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ARTICLE in VIBRATIONAL SPECTROSCOPY · JANUARY 2004

Impact Factor: 2 · DOI: 10.1016/j.vibspec.2003.05.003

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Raman and infrared spectroscopic study of  $C_{60}F_{18}$ ,  $C_{60}F_{36}$  and  $C_{60}F_{48}$ J.V. Rau<sup>a,b,\*</sup>, S. Nunziante Cesaro<sup>a</sup>, O.V. Boltalina<sup>b</sup>, V. Agafonov<sup>c</sup>, A.A. Popov<sup>b</sup>, L.N. Sidorov<sup>b</sup><sup>a</sup>*Dipartimento di Chimica, Università di Roma La Sapienza, Piazzale Aldo Moro 5, Roma 00185, Italy*<sup>b</sup>*Department of Chemistry, M. V. Lomonosov Moscow State University, 119899 Moscow, Russia*<sup>c</sup>*Faculté de Pharmacie, Laboratoire de Chimie Physique, 31 avenue Monge, 37200 Tours, France*

Received 14 February 2003; received in revised form 30 April 2003; accepted 5 May 2003

## Abstract

Vibrational spectroscopies have been employed to study the fluorofullerenes of formula  $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$ . For the first time, the Raman spectra of  $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$  as well as infrared (IR) spectra of their gaseous molecules isolated in cryogenic matrices have been obtained. The results were discussed and compared with the infrared spectra of the corresponding solids. In the case of  $C_{60}F_{18}$ , experimental data were supported by theoretical calculations.

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**Keywords:** Raman and FTIR spectroscopy; Matrix isolation; Fluorofullerenes;  $C_{60}F_{18}$ ;  $C_{60}F_{36}$ ;  $C_{60}F_{48}$ 

## 1. Introduction

The fullerenes—new allotropic forms of carbon—were discovered in 1985 [1]. The next step forward was the developing of a method of macroscopic preparation of fullerenes [2] so that they became available for the chemical reactivity and physical studies. It should be mentioned that spectroscopic methods played a key role in the first detection of fullerenes, particularly, observation of fullerenes in the gas phase was first made by mass spectrometry [1], whereas infrared (IR) spectroscopy data showed evidence for the presence of  $C_{60}$  in the graphitic soot in macroscopic quantities [2].

Due to its unique nature, a fullerene molecule can form a great variety of derivatives with various substituents attached either in the exo- or endo-positions of the cage. Among the exohedral derivatives, fluorofullerenes represent an important group of compounds both from the point of view of their properties and potential applications in material science as new functionality materials. The fluorofullerenes compositions range from  $C_{60}F_2$  to  $C_{60}F_{60}$ , and hyperfluorination (with  $F > 60$ ) accompanying the carbon cage rupture may occur. First attempts to fluorinate  $C_{60}$  resulted in a mixture of fluorofullerene products with a broad distribution of F atoms attached to the carbon cage [3]. Further studies were focused at the selective synthesis of

specific fluorofullerenes, which was achieved by optimization of the reaction conditions and careful choice of halogen donor. Thus, the first pure compound— $C_{60}F_{48}$ —was obtained as a main product of the reaction between  $C_{60}$  and  $F_2$  after studying effects of the experimental conditions including temperature, fluorine pressure, and concentration, fullerene sample history and time of the reaction on the yields and composition of the products [4].  $C_{60}F_{36}$  and  $C_{60}F_{18}$  compounds were synthesized in the solid-phase reaction of  $C_{60}$  with transition metal fluorides as fluorinating agents ( $MnF_3$  and  $K_2PtF_6$ , correspondingly) followed by the sublimation of volatile products [5,6]. For isolation of the specific products, the high performance liquid chromatography (HPLC) may be used. Structural determination of the mentioned fluorofullerenes was performed by  $^{19}F$  NMR and X-ray single crystal analysis.

At present only three fluorofullerene compounds— $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$ —can be prepared in relatively pure form ( $\geq 90\%$ ) with appreciable yields ( $\geq 50\%$ ) and in sufficient quantities, while the yields of other isolated species ( $C_{60}F_2$  [7],  $C_{60}F_{16}$  [8], and  $C_{60}F_{20}$  [9]) are small and require HPLC isolation.

The aim of the present work was to complete the spectroscopic characterization of  $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$  fluorofullerenes. The infrared spectra of the solid  $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$  have been reported in [5,6,10]. Raman spectroscopy data for fluorofullerenes and chlorofullerenes are not known, and are only available for brominated  $C_{60}$  derivatives:  $C_{60}Br_6$ ,  $C_{60}Br_8$ , and  $C_{60}Br_{24}$  [11]. This paper reports for the first time Raman spectroscopy data for the

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solid  $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$  and FTIR spectra of these species isolated in cryogenic matrices.

## 2. Experimental

### 2.1. Samples

The samples of  $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$  were synthesized following the procedures described elsewhere [4–6]. Mass spectrometry,  $^{19}\text{F}$  NMR, and chemical analyses were used for characterization of the compounds.  $C_{60}F_{18}$  (90% purity) and  $C_{60}F_{36}$  (95% purity) were purified by sublimation, whereas  $C_{60}F_{48}$  (95% purity) was used as prepared.  $C_{60}F_{18}$  is an isomerically pure compound ( $C_{3v}$  symmetry), with main impurity being  $C_{60}$  and trace amounts of  $C_{60}F_{17}CF_3$  and  $C_{60}F_{18}O$  as indicated by mass spectrometry.  $C_{60}F_{36}$  and  $C_{60}F_{48}$  samples represent mixtures of isomers:  $C_{60}F_{36}$  forms two major isomers  $C_3$  and  $T$  symmetry in approximate ratios 3:1, while  $C_{60}F_{48}$  has two isomers of  $D_3$  and  $S_6$  symmetries in the 1:1 ratio. For two latter fluorofullerenes main impurities include few percent of the species with lower F content as found by mass spectrometry:  $C_{60}F_{34}$  and  $C_{60}F_{46}$ , respectively.

### 2.2. Techniques

The Raman spectra were recorded with a Bruker FT Raman RTS100 spectrometer and a Dilor XY spectrometer using Nd:YAG and  $\text{Ar}^+/\text{Kr}^+$  lasers as excitation sources with wavelengths of 1064, 568.2, and 514.5 nm. Note that the line at  $84\text{ cm}^{-1}$  is a parasite one due to the instrumental error. All measurements were taken in a backscattering geometry. To avoid noticeable damage of samples during the experiments, the values of the power densities in the visible range were maintained at  $0.2\text{--}1.5\text{ W/cm}^2$ .

The apparatus for FTIR spectroscopic measurements consists of a cooling system-cryotip (Displex, Air Products and Chemicals 202 CSA) located in a home made high vacuum stainless steel shroud—connected under rotary vacuum to a Bruker IFS 113v Interferometer through a suitable IR-transparent CsI window. The vacuum chamber is in turn connected to a high temperature furnace. Matrix gas and evaporating species are condensed at  $T \approx 12\text{ K}$  on a gold-plated coldfinger. The coldfinger is allowed to rotate in such a way that having two reflecting surfaces one can carry out two series of measurements during the same experiment. Details of the apparatus are described elsewhere [12].

High-purity argon and nitrogen were used as isolating matrix gases with a flow rate of  $1\text{--}1.5\text{ mmol/h}$  through a standardized needle valve. All samples were vaporized from nickel Knudsen cells having an orifices of 1 mm in diameter. In order to heat the cell a tantalum liner was used. It was resistively heated by two water cooled copper electrodes connected to a power supply.

Each of three isolated fluorofullerenes  $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$  was loaded into the cell and vaporized. The

vaporization temperature ranged from 500 to 750 K, depositions lasted from 10 min to 1 h. The spectra were obtained by reflection. For routine spectra 200 scans were accumulated with a resolution of  $1\text{ cm}^{-1}$ . The examined spectral range was  $4000\text{--}200\text{ cm}^{-1}$ .

The spectra in diffuse reflectance have been obtained by means of a Bruker Equinox 55 Interferometer with a resolution of  $1\text{ cm}^{-1}$  accumulating 500 scans.

$\text{H}_2\text{O}$  and  $\text{CO}_2$  in traces have been detected at 1593.2, 3727.7 and at 662.2, 2347.1  $\text{cm}^{-1}$ , respectively.

### 2.3. DFT calculations of the IR vibrational frequencies of $C_{60}F_{18}$

Geometry optimization, force field, and IR intensities calculations of  $C_{60}F_{18}$  molecule were performed with the help of the quantum-chemical package PRIRODA [13] at DFT level of theory employing generalized gradient approximation of Perdew, Burke, and Ernzerhoff (PBE) [14] with TZ2P-quality  $\{6, 1, 1, 1, 1, 1/4, 1, 1/1, 1\}$  Gaussian basis set. Evaluation of Coulomb and exchange-correlation terms was accelerated by expansion of the electron density in an auxiliary uncontracted (10s/3p/3d/1f) basis sets. Cartesian force field was transferred to the system of redundant internal coordinates, built from all covalent bonds and valence angles of the molecule. Potential energy distribution (PED) analysis and normal mode visualization were performed with the program DISP [15], designed for the vibrational calculations. Comparison of the theoretical and experimental IR spectra demonstrated that calculated vibrational frequencies of  $C_{60}F_{18}$  were somewhat underestimated; hence they were scaled uniformly by an empirically revealed factor of 1.02.

## 3. Results and discussion

The interpretation of the spectroscopic data for  $C_{60}F_{48}$  and  $C_{60}F_{36}$  is complicated by the existence of isomeric forms for the both species.  $C_{60}F_{48}$ , indeed, consists of the two isoenergetic isomeric forms of  $D_3$  and  $S_6$  symmetry in the ratio of 1:1 [16–18].  $C_{60}F_{36}$  consists of the two isomers having  $C_3$  and  $T$  symmetry in the approximate ratio of 3:1 [19,20]. For this reason and in view of the great number of vibrational levels often lying in a tight spectral interval, obtained spectra have been analyzed with the aim of individualizing isomers without attempting an accurate assignment.

For  $C_{60}F_{18}$  the situation is less complicated. NMR spectroscopy [5,20] and a single crystal X-ray study [21,22] of  $C_{60}F_{18}$  (as a toluene solvate, more exactly) ascertained a single stable isomer of  $C_{60}F_{18}$  of “pseudocyclophane” arrangement having  $C_{3v}$  symmetry. In this molecule, all the fluorine atoms are bound only to one hemisphere of the  $C_{60}$  fullerene cage, the other hemisphere is nondistorted. Therefore, only in the case of  $C_{60}F_{18}$  the experimental investigation has been paralleled by a theoretical analysis

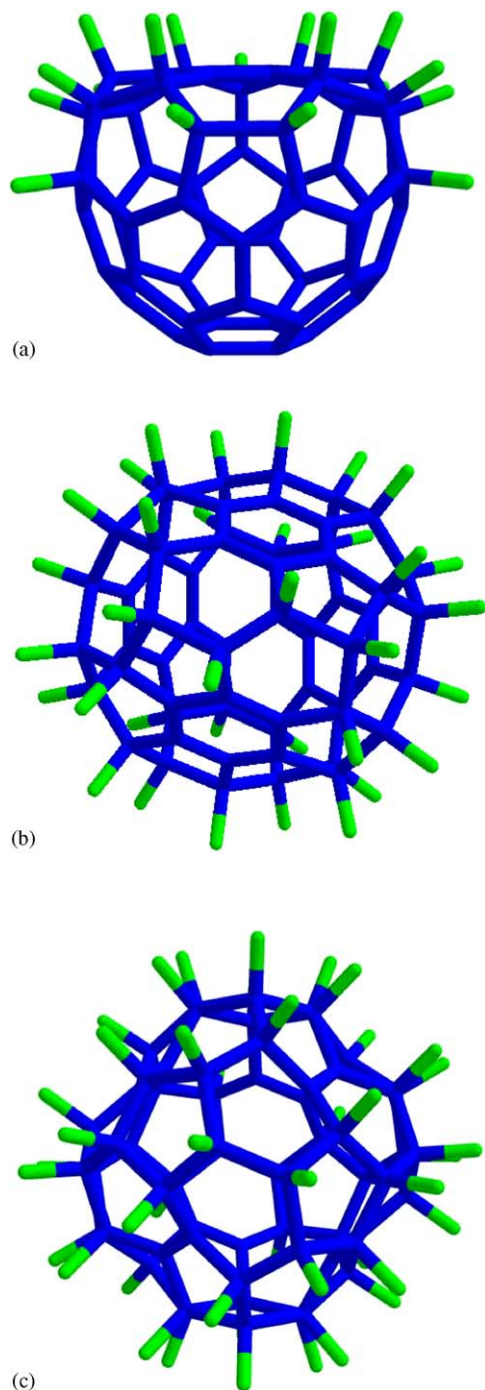


Fig. 1. (a) The structures of  $C_{60}F_{18}$ ; (b)  $C_{60}F_{36}$  (T symmetry isomer); and (c)  $C_{60}F_{48}$  ( $D_3$  symmetry isomer).

in order to achieve a better understanding of the spectroscopic data. The structures of  $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$  are presented in Fig. 1.

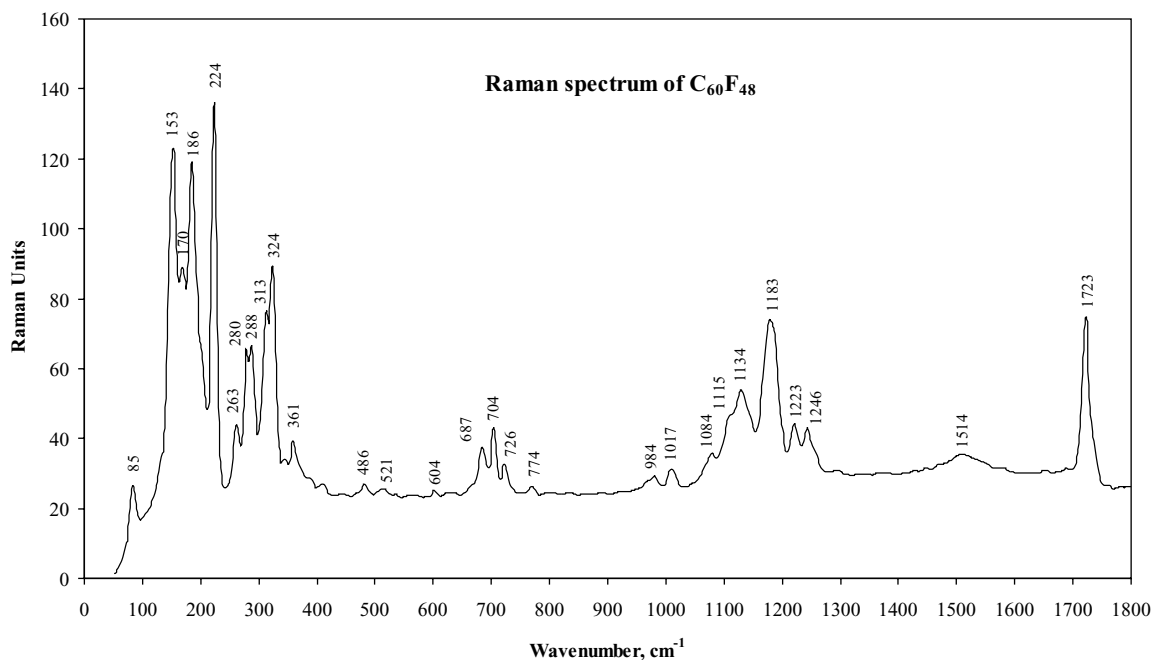
### 3.1. $C_{60}F_{48}$

According to the X-ray study data [23], the solid  $C_{60}F_{48}$  has tetragonal disordered structure which complicates its determination. However, the molecular structure determination

Table 1  
Experimental infrared and Raman vibrations of  $C_{60}F_{48}$

IR Ar matrix	IR solid (KBr pellet)	Raman
1241.8 m		1723 m
1239.1 m		1246 mw
1233.1 m	1238 s	
1229.6 m		
1217.7 mw		1223 mw
1214 m, sh	1215 ms	
1200.0 m	1199 ms	
1179 m,sh		1183 m
1173.1 s	1170 vs	
1167 m, sh		
1148.9 mw		
1143.7 ms	1142 s	
1127.5 m	1126 m, sh	1134 mw
1112.8 mw		1115 sh
1091.6 mw		
		1084 w
1074 w		
1070 w		
1060.4 m		
1033.8 vw		
1022.1 w		1017 w
992.9 vw		
982.5 vw		984 w
975.8 w		
968.6 w		
927.5 vw		
870.6 vw		
841.6 w		
801.7 w		774 w
776.0 mw		
771.6 m	771 ms	
757.4 w, sh		
753.7 m	754 m	
750.6 w, sh		
736.2 mw		
725.1 m		
723.1 m	724 s	726 mw
		704 m
680.3 mw		687 mw
677 w, sh		
651.1 m	650 ms	
638.7 mw		
630.6 w, sh		
626.6 m		
603.5 m	603 ms	604 vw
		521 w, br
		361 w
		324 m
		313 m
		288 m
		280 m
		263 mw
		224 s
		186 s
		170 m
		153 s
		85 mw

m: medium; w: weak; s: strong; sh: shoulder; mw: medium weak; ms: medium strong; m, sh: medium shoulder; w, br: weak broad; w, sh: weak shoulder; vs: very strong; vw: very weak.

Fig. 2. Raman spectrum of solid  $C_{60}F_{48}$ .

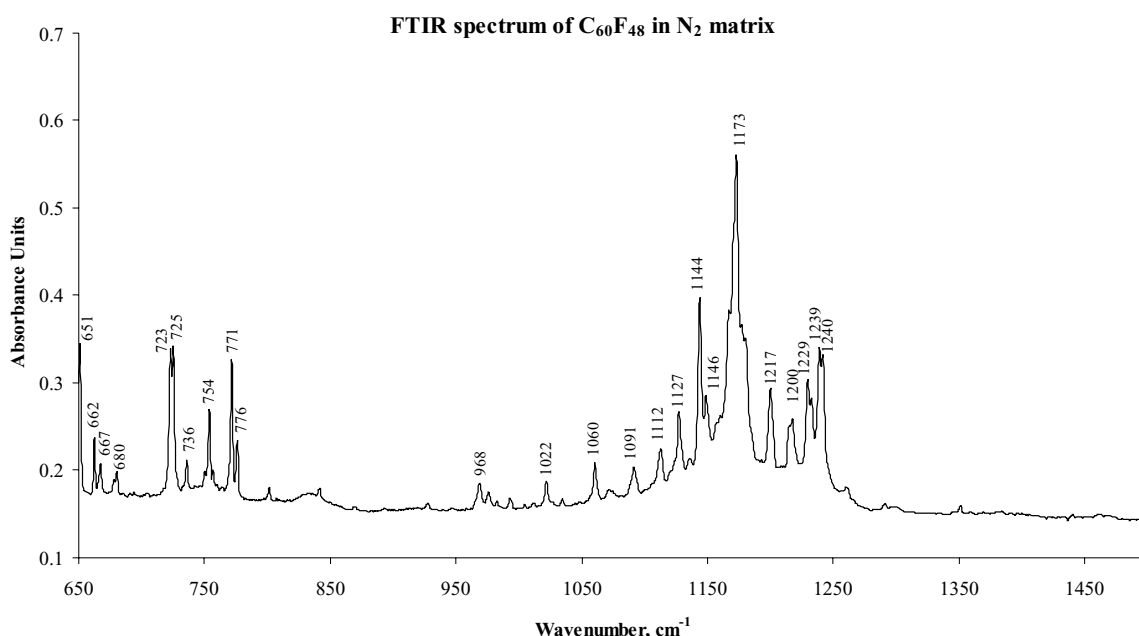
of  $C_{60}F_{48}$  was made using single crystals of solvate [16] and characterized by the presence of both  $D_3$  and  $S_6$  isoenergetic isomers, statistically disordered over two positions. Since both isomers of  $C_{60}F_{48}$  have very close energies [17] and structures, their spectra are expected to be similar.

The main feature of the infrared spectrum of the solid  $C_{60}F_{48}$  dispersed in KBr excess reported in [10] (see Table 1) consists of a six components multiplet lying in the spectral range where C–F stretching and skeleton modes are expected. Therefore, the interpretation of the spectral patterns is further

complicated by the overlapping of the modes that belong both to the same isomer and to the different ones.

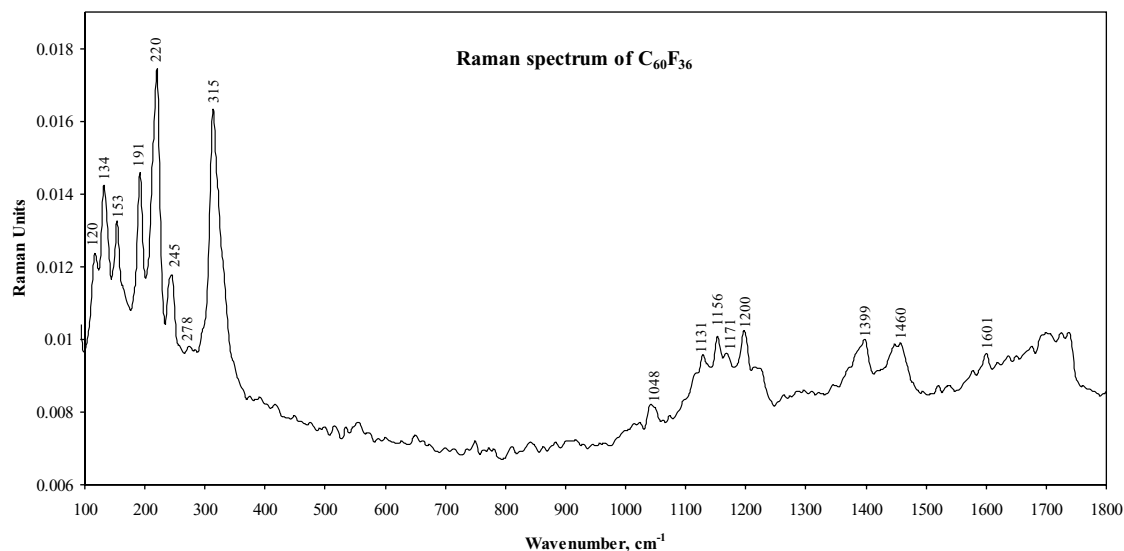
The Raman spectrum of the solid shows a medium intensity multiplet in the same region while the most prominent features are observed in the 400–100  $cm^{-1}$  range (Fig. 2).

The number of active bands individualized in the IR spectrum of matrix isolated molecules of  $C_{60}F_{48}$  (Fig. 3) is exceedingly higher than in the IR spectrum of solid (Table 1). Depositions at different vaporization temperature

Fig. 3. FTIR spectrum of  $N_2$  isolated  $C_{60}F_{48}$  molecules.

at 1161 and 1172  $\text{cm}^{-1}$ . At present, an assignment of the intense band at 1167.1  $\text{cm}^{-1}$  in Ar (1166.3  $\text{cm}^{-1}$  in  $\text{N}_2$ ) to the  $\text{C}_3$  isomer can be attempted due to its proximity to the main peak of this isomer in the solid state and because of its prevailing abundance. However, in the absence of the data on the vaporization behavior of each isomer, this assignment is only tentative.



Fig. 4. Raman spectrum of solid C<sub>60</sub>F<sub>36</sub>.

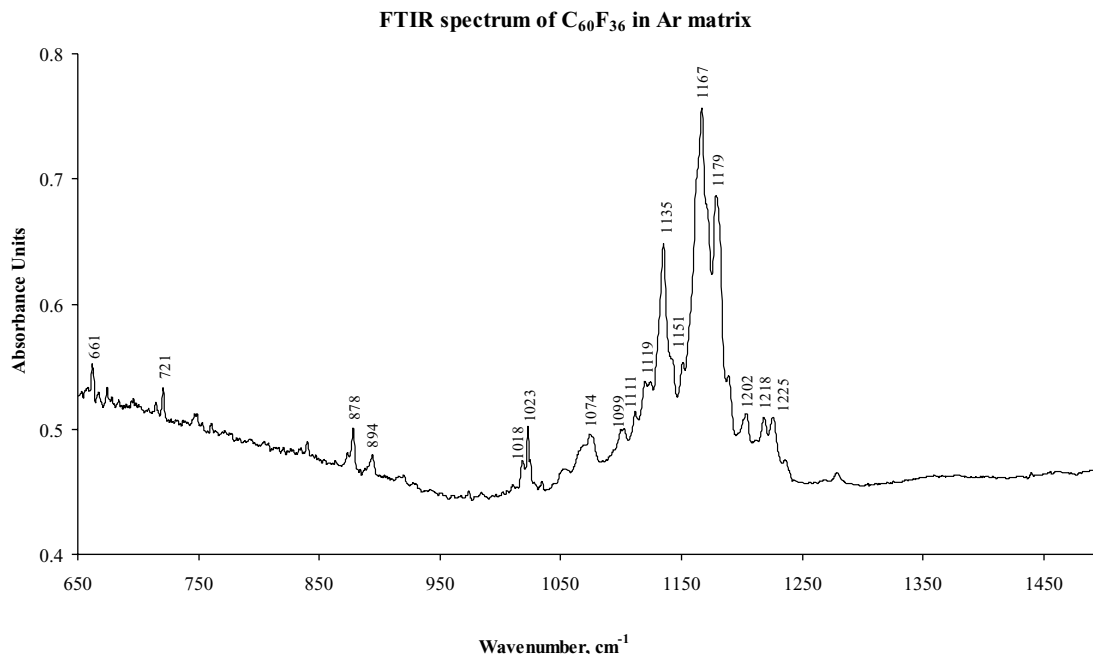
### 3.3. C<sub>60</sub>F<sub>18</sub>

The single crystal X-ray data of the C<sub>60</sub>F<sub>18</sub> solvates (in case of toluene solvate having a monoclinic cell of *P*2<sub>1</sub>/*n* symmetry) [21,22] have shown that the molecule represents a single C<sub>3v</sub> isomer, which fully agrees with the earlier interpretation of the solution NMR data [6]. The crystal structure of the pristine C<sub>60</sub>F<sub>18</sub> has recently been determined [22], revealing that solvent free C<sub>60</sub>F<sub>18</sub> crystallizes monoclinic forming slightly distorted hexagonal packing with the molecules oriented almost parallel to each other.

#### 3.3.1. Experimental Raman and IR spectroscopy data

The literature IR spectrum of C<sub>60</sub>F<sub>18</sub> in KBr pellet consists of a number of bands confirming, for their sharpness, the presence of a single isomer [6]. In this work, the sample dispersed in KBr in the approximate ratio of 1:500 has been analyzed using the diffuse reflectance technique. Obtained spectrum (Fig. 7) is identical to the literature one [6].

In addition, films have been obtained depositing the equilibrium vapor of C<sub>60</sub>F<sub>18</sub> on the coldfinger at 12 K without isolating gas. It is interesting to note that the spectrum

Fig. 5. FTIR spectrum of Ar isolated C<sub>60</sub>F<sub>36</sub> molecules.

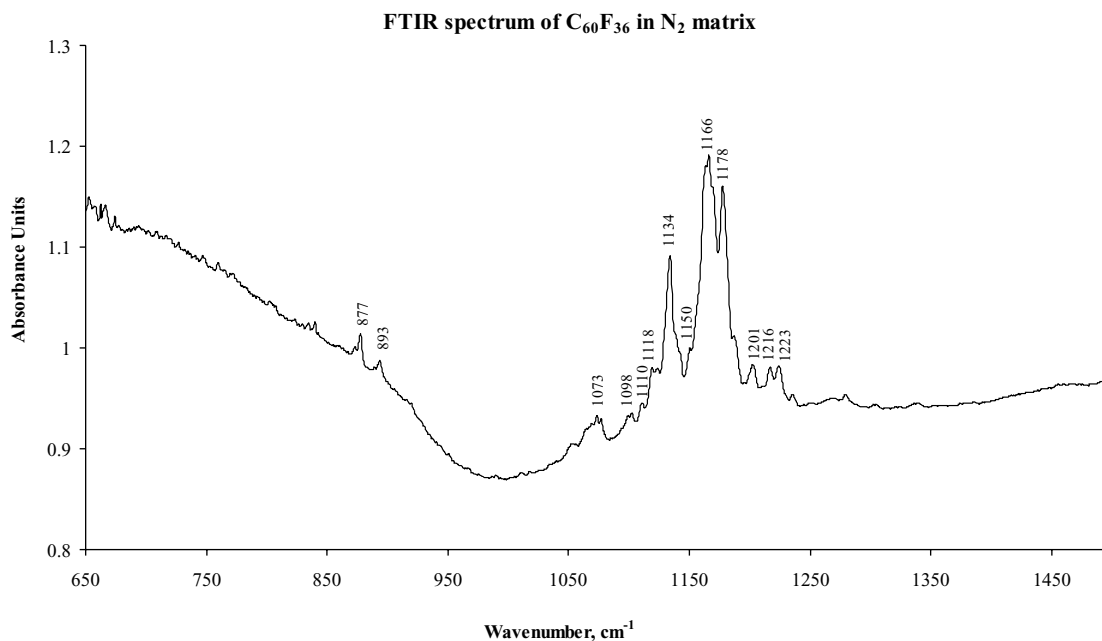


Fig. 6. FTIR spectrum of  $N_2$  isolated  $C_{60}F_{36}$  molecules.

observed after annealing cycles matched the patterns obtained on the solid sample dispersed in KBr.

As observed in case of  $C_{60}F_{48}$  and  $C_{60}F_{36}$ , also in the IR spectrum of  $C_{60}F_{18}$  the most intense infrared active bands lie in the  $1200\text{--}1000\text{ cm}^{-1}$  region (Fig. 8) while the Raman spectrum (Fig. 9) is characterized by a number of strong bands in the  $400\text{--}100\text{ cm}^{-1}$  interval and a very strong peak at  $1493\text{ cm}^{-1}$ , probably originating from pentagon pinch mode of  $C_{60}$  at  $1468\text{ cm}^{-1}$ , and its shift to the higher frequency manifests electron-withdrawing effect of the fluorine atoms.

As in previous cases, a medium intensity multiplet is present in the  $1200\text{--}1000\text{ cm}^{-1}$  range.

### 3.3.2. Theoretical calculations and spectra interpretation

The isolated  $C_{60}F_{18}$  molecule possesses  $C_{3v}$  symmetry, its 228 vibrations being distributed between the following distinct modes according to the irreducible representation:

$$\Gamma_{\text{vib}} = 41A_1 + 35A_2 + 76E.$$

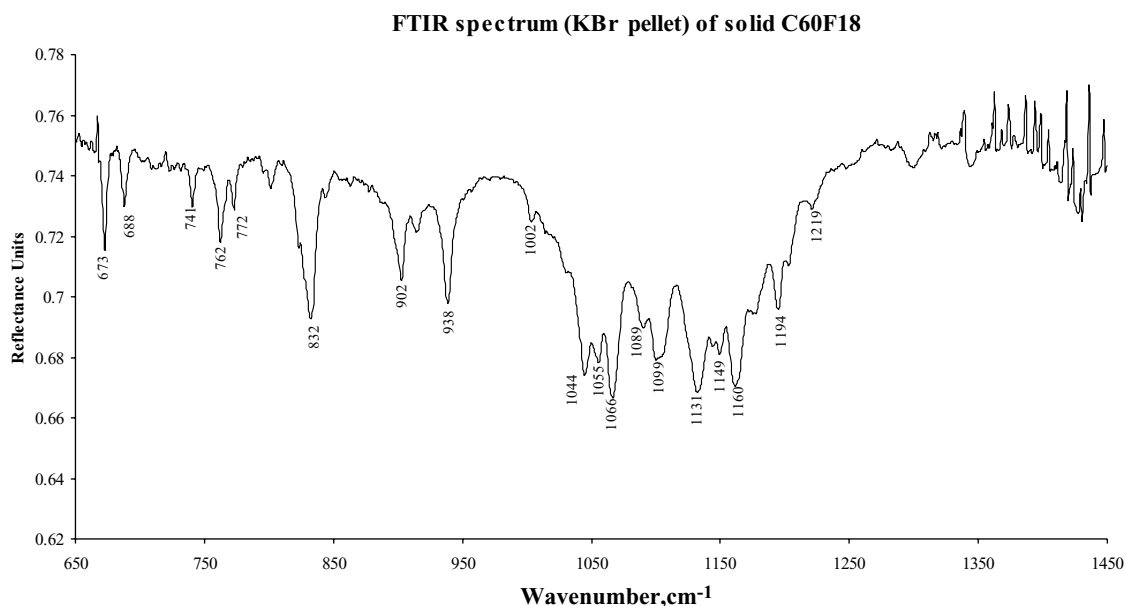
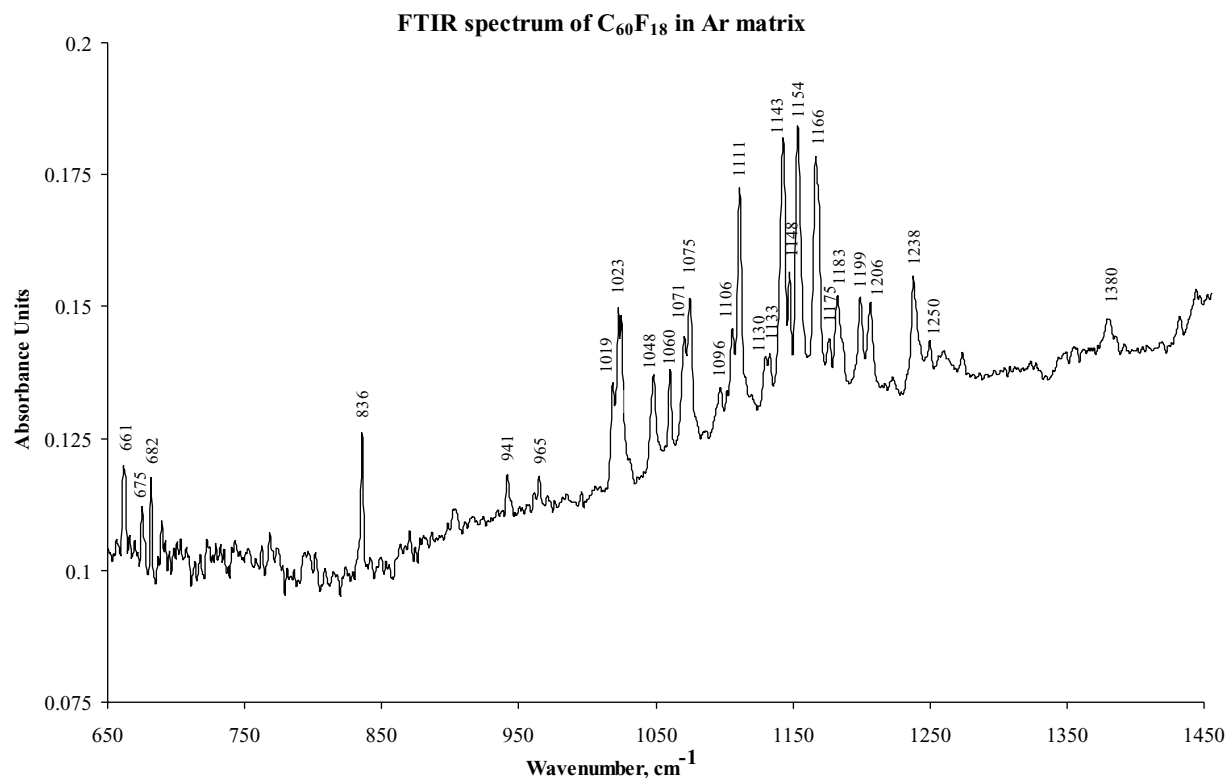


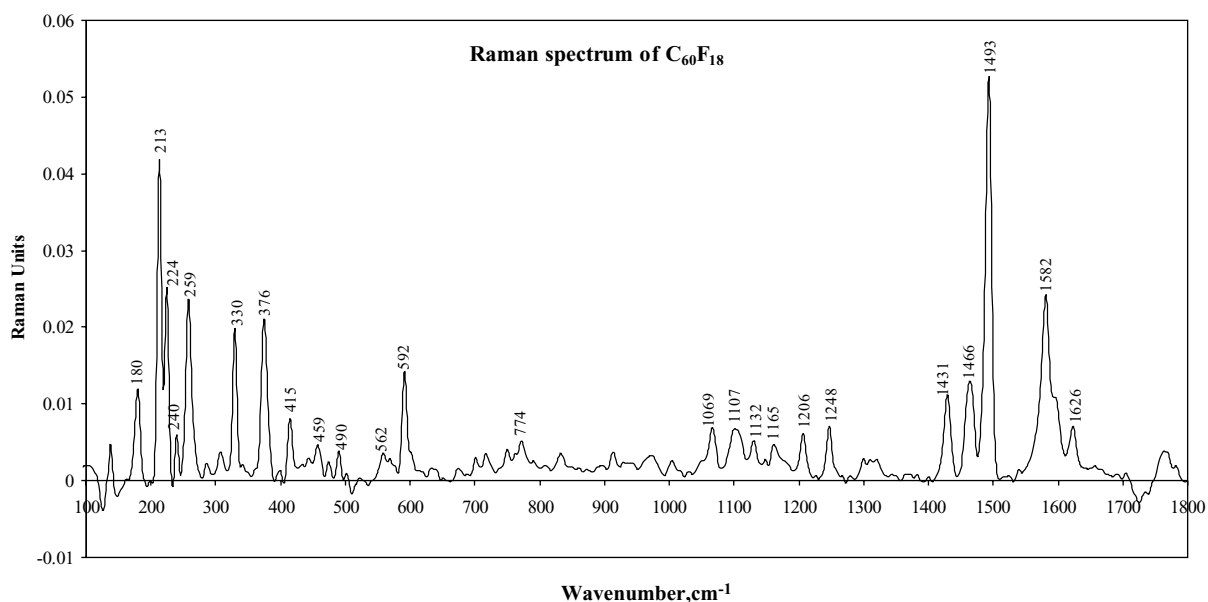
Fig. 7. Our FTIR spectrum of solid  $C_{60}F_{18}$  (KBr pellet).



Fig. 8. FTIR spectrum of Ar isolated C<sub>60</sub>F<sub>18</sub> molecules.

One hundred seventeen modes of A<sub>1</sub> and E symmetry should be both IR and Raman-active resulting in rather complicated spectra. Note that in the spectra of the crystalline phases of C<sub>60</sub>F<sub>18</sub>, some additional features may be observed because of the lower site-symmetry of the molecules in the lattice.

Because of the great number on bands, complete and reliable vibrational assignment for C<sub>60</sub>F<sub>18</sub> molecule requires additional calculations of the Raman intensities, however preliminary interpretations of the vibrational spectra of the fluorofullerene can be performed already at this stage.

Fig. 9. Raman spectrum of solid C<sub>60</sub>F<sub>18</sub>.

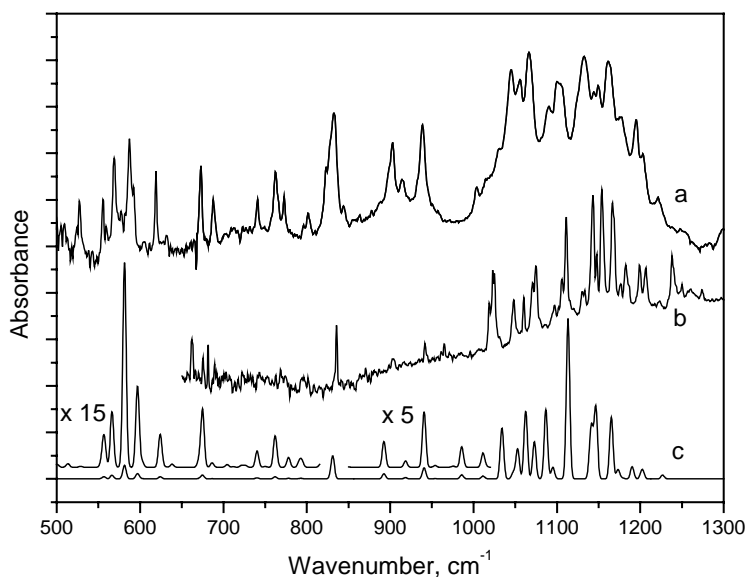


Fig. 10. Experimental and calculated IR spectra for  $C_{60}F_{18}$ : (a) solid  $C_{60}F_{18}$ , since it is a reflectance spectrum, intensities are only arbitrary and do not correspond to absorbance; (b) gaseous  $C_{60}F_{18}$  in Ar matrix; and (c) theoretical.

The calculated IR spectrum of  $C_{60}F_{18}$ , broadened by the Gaussian functions, is presented in Fig. 10 along with the experimental spectra.

IR spectra of  $C_{60}F_{18}$  are mostly dominated by a group of intense bands in the characteristic region of the C–F stretching vibrations. According to  $C_{3v}$  symmetry, stretches of 18 C–F bonds of the fluorofullerene molecule span the following irreducible representations:

$$\Gamma_{\text{vib}}(\text{CF}) = 4A_1 + 2A_2 + 6E,$$

formally resulting in 12 modes. Ten of them, belonging to  $A_1$  and E symmetry, are active both in IR and Raman scattering spectra. Meanwhile, some carbon skeleton vibrations, namely ordinary C–C stretches and CC(F)C deformations, also fall in this region. Hence, fluorofullerene modes around 900–1200  $\text{cm}^{-1}$  actually are of a mixed character, and C–F stretches are distributed among 20 or more of them with total C–F contribution not exceeding 30–50%. Table 3 presents calculated frequencies, IR intensities, C–F contribution to PED and tentative assignment of the  $C_{60}F_{18}$  modes in the 900–1200  $\text{cm}^{-1}$  region. Noteworthy, the most intense IR bands correspond to vibrations with the enhanced C–F contributions, whereas in the Raman spectrum these bands have moderate intensity.

Carbon skeleton vibrations can be seen in the IR spectra as a group of relatively weak features around 500–600  $\text{cm}^{-1}$ , but in the Raman spectrum they constitute most of the intense bands in the 400–1600  $\text{cm}^{-1}$  region. Highest frequency modes of  $C_{60}F_{18}$  correspond to C=C stretches and resemble tangential vibrations of the fullerene itself. Very strong Raman line at 1493  $\text{cm}^{-1}$  is attributed to the pentagon pinch mode of  $C_{60}$  at 1468  $\text{cm}^{-1}$ .

According to PED analysis, C–F bending bands are mostly located in the 150–350  $\text{cm}^{-1}$  region, and a medium-strong

Raman lines at 180, 213, 224, 259, 330, and 376  $\text{cm}^{-1}$  possess a significant contribution from CCF valence angles.

#### 4. Conclusion

Raman and FTIR spectroscopic studies of  $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$  species were performed. In this work, the Raman spectra of solid  $C_{60}F_{18}$ ,  $C_{60}F_{36}$ , and  $C_{60}F_{48}$  and the infrared spectra of gaseous molecules of the same compounds isolated in cryogenic matrixes are reported for the first time.

In the case of  $C_{60}F_{36}$  and  $C_{60}F_{48}$ , the analysis of the spectral patterns is complicated by the presence of isomeric forms. A great number of bands observed both in Raman and in the infrared spectra prevented an accurate assignment.

Attempts to separate the two isomers which constitute solid  $C_{60}F_{48}$  sample by varying temperatures of sublimation in our matrix-assisted FTIR studies were not successful. The way to resolve the problem seems to be in searching for the more elaborate separation techniques, which is a difficult task in view of the very close similarity in the structures and properties of the two isomers.

In the case of  $C_{60}F_{36}$ , isolation of a single isomer can be performed chromatographically and we plan further spectroscopic experiments with isomerically pure  $C_{60}F_{36}$  in the near future, however, even in the present study, a tentative assignment of the intense band at 1167.1  $\text{cm}^{-1}$  in Ar (1166.3  $\text{cm}^{-1}$  in  $N_2$ ) to the  $C_3$  isomer has been undertaken.

For a single isomer of  $C_{60}F_{18}$  theoretical calculation of IR spectrum was carried out. A good agreement between the theoretical and experimental data was achieved, and the interpretation of the spectra has been given. Ab initio calculations of Raman vibrational frequencies of  $C_{60}F_{18}$  are in progress.

Table 3

Calculated frequencies, IR intensities, CF contribution to PED, and tentative assignment of the C<sub>60</sub>F<sub>18</sub> modes in the 900–1200 cm<sup>-1</sup> region

Symmetry	Theory		Experiment			Potential energy distribution(%)			
	Frequency	Intensity (%)	IR Ar	IR solid (KBr pellet)	Raman	CF	C–C	CC(F)C	CCF
A1	1226.4	2.45	1239.2	1221.3		0.02	0.59	0.09	0.04
E	1203.0	2.93	1206.5			0.06	0.45	0.13	0.10
A1	1201.3	3.66	1199.2	1195.0		0.14	0.66	0.05	0.09
E	1189.9	7.85	1183.8			0.33	0.26	0.13	0.15
E	1178.2	0.62				0.06	0.39	0.29	0.13
A1	1173.0	5.98				0.48	0.23	0.09	0.09
E	1164.9	39.31	1167.2	1161.6	1165	0.17	0.40	0.11	0.08
A2	1148.9	0.00				0.17	0.48	0.11	0.10
A1	1146.3	44.96	1154.5	1149.4		0.37	0.23	0.20	0.12
E	1141.7	21.53	1143.3		1132	0.39	0.25	0.12	0.18
E	1139.7	15.96	1131.1	1132.6	1132	0.36	0.29	0.13	0.08
A2	1134.0	0.00				0.18	0.44	0.09	0.10
E	1112.9	100.00	1111.0	1100.7	1107	0.67	0.16	0.06	0.07
A1	1112.5	2.03				0.30	0.33	0.09	0.13
A2	1095.5	0.00				0.38	0.14	0.18	0.14
A2	1095.5	0.00				0.38	0.14	0.18	0.14
A1	1092.8	0.05		1090.4		0.35	0.40	0.10	0.04
A1	1086.4	44.03	1073.2	1066.6	1069	0.48	0.18	0.14	0.09
E	1072.6	23.63				0.37	0.23	0.17	0.13
E	1062.2	43.17	1060.4	1055.8		0.46	0.21	0.14	0.09
A2	1058.5	0.00				0.39	0.12	0.20	0.09
E	1052.5	19.11	1048.3	1045.1		0.43	0.27	0.11	0.10
A2	1048.2	0.00				0.18	0.24	0.32	0.11
A1	1047.3	4.09				0.34	0.35	0.10	0.12
E	1033.8	32.45	1023.4			0.24	0.44	0.14	0.06
A1	1014.2	0.14				0.20	0.32	0.23	0.10
E	1011.0	1.78				0.41	0.27	0.11	0.07
A1	975.1	0.14				0.24	0.25	0.23	0.12
E	940.4	7.09		938.7		0.22	0.36	0.09	0.10

Calculated frequencies are scaled by 1.02; calculated intensities are normalized to the highest intensity band at 1112.9 cm<sup>-1</sup>; C–CF bonds; C–C: ordinary CC bonds (both in “fullerene” and fluorinated fragments); CC(F)C–CCC angles with F-connected carbon in the vertex; CCF–CCF angles.

## Acknowledgements

Authors are grateful to Mr. P. Moscardelli for the technical assistance. Partial financial support of this research has been provided by the Volkswagen Stiftung (I77-855) and the Russian Foundation for Basic Research (grants no. 03-03-32756 and 03-03-32855).

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