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REGULAR ARTICLE

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Multi-level vibrational SCF calculations and FTIR measurements on furazan

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Abstract The structure and infrared spectrum of furazan (1,2,5-oxadiazole) were studied by vibrational SCF (VSCF) and configuration interaction (VCI) calculations based on a high quality potential derived from electronic structure calculations up to the CCSD(T)/aug-cc-pCVQZ level. In addition gas-phase FTIR measurements were performed, which allowed for several corrections in the spectrum of the first vibrational overtones. Excellent agreement was found between the computed and the experimental results.

1 Introduction

The ab initio calculation of vibrational spectra beyond the harmonic approximation usually requires substantial computational resources and is thus limited to small molecules only. The reason for this is a time-consuming scan of the potential energy surface around the equilibrium structure or the calculation of the third and fourth-order derivatives of the energy at the stationary point needed for a multi-dimensional Taylor expansion of the potential. The most popular approach for accounting of anharmonicity corrections is based on vibrational perturbation theory, which usually leads to very accurate results as long as the level of the underlying electronic structure calculations has been chosen properly [1]. Alternatively, variational self-consistent field approaches can be used for generating vibrational wave functions (VSCF) [2–4]. In analogy to electronic structure calculations, correlation effects can be accounted for subsequently by different approaches [5–7]. In this respect, vibrational configuration interaction (VCI) calculations have been performed within this study throughout.

VSCF theory for a polyatomic non-rotating and non-linear molecule usually is based with the Watson Hamiltonian [8] in dependence on the normal coordinates Q_i:

$$\hat{H} = \frac{1}{2}\sum_{\alpha\beta}\hat{\pi}_\alpha \mu_{\alpha\beta}\hat{\pi}_\beta - \frac{1}{8}\sum_\alpha \mu_{\alpha\alpha} - \frac{1}{2}\sum_i \frac{\partial^2}{\partial Q_i^2} + V(Q_1, \ldots, Q_N) \quad (1)$$

The first term in Eq. (1) – expressed in atomic units – is the Coriolis coupling operator, the second term is the mass-dependent Watson correction term to the potential, the third one represents the dominant contribution to the kinetic energy, and the last contribution is the problematic multi-dimensional potential energy surface. Using a grid representation of the potential, the number of electronic structure calculations increases dramatically for large molecules. For that very reason, an algorithm has been presented recently that introduces several approximations for speeding up the generation of the potential while allowing for control of the resulting errors [9]. As suggested by Carter et al. [10,11], within this approach the potential is represented by an incremental scheme rather than a Taylor expansion, i.e.,

$$V(Q_1, \ldots, Q_N) = \sum_i V_i(Q_i) + \sum_{i<j} V_{ij}(Q_i, Q_j) + \sum_{i<j<k} V_{ijk}(Q_i, Q_j, Q_k) + \cdots \quad (2)$$

with

$$V_i(Q_i) = V_i^0(Q_i) - V(0) \quad (3)$$

$$V_{ij}(Q_i, Q_j) = V_{ij}^0(Q_i, Q_j) - \sum_{r\in\{i,j\}} V_r(Q_r) - V(0) \quad (4)$$

Dedicated to Professor Hermann Stoll on occasion of his 60th birthday.

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Table 1 Equilibrium (r_e and θ_e) and vibrationally corrected (r_z and θ_z) geometrical parameters of furazan obtained from experimental data and CCSD(T)/aug-cc-pCVQZ calculations

Bond	$r_z^{\text{Exp a}}$	$r_e^{\text{Exp}}(z)^{\text{a}}$	r_e^{b}	r_e^{c}	$r_z^{\text{VSCF c}}$	$r_z^{\text{VCI c}}$
C–C	1.4237(20)	1.4183(30)	1.4167	1.4184	1.4262	1.4263
C=N	1.3084(10)	1.3044(20)	1.3035	1.3031	1.3075	1.3075
N–O	1.3756(10)	1.3677(30)	1.3661	1.3666	1.3751	1.3751
C–H	1.0732(10)	1.0729(10)	1.0749	1.0750	1.0798	1.0792
Angle	$\theta_z^{\text{Exp a}}$	$\theta_e^{\text{Exp}}(z)^{\text{a}}$	θ_e^{b}	θ_e^{c}	$\theta_z^{\text{VSCF c}}$	$\theta_z^{\text{VCI c}}$
C–C=N	108.90(5)	108.90(5)	108.77	108.77	108.82	108.82
C=N–O	105.45(6)	105.45(6)	105.58	105.57	105.56	105.56
N–O–N	111.30(7)	111.30(7)	111.30	111.32	111.24	111.24
H–C=N	120.88(8)	120.88(8)	120.86	120.92	120.97	120.98

[a] Taken from Ref. [19]
[b] Computational results taken from Ref. [19]
[c] This work

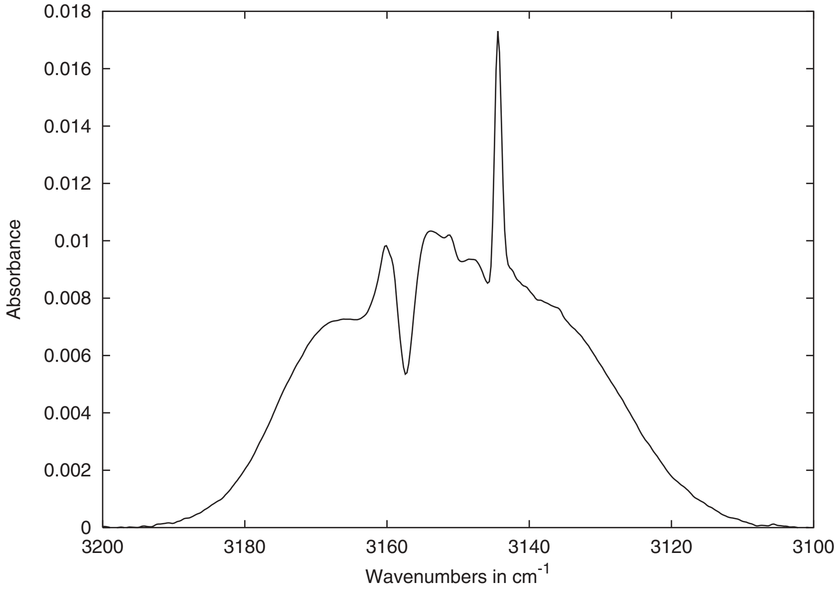

Fig. 1 Gas-phase FTIR spectrum of the C–H stretching region

$$
\begin{aligned}
V_{ijk}(Q_i, Q_j, Q_k) &= V^0_{ijk}(Q_i, Q_j, Q_k) \\
&\quad - \sum_{\substack{r,s\in\{i,j,k\}\\ r>s}} V_{rs}(Q_r, Q_s) \\
&\quad - \sum_{r\in\{i,j,k\}} V_r(Q_r) - V(0)
\end{aligned}
\tag{5}
$$

$$V_{ijkl}(Q_i, Q_j, Q_k, Q_l) = \cdots \tag{6}$$

$V(0)$ represents the total energy at the equilibrium geometry. Likewise, quantities with the superscript 0 denote the total energy as obtained from the electronic structure calculation at a distorted nuclear configuration. As the importance of the difference contributions, i.e., $V_i(Q_i)$, $V_{ij}(Q_i, Q_j)$, ... decreases with higher order, an hierarchical scheme has been introduced (see Ref. [9]), in which the most important 1D contributions are treated at the CCSD(T) level, while all other terms (2D and 3D) will be computed at the MP2 level only. This dual-level scheme resulted in deviations of up to four wavenumbers for some benchmark molecules and thus we now generalized the algorithm to allow for more flexible multi-level schemes, in which each contribution to the potential can be computed at a different theoretical level. We present here first calculations of a CCSD(T)-MP4(SDQ)-MP2 scheme for the 1D, 2D and 3D contributions. Although MP4(SDQ) scales with the sixth order with respect to the molecular size, this method is significantly faster than a CCSD calculation (which scales also with the sixth order) since it does not require an iterative solution of the amplitudes. Therefore, the MP4(SDQ) level must be considered a compromise between accuracy and computational cost. Moreover, the approximations introduced into the VSCF/VCI algorithm [9] were designed to represent fundamental vibrations best while higher excitations were not accounted for. However, in addition to our previous work we also consider first vibrational overtones in this study.

The vibrational spectrum of furazan (1,2,5-oxadiazole) has been studied experimentally by Christensen and Nielsen

Table 2 Experimental and computed fundamental modes of furazan

		Experiment				Calculated		
#	Sym.	Gas phase[a]	Vapour[b]	Liquid[b]	Solution[b]	Harm.	VSCF	VCI
ν_1	a_1	3157	3157	3148	3147	3293.5	3162.4	3158.8
ν_2		1418	1418	1420	1417	1459.1	1436.4	1420.1
ν_3		1316	1316	1312	1312	1339.6	1322.5	1312.7
ν_4		1036	1036	1035	1033	1059.8	1047.4	1039.8
ν_5		1005	1005	997	998	1025.2	1011.6	1002.6
ν_6		872	872	860	862	894.2	886.6	873.5
ν_7	a_2	–	–	824[c]	–	906.7	877.2	849.4
ν_8		–	–	635[d]	–	651.0	642.0	637.6
ν_9	b_2	3144	3144	3138	3134	3279.4	3127.4	3134.1
ν_{10}		1541	1541	1545	1540	1573.4	1546.5	1534.4
ν_{11}		1176	1175	1177	1173	1200.6	1191.0	1176.0
ν_{12}		953	953	949	948	959.2	947.2	948.6
ν_{13}		888	888[c]	–	–	882.8	915.6	891.1
ν_{14}	b_1	839	838	852	841	859.4	848.6	839.0
ν_{15}		–	631	622	623	641.8	631.0	631.2

[a] This work. As a total pressure of 1 bar has been used, we refer to the data as *gas phase* rather than *vapour*
[b] IR results of Christensen and Nielsen [12]
[c] See text for further details
[d] Obtained from a liquid-phase Raman spectrum [12]

[12] and Christensen et al. [13]. These authors assigned most of the fundamentals, vibrational overtones and combination bands. About 30 years later, El-Azhary used the scaled quantum-mechanical force field method (SQM) based on B3LYP/6-31G** calculations to fit the harmonic force constants to the experimental data of Christensen and Nielsen [12]. In contrast to the SQM approach, VSCF/VCI calculations are purely ab initio and thus free of any empirical scaling factors. Due to the work of these authors, furazan serves as an ideal benchmark molecule for computational approaches. In the course of studying the first vibrational overtones of furazan at the VCI level we realized significantly larger deviations from the experimental data than for the fundamental vibrations. This prompted us to remeasure the gas-phase FTIR spectrum of furazan. Based on this work, the position of a number of bands had to be shifted by up to six wavenumbers and two overtones were seen in the new gas-phase spectrum which were previously found in the liquid phase only.

2 Computational details

All electronic structure calculations, i.e., CCSD(T), MP4 (SDQ) and MP2, include core correlation effects and utilize a cc-pCVTZ basis set. Additional geometry optimizations were performed at the CCSD(T)/aug-cc-pCVQZ level (637 basis functions). Normal coordinates were obtained numerically from CCSD(T)/cc-pCVTZ calculations. The calculation of the potential included 1D, 2D and 3D contributions, resulting in 52 CCSD(T) single-point energy calculations, 1075 MP4(SDQ) calculations and 3576 MP2 energy determinations. Within the VSCF approach single-mode vibrational wave functions (modals) were generated from 16 distributed gaussians. Vibrational correlation effects were accounted for by a truncated VCI approach including configurations with at most four different excited modals (quadruple excitations) while restricting the maximum excitation level within one modal to the fourth root. In addition, the overall excitation level was restricted to six. This resulted in VCI matrices of 8726 (a_1), 8735 (b_2), and 6770 (a_2 and b_1) configurations. The eigenvalues of the VCI matrices were obtained from an iterative Davidson-Lanczos type algorithm as proposed by Carter et al. [15]. Vibrational states in the fingerprint region usually did not require more than five or six iterations, while due to the dense eigenvalue spectrum at higher energies those states corresponding to C–H stretches needed more than ten iterations. All calculations presented here have been performed with a development version of the MOLPRO package of ab initio programs [16].

3 Experimental details

The preparation of furazan was carried out in analogy to the literature [17]. About 2.00 g (22.7 mmol) of glyoxime (recrystallized from methanol) and 2.86 g (28.6 mmol) of succinic anhydride were placed in a 50 ml round bottom flask, equipped with a distillation head and a magnetic stirrer. The mixture was heated to 423 K. With the melting of the reactants the exothermic reaction started and the crude furazan was collected in a second flask connected by the distillation bridge. Dry sodium sulfate was added to the crude product and furazan was condensed to a third flask. To remove the remaining impurities molecular sieve (4 Å) was added and the product was carefully condensed into a fourth flask under reduced pressure. About 633 mg of furazan (9.04 mmol, 40%) was collected as a colorless liquid. ^{1}H NMR ($CDCl_3$, 500 MHz): = 8.35 (s, 2 H). ^{13}C NMR ($CDCl_3$, 125 MHz): = 140.72 (d, 2 C).

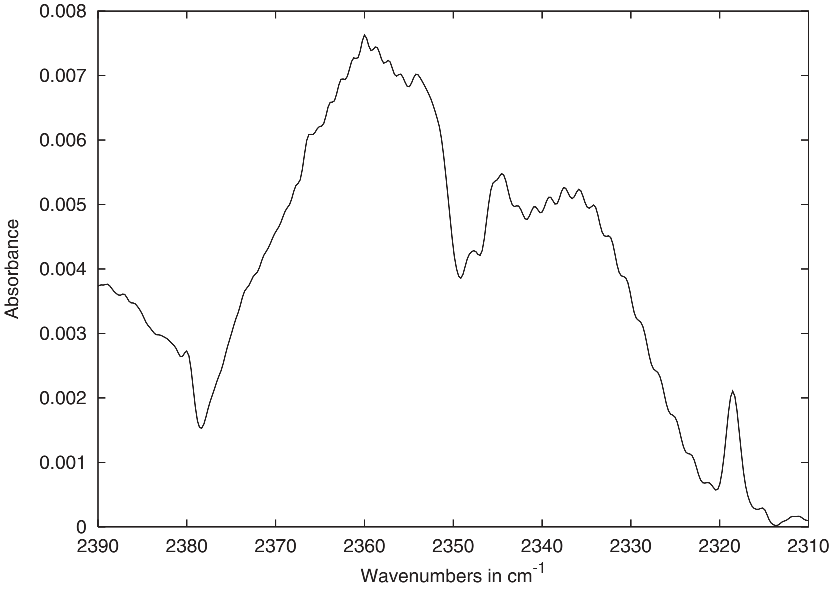

Fig. 2 Gas-phase FTIR spectrum in the region of the $2v_{11}$ overtone

The IR spectrum of furazan was measured with a Nicolet Magna 560 spectrometer. Furazan was evaporated in an evacuated temperature-controlled quartz cell ($V = 209\,\mathrm{L}$) equipped with a long path White mirror system with an optical pathlength of 2904 cm. The spectrum was recorded at 298 K with a spectral resolution of 1 cm^{-1} at a total pressure of 1 bar and nitrogen as a buffer gas with a furazan concentration of approximately 5×10^{15} cm^{-3}. About 3600 interferograms were accumulated.

4 Results and discussion

4.1 Geometry

The geometry of furazan has been studied before by both experimental and computational approaches [18,19]. In particular Vazquez et al. [19] performed extensive CCSD(T) calculations in order to obtain most accurate results for this molecule. Likewise, based on the IR spectrum of Christensen and Nielsen [12] these authors provide r_z, r_0, r_s and r_m values for the bond lengths of furazan and correct the r_z values to deduce r_e values which can directly be compared with the CCSD(T) results. In this study here, geometrical optimizations were performed at the CCSD(T)/aug-cc-pCVQZ and CCSD(T)/cc-pCVTZ levels including core-correlation effects. Note that the use of core-valence basis sets is mandatory in combination with all-electron calculations in order to minimize basis set superposition errors. For more details concerning the accurate calculation of equilibrium structures see the recent work of Botschwina [20]. Vibrational corrections were obtained from VSCF and VCI calculations, and thus r_e and r_z values are provided for all geometrical parameters. As the vibrational corrections refer to the cc-pCVTZ basis set only, the corresponding shifts in the geometrical parameters were transferred to the more accurate CCSD(T)/aug-cc-pCVQZ geometry. Both computed and experimental results are shown in Table 1. The VCI r_z results must in principle be considered to be superior to the VSCF results, but the differences are very small. The agreement between the calculated and the experimental r_e and r_z values is excellent. The only meaningful deviations were found for the C–H bond length. However, while our computed value is in perfect agreement with the computed result of Vazquez et al. [19] , the experimental values are consistently shorter. In particular, for this bond the VCI vibrational corrections are significantly larger than those given by Vazquez et al. [19]. According to these authors the anharmonicity of the C–H stretching is unusually small which results in r_z values being very close to the equilibrium bond lengths r_e. However, our calculations do not support this result.

4.2 Fundamental vibrations

Computed and experimental results for the fundamental vibrations are listed in Table 2. Our experimentally determined fundamentals are in perfect agreement with those of Christensen and Nielsen [12]. The a_2 modes could not be seen in the gas-phase spectrum due to their IR-inactivity and the two bands below 650 cm^{-1} were out of range, because our equipment is restricted to a range between 650 and 4000 cm^{-1}. The two C–H stretching modes, which were seen by Christensen and Nielsen [12] as a complex band at 3150 cm^{-1} only, could now be resolved and were found to be exactly at those positions which were deduced by these authors (see Fig. 1). The harmonic CCSD(T)/cc-pCVTZ frequencies differ from the experimental values by −0.6% up to +4.3%. Consequently, uniform scaling of the harmonic frequencies by a constant factor is of very limited use for this molecule.

Table 3 Experimental and computed first vibrational overtones of furazan

	Experiment				Calculated		
#	Gas phase[a]	Vapour[b]	Liquid[b]	Solution[b]	Harm.	VSCF	VCI
$2\nu_1$	–	–	–	–	6587.0	6270.1	–[c]
$2\nu_2$	2824	2823	2827	–	2918.2	2862.0	2830.8
$2\nu_3$	2629	2628	2620	–	2679.2	2641.0	2632.1
$2\nu_4$	2068	2067	2065	–	2119.6	2090.4	2077.1
$2\nu_5$	2004	2002	1987	–	2050.4	2017.5	2002.7
$2\nu_6$	–	–	–	–	1788.4	1770.0	1749.3
$2\nu_7$	–	–	–	–	1813.4	1772.4	1704.2
$2\nu_8$	1276	1283	1270	1268	1302.0	1286.0	1270.4
$2\nu_9$	–	–	–	–	6558.8	6183.4	6228.8
$2\nu_{10}$	3054	–	3062	–	3146.8	3080.1	3053.2
$2\nu_{11}$	2349	–	2344	–	2401.2	2380.8	2346.4
$2\nu_{12}$	1907	1904	1895	–	1918.4	1894.2	1897.7
$2\nu_{13}$	1774	1773	–	1780	1765.6	1846.9	1786.8
$2\nu_{14}$	1654	1652[d]	1621[d]	–	1718.8	1675.6	1662.4
$2\nu_{15}$	1259	1265	1239	–	1283.6	1260.4	1259.1

[a] This work. As a total pressure of 1 bar has been used, we refer to the data as *gas phase* rather than *vapour*

[b] IR results of Christensen and Nielsen [12]

[c] See text for details

[d] Assigned by Christensen and Nielsen [12] as ν_7 overtone

The agreement of the VCI results with the experimental values is excellent. The largest deviation was found for the $9b_2$ C–H stretching mode with 9.9 cm^{-1} (0.3%), while the mean absolute deviation for all those modes which could be clearly assigned in the gas-phase spectrum did not exceed 3.0 cm^{-1}.

Of particular interest is the IR-inactive $7a_2$ band, which was seen by Christensen and Nielsen [12] in the liquid-phase Raman spectrum as a shoulder at 820 cm^{-1} and at 824 cm^{-1} in the liquid-phase IR spectrum. Our VCI calculations predict this mode to be at 849.4 cm^{-1} which would result in an exceptionally large deviation of about 30 cm^{-1}. As the observed fundamental vibration occurs in the region of the very strong $14b_1$ and $6a_1$ modes, most likely the authors of Ref. [14] deduced the assignment of the $7a_2$ band from the corresponding overtones and combination bands rather than by identifying the fundamental mode itself. However, the overtones of the $14b_1$ and $6a_1$ modes are not provided and thus the question arises if the assignment of the $7a_2$ band is correct. We computed the overtones of the $7a_2$ and $14b_1$ bands at 1704.2 cm^{-1} and 1662.4 cm^{-1}, respectively. The latter value (overtone of $14b_1$) would be in nice agreement with the observed value of the $7a_2$ overtone at 1654 cm^{-1} and thus there is certain evidence of a misassignment for the $7a_2$ mode. As a consequence, several of the combination bands assigned by Christensen and Nielsen [12] would also require a reassignment. However, almost all of these combination bands can be explained by replacing the $7a_2$ mode by the $14b_1$ mode. Note that in many cases the band type (i.e., A, B and C) could not be determined precisely and thus it provides little help in the symmetry assignment. In order to resolve this problem definitely even more accurate calculations including all combination bands or refined measurements are necessary.

Further discussion requires the symmetry assignment of the fundamental modes at 824 and 888 cm^{-1} (experimental values, Table 2). In their first paper, Christensen and Nielsen [12] assigned the mode at 824 cm^{-1} (ν_7) to have a_2 symmetry but interchanged the assignment in their second paper [13] with the mode at 888 cm^{-1} (ν_{13}). The latter one is the assignment used by El-Azhary [14] and Vazquez et al. [19] in their computational work. Harmonic calculations clearly support this assignment (see Table 2) as the a_2 mode is about 24 cm^{-1} above the b_2 mode. However, due to opposite anharmonic shifts (-57.3 versus $+8.3$ cm^{-1}) VSCF and VCI calculations interchange the order of these two modes and now shift the a_2 mode below the b_2 fundamental. Therefore, we believe that the original assignment of Christensen and Nielsen [12] was correct and that the mode at 888 cm^{-1} indeed belongs to the b_2 irreducible representation, which is supported by the fact that this mode shows a certain – though weak – intensity in the gas phase.

4.3 Vibrational Overtones

Positions of the remeasured and computed first vibrational overtones are summarized in Table 3. In the experimental spectrum, all overtones show B-type bands with P- and R-branches and hence the tabulated positions were obtained from the intensity minima. The assignment of Christensen and Nielsen [12] could be augmented by the overtones of the $10b_2$ and $11b_2$ bands at 3054 and 2349 cm^{-1}, respectively (see Fig. 2). These values differ by 8 and 5 cm^{-1} from the Raman data in the liquid phase and thus provide a significantly improved reference for the calculations. Likewise, shifts of two and six wavenumbers were obtained for the overtones of the b_1 modes. Accepting the new assignment of the $14b_1$ overtone at 1654 cm^{-1} (experimentally; see the previous discussion) the mean absolute deviation of the VCI results is 5.4 cm^{-1}. Note that the calculation of the potential (Eq. 2) has been taylored for the determination of fundamentals and thus the outer regions of the potential (i.e., those belonging to the largest elongations) were obtained from extrapolation schemes rather than accurate electronic structure calculations. As the wave function of a vibrational overtone stretches over a broader region than the corresponding fundamental, the former depends much more on the accuracy of the outer regions. Consequently, the agreement obtained here must still be considered to be very good. In particular, significant deviations must be expected for the overtones of the two C–H stretches as the gap between the eigenvalues belonging to different quantum numbers is largest. Unfortunately, we are not able to provide a definite VCI result for the overtone of ν_1, because two VCI roots (6203.7 and 6262.4 cm^{-1}) with almost identical (but very low) contributions of the $2\nu_1$ configuration could be detected. Therefore, a corresponding number has not been provided in Table 3. According to the calculations, the $2\nu_6$ and $2\nu_7$ overtones should occur at 1749.3 and 1704.2 cm^{-1}. In agreement with the results of Christensen and Nielsen [12], we were not able to assign any modes in that region based on our experimental results. However, most likely this is due to very low intensities rather than inaccurate computational results.

5 Summary and conclusions

The infrared spectrum of furazan (1,2,5-oxadiazole) has been computed at the vibrational CI level and has been remeasured in the gas phase. On the basis of both results, several corrections and additions to existing assignments were made. The agreement between the computational and the experimental results is excellent. The mean absolute deviation for the fundamental modes is as low as 3.0 and 5.4 cm^{-1} for the first vibrational overtones. Consequently, the approximation of the potential by a CCSD(T)-MP4(SDQ)-MP2 multi-level scheme within VSCF/VCI calculations must be considered to yield very accurate results while significantly reducing the computational cost. Moreover, this study presents the first test on the calculation of vibrational overtones based on a VSCF/VCI algorithm including several approximations which were orginally designed for a proper prediction of fundamental modes. Although the agreement for the vibrational overtones is still very good, we recommend a more accurate representation of the outer regions of the potential for these kinds of calculations.

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References

1. Clabo DA Jr, Allen WD, Remington RB, Yamaguchi Y, Schaefer HF (1988) Chem Phys 123:187
2. Bowman JM (1986) Acc Chem Res 19:202
3. Bowman JM (1978) J Chem Phys 68:608
4. Gerber R, Ratner M (1988) Adv Chem Phys 70:97
5. Christoffel KM, Bowman JM (1982) Chem Phys Lett 85:220
6. Bowman JM, Christoffel K, Tobin F (1979) J Phys Chem 83:905
7. Christiansen O (2004) J Chem Phys 120:2149
8. Watson JKG (1968) Mol Phys 15:479
9. Rauhut G (2004) J Chem Phys 121:9313
10. Carter S, Culik SJ, Bowman JM (1997) J Chem Phys 107:10459
11. Carter S, Bowman JM, Harding LB (1997) Spectrochim Acta A 53:1179
12. Christensen DH, Nielsen OF (1967) J Mol Spectrosc 24:477
13. Christensen DH, Jensen PW, Nielsen JT, Nielsen OF (1973) Spectrochim Acta A 29:1393
14. El-Azhary AA (1996) Spectrochim Acta A 52:33
15. Carter S, Bowman JM, Handy NC (1998) Theor Chim Acta 100:191
16. MOLPRO, Version 2002.9, is a package of ab initio programs written by H.-J. Werner and P. J. Knowles, with contributions from R.D. Amos, A. Bernhardsson, A. Berning, P. Celani, D.L. Cooper, M.J.O. Deegan, A.J. Dobbyn, F. Eckert, C. Hampel, G. Hetzer, T. Korona, R. Lindh, A. W. Lloyd, F.R. Manby, W. Meyer, S.J. McNicholas, M.E. Mura, A. Nicklass, P. Palmieri, K. Peterson, P. Pulay, G. Rauhut, M. Schütz, U. Schumann, H. Stoll, A.J. Stone, R. Tarroni, and T. Thorsteinsson., (see `http://www.molpro.net/`)
17. Olofson RA, Michelman JS (1965) J Org Chem 30:1854
18. Stiefvater O (1988) Z Naturforsch A 43:597
19. Vazquez J, Demaison J, Lopez-Gonzalez JJ, Boggs JE, Rudolph HD, J Mol Spectrosc 207:224
20. Botschwina P (2005) Mol Phys 103:1441