

## Review Article

# IR and UV/VIS Spectroscopic Characterization of the Higher Fullerene C<sub>76</sub>-D<sub>2</sub> for Its Quantitative and Qualitative Determination

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The only stable isomer of the higher fullerene C<sub>76</sub> of D<sub>2</sub> symmetry was isolated from carbon soot by the new and advanced extraction and chromatographic methods and processes. Characterization of the isolated C<sub>76</sub>-D<sub>2</sub> was performed by the IR(KBr) and UV/VIS method in the absorption mode. All of the experimentally observed infrared and electronic absorption bands are in excellent agreement with the theoretical calculations for this fullerene. The molar absorptivity  $\epsilon$  and the integrated molar absorptivity  $\Psi$  of the observed entire new series of various characteristic, both deconvoluted and convoluted IR absorption bands of the C<sub>76</sub>-D<sub>2</sub> isomer, in different integration ranges were determined. In addition, the molar extinction coefficients of its UV/VIS absorption bands were determined. The obtained novel IR and UV/VIS spectroscopic parameters are significant for the quantitative assessment of C<sub>76</sub>-D<sub>2</sub>. All the presented data are important both for its qualitative and quantitative determination, either in natural resources on Earth and in space or in artificially synthesized materials, electronic and optical devices, optical limiters, sensors, polymers, solar cells, nanophotonic lenses, diagnostic and therapeutic agents, pharmaceutical substances, for targeted drug delivery, incorporation of metal atoms, in biomedical engineering, industry, applied optical science, batteries, catalysts and so forth.

## 1. Introduction

Fullerenes C<sub>60</sub> and C<sub>70</sub> were first detected in space [1–14] and quantified [5, 6] by means of IR spectroscopy [1–27]. They were found in a series of space environments and astrophysical objects [1–27], such as certain planetary [4–7] and protoplanetary nebulae [7], carbon-rich stars including also R-Coronae Borealis stars [8, 9], postasymptotic giant branch stars, and young stellar objects [10], in the interstellar medium, in reflection nebulae [1–3, 11–14], as well as in some resources on Earth [3, 15].

For the identification of the basic fullerenes, the knowledge of the infrared band position and band widths as well

as the evolution of these parameters with temperature was necessary [1–25]. Quantitative assessment of fullerenes C<sub>60</sub> and C<sub>70</sub> required knowledge about intensities of their IR absorption bands [3, 5, 6, 26–28].

Their relative abundance in space, for example, an abundance of about 0.35% in certain planetary nebulae, was estimated through the molar absorptivity and integrated molar absorptivity of the infrared maxima measured in laboratory [5, 6].

Another useful method for the identification and quantitative determination of fullerenes can be electronic absorption spectroscopy due to their transitions in the spectral range comprised between 190 and 1500 nm,

where it is known that the space is rich in a number of yet unassigned electronic transitions belonging to molecules and radicals [28, 29].

It should be expected also that the higher fullerenes can be found and quantified in space because of their exceptional stability toward high temperatures and cosmic rays [1–3, 30–34], as well as the possibilities of their formation through coalescence of smaller fullerenes by laser ablation of carbon and dehydrogenation of hydrogenated fullerenes, fulleranes [1–3, 30–37].

The IR and electronic absorption spectra as well as their dependence on temperature that are necessary for the qualitative detection of the higher fullerenes, such as  $C_{76}\text{-D}_2$ , the only stable  $C_{76}$  isomer of  $D_2$  symmetry [1–3, 38–61], isolated by the new advanced chromatographic methods [2, 3, 38–45], were studied in the previous works [2, 3, 38–61].

It is important to mention that all of the experimentally observed infrared and electronic absorption bands of the isolated  $C_{76}\text{-D}_2$  in this research [2, 3, 38–44] are in excellent agreement with the theoretical calculations for this molecule [46–49].

The aim of this study was to determine the novel IR and UV/VIS spectroscopic parameters that are necessary for the quantitative assessment of  $C_{76}\text{-D}_2$ .

In the previous work [3], the molar extinction coefficients and the integrated molar extinction coefficients of the main convoluted or integral IR absorption bands with some shoulders of this fullerene were determined and reported together with the relative intensities.

Excellent agreement was found between the relative intensities of the main characteristic absorption maxima calculated from  $\epsilon_\lambda$  and from the  $\Psi_\lambda$  values in adequate integration ranges [3].

In this article, the molar absorptivity and the integrated molar absorptivity of the entire series of all the observed various characteristic and new deconvoluted or separated absorption maxima and shoulders were determined. In addition, the integrated molar absorptivity of several convoluted absorption bands with some shoulders of  $C_{76}\text{-D}_2$  in different and new relevant integration ranges were determined. The molar extinction coefficients of its UV/VIS absorption bands were also determined.

The molar absorptivity and the integrated molar absorptivity in the applied integration ranges of the corresponding main and characteristic absorption bands, both separated and integral, in all the IR and UV/VIS spectra of the chromatographically purified  $C_{76}\text{-D}_2$  samples from this research [2, 3, 38–44] are in excellent agreement.

The obtained new research results in the recent [3] and current IR and UV/VIS spectroscopic study of the higher fullerene  $C_{76}\text{-D}_2$  are important for its quantitative determination.

All the presented IR and UV/VIS data will significantly contribute to better understanding of the spectroscopic properties of  $C_{76}\text{-D}_2$ , which is important both for its identification and quantitative assessment, either in natural resources or in artificially synthesized materials.

## 2. Experimental Methods

In the first phase of this research,  $C_{60}$ ,  $C_{70}$  [21–23], and the higher fullerenes, mainly  $C_{76}$  and  $C_{84}$  [2, 3, 38–45], were Soxhlet extracted with a series of different and previously unapplied solvents or combinations of solvents from the samples of the carbon soot produced by an electric arc (MER Corporation, Tucson, USA). The extraction procedures were performed until the complete disappearance of color in a Soxhlet extraction thimble. Solvents used were *n*-heptane, toluene, chlorobenzene, *p*-xylene, a mixture of *o/m/p*-xylene, and pyridine, as well as the successive use of toluene and chlorobenzene and *p*-xylene and pyridine. The yields as well as the compositions of all the extracts were determined by spectroscopic and chromatographic methods. The procedures for increases of fullerene yields and for additional selective extraction of higher order fullerenes were found [2, 3, 21–23, 38–45].

In the second phase,  $C_{60}$ ,  $C_{70}$ , and the higher fullerenes  $C_{76}$  and  $C_{84}$  (the only stable  $C_{60}\text{-Ih}$ ,  $C_{70}\text{-D5h}$ , and  $C_{76}\text{-D}_2$  isomers of the first three mentioned fullerenes and the most abundant, stable  $C_{84}$  isomer of  $D_2$  symmetry) were chromatographically separated from the obtained extracts of the carbon soot on the activated  $\text{Al}_2\text{O}_3$  columns by new and advanced methods [2, 3, 38–45].

The main difference and advantage of these methods [2, 3, 38–45], in comparison to previous methods under pressure [53–61], is the isolation of the purified stable isomers of the higher fullerenes  $C_{76}$  and  $C_{84}$  (the  $C_{76}\text{-D}_2$  and  $C_{84}\text{-D}_2$ :22 isomers) successively after the basic fullerenes in one phase of each of the processes under atmospheric pressure and smaller flow of 1.5 mL/min in increased milligram yields. The elution was performed continuously with several different original, defined gradients of solvents: from pure hexane or 5% toluene in hexane to pure toluene. The amounts of the initial materials used were as follows: fullerene extracts, 10 mg, and finely granulated  $\text{Al}_2\text{O}_3$ , 50 g, activated for 2 h at 105°C, and eluent (1.5 to 1.75 L) per chromatographic separation [2, 3, 38–45]. Starting from 10 mg of the soluble soot extract, in average ca. 1 mg of  $C_{76}$  and ca. 1 mg of  $C_{84}$  were isolated in purified form per one chromatographic process or up to few milligrams in some cases. The time spent on the purification processes was from 16.7 to 19.4 h [3, 42, 43].

The other advantages of the developed methods [2, 3, 38–45], in comparison to previous methods [53–61], are the use of significantly smaller amounts of the initial materials as well as less expensive laboratory equipment. In these methods [2, 3, 38–45], the entire materials and energy expense, the time spent on the purification processes, and environmental pollution were decreased using smaller amounts of less toxic solvents. The yields and the purities of the isolated fullerenes were increased or maximized [2, 3, 42, 43].

Purification of the higher fullerenes under pressure on a preparative scale, either by flash chromatography or by HPLC, generally required larger amounts of the initial materials repeated chromatography, and the fullerenes

were obtained in smaller yields [53–61] compared to our results [2, 3, 38–45]. This was discussed and presented in more detail in the previous articles [3, 42, 43].

**2.1. Measurement of the IR Spectra, the Molar Absorptivity, and Integrated Molar Absorptivity of Deconvoluted and Convolved Absorption Bands of  $C_{76}\text{-D}_2$ .** The IR spectra of the  $C_{76}\text{-D}_2$  samples, isolated by the new and advanced chromatographic methods and processes [2, 3, 38–44], were recorded on a Thermo Scientific FT-IR spectrometer Nicolet IR-6700 by the KBr disk technique in the range of 400–2000  $\text{cm}^{-1}$  at a resolution of 1  $\text{cm}^{-1}$  in the transparence mode formerly for its qualitative detection [2]. In the previous [3] and this article, the IR spectra of the isolated  $C_{76}\text{-D}_2$  samples were recorded in the absorption mode for determination of novel parameters for its quantitative determination.

Chromatographically isolated  $C_{76}\text{-D}_2$  sample (0.196 mg) was mixed with 100.4 mg of KBr. The obtained powder was compressed at 4 tons/ $\text{cm}^2$  with the Perkin Elmer press. The resulting pellet was placed in the FT-IR spectrometer. Measurement of the intensities (heights) of the entire new series of  $C_{76}\text{-D}_2$  absorption bands as well as of the integrated intensities of both all deconvoluted absorption maxima and shoulders and of convoluted absorption bands with some shoulders of this fullerene in different integration ranges with automatic subtraction of the baseline was made possible through the OMNIC software from Thermo Scientific, dedicated to the FT-IR spectrometer. The method and software used in this study have also been recently used for the measurement of relative intensities of IR absorption bands of the basic fullerenes  $C_{60}$ ,  $C_{70}$ , and their hydrogenated derivative fullerenes [25–27], as well as of the main convoluted absorption bands of the higher fullerenes  $C_{76}\text{-D}_2$  and  $C_{84}\text{-D}_{22}$  [3].

The mass of the resulting pellet was 100.6 mg, and the percentage of carbon determined by the elemental analysis was 0.195. Its measured thickness ( $b$ ) was 1.205 mm  $\sim$  0.1205 cm, diameter ( $R$ ) was 0.7 cm, and the half diameter ( $r$ ) was 0.35 cm.

The volume of the pellet ( $V$ ) was determined from the abovementioned  $r$  and  $b$  parameters by the equation  $V = r^2 \pi b$ . The obtained values of the volume and the thickness of the pellet were also confirmed using KBr density (2.753  $\text{g}/\text{cm}^3$ ) [3, 26] and the mass of the pellet.

Concentration ( $c$ ) of fullerene  $C_{76}$  in this pellet was calculated using the above given mass of  $C_{76}$  in the pellet, its molar mass of 912.76  $\text{g}/\text{mol}$ , and the volume of the pellet. The  $(bc)^{-1}$  value determined for the applied  $C_{76}\text{-D}_2$  sample in KBr pellet from the abovementioned experimental parameters was 1409.9  $\text{L cm}^{-1} \text{ mol}^{-1}$ , ca. 1410  $\text{L cm}^{-1} \text{ mol}^{-1}$ .

**2.2. Measurement of the UV/VIS Spectra and the Molar Absorptivity of Absorption Bands of  $C_{76}\text{-D}_2$ .** The UV/VIS spectra of the chromatographically isolated  $C_{76}\text{-D}_2$  samples by the new improved methods were recorded on the GBC Cintra 40 spectrophotometer in the region from 200 to 900 nm for its qualitative detection previously [2, 38–43], as well as for the quantitative

determination in this article. Solutions of fullerene  $C_{76}$  in hexane, conc.  $10^{-5} \text{ mol}/\text{dm}^3$  were used. The thickness of the cuvette was 1 cm.

The  $(bc)^{-1}$  value determined for the  $C_{76}\text{-D}_2$  sample in  $n$ -hexane from the abovementioned experimental parameters was 100,000  $\text{L cm}^{-1} \text{ mol}^{-1}$ .

### 3. Results and Discussion

In this article, the molar absorptivity and the integrated molar absorptivity of the observed series of various characteristic and new for both deconvoluted and convoluted IR absorption bands in different integration ranges of the  $C_{76}\text{-D}_2$  isomer were determined. The molar absorptivity of its UV/VIS absorption bands was also determined.

The original characteristic and new IR spectrum of the chromatographically isolated  $C_{76}\text{-D}_2$  sample are obtained in the absorption mode in this article, Figure 1, in order to find the abovementioned novel parameters for its quantitative determination. This spectrum was previously provided in transparence mode [2] for its qualitative determination.

The main three most intense dominant  $C_{76}$  maxima registered in this research [2, 3, 38–44] appear at 967  $\text{cm}^{-1}$ ; 1082  $\text{cm}^{-1}$  with the shoulders at 1122, 1101, 1056, and 1024  $\text{cm}^{-1}$ ; and at 1187  $\text{cm}^{-1}$  with the shoulders at 1209 and 1162  $\text{cm}^{-1}$  in the central part of the region relevant for the identification of fullerenes from ca. 400 to 1800  $\text{cm}^{-1}$ . Characteristic absorption bands unique to  $C_{76}$  are present in the first relevant part of the spectrum at 892 and 823  $\text{cm}^{-1}$  with a neighboring band at 789  $\text{cm}^{-1}$ , at 705  $\text{cm}^{-1}$  with the shoulders at 743 and 729  $\text{cm}^{-1}$ , at 646  $\text{cm}^{-1}$  with a shoulder at 661  $\text{cm}^{-1}$ , followed by a maximum at 603  $\text{cm}^{-1}$ . Several other  $C_{76}$  absorption bands appear at 533  $\text{cm}^{-1}$  with a shoulder at 555  $\text{cm}^{-1}$ , at 487  $\text{cm}^{-1}$  with a shoulder at 507  $\text{cm}^{-1}$ , at 436  $\text{cm}^{-1}$  with a shoulder at 461  $\text{cm}^{-1}$ , and at 405  $\text{cm}^{-1}$ . Pronounced and intense maxima are present in the higher frequency region at 1386  $\text{cm}^{-1}$  with the shoulders at 1399 and 1364  $\text{cm}^{-1}$ , at 1461  $\text{cm}^{-1}$  with a neighboring band at 1493  $\text{cm}^{-1}$ , and at 1633 and 1734  $\text{cm}^{-1}$  with the shoulders at 1681  $\text{cm}^{-1}$  and 1713  $\text{cm}^{-1}$ , respectively. Maximum at 1312  $\text{cm}^{-1}$  appears, followed by the bands at 1276  $\text{cm}^{-1}$ , with a shoulder at 1291  $\text{cm}^{-1}$  and at 1247  $\text{cm}^{-1}$ . Weak absorption features are also observed at 1552, 1533, and 1339  $\text{cm}^{-1}$ . Complete absorption [2] in this spectrum corresponds to the theoretical predictions for  $C_{76}\text{-D}_2$ , as well as for its dianion [46, 47].

The IR spectra of all the chromatographically isolated  $C_{76}\text{-D}_2$  samples from this research have similar properties. All the observed vibrational frequencies and the general pattern of these spectra [2, 3, 38–44] are in agreement with the semiempirical QCFF/PI and DFT theoretical calculations for  $C_{76}\text{-D}_2$ , as well as for its dianion  $C_{76}\text{-D}_2^{2-}$  [2, 3, 42–44, 46, 47].

From the presented IR absorption spectrum Figure 1, the values of absorbance  $A_\lambda$  have been determined for all the separated absorption maxima and shoulders using the OMNIC software subtracting automatically the base line. Determination of molar absorptivity of the entire series of deconvoluted IR absorption bands of the  $C_{76}\text{-D}_2$  isomer at a given wave

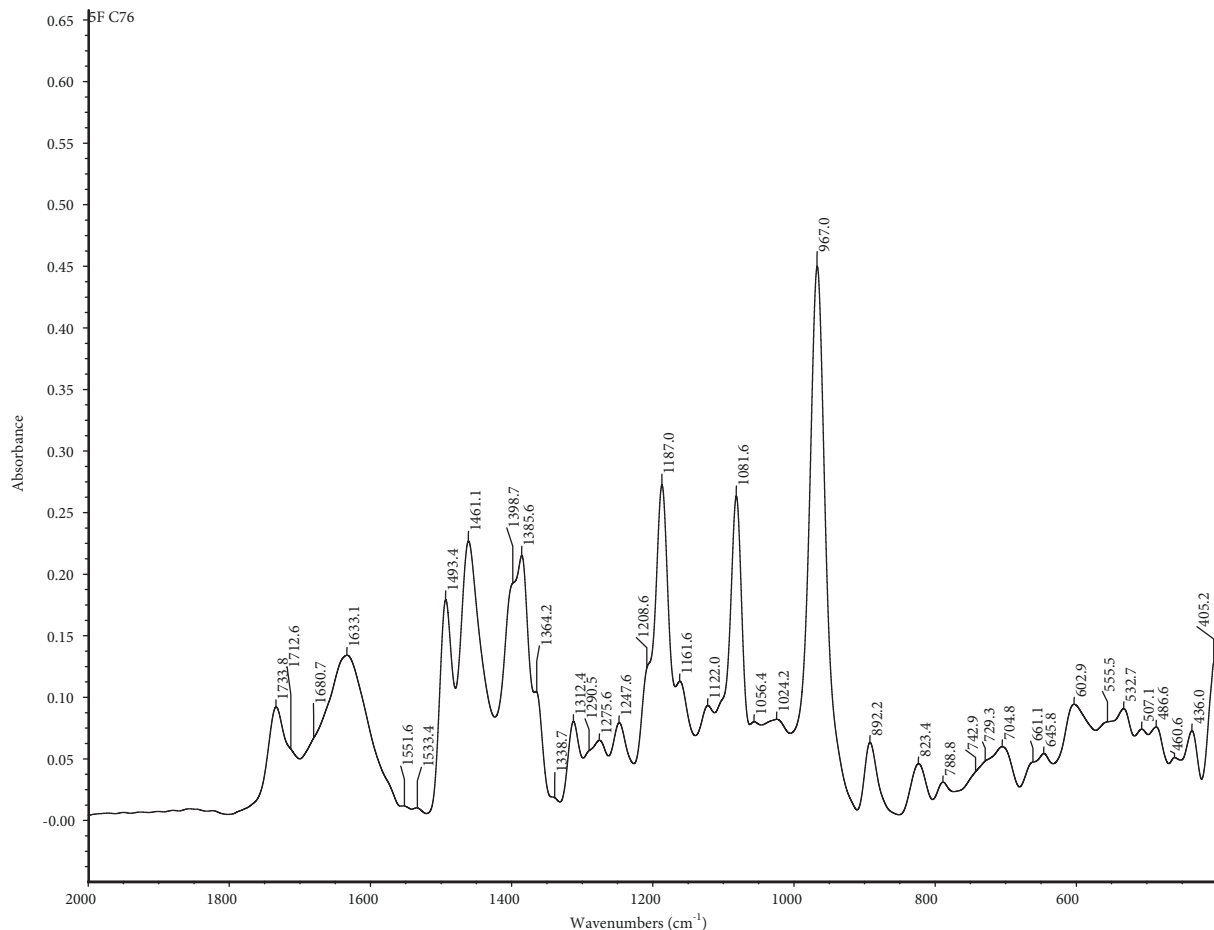


FIGURE 1: The IR(KBr) absorption spectrum of the isolated  $C_{76}-D_2$  sample.

number  $\varepsilon_\lambda$  was achieved through (1), previously applied for its main convoluted infrared absorption bands for  $C_{60}$  and  $C_{70}$ , as well as hydrogenated fullerenes [3, 25–27, 62], according to Lambert and Beer law using the absorbance  $A_\lambda$  read at a given wave number.

$$\varepsilon_\lambda = A_\lambda (bc)^{-1}. \quad (1)$$

It was found that the peak height measurements that correspond to the absorbance  $A$  are sensitive to changes in the resolution of the spectrometers used [25–27, 62] and to changes in temperature and smaller chemical shifts of characteristic absorption bands (within  $1-3 \text{ cm}^{-1}$ ) in some cases. Theoretical calculations [46, 47] also predict the possibility of appearance of very close or different out of the numerous possible IR vibration modes  $C_{76}-D_2$ . The measurement of the integrated intensity that represents the area below a corresponding absorption band measured in adequate integration range is much less sensitive to instrumental resolution [25–27, 62] and temperature as well as smaller shifts of absorption bands than the peak height measurement.

Thus in this article also, the integrated intensity of both deconvoluted and convoluted absorption bands in different integration ranges was determined from the

presented infrared spectrum in a mode of the isolated  $C_{76}-D_2$  sample, Figure 1, using the OMNIC software and subtracting automatically the baseline. The integrated molar absorptivity expressed in  $\text{cm mol}^{-1}$  or  $10^{-5} \text{ Km mol}^{-1}$  was calculated by (2), previously applied for its main convoluted absorption bands for the basic fullerenes as well as for fullerenes [3, 25–27, 62].

$$\Psi = \int \varepsilon_\lambda d\lambda. \quad (2)$$

In this equation,  $\lambda$  is the wavelength, and  $\varepsilon_\lambda$  is the molar absorptivity integrated over the whole band. In practice, by substituting (1) into (2), we get [3, 25–27, 62]

$$\Psi = (bc)^{-1} \int A_\lambda d\lambda. \quad (3)$$

The molar absorptivity and the integrated molar absorptivity in adequate integration range calculated according to (1) and (2) of all the observed [2, 3] deconvoluted absorption bands of the higher fullerene  $C_{76}-D_2$  in this spectrum are reported in Table 1.

The integrated molar absorptivity of convoluted absorption maxima with some absorption shoulders of  $C_{76}-D_2$  in determined, different, and new relevant integration ranges

TABLE 1: The molar absorptivity and the integrated molar absorptivity in adequate integration range of deconvoluted absorption bands of  $C_{76}\text{-D}_2$ .

$\nu^{\text{a,b}}$ ( $\text{cm}^{-1}$ )	$\epsilon_\lambda$ ( $\text{L cm}^{-1} \text{ mol}^{-1}$ )	Int. range ( $\text{cm}^{-1}$ )	$\Psi$ ( $\text{Km mol}^{-1}$ )
1733.8	129.711	1758–1721	1.097
1712.6	81.774	1721–1699	0.017
1680.7	91.643	1684–1678	0.004
1633.1	188.927	1678–1573	6.549
1551.6	16.919	1562–1543	0.022
1533.4	14.099	1542–1513	0.025
1493.4	252.372	1512–1481	2.242
1461.1	320.047	1478–1432	3.953
1398.7	270.701	1416–1396	0.265
1385.6	303.128	1393–1371	0.850
1364.2	146.630	1368–1349	0.230
1338.7	29.608	1349–1326	0.024
1312.4	112.792	1326–1300	0.884
1290.5	81.774	1296–1283	0.010
1275.6	91.643	1282–1263	0.096
1247.6	111.382	1260–1231	0.568
1208.6	174.828	1222–1202	0.234
1187.0	384.903	1200–1168	3.423
1161.6	159.319	1167–1141	0.254
1122.0	131.121	1139–1112	0.219
1101.0	140.990	1110–1099	0.028
1081.6	370.804	1098–1063	3.810
1056.4	112.792	1062–1048	0.027
1024.2	115.612	1039–1005	0.179
967.0	634.455	996–926	13.765
892.2	88.824	908–871	1.107
823.4	64.855	848–809	1.376
788.8	43.707	803–774	0.219
742.9	54.986	750–736	0.010
729.3	67.675	736–717	0.014
704.8	84.594	715–679	0.460
661.1	66.265	678–655	0.240
645.8	76.135	655–632	0.031
602.9	132.531	627–575	1.246
555.5	112.792	570–548	0.038
532.7	126.891	545–520	0.300
507.1	104.333	518–499	0.062
486.6	107.152	499–471	0.344
460.6	71.905	469–453	0.037
436.0	102.923	450–422	0.637
405.2	179.057	421–400	1.799

<sup>a</sup>[2]. <sup>b</sup>[3].

for its quantitative determination as well as identification is presented in Table 2.

The molar absorptivity and the integrated molar absorptivity in the mentioned adequate integration ranges of the

TABLE 2: The integrated molar absorptivity in determined integration ranges of convoluted absorption maxima with some absorption shoulders of  $C_{76}\text{-D}_2$ .

$\nu$ ( $\text{cm}^{-1}$ )	Int. range ( $\text{cm}^{-1}$ )	$\Psi$ ( $\text{Km mol}^{-1}$ )
1733.8–1712.6	1757–1699	2.163
1633.1–1680.7	1683–1573	6.861
1461.1–1493.4	1512–1432	9.907
1385.6–1398.7	1423–1371	4.457
1385.6–2 ab. shoulders <sup>a</sup>	1421–1349	13.163
1275.6–1290.5	1298–1264	0.341
1187.0–2 ab. shoulders <sup>b</sup>	1222–1143	8.481
1081.6–4 ab. shoulders <sup>c</sup>	1139–1004	7.979
704.8–742.9	774–681	2.168
645.8–661.1	678–632	0.587
532.7–555.5	571–518	0.735
486.6–507.1	518–470	0.746
436.0–460.6	468–422	0.946

<sup>a</sup>Absorption maximum at  $1386 \text{ cm}^{-1}$  with two absorption shoulders at  $1399$  and  $1364 \text{ cm}^{-1}$ . <sup>b</sup>Absorption maximum at  $1187 \text{ cm}^{-1}$  with two absorption shoulders at  $1209$  and  $1162 \text{ cm}^{-1}$ . <sup>c</sup>Absorption maximum at  $1081.6 \text{ cm}^{-1}$  with four absorption shoulders at  $1122$ ,  $1101$ ,  $1056$ , and  $1024 \text{ cm}^{-1}$ .

corresponding main and characteristic absorption bands, both deconvoluted and convoluted, in all the obtained IR spectra of the chromatographically purified  $C_{76}\text{-D}_2$  samples from this research [2, 3, 38–44] are in excellent agreement.

In this article also, the original UV/VIS spectrum of the chromatographically isolated  $C_{76}\text{-D}_2$  sample previously applied for its identification [39, 40] is presented in Figure 2 for determination of the abovementioned parameters for its quantitative assessment.

Relevant  $C_{76}$  absorption maxima [2, 38–43] of decreased relative intensity in comparison to the spectra of the previous fractions  $C_{60}$  and  $C_{70}$  [21–23] appear at  $258$  and  $328 \text{ nm}$  [39, 40]. An inflection point occurs at  $210 \text{ nm}$ , whereas the most intense dominant UV absorption is moved to the region below  $200 \text{ nm}$ , which is characteristic for  $C_{76}$ . Pronounced  $C_{76}$  absorption shoulder is present at  $275 \text{ nm}$  followed by less intense shoulders at  $358$  and  $378 \text{ nm}$ . In the visible part, weak absorption band appears at  $405 \text{ nm}$ ; the absorption is prolonged to  $900 \text{ nm}$ . Complete absorption in this spectrum [39, 40] corresponds to the theoretical predictions for  $C_{76}\text{-D}_2$  [48, 49].

The UV/VIS spectra of all the chromatographically isolated  $C_{76}\text{-D}_2$  samples from this research have similar properties. All the observed absorption bands and the general pattern of these spectra [2, 3, 38–44] are in agreement with the semiempirical QCFF/PI and DFT theoretical calculations for  $C_{76}\text{-D}_2$  [2, 42, 43, 48, 49].

From the UV/VIS spectrum [39, 40] presented in Figure 2, the values of absorbance  $A_\lambda$  of the absorption bands of  $C_{76}$  have been determined. The values of molar absorptivity  $\epsilon_\lambda$  were calculated according to (1) previously applied for the basic fullerenes and their radical cations as well as fullerenes [28, 29, 62] and reported in Table 3.

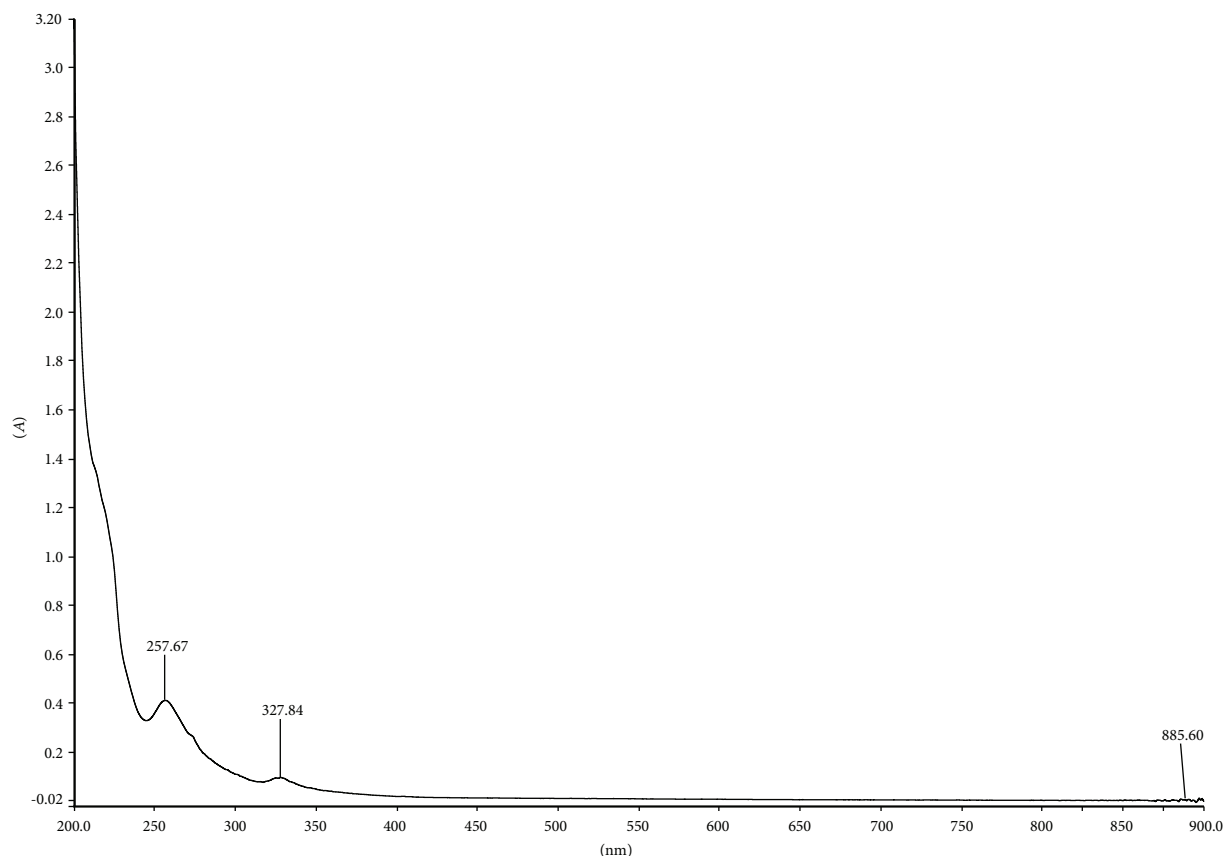


FIGURE 2: The UV/VIS spectrum of the isolated  $C_{76}$ - $D_2$  sample [39, 40].

TABLE 3: The molar absorptivity of absorption bands of  $C_{76}$ - $D_2$ .

$\lambda^{a,b}$ (nm)	$\epsilon_\lambda$ ( $L\text{ cm}^{-1}\text{ mol}^{-1}$ )
210.0	140,000
257.7	41,500
275.0	26,500
327.8	11,000
358.0	6000
378.0	4500
405.0	3100

<sup>a</sup>[39]. <sup>b</sup>[40].

The molar absorptivity of the observed main and characteristic absorption bands in all the obtained UV/VIS spectra of the chromatographically purified  $C_{76}$ - $D_2$  samples from this research [2, 38–43] is in excellent agreement.

The aforementioned change of the spectral parameters of the  $C_{76}$ - $D_2$  isomer compared to  $C_{60}$  and  $C_{70}$  can also lead to changes of refraction features that can be useful for its application in the fullerene-based optoelectronic materials and devices, such as nanophotonic lenses with advanced properties. The results of the recent investigations [63–67] show also that fullerene nanomaterials incorporated in standard, basic (commercial) materials, such as poly(methyl methacrylate) for the rigid gas permeable and poly(2-

hydroxyethyl methacrylate) for the soft contact lenses, improve their wettability.

#### 4. Conclusion

In this study, the only stable isomer of the higher fullerene  $C_{76}$  of  $D_2$  symmetry was isolated from the carbon soot by new and advanced extraction and chromatographic methods and processes [2, 3, 38–44]. The original and new IR and UV/VIS spectra [39, 40] of the isolated  $C_{76}$ - $D_2$  sample were obtained in the absorption mode over the relevant regions from 400 to  $2000\text{ cm}^{-1}$ , as well as from 200 to 900 nm, and presented for determination of novel parameters for its quantitative assessment.

All of the experimentally observed infrared and electronic absorption bands of the isolated  $C_{76}$ - $D_2$  samples from this research [2, 3, 38–44] are in excellent agreement with the theoretical calculations for this molecule [46–49], which is important for the qualitative detection [2, 3].

In the previous article [3], the molar extinction coefficients and the integrated molar extinction coefficients of the main convoluted IR absorption bands of the higher fullerene  $C_{76}$ - $D_2$  were determined and reported together with the relative intensities.

Excellent agreement was obtained between the relative intensities of the main absorption maxima calculated from  $\epsilon_\lambda$  and from the  $\Psi_\lambda$  values in adequate integration ranges [3].

In this article, the molar absorptivity and the integrated molar absorptivity of the entire series of the observed various characteristic and new deconvoluted IR absorption maxima and shoulders of the isolated  $C_{76}$ -D<sub>2</sub> isomer were determined at room temperature in the KBr matrix. In addition, the integrated molar absorptivity of several convoluted absorption bands with some shoulders in different and relevant integration ranges was determined. The molar absorptivity of its UV/VIS absorption bands was also determined.

It should be mentioned that the molar extinction coefficients and the integrated molar extinction coefficients in the mentioned adequate integration ranges of the corresponding main and characteristic absorption bands, both separated and convoluted, in all the IR and UV/VIS spectra of the chromatographically purified  $C_{76}$ -D<sub>2</sub> samples from this research [2, 3, 38–44] are in excellent agreement.

The obtained new IR and UV/VIS spectroscopic results and parameters of the higher fullerene  $C_{76}$ -D<sub>2</sub> are important for its quantitative determination.

All the presented data will significantly contribute to better understanding of the IR and UV/VIS spectroscopic properties of the  $C_{76}$ -D<sub>2</sub> isomer. This is important both for its identification and quantitative assessment, either in natural resources or in artificially synthesized materials, electronic and optical devices, optical limiters, sensors, polymers, solar cells, nanophotonic lenses, diagnostic and therapeutic agents such as for diabetes, incorporation of metal atoms, targeted drug delivery in biomedical engineering, industry, applied optical science, batteries, catalysts, synthesis of diamond, and so forth.

## Additional Points

Figure 2 is an intellectual property of Tamara Jovanovic and Djuro Koruga. The new technological process for extraction, chromatography, and characterization of the basic and the higher fullerenes from carbon soot, the intellectual property office of Serbia, Belgrade, no. 985/09 A-59/09, 2009.

## Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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