which occur for higher frequencies, are not shown in the figures.

It is interesting to note, at all graphics, the resemblance between the curves obtained at the SCF and

Table 4
Coefficients of the quadratic fit and relative root-mean-square deviation for frequency dependent electric properties of the NaF molecule (in atomic units)

		$\alpha_{xx}(\omega;\omega)$	$\alpha_{zz}(\omega;\omega)$	$\beta_{xxz}(-\omega;\omega,0)$	$\beta_{zxx}(-\omega;\omega,0)$	$\beta_{zzz}(-\omega;\omega,0)$	$\beta_{xxz}(-2\omega;\omega,\omega)$	$\beta_{zxx}(-2\omega;\omega,\omega)$	$\beta_{zzz}(-2\omega;\omega,\omega)$
el	a	4.462	4.429	25.52	22.24	25.35	60.86	68.30	71.53
	b	51.87	48.34	973.8	547.7	777.8	4825	8920	8453
	δ	0.00004	0.00004	0.002	0.0007	0.001	0.001	0.003	0.003
zpva	a	14.50	14.05	33.65	32.06	30.05	83.93	80.52	67.17
	b	448.7	328.1	2354	1306	1440	13333	23453	18597
	δ	0.001	0.001	0.006	0.002	0.002	0.004	0.01	0.007

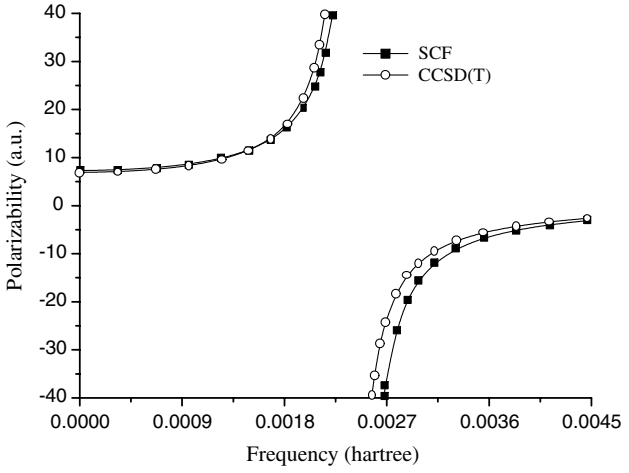

Fig. 1. Pure vibrational contribution to $\alpha_{zz}(-\omega;\omega)$ calculated at the SCF and CCSD(T) levels.

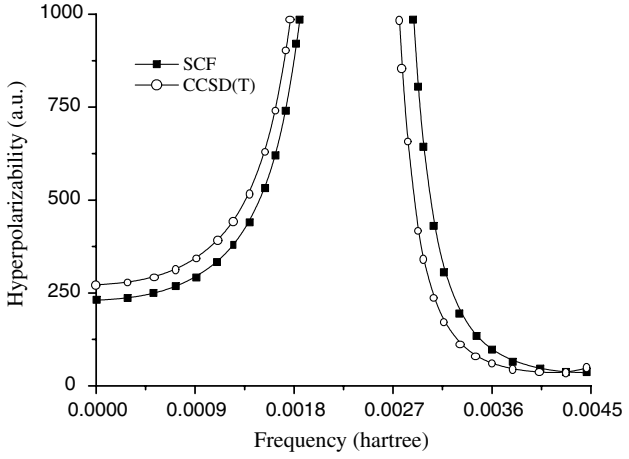

Fig. 2. Pure vibrational contribution to $\beta_{zzz}(-\omega;\omega,0)$ calculated at the SCF and CCSD(T) levels.

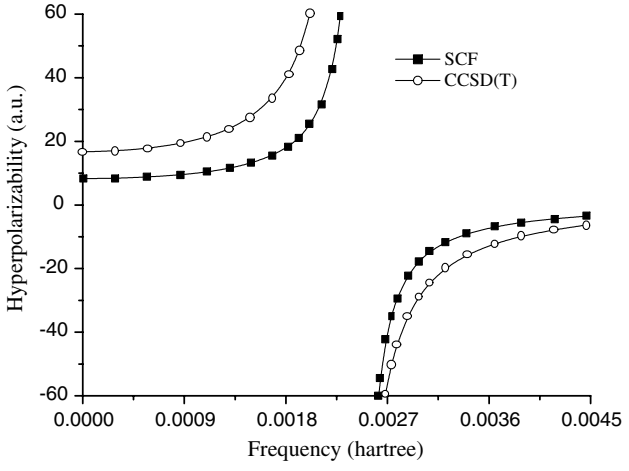

Fig. 3. Pure vibrational contribution to $\beta_{xxz}(-2\omega;\omega,\omega)$ calculated at the SCF and CCSD(T) levels.

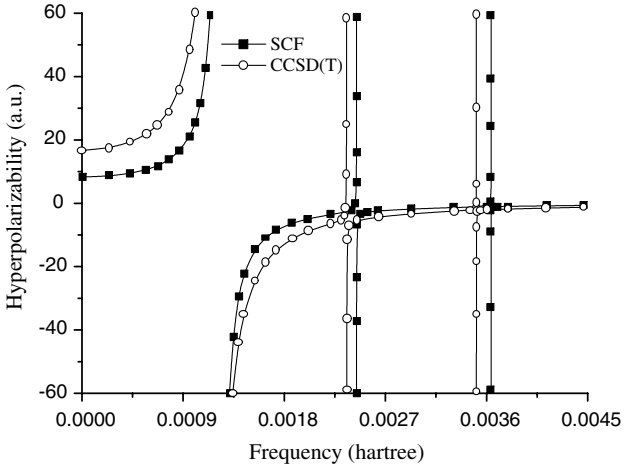

Fig. 4. Pure vibrational contribution to $\beta_{zxx}(-2\omega;\omega,\omega)$ calculated at the SCF and CCSD(T) levels.

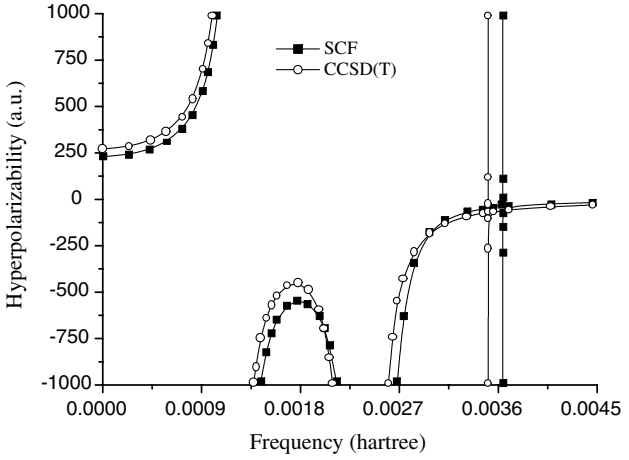

Fig. 5. Pure vibrational contribution to $\beta_{zzz}(-2\omega;\omega,\omega)$ calculated at the SCF and CCSD(T) levels.

CCSD(T) levels. Correlated curves tend to be displaced to the left in relation to the SCF curves because the inclusion of the electron correlation effects decrease the calculated values of the resonance frequencies. Fig. 1 shows the results obtained for the pv contribution to the dipole polarizability. One can see that the electron correlation effects are small for this property. For frequencies varying from 0.0 to 0.0018 hartree, the difference between correlated and SCF values remains below 6%. This difference increases when ω approaches the resonance frequency. Results obtained for the pv contributions to the hyperpolarizability are presented in Figs. 2–5. The resemblance between the SCF and CCSD(T) curves, also observed in these figures, is not impaired by the more important electron correlation corrections to the hyperpolarizability.

4. Conclusions

In this work, we have reported calculations of the vibrational corrections to the dynamic polarizability and hyperpolarizability of the NaF molecule for frequencies varying from 0 to 0.12 hartree. Results obtained have shown that the relative importance of the zpva contribution is small and practically independent of the frequency. Electronic and zpva contributions present a similar frequency dependence and are practically constant on the range of vibrational frequencies.

Previous results obtained in the static limit [8] have shown that the pure vibrational contribution play an important role on the determination of α_{zz} and β_{xxz} and represents the dominant term for β_{zzz}. Results presented in this work show that this contribution is even more important for the dynamic electric properties on the range of vibrational frequencies. In contrast, the pv contribution is very small for frequencies on the visible region, except for $\beta_{xxz}(-\omega;\omega,0)$ and $\beta_{zzz}(-\omega;\omega,0)$.

Correlated calculations performed at the CCSD(T) level show that the electron correlation effects have a minor impact on the pv contribution to the polarizability. These effects even being more expressive for the hyperpolarizability, do not spoil the resemblance between the SCF and CCSD(T) curves, also observed for this property.

We have not included electron correlation effects on the calculations of the electronic and zpva contributions. These effects being significant in the static limit [8], are expected to be also important for the dynamic properties. It has been suggested [23] that if the properties present a regular frequency dependence, if the optical frequency is quite smaller than the first electronic transition frequency and if the static electron correlation effects are small, the dynamic electron correlation contributions could be inferred from the corresponding static contributions by scaling and/or addition procedures. Regarding the dipole polarizability, one can see that all the above mentioned conditions are satisfied on the range of frequencies considered here. On the other hand, as the static electron correlation effects are large for the hyperpolarizability [8], we do not expect that scaling and/or addition approximations would provide reliable estimates for this property. A clear-cut statement on this issue however would be premature without having in hands the results of a correlated calculation for the electronic contributions.

Even considering that the results presented in this work refer solely to the NaF molecule, it is worthwhile stressing that previous results [6–8,24] have shown that, as regards electric properties, diatomic ionic molecules present a very similar behavior. This allow us to infer that most of the conclusions presented here could also be extended for other ionic systems.

Acknowledgements

The authors gratefully acknowledge the financial support of the CAPES, CNPq and FUNAPE/UFG Brazilian agencies.

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