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A DFT modeling of the uranium trioxide vibration spectra characteristics

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Abstract

Results of DFT calculations of structure and vibrational IR and Raman spectra of uranium trioxide in the isolated state as well as in the surroundings of 30 neon and argon atoms are presented. It is found that the uranium trioxide molecule can exist in two conformers: Y-shaped and T-shaped. The degree of anharmonicity of UO stretching vibration in simple uranium oxides is defined. Characteristics of the computed vibration spectra are, generally, in a good agreement with the experimental data. Interpretation of the α-uranium trioxide Raman spectrum is realized on the basis of the calculations.

Keywords: Density Functional Theory; Effective Core Potential; Raman spectrum; Uranium oxides; Matrix isolation; Vibration anharmonicity

1. Introduction

Uranium–oxygen compounds demonstrate the highest strength and thermodynamic stability. They are also very important in the nuclear fuel production. There are several technologically proven methods to extract them from various uranium compounds [1]. However, in some cases certain difficulties of instrumental character may occur while deriving uranium oxide nanoclusters. Thus, physical properties of the uranium trioxide received, for example, from uranyl nitrate, depend on temperature of the sample incineration and rate of the temperature increase [1]. Slow or fast heating of uranyl nitrate hexahydrate in the range of 350–400 ºC results in formation of uranium trioxide with the bulk weight of 2.8–4.2 g/cm^3, respectively. Sizes of trioxide uranium crystals herewith make up about 1 micron.

The last decades' studies [2] have confirmed the possibility of existence of UO monoxide as well as the U_2O_5, U_3O_7, U_4O_9 formations along with the three previously known oxides (dioxide UO_2, triuranium octoxide U_3O_8, trioxide UO_3). These compounds have also proved not to be stoichiometrical, producing, in fact, a variety of nonstoichiometrical forms. In the uranium–oxygen system, a few homogeneous regions with a variable composition of uranium and oxygen have been discovered, and the hypothesis has been made referring to the existence of certain phases with some of them being unstable. Exact definition of the structure of metastable phases is of great interest in connection with technological problems of conservation and further disposal of radioactive waste (in particular, due to the process of UO_2 oxidizing to the U_3O_7 and U_3O_8 formations in the open air) [3].

From the stated above follows, that identification of separate components of the uranium–oxygen complex system appears to be a difficult problem. At this point, modeling of the structure of separate components and calculation of their vibrational spectra can be rather useful.

Vibration IR spectra of the uranium simple oxides (neutral UO, UO_2, UO_3 and some ions) have been investigated for the molecular systems isolated in the low-temperature matrices of noble gases and nitrogen [4–8]. As it is well-known (see, for example, [9]), spectral shifts of vibrational frequencies for the molecular systems in the matrix isolation in respect to a gas phase are, generally, insignificant, allowing to interpret results of such investigations by means of the calculations, performed for monomeric forms of noninteracting molecular systems (i.e. for the gas phase model). Nevertheless, according to [10], values of spectral shifts for the matrix isolation can reach in some cases 20–30 cm^{-1} and even more. Moreover, one may observe the spectral shifts for stretching vibrations tending to increase with respect to the gas phase among the Ne → Ar → Kr isolating matrices in the majority of the molecular systems, explored in such environment [11]. Despite the evident reason for the spectral shifts (interaction with matrix atoms), actual mechanisms can be different: formation of chemical bonds with the matrix environment of a molecule, reduction (elongation) of bonds, decrease in the effect of anharmonicity of vibrations, etc. The analysis of vibration spectra of uranium mono- and dioxide has revealed [4, 8] the anomalously large long-wave (~70 and ~140 cm^{-1}, respectively) shifts of the frequencies of UO stretching vibration in the argon or krypton matrix with regard to the neon one. On the basis of calculations of the electronic structure of the given formations, the hypothesis has been made on the presence of a strong interaction of the isolated molecules with atoms of the matrices, resulting in the variation of the molecule ground electronic term [8, 12, 13].

In the given paper, following quantum chemical calculations for several simple uranium oxides, the interpretation of the Raman spectrum α-UO_3 in a crystalline state has been realized as well as the influence of various factors on the values of frequencies in vibration spectra of the particular compound has been analyzed.

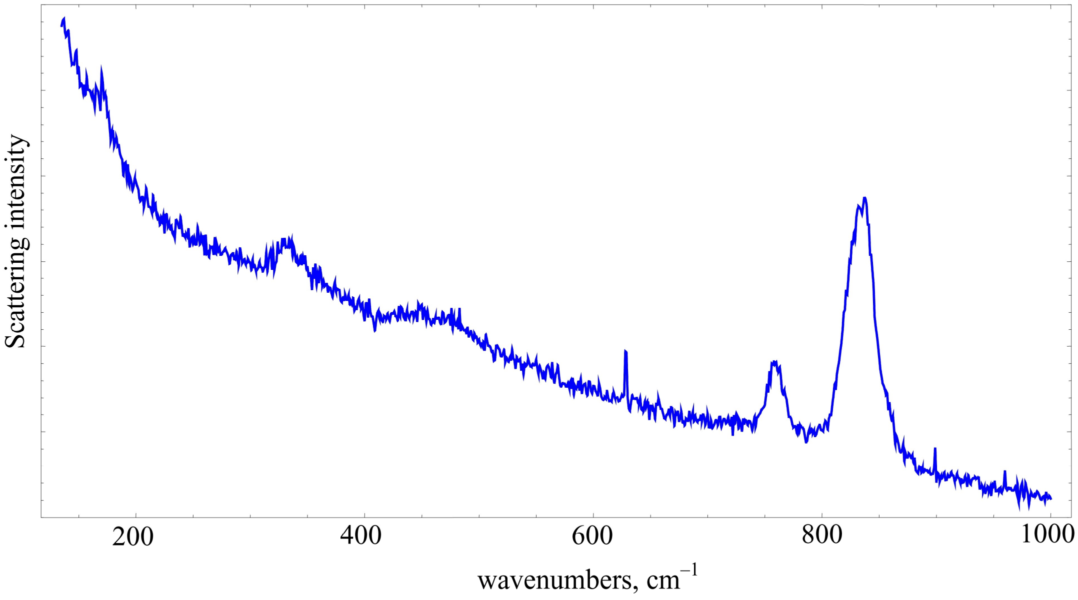

Figure 1. The Raman spectrum of the crystal α-UO_3.

Table 1. The calculated structural parameters of uranium trioxide UO_3.

	cc-pVDZ				cc-pCVDZ		cc-pCVTZ		cc-pCVQZ	
	UO_3, T-form	UO_3, Y-form	$UO_3 \cdot Ne_{30}$	$UO_3 \cdot Ar_{30}$	T-form	Y-form	T-form	Y-form	T-form	Y-form
UO(1) bond length, Å	1.804	1.830	1.830	1.833	1.804	1.830	1.800	1.829	1.800	1.830
UO(3) bond length, Å	1.867	1.804	1.807	1.807	1.868	1.804	1.867	1.806	1.871	1.804
O(1)UO(2) angle, deg	156.3	88.7	87.1	88.4	156.3	88.7	159.2	87.8	157.8	88.5
O(1)UO(3) angle, deg	101.8	135.6	136.5	135.8	101.8	135.6	100.4	136.1	101.1	135.8

2. Experiment and calculation procedure

The uranium trioxide provided on the commercial basis by V. G. Hlopin Radium Institute (St.-Petersburg, Russia) was used as the sample for registration of Raman spectrum. The Raman spectrum was registered at room temperature for fine crystals pressed into a capillary tube on DFS-52 double monochromator under excitation by the second harmonics (532 nm) of the Nd:YAG laser.

Optimization of the equilibrium structure as well as computations of the force fields, vibrations frequencies and intensities in the IR and Raman spectra in the harmonic approximation of the isolated molecules of uranium mono- di- and trioxides (UO, UO_2 and UO_3), and trioxide uranium molecule in the surroundings of neon and argon atoms were accomplished by means of GAMESS-US quantum chemical package [14, 15]. Visualization of the results was performed utilizing MacMolPlt [16] and ORTEP [17] programs. The relativistic effective core potential (RECP) LANL2DZ [18] that replaced the 78 inner electrons was used for the uranium atom. One has employed DZ-basis sets specifically elaborated for the particular RECP to include remaining electrons of the uranium atom. Description of oxygen, neon and argon atoms was realized on the basis of standard all-electron correlated consistent Dunning basis sets cc-pVnZ and cc-pCVnZ (n = D, T, Q) [19]. The RECP and the corresponding basis sets were generated using the Extensible Computational Chemistry Environment Basis Set Database [20–22]. The hybrid exchange-correlation functional B3LYP was also used in all calculations [23–25].

Calculations of the vibration states energies of the uranium monoxide in the anharmonic approximation were carried out applying the double-stage numerical algorithm [26]: determination of the energy intervals containing one level as the first stage and evaluation of energy eigenvalues with the specified accuracy as the second stage.

3. Results and Discussion

α-UO_3 Raman spectrum in the region of 130–1000 cm^{-1} is shown in Figure 1. In this region one can observe in a spectrum six lines of scattering: 836, 760, 476, 446, 332 and 171 cm^{-1}. Peak near 630 cm^{-1} is a stray spike (instrumental noise).

The calculated values of geometrical parameters of the uranium trioxide isolated molecule utilizing various basis sets are given in Table 1. All variants of the calculations lead to a flat, close to T-like, shape of the molecule (T-form) of symmetry C_{2v} (value of the bend of O(1)=U=O(2) “uranyl” fragment falls in the range of 156-160°) for the equilibrium configuration. This result qualitatively agrees with the structural data obtained due to the analysis of trioxide spectra in the matrix isolation [5, 6]. To reveal specific features of the matrix isolation influence on the structure and vibration spectrum of UO_3, the model calculations, reproducing the matrix environment of the molecule, are made. For this purpose, the uranium trioxide molecule is put into the

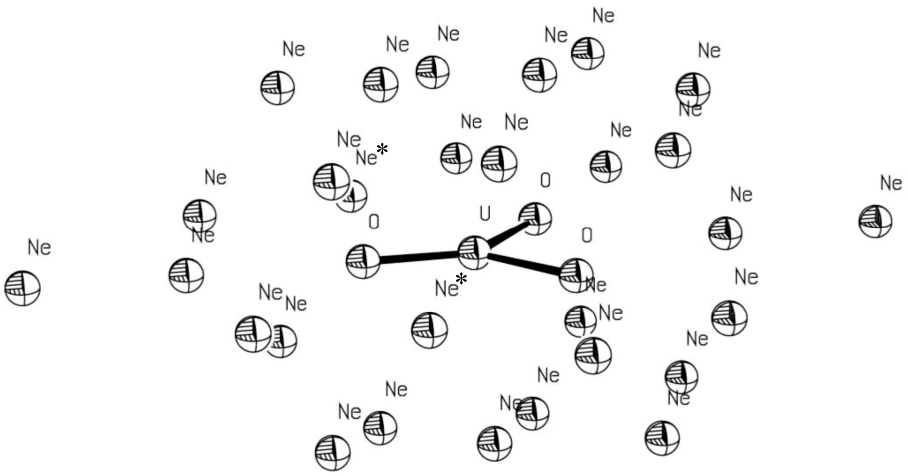

Figure 2. The uranium trioxide molecule in the surroundings of 30 neon atoms.

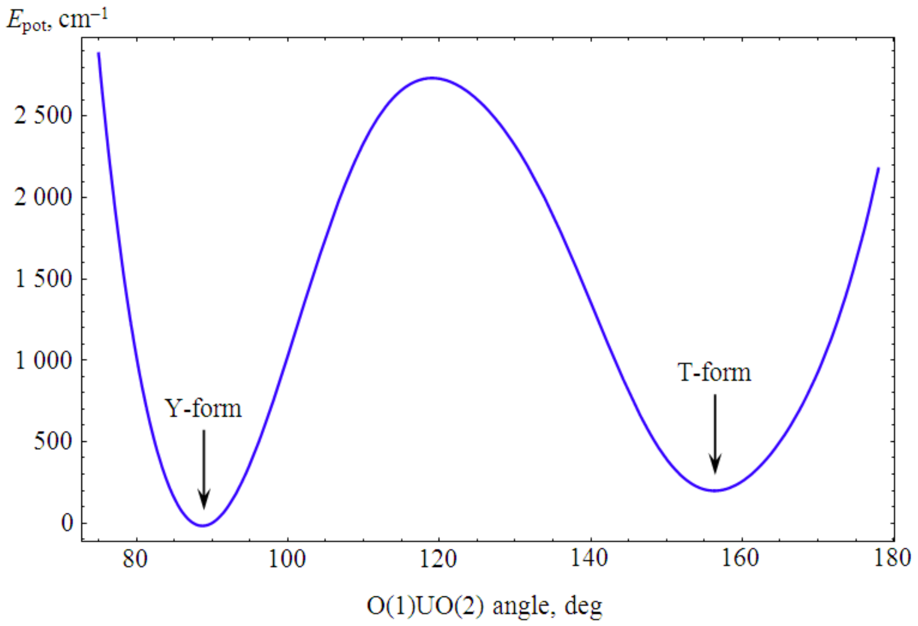

Figure 3. Potential energy of the UO_3 molecule as a function of the O(1)UO(2) angle according to the results of calculation the LANL2DZ/B3LYP/cc-pVDZ level of theory.

surroundings of 30 neon atoms (the $UO_3{\cdot}Ne_{30}$ cluster), and a full geometrical optimization is achieved (Figure 2). As a result, one has the configuration of the uranium trioxide molecule, differing from the gas phase model (see Table 1): bonds of the O(1)=U=O(2) "uranyl" fragment have been apparently extended, while the UO(3) bond, on the contrary, has reduced; the angle of O(1)=U=O(2) has considerably decreased, and the molecule structure in the cluster appears to be closer to the Y-type shape. Analogous calculations have been made for the argon matrix model (the $UO_3{\cdot}Ar_{30}$ cluster). In this case, one has the similar configuration of the cluster and molecule (see Table 1).

This result points to a significant deformation of the molecular configuration in the matrix isolation. To elucidate the cause of such a deformation, the potential energy of a free UO_3 molecule was computed as a function of the angle between two "uranyl" bonds O(1)=U=O(2) over the range 70–177.5º by steps of 2.5º. The computations have been performed with "freezing" of the angles O(1)UO(3) and O(2)UO(3) and with optimization of the remaining molecular geometrical parameters. The result of these computations (see Figure 3) was rather unexpected: apart from the minimum associated with the T-shaped molecule (156.3º), the potential curve reveals another minimum corresponding to the Y-shaped (Y-form) molecule (88.7º). The Y-shape parameters (Table 1) were determined by a complete geometrical optimization with the initial setting of the angle O(1)=U=O(2) to about 90º. The computations, in all the bases used, have resulted in a stable Y-shaped molecular configuration (the computed spectrum demonstrated the absence of imaginary frequencies; see Tables 1 and 2). For the cc-pVDZ basis set, the T-shape energy is higher than the Y-shape energy by 205 cm^{-1}. A height of the potential barrier between these two forms comes to 2731 cm^{-1}, and it corresponds to an angle of 120º (Figure 3).

Table 2. Spectral characteristics of uranium trioxide UO_3.

Assignment and symmetry species	Experiment				Calculation											
	IR, matrix isolation			Raman	cc-pVDZ				cc-pCVDZ		cc-pCVTZ		cc-pCVQZ		‹*I*›, IR	‹*I*›, Raman
	Ne [8]	Ar [5, 6]	Kr [5]		UO_3, T-form	UO_3, Y-form	$UO_3 \cdot Ne_{30}$	$UO_3 \cdot Ar_{30}$	T-form	Y-form	T-form	Y-form	T-form	Y-form		
ν_1 (ν_s OUO), A_1	—	—	—	836	846	836	826	823	850	836	848	824	840	824	0.04	1.00
ν_2 (ν UO), A_1	760.3	745.7	740.7	760	757	759	761	752	759	756	749	748	739	737	0.52	0.51
ν_3 (δ_s OUO), A_1	—	186.2	—	171	208	312	323	297	208	312	224	307	204	306	0.06	0.01
ν_4 (ν_a OUO), B_1	865.3	852.6	848.1	—	882	877	878	870	888	879	886	871	877	863	1.00	0.10
ν_5 (δ_a OUO), B_1	—	211.6	—	—	257	254	46	48	257	254	193	198	220	220	0.13	0.00
ν_6 (δ out-of-plane), B_2	—	151.5	—	—	103	180	234	215	103	181	55	106	24	46	0.10	0.09

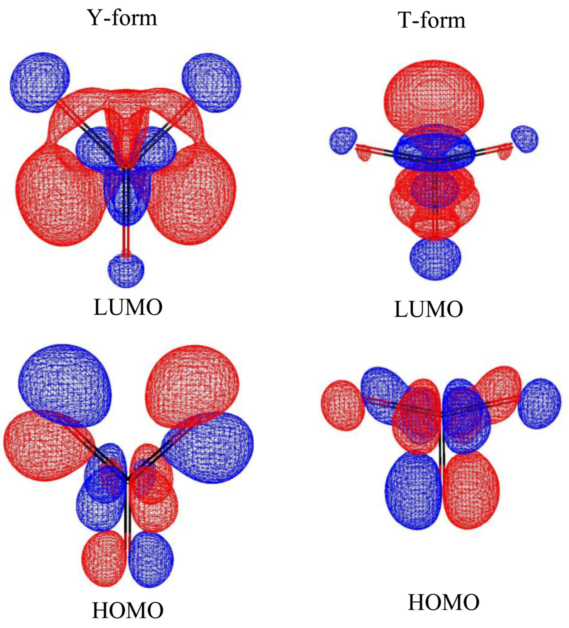

Figure 4. The atomic orbital compositions of the frontier molecular orbitals for two forms of UO_3.

Not discarding the possibility for artificial origin of this phenomenon, we assume that the existence of two stable forms of a free UO_3 molecule is caused by an ambiguous hybridization of the electron density for a uranium atom in the case of UO bonding. The differences in hybridization, in turn, lead to different directivity of chemical bonds. In any case, the form of the frontier molecular orbitals (HOMO and LUMO) for two hypothetical conformers of UO_3 (Figure 4) suggests different hybridizations for the Y- and T-shaped configurations.

As the clusters $UO_3 \cdot Ne_{30}$ and $UO_3 \cdot Ar_{30}$ were optimized with the initial setting of a T-shaped configuration for uranium trioxide, whereas the final configuration was associated with the Y-shaped one, a single equilibrium configuration (Y-form) of UO_3 was realized in the environment of noble gas atoms. This is indirectly demonstrated by the absence of frequencies attributed to the second form in IR spectra for uranium trioxide in the matrix isolation [5, 6, 8]. In this way it is assumed that the nearest neighbors of uranium trioxide in simulated clusters (two atoms of neon or argon in the molecular plane which are marked by asterisks in Figure 2) are responsible for the transformation of the T-shaped molecule to the Y-form. The definitive answer to the question concerning the existence of two different configurations of uranium trioxide may be given, for example, by recording of vibrational spectra for such compound in the gaseous phase and at temperatures enabling thermal separation of these two hypothetical forms.

The observational and calculated spectral characteristics of uranium trioxide are presented in Table 2 (the frequencies are specified in cm^{-1}, the band and line intensities are normalized to the peak values in the corresponding spectra). The band and line intensities are averaged since they are hardly varying on going from one basis set to the other. When a molecule of UO_3 is in the environment of Ne or Ar atoms, an intensity of the vibration ν_4 is slightly increased (within an order of magnitude) and that of the vibration ν_1 is lowered. All frequencies (observational and calculated) are given for the ^{16}O isotope.

Deriving with the help of quantum chemistry techniques, vibration frequencies of the molecules, in general, turn out to be higher than the experimentally measured values for the gas phase. As it is well-known, the main reasons for such a discrepancy in frequencies are the following: 1) failure to account for electron correlation; 2) usage of an incomplete basis set; 3) the anharmonicity of vibrations of real molecular systems; 4) failure to include the relativistic corrections for the inner-shell electrons of heavy atoms. While modeling a spectrum of the condensed phase or a molecule in the matrix isolation, one has also to consider the environment influence.

Let us look at each cause in more details. The effect of the 1st and 4th ones is supposed to be inappreciable due to the correlated consistent basis sets and correlation functionals in the first case and the relativistic corrections for the effective core potentials in the second case.

Here, the influence of anharmonicity should be viewed in two aspects. On one hand, as everyone knows, in the presence of essential effect of the anharmonicity, vibration frequencies reduce significantly with regard to the values obtained in the harmonic approximation. On the other hand, in the matrix isolation, as the authors [10] stress, the additional potential of repulsion, arising in the environment of a molecule, makes the potential energy function approach the parabolic form, thereby reducing the anharmonicity. In this case, molecular vibration frequencies in the matrix isolation will increase and, probably, correspond to the harmonic values.

To define a degree of the vibration anharmonicity of UO stretch modes in simple uranium oxides, one had to specify the form of the potential energy function of interaction of uranium and oxygen atoms for uranium monoxide

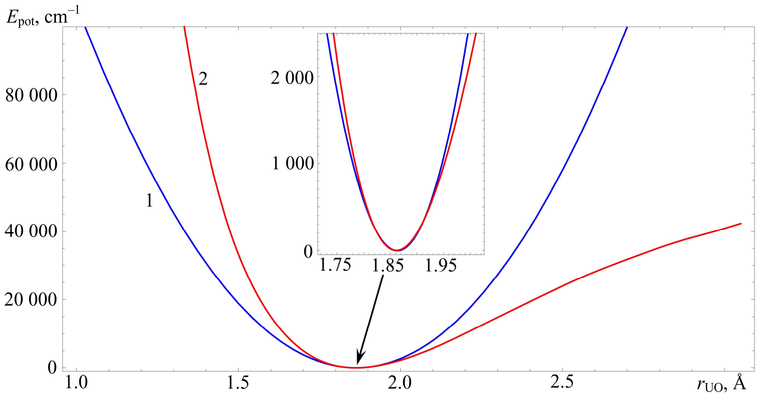

Figure 5. Potential energy function of the interaction between uranium and oxygen atoms in the uranium monoxide molecule according to the results of calculation the LANL2DZ/B3LYP/cc-pCVTZ level of theory in harmonic (1) and anharmonic (2) approximations. The insert demonstrates the forms of functions near the equilibrium.

employing the cc-pVDZ and cc-pCVTZ basis sets. The potential energy was calculated in the range of 1.40–3.40 Å in the first basis set and 1.05–3.50 Å — in the second basis set with the step of 0.01 Å near the equilibrium (1.70–1.90 and 1.75–2.00 Å, respectively) and 0.10 Å — for the other regions. Further, according to the algorithm [26], the numerical evaluation of vibration Schrödinger equation was made with the reduced mass of UO molecule and two forms of the potential energy functions: the parabola reconstructed from the force constant value, and the dependence, resulted from a point-by-point calculation of the total energy (Figure 5). Numerical evaluation reproduces the harmonic frequencies, obtained by means of GAMESS (860 and 802 cm^{-1} for cc-pVDZ and cc-pCVTZ basis sets, respectively), with the required accuracy, thus confirming the validity of the computational algorithm. The calculated frequencies of a fundamental transition in the anharmonic approximation turn out to be lower than the harmonic values for the cc-pVDZ and cc-pCVTZ basis sets by 4 and 9 cm^{-1} (amounting to 0.5 and 1.1 %), respectively. As follows from the graphs, presented in Figure 5, close to the equilibrium, forms of the two functions differ insignificantly, and that is the reason for a smallness of the anharmonicity effect for the fundamental of stretching UO modes.

Possibilities of estimating the influence of the second cause (size of a basis set) are essentially reduced by the limited description of the outer-shell electrons of the uranium atom within the ECP approximation. In this case, to adequately characterize oxygen and neon atoms, one has to utilize double split (DZ) basis due to their better balance with functions of the outer-shell electrons of the uranium atom. Nevertheless, influence of the quantitative and qualitative composition of basis sets on spectral characteristics of the systems under study can be traced down in a series of the calculations performed with the help of the cc-pVnZ and cc-pCVnZ correlated consistent basis sets. Calculation results show that the frequencies of uranium oxides with unsaturated bonds of the U atom (mono- and dioxide) are mostly affected by a basis set size. Transition from the double split basis to the triple split one lowers the harmonic frequency for monoxide by 58 cm^{-1} (from 860 to 802 cm^{-1}) making up ~ 7 % of the original value. For dioxide, decrease in the frequency of the OUO asymmetric stretching mode (the most intensive in the spectrum) appears to be rather considerable, too: 39 cm^{-1} (from 857 to 818 cm^{-1}, or 4.5 %). Employing the quadruple zeta basis set for the oxygen atom also leads to reduction of the harmonic frequencies, however, their variations regarding the values for the triple zeta basis are apparently lower: 5 cm^{-1} (from 802 to 797 cm^{-1}, or 0.6 %) for UO and 7 cm^{-1} (from 818 to 811 cm^{-1}, or 0.9 %) for UO_2. The calculated frequencies of uranium trioxide, in general, follow the same trend with much smaller absolute variations of the frequency values (Table 2). Moreover, the frequency of δ_a OUO bending asymmetric mode tends to be appreciably underestimated in the calculations applying TZ and QZ basis sets. One should also note, usage of the correlated consistent basis sets, accounting for the correlation of not only valence electrons (cc-pVnZ) but also core ones (cc-pCVnZ), either keep vibration frequencies unchanged or slightly raise them (see Table 2).

The calculated uranium trioxide spectrum in the surroundings of neon atoms (Figure 2) mostly meets the observational features: spectral shifts of the frequencies of stretching vibrations match the experimental values for the similar compounds [11], and two frequencies out of three have been shifted to the long-wave region. One can observe the full correspondence to the observational trends for the argon matrix model: the frequencies of all stretching vibrations are drifting to the long-wave region, and the spectral shifts turn out to be higher than those of the neon matrix. However, it should be pointed out here, assignment of the stretching modes to ν_s OUO, ν_a OUO and ν UO for UO_3 in the environment of neon or argon atoms has somewhat the arbitrary character as the forms of normal vibrations of UO bonds in the $UO_3{\cdot}Ne_{30}$ or $UO_3{\cdot}Ar_{30}$ clusters essentially differ from the likes of the isolated molecule.

The symmetric stretching mode ν_s OUO is not observed in the IR spectra of uranium trioxide [5, 6, 8], and according to the calculation data, intensity of the corresponding band is minimal. In contrast, the most intensive line is just assigned to same vibration in the calculated Raman spectrum. The opposite behavior (see Table 2) is quite typical for the asymmetric stretching mode ν_a OUO. Thus, on the basis of the performed calculations, one may state, that the most intensive line 836 cm^{-1} in the Raman spectrum (Figure 1) is assigned to the ν_s OUO (ν_1) symmetric mode, while the line 760 cm^{-1} is attributed to the stretching mode ν UO (ν_2).

The frequencies of deformation vibrations for $UO_3{\cdot}Ne_{30}$ and $UO_3{\cdot}Ar_{30}$ clusters compared with the T-form of the molecule show multidirectional shifts: frequencies ν_3 and ν_6 are shifted to shorter wavelengths, ν_5 — to the long-wavelength. All frequencies shifts are of considerable magnitude (100–200 cm^{-1}), and this seems unlikely. Compared with the Y-form of the free molecule the frequencies of deformation vibrations in the clusters are also shifted to longer wavelengths as well as the short-wavelength region. Excluding from consideration (as an artifact) the very large (over 200 cm^{-1}) long-wave shift of the ν_5 vibration, we can conclude that low-frequency modes, in contrast to the high frequency tend to increase their frequency in the matrix isolation. This conclusion is consistent with the data [10]. In this case, we can assume that the line 171 cm^{-1} in the Raman spectrum corresponds to the ν_3 mode (186.2 cm^{-1} in the IR spectra [5, 6]).

Weak lines in the region of 330–480 cm^{-1}, observed in the Raman spectrum (Figure 1), are confirmed neither by the matrix isolation IR spectra, nor by the calculation data for gas phase and Ne and Ar clusters models. One can assume that these lines are due to the crystalline structure of the sample. The final answer to this question requires additional studies.

4. Conclusions

Interpretation of the Raman spectrum of crystal α-uranium trioxide is realized on the basis of DFT calculations of uranium simple oxides electronic structure. Influence of various factors over the structural and spectral characteristics of molecular uranium trioxide is analyzed. It is assumed that the two hypothetical stable conformers of the uranium trioxide molecule (T-shaped and Y-shaped) are due to different hybridizations of the uranium atomic orbitals. As has been determined, stretching modes of UO bonds have a low degree of anharmonicity. Calculated on the basis of the model T-type structure of molecular uranium trioxide, the features of IR and Raman vibration spectra, in general, adequately reproduce the experimental data. Results of the UO_3 vibration analysis can be used for analytical matters.

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