

Article

Determination of New IR and UV/VIS Spectroscopic Parameters of the C₈₄-D₂:22 Isomer for Its Quantitative Assessment, Identification and Possible Applications

Tamara Jovanović

Department of Biomedical Engineering, Faculty of Mechanical Engineering, University of Belgrade, Kraljice Marije 16, 11120 Belgrade, Serbia; tamara.jovanovic@sbb.rs

Abstract: The stable isomers of the higher fullerenes C₇₆-D₂ and C₈₄-D₂:22, as well as fullerenes C₆₀ and C₇₀ were isolated from carbon soot by the new and improved extraction and chromatographic methods and processes. Characterizations of the C₈₄-D₂:22 isomer in this study were performed by infrared and electronic absorption spectroscopy. All of the experimentally observed IR and UV/VIS bands were in excellent agreement with the semi-empirical, DFT and TB potential theoretical calculations for this molecule. The molar extinction coefficients and the integrated molar extinction coefficients of the observed larger number of completely separated infrared absorption maxima and shoulders of fullerene C₈₄-D₂:22, as well as of its main convoluted maxima, in different and new relevant entire integration ranges, including neighboring, and all surrounding absorption shoulders were determined and their relative intensities compared. In addition, the molar absorptivity of the electronic absorption bands of this carbon cluster was found. The new IR and UV/VIS spectroscopic parameters that are significant for the quantitative determination, identification and numerous possible applications of C₈₄-D₂:22 are obtained and their changes compared to C₇₆-D₂ observed. Isolated and characterized C₈₄-D₂:22, as well as other fullerenes from this research can be used in electronic, optical, chemical and biomedical devices, superconductors, semiconductors, batteries, catalysts, polymers, sensors, solar cells, nanophotonic lenses with better optical transmission, refraction and wettability, diagnostic and therapeutic pharmaceutical substances, such as those against diabetes, cancer, neurodegenerative disorders, free radical scavenging, radio nuclear, antibacterial and antiviral agents that can inhibit HIV 1, HSV, COVID-19, influenza, malaria and so forth.

Keywords: higher fullerene; C₈₄-D₂:22 isomer; chromatographic isolation; IR and UV/VIS spectroscopic parameters; applications



Citation: Jovanović, T. Determination of New IR and UV/VIS Spectroscopic Parameters of the C₈₄-D₂:22 Isomer for Its Quantitative Assessment, Identification and Possible Applications. *Crystals* **2021**, *11*, 757. <https://doi.org/10.3390/cryst11070757>

Academic Editor: Yoshikazu Yoshida

Received: 4 June 2021

Accepted: 22 June 2021

Published: 28 June 2021

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



Copyright: © 2021 by the author. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

1. Introduction

The presence of the basic fullerenes was confirmed in various space environments, objects and their shells [1–8], as well as in the interstellar medium [9–11] and some resources on Earth [12–27], by means of IR and UV/VIS spectroscopy [1–41].

It can be assumed that the higher fullerenes also exist in space, due to their extraordinary thermodynamic stability, persistence toward high energy γ radiation [19–23,42–50] and corpuscular collisions. Their formation is possible through the coalescence of smaller carbon clusters [22,23], as well as by decomposition of some derivatives, such as dehydrogenation of hydrogenated fullerenes, fullerenes [19–27,46–53].

Applications of the infrared and electronic absorption spectroscopy for the identification of C₆₀ and C₇₀ and the higher fullerenes [19–44,54–72], such as the only stable C₇₆-D₂ isomer [54–57,62–64] and C₈₄-D₂:22, the most abundant, stable C₈₄ isomer of D₂ symmetry [57–64], isolated by the new, improved extraction and chromatographic methods and processes from the carbon soot [20–23,33–43], were studied in the previous works [19–44,54–73].

The aim of this study was to determine the new IR and UV/VIS spectroscopic parameters that are important for the quantitative assessment, as well as for the identification and possible applications of the higher fullerene C₈₄-D₂:22.

The IR spectrum of the sample of C₈₄-D₂:22, isolated in one of the original advanced processes [36], recorded in the absorption mode on a Thermo Scientific FT-IR spectrometer, over the relevant region from 400 to 2000 cm⁻¹, and the UV/VIS spectrum recorded on a GBC Cintra spectrophotometer, from 200 to 900 nm, previously applied for its identification [26,27,39], were used and presented in this article for determination of the new parameters.

All of the experimentally observed IR and UV/VIS maxima [20–22] and the general pattern of the obtained spectra of the isolated C₈₄-D₂:22 samples from our research, which showed similar properties [20,21,26,27,36–41,43], are in excellent agreement with the theoretical predictions for this fullerene, with numerous possible absorption bands [20,21,26,27,36–41,43,54–64].

In the previous study [22,23] and this study, the molar absorptivity and the integrated molar absorptivity of the observed entire series of a larger number, then formerly [20,21], of various characteristic and new completely separated IR absorption maxima and shoulders of the higher fullerenes C₇₆-D₂ [22,23] and C₈₄-D₂:22, out of the numerous possible vibrational modes [54–61], were determined.

In addition, the molar extinction coefficients and the integrated molar extinction coefficients of several main and characteristic absorption maxima of these fullerenes, in the appropriate, different integration ranges were reported and their relative intensities compared [20–23].

In this article, the molar absorptivity and the integrated molar absorptivity of the main convoluted absorption maxima of C₈₄-D₂:22, in new, proportionally larger integration ranges, compared to previous measurements for this molecule [20,21], including neighboring, and all surrounding absorption shoulders were determined. The relative intensities of the main, completely convoluted infrared absorption maxima, computed from ϵ_λ and from ψ_λ , were compared.

The molar extinction coefficients of the UV/VIS absorption bands of carbon clusters C₇₆-D₂ [22,23] and C₈₄-D₂:22 were also found. Such infrared and electronic absorption properties and parameters that are important for the quantitative determination, which were previously investigated and found for C₇₆-D₂, as well as for C₆₀, C₇₀ and fullerenes showed different properties [15–18,20–23,44,45].

It is important to mention that excellent agreement is found between the relative intensities of the molar absorptivity and integrated molar absorptivity of the main, completely convoluted infrared absorption maxima of C₈₄-D₂:22, with all surrounding absorption shoulders, in the applied corresponding new entire, proportionally larger integration ranges in this article, in comparison to previous measurements [20,21].

Excellent agreement was also found between the relative intensities of several main and characteristic IR absorption bands of this fullerene, computed from ϵ_λ and from ψ_λ values, in the previous work [20,21], in the appropriate, proportionally smaller integration ranges.

The molar extinction coefficients and the integrated molar extinction coefficients in the applied integration ranges in the previous [20,21] and this study of the corresponding IR and UV/VIS bands in all the obtained spectra of the chromatographically isolated C₈₄-D₂:22 samples from this research [20,21,26,27,36–41,43] are in excellent agreement.

The obtained novel IR and UV/VIS spectroscopic parameters for the higher fullerene C₈₄-D₂:22 are significant for its quantitative assessment, as well as for the identification and numerous possible applications.

Further changes of its spectral properties and parameters, in comparison to C₇₆-D₂ [20–23], can be used for its incorporation in nanophotonic materials and devices, such as special lenses [22,23] with improved optical absorption in the UV region and transmission in the visible part, refraction features and wettability.

Isolated and characterized $C_{84}\text{-D}_2:22$, as well as fullerenes C_{60} , C_{70} and $C_{76}\text{-D}_2$ of high purity, in increased yields [43], by the new advanced processes from this research [20–27,33–43] have important physical, chemical, biological, antioxidant, anti-inflammatory, biocompatible and nontoxic properties. These carbon clusters are significant for the applications in electronic, optical, and biomedical devices [20,21], sensors, as well as for the preparation of medicinal formulations for targeted drug delivery, including those against diabetes, cancer, neurodegenerative diseases, free radical scavenging, radioactive, antibacterial and antiviral agents, such as for HIV 1, HSV and COVID-19.

2. Experimental Methods

Measurement of the Molar Absorptivity, and Integrated Molar Absorptivity of Deconvoluted and Convolved Absorption Bands of $C_{84}\text{-D}_2:22$. The IR spectrum of the $C_{84}\text{-D}_2:22$ sample, isolated in one of the original, advanced extraction and chromatographic processes [36], was measured on a Thermo Scientific FT-IR spectrometer Nicolet IR-6700, by the KBr pellet technique, in the region from 400 to 2000 cm^{-1} , at a resolution of 1 cm^{-1} and room temperature, in the absorption mode, in order to find the new parameters for its quantitative assessment, as well as in the transparency mode previously [43] for its qualitative detection.

Sample of $C_{84}\text{-D}_2:22$ (0.312 mg) was mixed with 76.3 mg of KBr, the resulting powder was compressed into a pellet with the hydraulic Perkin Elmer press, at 4 t/ cm^2 and placed in the FT-IR spectrometer.

In this article, the molar absorptivity and the integrated molar absorptivity of the observed series of a larger number, compared to the previous study [20,21], of completely separated infrared absorption maxima and shoulders from the presented spectrum of the isolated sample of $C_{84}\text{-D}_2:22$ were measured on a Thermo Scientific FT-IR spectrometer with the OMNIC software and automatic subtraction of the baseline.

In addition, the molar absorptivity of the main convoluted absorption maxima of this molecule, in different and new relevant entire, proportionally larger integration ranges, compared to previous measurements [20,21], including neighboring, and all surrounding absorption shoulders was measured on the same spectrometer.

In the previous study, the molar extinction coefficients and the integrated molar extinction coefficients of the main and characteristic infrared maxima, inadequate, proportionally smaller integration ranges, compared to this study, were determined from the presented spectrum of the sample of $C_{84}\text{-D}_2:22$ [20,21], isolated in another original, advanced process [38], recorded in a-mode on a Thermo Scientific FT-IR spectrometer [20,21].

The mass of the obtained KBr pellet in this work, with the applied sample of $C_{84}\text{-D}_2:22$, was 76.6 mg, and the percentage of carbon determined by the elemental analysis was 0.407%. Its measured thickness (b) was 0.72 mm, ~ 0.07 cm, diameter (R) was 0.7 cm and the half diameter (r) was 0.35 cm, similarly to the previously obtained KBr pellet with the $C_{76}\text{-D}_2$ sample [22,23].

The volume of this pellet (V), determined from the abovementioned parameters by the equation $V = r^2\pi b$ was 0.0278 cm^3 . Concentration (c) of fullerene $C_{84}\text{-D}_2:22$ in this pellet computed from the above-mentioned mass of $C_{84}\text{-D}_2:22$ in the pellet, its molar mass of 1008.84 g/mol, and the volume of the pellet was 0.01 mol/L. The $(bc)^{-1}$ value determined for the applied $C_{84}\text{-D}_2:22$ sample in KBr pellet from the abovementioned experimental parameters was 1428.6 $\text{L cm}^{-1} \text{mol}^{-1}$, ca 1429 $\text{L cm}^{-1} \text{mol}^{-1}$. The $(bc)^{-1}$ value for the applied $C_{76}\text{-D}_2$ sample in the previous IR study [22,23] was obtained by a similar procedure. The above-mentioned infrared spectroscopic parameters that were investigated and presented for the isolated $C_{76}\text{-D}_2:22$ previously [20–23] showed distinct properties.

Measurement of the Molar Absorptivity of Absorption Bands of $C_{84}\text{-D}_2:22$. The electronic absorption spectrum of the $C_{84}\text{-D}_2:22$ sample was measured on the GBC Cintra 40 spectrophotometer, in the range of 200–900 nm, at a resolution of 1 nm, at ambient condi-

tions, for its qualitative detection previously [26,27,39], and presented for the determination of the new parameters for its quantitative assessment in this study.

Solutions of fullerene C₈₄-D₂:22 in hexane, conc. 10⁻⁵ mol/dm³ were used. The thickness of the cuvette was 1 cm. The (bc)⁻¹ value determined for the C₈₄-D₂:22 sample from the above-mentioned parameters was 100.000 L cm⁻¹ mol⁻¹. The (bc)⁻¹ value for the applied C₇₆-D₂ sample in the previous UV/VIS study [22,23] was obtained by a similar procedure. The molar extinction coefficients of absorption bands of C₇₆-D₂ [22,23] showed distinct properties.

3. Results and Discussion

The new IR and UV/VIS spectroscopic parameters that are important for the quantitative assessment, as well as for the identification and possible applications of the higher fullerene C₈₄-D₂:22 were determined in this study.

In the previous [22,23] and this article, the molar absorptivity and the integrated molar absorptivity of the observed entire new series of a larger number, then formerly [20,21], of various characteristic, completely deconvoluted IR absorption bands of the isolated C₇₆-D₂ [22,23] and C₈₄-D₂:22 isomer were determined.

Besides that, the molar extinction coefficients and the integrated molar extinction coefficients of several main and characteristic absorption maxima of these carbon clusters, in the appropriate, different integration ranges were reported [20–23].

In this article, the molar absorptivity of the main convoluted absorption maxima of C₈₄-D₂:22, including neighboring, and all surrounding absorption shoulders was determined, in new entire, proportionally larger integration ranges, compared to previous measurement [20,21]. The molar extinction coefficients of the UV/VIS absorption bands of C₇₆-D₂ [22,23] and C₈₄-D₂:22 were also found.

The new, characteristic infrared spectrum of the sample of C₈₄-D₂:22, isolated in one of the original, advanced processes [36], was recorded in the absorption mode, on a Thermo Scientific FT-IR spectrometer, Figure 1, for determination of the abovementioned novel parameters for its quantitative assessment, as well as in transparency mode previously [43] for its qualitative detection.

The main absorption bands [43] in this spectrum appear in the region relevant for the identification of C₈₄-D₂:22 [41], from ca. 1050 to 1800 cm⁻¹. The dominant absorption maximum is observed at 1384.6 cm⁻¹ with a shoulder band at 1399.8 cm⁻¹. Intense and pronounced maxima are also present at 1731.6 cm⁻¹ with a neighbor shoulder at 1699.8 cm⁻¹, at 1615.8 cm⁻¹ with a neighbor at 1601.6 cm⁻¹, at 1263.8 cm⁻¹ with a neighboring at 1284.1 cm⁻¹, as well as in the middle part of the spectrum at 1186 and 1122 cm⁻¹. In the next region relevant for C₈₄-D₂:22, from ca. 400 to 850 cm⁻¹, pronounced maxima corresponding to this molecule are present at 842.1 cm⁻¹ with the neighboring bands at 823.1, 800.9 and 777.5 cm⁻¹, at 743.1 cm⁻¹ with the neighboring bands at 711.3 and 700.0 cm⁻¹, and at 476.0 cm⁻¹ with the neighbors at 463.6, 451.2 and 439.8 cm⁻¹. Several features also appear at 632.4, 419.2 and 401.0 cm⁻¹. The infrared absorption bands [41] in the spectrum, shown in Figure 1, correspond to C-C vibration modes that are in agreement with the theoretical predictions for C₈₄-D₂:22 [59–61].

From the IR absorption spectra presented in the recent article [22,23], and in this article in Figure 1, the values of absorbance A_λ were determined for all the separated absorption maxima and shoulders of C₇₆-D₂ [22,23] and C₈₄-D₂:22. Determination of molar extinction coefficients of separated infrared bands of C₇₆-D₂ [22,23] and of C₈₄-D₂:22 was achieved according to Lambert and Beer law, using the absorbance A_λ read at a given wave number, through the Equation (1) [74], which was also applied in the previously mentioned investigations [15–18,20–23].

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

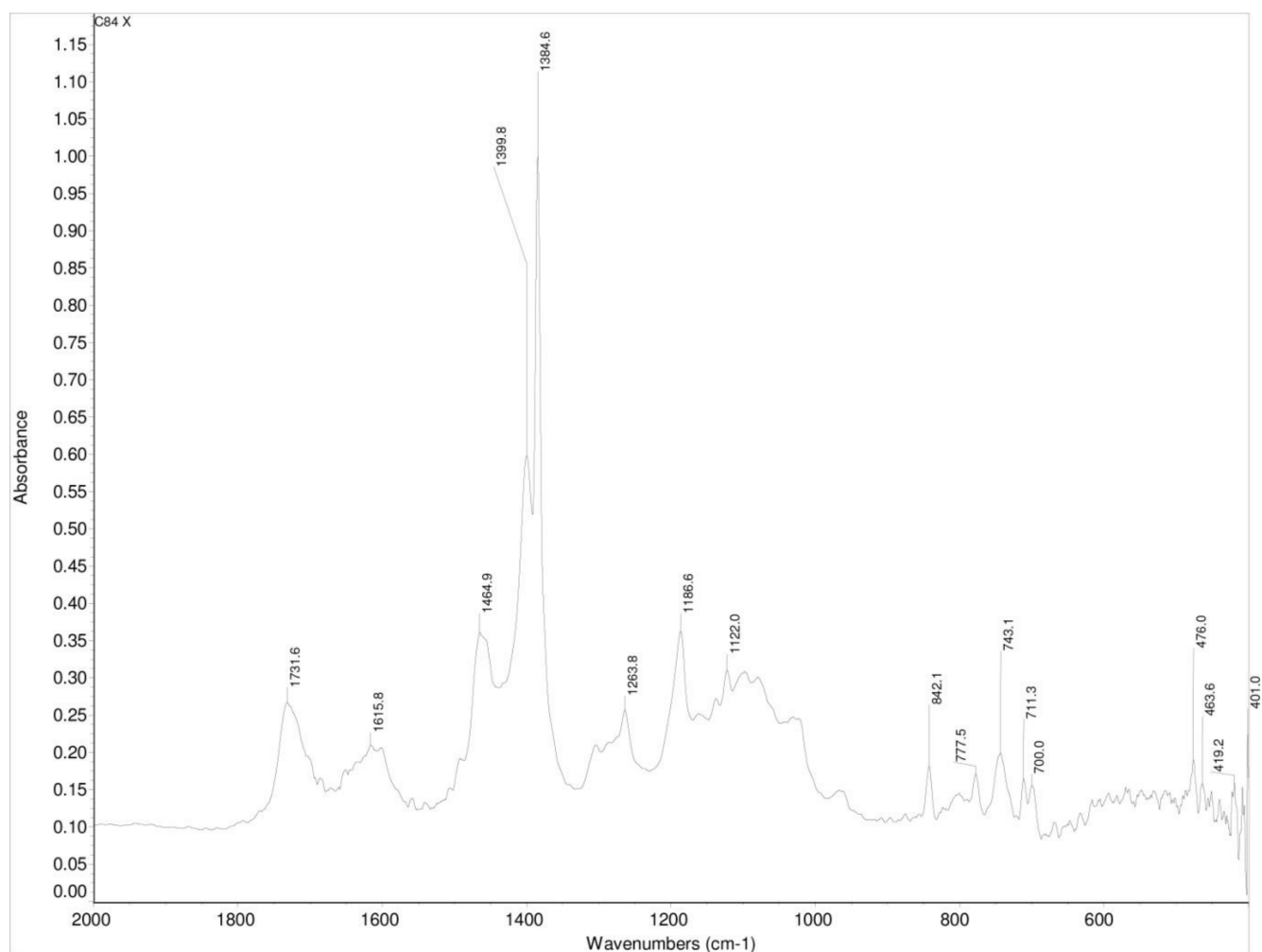


Figure 1. The infrared spectrum of the C₈₄-D₂:22 sample, isolated in the original, advanced processes [36], recorded on a Thermo Scientific FT-IR spectrometer, in the absorption mode.

In the previous [22,23] and this article also, the integrated molar absorptivity of deconvoluted absorption maxima and shoulders, as well as of convoluted absorption maxima, with neighboring, and all surrounding shoulders, in the entire integration range, was determined from the presented infrared absorption spectra of the isolated C₇₆-D₂ [22,23] and of the sample of C₈₄-D₂:22, Figure 1. The integrated intensity expressed in cm mol⁻¹ or 10⁻⁵ Km mol⁻¹ was computed by Equation (2) [72], applied in the previous studies [15–18,20–23].

$$\psi = (bc)^{-1} \int A_{\lambda} d\lambda \quad (2)$$

The molar extinction coefficients and the integrated molar extinction coefficients in adequate integration range, calculated by the Equations (1) and (2), of deconvoluted infrared absorption bands of C₇₆-D₂ were presented previously [22,23] and of the observed separated absorption bands of C₈₄-D₂:22 in the presented spectrum, Figure 1, in this article in Table 1. The integrated molar absorptivity of several absorption maxima with neighboring absorption shoulders of C₈₄-D₂:22 are also reported in this table.

Table 1. The molar extinction coefficients and the integrated molar extinction coefficients in the appropriate integration range of separated IR absorption maxima and shoulders of C₈₄-D₂:22, as well as of several convoluted maxima with neighboring absorption shoulders of this molecule.

ν^a (cm ⁻¹)	ϵ_λ (L cm ⁻¹ mol ⁻¹)	Int. Range (cm ⁻¹)	ψ (Km mol ⁻¹)
1731.6	380.114	1710–1757	3.182
1699.8	271.510	1694–1710	0.113
1686.1	238.643	1679–1693	0.129
1601.6–1615.8		1585–1626	1.205
1615.8	298.661	1605–1626	0.177
1601.6	294.374	1586–1605	0.260
1558.5	195.773	1552–1562	0.126
1541.0	187.199	1535–1547	0.054
1506.0	211.492	1501–1513	0.083
1491.5	212.921	1486–1500	0.234
1454.2–1464.9		1446–1479	3.135
1464.9	514.440	1460–1480	0.683
1454.2	498.721	1446–1459	0.133
1399.8	854.542	1392–1419	2.185
1384.6	1429.000	1371–1392	5.990
1304.2	291.516	1294–1308	0.057
1263.8–1284.1		1250–1294	1.420
1284.1	297.232	1278–1294	0.047
1263.8	365.824	1250–1272	0.710
1186.6	517.298	1170–1218	3.700
1160.8	358.679	1146–1170	0.236
1137.7	388.688	1131–1146	0.157
1122.0	441.561	1115–1131	0.410
1098.2	438.703	1091–1114	0.292
1079.9	428.700	1069–1084	0.170
1059.5	375.112	1050–1069	0.110
842.1	258.649	833–851	0.800
823.1	180.054	817–832	0.084
800.9	204.347	792–813	0.206
777.5–2 ab.shoulders		768–832	2.131
777.5	244.359	768–784	0.476
743.1	282.942	724–763	2.256
700.0–711.3		687–716	1.776
711.3	234.356	705–716	0.353
700.0	221.495	687–704	0.489
632.4	168.622	626–637	0.184
476.0	270.081	468–481	0.433
463.6	242.930	458–470	0.349
419.2	200.060	415–426	0.473

^a [43].

The molar absorptivity and the integrated molar absorptivity were calculated by the Equations (1) and (2) for the main convoluted absorption maxima of C₇₆-D₂ [20–23] and of C₈₄-D₂:22, in adequate integration ranges applied previously [20,21], as well as in the new integration ranges in this study, with all surrounding absorption shoulders, from the presented spectrum in Figure 1, and reported in Table 2. The relative intensities of the main, completely convoluted C₈₄-D₂:22 maxima, computed from ϵ_λ and from ψ_λ values are compared in this table.

Table 2. The molar extinction coefficients and the integrated molar extinction coefficients of the main convoluted IR maxima of C₈₄-D₂:22, in the appropriate entire integration ranges, with all surrounding absorption shoulders, and their relative intensities.

ν^a (cm ⁻¹)	ϵ_λ (L cm ⁻¹ mol ⁻¹)	Rel. int. [ϵ_λ]	Int. Range (cm ⁻¹)	ψ (Km mol ⁻¹)	Rel. int. [ϵ_λ]
1731.6	380.114	26.6	1694–1757	4.261	26.3
1615.8	298.661	20.9	1585–1650	3.371	20.8
1464.9	514.440	36.0	1433–1533	5.682	35.1
1384.6	1429.000	100.0	1370–1419	16.193	100.0
1263.8	365.824	25.6	1250–1328	4.084	25.2
1186.6	517.298	36.2	1146–1220	5.859	36.2
1122.0	441.561	30.9	1050–1146	4.971	30.7
842.1	258.649	18.1	768–851	2.930	18.1
743.1	282.942	19.8	690–763	3.196	19.7
476.0	250.075	17.5	426–504	2.841	17.5

^a [43].

It can be seen from the table that excellent agreement is found between the relative intensities of the main, completely convoluted infrared absorption maxima of C₈₄-D₂:22, computed from ϵ_λ and from ψ_λ , in the applied new entire, larger integration ranges, then in previous studies [20,21], taking as 100 the most intense band at 1384.6 cm⁻¹ with a shoulder at 1399.8 cm⁻¹, Table 2.

Excellent agreement was also found in the previous article [20,21] between the relative intensities of several main and characteristic IR absorption maxima of this molecule, calculated from ϵ_λ and from ψ_λ , in the appropriate, proportionally smaller integration ranges [20,21], compared to this study, taking as 100 the most intense band at 1384.5 cm⁻¹ in the spectrum of the C₈₄-D₂:22 sample [20,21].

The molar extinction coefficients and the integrated molar extinction coefficients, in the applied integration ranges in the previous [20,21] and this study, of the corresponding IR bands, in all the obtained spectra of the chromatographically purified C₈₄-D₂:22 samples from this research [20,21,26,27,36–41,43] are in excellent agreement.

In the former study, the original, characteristic electronic absorption spectrum of the chromatographically isolated C₇₆-D₂ sample was used [22,23], and in this study, the UV/VIS spectrum of the isolated C₈₄-D₂:22 sample, previously applied for its identification [26,27,39], is presented in Figure 2, for determination of the above-mentioned novel parameters for its quantitative assessment.

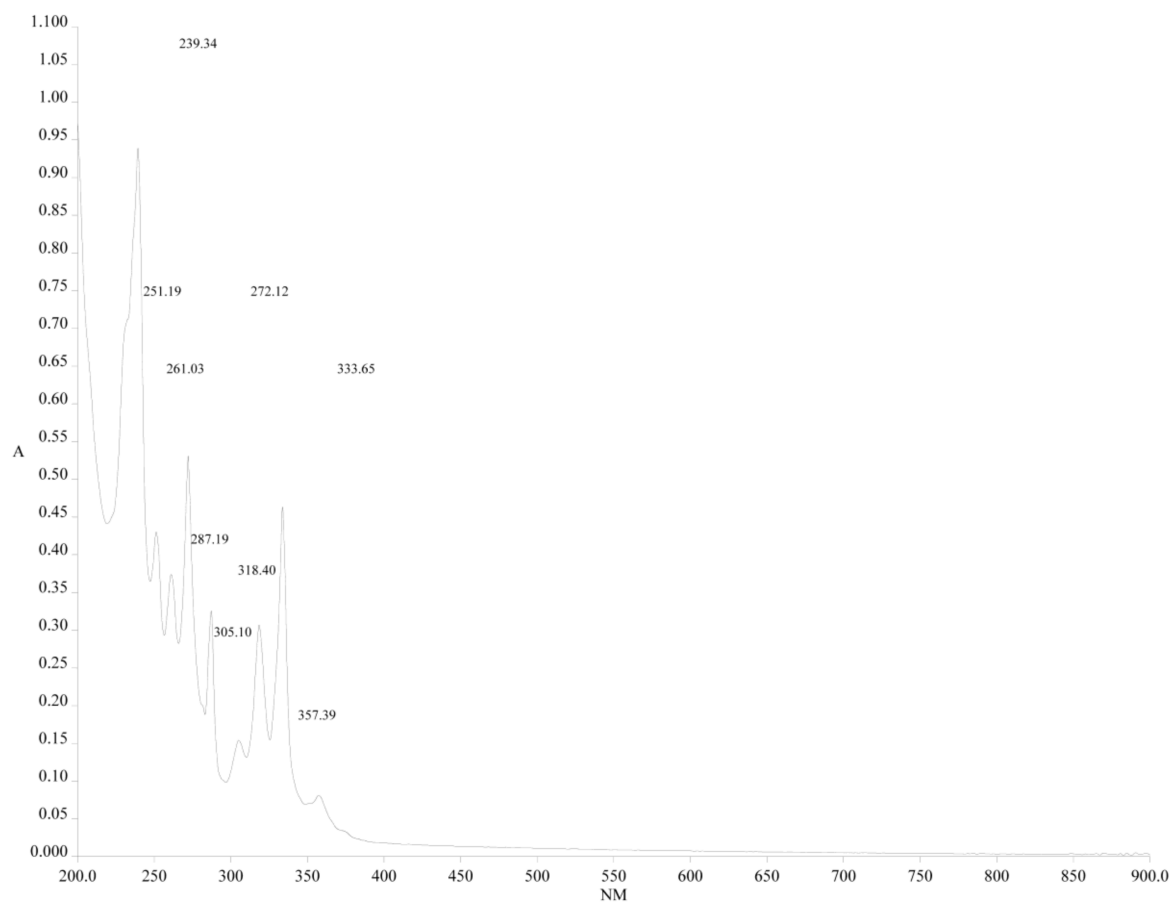


Figure 2. The electronic absorption spectrum of the $C_{84}\text{-D}_2:22$ sample [26,27,39], for determination of molar extinction coefficients.

A series of the electronic absorption maxima attributed to $C_{84}\text{-D}_2:22$ appears in this spectrum [26,27,39] in the UV region, from 200 to 400 nm, at 200.00, 230.11, 239.34, 251.19, 261.03 and 272.12 nm, followed by the bands at 287.19, 305.10, 318.40, 333.65 and 357.39 nm, as well as weak decreasing absorption in the visible part extended to 900 nm. The electronic absorption bands in the spectrum [26,27,39], shown in Figure 2, correspond to the electronic transitions from HOMO to LUMO that are in agreement with the theoretical calculations for this molecule [60–62].

Absorbance A_λ of the electronic absorption bands was determined from the UV/VIS spectrum of $C_{76}\text{-D}_2$ previously [22], and from the UV/VIS spectrum of $C_{84}\text{-D}_2:22$ [26,27,39], presented in Figure 2, in the current study. Molar absorptivity ϵ_λ was calculated according to Equation (1) for $C_{76}\text{-D}_2$ [22] and for $C_{84}\text{-D}_2:22$, and reported for this molecule in Table 3.

The molar extinction coefficients of the corresponding UV/VIS bands in all the obtained electronic absorption spectra of the chromatographically purified $C_{84}\text{-D}_2:22$ samples from this research [26,27,36–41,43] are in excellent agreement.

The appearance of a larger number of characteristic, intense and pronounced absorption bands in the mentioned spectral regions, fine structure, as well as a general increase in molar absorptivity and integrated molar absorptivity in the IR and UV/VIS spectra of $C_{84}\text{-D}_2:22$, in relation to $C_{76}\text{-D}_2$ and basic fullerenes [15–18,20–23,44,45] indicate a decrease in the symmetry of $C_{84}\text{-D}_2:22$ compared to these fullerenes.

Table 3. The molar extinction coefficients of the UV/VIS bands of C₈₄-D₂:22.

λ ^{a,b} (nm)	ϵ_{λ} (L cm ⁻¹ mol ⁻¹)
200.00	97,000
230.11	71,500
239.34	94,000
251.19	42,500
261.03	37,000
272.12	53,000
287.19	32,500
305.10	15,000
318.40	31,000
333.65	46,000
357.39	8000

^a [26,27]; ^b [39].

The aforementioned changes of the spectroscopic parameters of C₈₄-D₂:22, in comparison to C₇₆-D₂ [20–23] can also lead to further changes and improvement of the refraction and wettability features. This can be used for its applications in nanophotonic materials and devices, such as special lenses with improved optical absorption of UV rays, transmission in the visible part, and other physical properties. Recent investigations [22–25,75–77] indicate that incorporation of fullerene-based materials in standard polymers for the rigid and soft contact lenses generally enhances their optoelectronic and mechanical properties.

4. Conclusions

The only stable C₇₆-D₂ isomer and the most abundant stable C₈₄-D₂ isomer, as well as the basic fullerenes C₆₀ and C₇₀ were isolated from the carbon soot by new and advanced extraction and chromatographic methods and processes [20–23,36–43].

The infrared spectrum of the sample of C₈₄-D₂:22, isolated in one of the original advanced processes [36], recorded in the absorption mode on a Thermo Scientific FT-IR spectrometer, over the relevant region from 400 to 2000 cm⁻¹, and the electronic absorption spectrum recorded on a GBC Cintra spectrophotometer, from 200 to 900 nm, previously applied for its identification [26,27,39], were presented in this study for determination of new parameters for its quantitative assessment, as well as identification and possible applications.

All of the experimentally observed IR and UV/VIS absorption bands of the isolated C₈₄-D₂:22 samples from this research [20,21,26,27,36–41,43] are in excellent agreement with the semi-empirical QCFF/PI, DFT and TB potential theoretical calculations for this molecule [20,21,26,27,36–41,43,59–64].

In the previous [22,23] and this article, the molar absorptivity and the integrated molar absorptivity of the observed entire series of a larger number, then formerly [20,21], of various characteristic and new, completely deconvoluted IR absorption maxima and shoulders of the isolated C₇₆-D₂ [22,23] and C₈₄-D₂:22 isomer were determined.

In addition, the molar extinction coefficients and the integrated molar extinction coefficients of several main and characteristic absorption maxima of these molecules in the appropriate, different integration ranges were determined and reported together with the relative intensities [20–23].

In this article, the molar absorptivity and the integrated molar absorptivity of the main convoluted absorption maxima of C₈₄-D₂:22, in new, proportionally larger integration ranges, compared to the previous studies [20,21], including neighboring, and all surrounding absorption shoulders were determined and their relative intensities compared.

The molar extinction coefficients of the UV/VIS absorption bands of carbon clusters $C_{76}-D_2$ [22,23] and $C_{84}-D_2:22$ were also obtained. The above-mentioned infrared and electronic absorption parameters that were investigated and presented for $C_{76}-D_2:22$ previously [20–23] showed distinct properties.

It is important to emphasize that in this article the excellent agreement is obtained between the relative intensities of the main, completely convoluted IR maxima of $C_{84}-D_2:22$, with all surrounding absorption shoulders, in the applied new entire, proportionally larger integration ranges, then previously [20,21], computed from the ϵ_λ and from the ψ_λ values, taking as 100 the most intense vibration mode of this fullerene at 1384.6 cm^{-1} , with a neighboring shoulder at 1399.8 cm^{-1} .

Excellent agreement was also found in the previous article [20,21] between the relative intensities of several main and characteristic IR absorption maxima of this molecule, calculated from ϵ_λ and from ψ_λ , in adequate, proportionally smaller integration ranges, taking as 100 the most intense band at 1384.5 cm^{-1} in the presented spectrum of the isolated sample of $C_{84}-D_2:22$.

It should be mentioned that the molar extinction coefficients and the integrated molar extinction coefficients in the applied integration ranges in the previous [20,21] and this study of the corresponding main and characteristic absorption bands in all the IR and UV/VIS spectra of the chromatographically purified $C_{84}-D_2:22$ samples from this research [20,21,26,27,36–41,43] are in excellent agreement.

The new spectroscopic results and parameters obtained for this carbon cluster are significant for its quantitative assessment, as well as for the identification and numerous possible applications. The observed further changes of its spectral properties and parameters, compared to $C_{76}-D_2$ [20–23], can be useful for the applications in optoelectronic materials and devices with advanced properties, such as nanophotonic lenses with improved optical absorption in the UV region and transmission in the visible part, as well as with enhanced refraction and wettability features.

Isolated and characterized $C_{84}-D_2:22$ and other fullerenes of high purity, in increased yields [38], by the new improved methods and processes from this research [20–27,33–43] can be used in electronic, optical, chemical and biomedical devices, superconductors, semiconductors, catalysts, batteries, synthesis of diamond, biosensors, optical limiters, diagnostic and therapeutic medicinal formulations, such as those against diabetes, cancer, neurodegenerative disorders, free radical scavenging, incorporation of metal atoms, radio nuclear therapy, antibacterial and antiviral agents that can inhibit for example HIV 1, HSV, COVID-19, influenza and malaria, due to their important antioxidant, anti-inflammatory, biocompatible and nontoxic properties.

Additional Points: Figure 2 is an intellectual property of Tamara Jovanovic and Djuro Koruga: The new technological process for obtaining the higher fullerenes of high purity from carbon soot, The Intellectual Property Office of the Republic of Serbia, Belgrade, no. 2693/09 A-165/09, 2009.

Funding: This research and the APC was funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia and the University of Belgrade, The integrated project of the Ministry of Education, Science and Technological Development of the Republic of Serbia and the Faculty of Mechanical Engineering, University of Belgrade, subproject III 45009.

Institutional Review Board Statement: This study did not involve humans or animals.

Informed Consent Statement: This article does not describe a study involving humans.

Data Availability Statement: There are no publicly archived datasets.

Acknowledgments: The author is grateful to the Ministry of Education, Science and Technological Development of the Republic of Serbia and the University of Belgrade for financial support of this research (The integrated project of the Ministry of Education, Science and Technological Development of the Republic of Serbia and the Faculty of Mechanical Engineering, University of Belgrade, subproject III 45009).

Conflicts of Interest: The author declares that there are no conflict of interest regarding the publication of this paper.

References

1. Cami, J.; Bernard-Salas, J.; Peeters, E.; Malek, S.E. Detection of C₆₀ and C₇₀ in a Young Planetary Nebula. *Science* **2010**, *329*, 1180–1182. [[CrossRef](#)]
2. García-Hernández, D.A.; Iglesiasgroth, S.; Acosta-Pulido, J.A.; Manchado, A.; García-Lario, P.; Stanghellini, L.; Villaver, E.; Shaw, R.; Cataldo, F. The formation of fullerenes: Clues from new C₆₀, C₇₀, and (possible) planar C₂₄ detections in Magellanic cloud planetary nebulae. *Astrophys. J.* **2011**, *737*, L30. [[CrossRef](#)]
3. García-Hernández, D.A.; Villaver, E.; García-Lario, P.; Acosta-Pulido, J.A.; Manchado, A.; Stanghellini, L.; Shaw, R.; Cataldo, F. Infrared study of fullerene planetary nebulae. *Astrophys. J.* **2012**, *760*, 107. [[CrossRef](#)]
4. Zhang, Y.; Kwok, S. Detection of C₆₀ in the protoplanetary nebula IRAS 01005 + 7910. *Astrophys. J.* **2011**, *730*, 126. [[CrossRef](#)]
5. Clayton, G.; Kelly, D.M.; Lacy, J.H.; Little-Marenin, I.R.; Feldman, P.A.; Bernath, P.F. A Mid-Infrared Search for C₆₀ in R Coronae Borealis Stars and IRC + 10216. *Astron. J.* **1995**, *109*, 2096. [[CrossRef](#)]
6. García-Hernández, D.A.; Rao, N.K.; Lambert, D.L. Are C₆₀ molecules detectable in circumstellar shells of r corone borealis stars? *Astrophys. J.* **2011**, *729*, 126. [[CrossRef](#)]
7. Roberts, K.R.G.; Smith, K.T.; Sarre, P.J.; Migaszewski, C.; Goździewski, K.; Hinse, T.C. Detection of C₆₀ in embedded young stellar objects, a Herbig Ae/Be star and an unusual post-asymptotic giant branch star. *Mon. Not. R. Astron. Soc.* **2012**, *421*, 3277–3285. [[CrossRef](#)]
8. Sellgren, K.; Werner, W.M.; Ingalls, G.J.; Smith, T.J.D.; Carleton, T.M.; Joblin, C. Confirmation of C₆₀ in the reflection nebula NGC 7023. *EAS Publ. Ser.* **2011**, *46*, 209–214. [[CrossRef](#)]
9. Herbig, G.H. The Search for Interstellar C₆₀. *Astrophys. J.* **2000**, *542*, 334–343. [[CrossRef](#)]
10. Iglesias-Groth, S. Fullerenes and the 4430 Å Diffuse Interstellar Band. *Astrophys. J.* **2007**, *661*, L167–L170. [[CrossRef](#)]
11. Foing, B.H.; Ehrenfreund, P. Detection of two interstellar absorption bands coincident with spectral features of C₆₀⁺. *Nat. Cell Biol.* **1994**, *369*, 296–298. [[CrossRef](#)]
12. Hameroff, S.; Withers, J.; Loufty, R.; Sundareshan, M.; Koruga, D. *Fullerene C₆₀: History, Physics, Nanobiology, Nanotechnology*; Elsevier Science Publishers: Amsterdam, The Netherlands, 1993.
13. Hirsch, A.; Brettreich, M. *Fullerenes: Chemistry and Reactions*; Wiley-VCH: Stuttgart, NY, USA, 2005.
14. Cataldo, F.; Iglesias-Groth, S.; Manchado, A. Low and High Temperature Infrared Spectroscopy of C₆₀ and C₇₀ Fullerenes. *Full Nanotub. Carbon Nanostruct.* **2010**, *18*, 224–235. [[CrossRef](#)]
15. Iglesias-Groth, S.; Cataldo, F.; Manchado, A. Infrared spectroscopy and integrated molar absorptivity of C₆₀ and C₇₀ fullerenes at extreme temperatures. *Mon. Not. R. Astron. Soc.* **2011**, *413*, 213–222. [[CrossRef](#)]
16. Cataldo, F.; Iglesias-Groth, S.; Manchado, A. On the Molar Extinction Coefficient and Integrated Molar Absorptivity of the Infrared Absorption Spectra of C₆₀ and C₇₀ Fullerenes. *Full Nanotub. Carbon Nanostruct.* **2012**, *20*, 191–199. [[CrossRef](#)]
17. Cataldo, F.; Iglesias-Groth, S.; Manchado, A. Molar extinction coefficient of fullerenes and related hydrogenated derivatives “fulleranes”. *Proc. Int. Astron. Union* **2011**, *7*, 324–325. [[CrossRef](#)]
18. Cataldo, F.; Iglesias-Groth, S.; García-Hernández, D.A.; Manchado, A. Determination of the Integrated Molar Absorptivity and Molar Extinction Coefficient of Hydrogenated Fullerenes. *Full Nanotub. Carbon Nanostruct.* **2013**, *21*, 417–428. [[CrossRef](#)]
19. Cataldo, F.; Hafez, Y.; Iglesias-Groth, S. FT-IR spectra of fullerenes C₇₆, C₇₈ and C₈₄ at temperatures between –180°C and +250°C. *Fuller. Nanotub. Carbon Nanostruct.* **2014**, *22*, 901–913. [[CrossRef](#)]
20. Jovanovic, T.; Koruga, D.; Jovančević, B.; Koruga, D. The IR Spectra, Molar Absorptivity, and Integrated Molar Absorptivity of the C₇₆-D₂ and C₈₄-D₂:22 Isomers. *J. Nanomater.* **2017**, *2017*, 4360746. [[CrossRef](#)]
21. Jovanovic, T.; Koruga, D.; Jovancevic, B. IR Spectroscopic Characterization of the C₇₆-D₂ and C₈₄-D₂:22 Isomers for their Qualitative and Quantitative Determination. In *Recent Developments in Engineering Research Vol. 10*; Elangovan, P., Ed.; Sciencedomain International, Book Publisher International: London, UK, 2020; pp. 138–153. ISBN 978-81-949988-1-5. 978-81-949988-1-5 or 978-93-90516-95-7.
22. Jovanovic, T.; Koruga, D.; Mitrovic, A.; Stamenkovic, D.; Devic, G. IR and UV/VIS spectroscopic characterization of the higher fullerene C₇₆-D₂ for its quantitative and qualitative determination. *J. Nanomater.* **2018**, *2018*, 6862710. [[CrossRef](#)]
23. Jovanovic, T.; Koruga, D.; Mitrovic, A.; Stamenkovic, D.; Devic, G. Chapter IR and UV/VIS spectroscopic characterization of the higher fullerene C₇₆-D₂ for its quantitative and qualitative determination. In *Top 5 Contributions in Nanotechnology*; Lakshmi, S., Ed.; Avid Science: Berlin, Germany, 2019; pp. 2–26. ISBN 978-93-88170-59-8.
24. Jovanovic, T.; Koruga, D.; Jovancevic, B.; Stamenkovic, D. IR Spectroscopy of the Higher Fullerene C₇₆-D₂ for its Qualitative and Quantitative Determination. In *Proceedings of the International Conference on Experimental and Numerical Investigations and New Technologies CNN TECH 2017*, Zlatibor, Serbia, 2–5 July 2017; p. 24, ISBN 978-86-7083-938-0.
25. Jovanovic, T.; Koruga, D.; Debeljkovic, A.; Stamenkovic, D.; Sakota-Rosic, M.T.J.; Cvetkovic, M. IR Spectroscopy of the Higher Fullerene C₈₄-D₂:22 for its Qualitative and Quantitative Determination. In *Proceedings of the International Conference on Experimental and Numerical Investigations and New Technologies CNN TECH 2018*, Zlatibor, Serbia, 4–7 July 2018; p. 19, ISBN 978-86-7083-979-3.

26. Jovanovic, T.; Koruga, D.; Jovancicevic, B. Recent advances in IR and UV/VIS spectroscopic characterization of the C₇₆ and C₈₄ isomers of D₂ symmetry. *J. Nanomater.* **2014**, *2014*, 701312. [[CrossRef](#)]
27. Jovanovic, T.; Koruga, D.; Jovancicevic, B. Chapter Recent advances in IR and UV/VIS spectroscopic characterization of the C₇₆ and C₈₄ isomers of D₂ symmetry. In *Top 5 Contributions in Nanotechnology*; Lakshmi, S., Ed.; Avid Science: Berlin, Germany, 2019; pp. 2–35, ISBN 978-93-88170-59-8.
28. Krätschmer, W.; Lamb, L.D.; Fostiropoulos, K.; Huffman, D.R. Solid C₆₀: A new form of carbon. *Nat. Cell Biol.* **1990**, *347*, 354–358. [[CrossRef](#)]
29. Krätschmer, W.; Fostiropoulos, K.; Huffman, D.R. The infrared and ultraviolet absorption spectra of laboratory-produced carbon dust: Evidence for the presence of the C₆₀ molecule. *Chem. Phys. Lett.* **1990**, *170*, 167–170. [[CrossRef](#)]
30. Cox, D.M.; Behal, S.; Disko, M.; Gorun, S.M.; Greaney, M.; Hsu, C.S.; Kollin, E.B.; Millar, J.; Robbins, J. Characterization of C₆₀ and C₇₀ clusters. *J. Am. Chem. Soc.* **1991**, *113*, 2940–2944. [[CrossRef](#)]
31. Bethune, D.S.; Meijer, G.; Tang, W.C.; Rosen, H.J.; Golden, W.G.; Seki, H.; Brown, C.A.; de Vries, M.S. Vibrational Raman and infrared spectra of chromatographically separated C₆₀ and C₇₀ fullerene clusters. *Chem. Phys. Lett.* **1991**, *179*, 181–186. [[CrossRef](#)]
32. Hare, J.P.; Dennis, T.J.; Kroto, H.W.; Taylor, R.; Allaf, A.W.; Balm, S.; Walton, D.R.M. The IR spectra of fullerene-60 and -70. *J. Chem. Soc. Chem. Commun.* **1991**, 412–413. [[CrossRef](#)]
33. Jovanovic, T.; Koruga, D.; Jovancicevic, B.; Simić-Krstić, J. Modifications of Fullerenes Extractions and Chromatographies with Different Solvents. *Full Nanotub. Carbon Nanostruct.* **2003**, *11*, 383–394. [[CrossRef](#)]
34. Jovanovic, T.; Koruga, D.; Polić, P.; Dević, G. Extraction, Separation and Characterization of Fullerenes from Carbon Soot. *Mater. Sci. Forum* **2002**, *413*, 59–64. [[CrossRef](#)]
35. Jovanovic, T.; Koruga, D.; Jovančičević, B.; Simić-Krstić, J. Improvement in separation of nanostructured carbon clusters C₆₀ and C₇₀. *Int. J. Nanosci.* **2003**, *2*, 129–140. [[CrossRef](#)]
36. Jovanovic, T.; Koruga, D.; Jovancicevic, B.; Simić-Krstić, J. Advancement of the Process for Extraction, Chromatography and Characterization of Fullerenes. *Full Nanotub. Carbon Nanostruct.* **2009**, *17*, 135–150. [[CrossRef](#)]
37. Jovanovic, T.; Koruga, D.; Jovancicevic, B.; Vajs, V.; Dević, G. Comparative Spectroscopic Characterization of the Basic and the Higher Fullerenes. *Full Nanotub. Carbon Nanostruct.* **2013**, *21*, 64–74. [[CrossRef](#)]
38. Jovanovic, T.; Koruga, D.; Jovancicevic, B. Isolation and Characterization of the Higher Fullerenes from Carbon Soot. *Full Nanotub. Carbon Nanostruct.* **2011**, *19*, 309–316. [[CrossRef](#)]
39. Jovanovic, T.; Koruga, D. *The New Technological Process for Obtaining the Higher Fullerenes of High Purity from Carbon Soot*; no. 2693/09 A-165/09; The Intellectual Property Office: Belgrade, Serbia, 2009.
40. Jovanovic, T.; Koruga, D.; Jovancicevic, B. Advances in Chromatographic Separation on Al₂O₃ and Spectroscopic Characterization of the Higher Fullerenes. *Full Nanotub. Carbon Nanostruct.* **2014**, *22*, 384–396. [[CrossRef](#)]
41. Jovanovic, T.; Koruga, D. Recent advances in chromatographic separation and spectroscopic characterization of the higher fullerenes C₇₆ and C₈₄. *Recent Pat. Nanotechnol.* **2014**, *8*, 62–75. [[CrossRef](#)]
42. Jovanovic, T.; Koruga, D. The electronic structure and vibrational frequencies of the stable C₇₆ isomer of D₂ symmetry: Theory and experiment. *Chem. Phys. Lett.* **2013**, *577*, 68–70. [[CrossRef](#)]
43. Jovanovic, T.; Koruga, D.; Jovancicevic, B. The electronic structure and vibrational frequencies of the stable C₈₄ isomer of D₂ symmetry: Theory and experiment. *Diam. Relat. Mater.* **2014**, *44*, 44–48. [[CrossRef](#)]
44. Cataldo, F.; García-Hernández, D.A.; Machado, A.; Iglesias-Groth, S. Spectroscopy of Fullerenes, Fullerenes and PAHs in the UV, Visible and Near Infrared Spectral Range. *Proc. Int. Astron. Union* **2013**, *9*, 294–296. [[CrossRef](#)]
45. Cataldo, F.; Iglesias-Groth, S.; Hafez, Y. On the molar extinction coefficients of the electronic absorption spectra of C₆₀ and C₇₀ fullerenes radical cation. *Eur. Chem. Bull.* **2013**, *2*, 1013–1018.
46. Cioslowski, J. Heats of formation of higher fullerenes from ab initio Hartree–Fock and correlation energy functional calculations. *Chem. Phys. Lett.* **1993**, *216*, 389–393. [[CrossRef](#)]
47. Cataldo, F.; Strazzulla, G.; Iglesias-Groth, S. Stability of C₆₀ and C₇₀ fullerenes toward corpuscular and γ radiation. *Mon. Not. R. Astron. Soc.* **2009**, *394*, 615–623. [[CrossRef](#)]
48. Iglesias-Groth, S. Hydrogenated fullerenes and the anomalous microwave emission of the dark cloud LDN 1622. *Mon. Not. R. Astron. Soc.* **2006**, *368*, 1925–1930. [[CrossRef](#)]
49. Cataldo, F.; Iglesias-Groth, S. On the action of UV photons on hydrogenated fullerenes C₆₀H₃₆ and C₆₀D₃₆. *Mon. Not. R. Astron. Soc.* **2009**, *400*, 291–298. [[CrossRef](#)]
50. Cataldo, F.; Iglesias-Groth, S. *Fullerenes: The Hydrogenated Fullerenes*; Springer: Berlin, Germany, 2009.
51. Yeretzyan, C.; Hansen, K.; Diederich, F.; Whetten, R.L. Fran Coalescence reactions of fullerenes. *Nat. Cell Biol.* **1992**, *359*, 44–47. [[CrossRef](#)]
52. Kubler, B.; Millon, E.; Gaumet, J.J.; Muller, J.F. Formation of high mass C_n clusters (n > 100) by laser ablation/desorption coupled with mass spectrometry. *Fuller. Sci. Technol.* **1996**, *4*, 1247–1261. [[CrossRef](#)]
53. Cataldo, F.; Keheyani, Y. On the mechanism of carbon clusters formation under laser irradiation. the case of diamond grains and solid C₆₀ fullerene. *Full Nanotub. Carbon Nanostruct.* **2002**, *10*, 313–332. [[CrossRef](#)]
54. Orlandi, G.; Zerbetto, F.; Fowler, P.W.; Manolopoulos, D.E. The electronic structure and vibrational frequencies of the stable C₇₆ isomer of D₂ symmetry. *Chem. Phys. Lett.* **1993**, *208*, 441–445. [[CrossRef](#)]

55. Hampe, O.; Neumaier, M.; Boese, A.D.; Lemaire, J.; Niedner-Schatteburg, G.; Kappes, M.M. Infrared multiphoton electron detachment spectroscopy of C_{76}^{2-} . *J. Chem. Phys.* **2009**, *131*, 124306. [[CrossRef](#)]
56. Manolopoulos, D.E. Faraday communications. Proposal of a chiral structure for the fullerene C_{76} . *J. Chem. Soc. Faraday Trans.* **1991**, *87*, 2861–2862. [[CrossRef](#)]
57. Manolopoulos, D.E.; Fowler, P.W. Molecular graphs, point groups, and fullerenes. *J. Chem. Phys.* **1992**, *96*, 7603–7614. [[CrossRef](#)]
58. Manolopoulos, D.E.; Fowler, P.W.; Taylor, R.; Kroto, H.W.; Walton, D.R.M. Faraday communications. An end to the search for the ground state of C_{84} ? *J. Chem. Soc. Faraday Trans.* **1992**, *88*, 3117–3118. [[CrossRef](#)]
59. Negri, F.; Orlandi, G.; Zerbetto, F. Prediction of the structure and the vibrational frequencies of a C_{84} isomer of D_2 symmetry. *Chem. Phys. Lett.* **1992**, *189*, 495–498. [[CrossRef](#)]
60. Bettinger, H.F.; Scuseria, G.E. The infrared vibrational spectra of the two major C_{84} isomers. *Chem. Phys. Lett.* **2000**, *332*, 35–42. [[CrossRef](#)]
61. Zhang, B.L.; Wang, C.Z.; Ho, K.M. Vibrational spectra of C_{84} isomers. *Phys. Rev. B* **1993**, *47*, 1643–1646. [[CrossRef](#)]
62. Harigaya, K.; Abe, S. Optical absorption spectra and geometric effects in higher fullerenes. *J. Phys. Condens. Matter* **1996**, *8*, 8057–8066. [[CrossRef](#)]
63. Saito, S.; Sawada, S.-I.; Hamada, N. Electronic and geometric structures of C_{76} and C_{84} . *Phys. Rev. B* **1992**, *45*, 13845–13848. [[CrossRef](#)]
64. Ehrler, O.T.; Furche, F.; Weber, J.M.; Kappes, M.M. Photoelectron spectroscopy of fullerene dianions $C_{76}(2-)$, $C_{78}(2-)$, $C_{84}(2-)$. *J. Chem. Phys.* **2005**, *122*, 094321. [[CrossRef](#)]
65. Diederich, F.; Ettl, R.; Rubin, Y.; Whetten, R.L.; Beck, R.; Alvarez, M.; Anz, S.; Sensharma, D.; Wudl, F.; Khemani, K.C.; et al. The Higher Fullerenes: Isolation and Characterization of C_{76} , C_{84} , C_{90} , C_{94} , and $C_{70}O$, an Oxide of D_{5h} - C_{70} . *Science* **1991**, *252*, 548–551. [[CrossRef](#)]
66. Jinno, K.; Matsui, H.; Ohta, H.; Saito, Y.; Nakagawa, K.; Nagashima, H.; Itoh, K. Separation and identification of higher fullerenes in soot extract by liquid chromatography-mass spectrometry. *Chromatographia* **1995**, *41*, 353–360. [[CrossRef](#)]
67. Jinno, K.; Sato, Y.; Nagashima, H.; Itoh, K. Separation and identification of higher fullerenes by high-performance liquid chromatography coupled with electrospray ionization mass spectrometry. *J. Microcolumn Sep.* **1998**, *10*, 79–88. [[CrossRef](#)]
68. Kikuchi, K.; Nakahara, N.; Honda, M.; Suzuki, S.; Saito, K.; Shiromaru, H.; Yamauchi, K.; Ikemoto, I.; Kuramochi, T.; Hino, S.; et al. Separation, Detection, and UV/Visible Absorption Spectra of Fullerenes; C_{76} , C_{78} , and C_{84} . *Chem. Lett.* **1991**, *20*, 1607–1610. [[CrossRef](#)]
69. Kikuchi, K.; Nakahara, N.; Wakabayashi, T.; Honda, M.; Matsumiya, H.; Moriwaki, T.; Suzuki, S.; Shiromaru, H.; Saito, K.; Yamauchi, K.; et al. Isolation and identification of fullerene family: C_{76} , C_{78} , C_{82} , C_{84} , C_{90} and C_{96} . *Chem. Phys. Lett.* **1992**, *188*, 177–180. [[CrossRef](#)]
70. Ettl, R.; Chao, I.; Diederich, F.; Whetten, R.L. Isolation of C_{76} , a chiral (D_2) allotrope of carbon. *Nat. Cell Biol.* **1991**, *353*, 149–153. [[CrossRef](#)]
71. Michel, R.H.; Schreiber, H.; Gierden, R.; Hennrich, F.; Rockenberger, J.; Beck, R.D.; Kappes, M.M.; Lehner, C.; Adelman, P.; Armbruster, J.F. Vibrational spectroscopy of purified C_{76} . *Ber. Bunsenges. Phys. Chem.* **1994**, *98*, 975–978. [[CrossRef](#)]
72. Avent, A.G.; Dubois, D.; Pénicaud, A.; Taylor, R. The minor isomers and IR spectrum of [84]fullerene. *J. Chem. Soc. Perkin Trans.* **1997**, *2*, 1907–1910. [[CrossRef](#)]
73. Dennis, T.J.S.; Hulman, M.; Kuzmany, H.; Shinohara, H. Vibrational Infrared Spectra of the Two Major Isomers of [84]Fullerene: $C_{84}\{D_2(IV)\}$ and $C_{84}\{D_2d(II)\}$. *J. Phys. Chem. B* **2000**, *104*, 5411–5413. [[CrossRef](#)]
74. Colthup, N.B.; Daly, L.H.; Wiberley, S.E. *Introduction to Infrared and Raman Spectroscopy*; Elsevier BV: Amsterdam, The Netherlands, 1975.
75. Jovanović, T.; Koruga, D. Optical absorption properties and applications of fullerenes. In Proceedings of the 14th Yugoslav Materials Research Society Conference “YUCOMAT ‘12”, Materials Research Society of Serbia, Herceg Novi, Montenegro, 3–7 September 2012; p. 122.
76. Stamenković, D.; Jagodić, N.; Conte, M.; Ilanković, N.; Jovanović, T.; Koruga, D. Optical properties of nanophotonic contact lenses. In Proceedings of the 12th Yugoslav Materials Research Society Conference “YUCOMAT ‘10”, Materials Research Society of Serbia, Herceg Novi, Montenegro, 6–10 September 2010; p. 177.
77. Jovanović, T.; Koruga, D.; Jovančević, B.; Mitrović, A.; Stamenković, D.; Rakonjac, I. Comparative spectroscopic characterization of fullerene nanomaterials. In Proceedings of the 19th Yugoslav Materials Research Society Conference “YUCOMAT ‘17” of Materials Research Society of Serbia, Herceg Novi, Montenegro, 4–8 September 2017; p. 107.