Data Article

Electron spectrosopies of 3-hydroxyflavone and 7-hydroxyflavone in MCM-41 silica nanoparticles and in acetonitrile solutions. Experimental data and DFT/TD-DFT calculations

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A B S T R A C T

The data presented here concern the photophysical characterization of luminescent MCM-41 nanoparticles doped with 3-hydroxyflavone and 7-hydroxyflavone, two fluorescent flavonoids. UV-Vis and fluorescence spectra obtained on freshly-prepared samples and aged (2 months exposed to air) samples are shown. The effect of light exposure is also studied. In parallel, experiments have been carried out in acetonitrile solutions of the two flavonoids as a term of comparison. Time-dependent density functional theory calculations have also been used to simulate UV-Vis and emission spectra of different species for both flavonoids (neutral molecule, tautomer, cationic and anionic forms), taking into account the

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effect of the surrounding medium (solvent). Density functional theory calculations of vibrational spectra (IR, Raman) of neutral and tautomeric species of 3HF and 7HF are also provided.

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### Specifications Table

| Subject | Physical Chemistry |
|---------|--------------------|
| Specific subject area | Electronic spectroscopy, photophysics |
| Type of data | Spectra |
| How data were acquired | UV-Vis spectra were recorded with an Agilent Cary5000 spectrophotometer. An integrating sphere was used to record reflectance. Spectra were reconstructed through Kubelka-Munk transform. Steady-state photoluminescence spectra of flavonoids in silica NPs were recorded with Edinburgh instruments FLS980 spectrofluorimeter (excitation source: Xenon arc lamp). Photobleaching tests were performed by doing repeated emission scans of the samples in 3-minute intervals. The computer codes ORCA [1] and Gaussian09 Revision A.02 [2] were used in DFT and TD-DFT calculations. |
| Data format | Raw |
| Parameters for data collection | UV-Vis and fluorescence spectra of 3HF and 7HF in different environments and under different conditions (air exposure, UV exposure). Simulation of UV-Vis and fluorescence spectra (by TD-DFT calculations) of 3HF and 7HF in gas phase and acetonitrile (MeCN). |
| Description of data collection | UV-Vis and fluorescence spectra from 3-hydroxyflavone (3HF) and 7-hydroxyflavone (7HF) embedded in MCM-41 silica nanoparticles before and after 2 months of exposure to air at 298 K. Evolution of fluorescence spectra of 3HF and 7HF in MCM-41 matrices and in Acetonitrile (MeCN) solutions under UV irradiation. Simulation via TD-DFT calculations of absorption and fluorescence spectra of neutral, anionic, cationic, tautomeric forms of 3HF and 7HF in gas phase and in MeCN. |
| Data accessibility | With the article |
| Related research article | Landström A, Leccese S, Abadian H, Lambert J-F, Concina I, Protti S, Ari Paavo Seitsonen AP, Mezzetti A, "Fluorescent silica MCM-41 nanoparticles based on flavonoids: Direct post-doping encapsulation and spectral characterization. Dyes and Pigments 185 (2021) 108870, for a co-submission research article. https://doi.org/10.1016/j.dyepig.2020.108870 |

### Value of the Data

- UV-Vis and fluorescence spectra of 3HF and 7HF in MCM-41 silica nanoparticles (NPs) remain fluorescent after 2 month of air exposure at room temperature. In the case of 7HF silica NPs, the fluorescence spectrum is modified compared to the spectrum of freshly-prepared 7HF silica NPs.
- Fluorescence spectra recorded at different time of UV irradiation show the effect of photodecomposition in the emission properties of MCM-41 flavonoid-doped NPs and of flavonoid solutions in MeCN.
- TD-DFT calculations of UV-Vis and fluorescence spectra (in vacuum and in MeCN) of 3HF and 7HF both in neutral, tautomeric, anionic, cationic forms are reported. They can be useful in
Fig. 1. F(R) spectrum (approximately equivalent to UV-Vis absorbance spectrum) of aged (2 months of air exposure at 298K) 3HF-doped MCM-41 NPs. F(R) spectrum of freshly-prepared 3HF-doped MCM-41 NPs is shown in Fig. 3 of the related research paper [6]. F(R) is the Kubelka-Munk transform of the reflectance R, \( F(R) = \frac{(1-R)^2}{2R} \).

- The interpretation of experimental absorption and fluorescence spectra of 3HF and 7HF and in the assessment of environmental effects on these spectra.
- TD-DFT simulation of electronic spectra and DFT simulation of vibrational spectra of 3HF and 7HF in vacuum and in MeCN can be useful in the interpretation of experimental FTIR and Raman spectra of 3HF and 7HF and in the assessment of environmental effects on these spectra.

1. Data Description

3HF and 7HF are fluorescent molecules widely used in biophysics and analytical chemistry [3–5]. In this work and in the related research article [6] the fluorescence properties of these two flavonoids inside MCM-41 silica NPs have been studied. The spectra presented here focus first on the effect of air exposure on the emission properties of the NPs. Figs. 1 and 2 show the UV-Vis spectra after 2 months of air exposure. Only minimal changes are observed compared to the spectra recorded on freshly-prepared NPs (reported in [6]). In Figs. 3 and 4 the emission spectra of aged flavonoid-doped NPs are reported. These two figures show that both kind of NPs remain fluorescent. For 3HF-doped aged NPs a slight attenuation of the fluorescent intensity is observed compared to freshly-prepared 3HF-doped NPs [6], without almost any modification of the spectral shape. For 7HF-doped NPs, 2 months of air exposure modify quite strongly the shape of the emission spectra.

Figs. 5 and 6 show the effect of UV irradiation exposure of the fluorescent properties of the two kinds of flavonoid-doped NPs. For a comparison, Figs. 7 and 8 show the same kind of experiment for 3HF and 7HF in MeCN solutions. Fig. 8 shows that for 7HF in MeCN UV exposure lead to an increase of emission at \( \sim 375 \) nm.

Table 1 reports the results of TD-DFT calculations used to simulate absorption and fluorescence spectra of 3HF and 7HF in different forms (neutral, tautomeric, anionic, cationic). The results obtained in gas phase and in MeCN are compared.
Table 2 contains the most intense bands in the computed IR and Raman spectra of 3HF and 7HF in neutral and tautomeric forms; also in this case results obtained in gas phase and in MeCN are compared.

Fig. 9 helps to better understand data reported in Tables 1 and 2.
2. Experimental Design, Materials and Methods

**Chemicals.** 3HF and 7HF were purchased from Sigma-Aldrich and recrystallized from cyclohexane. Acetonitrile (MeCN) for post-doping procedure was of spectroscopic grade. Fluorescence analysis were carried out using anhydrous MeCN.

**Synthesis of silica NPs.** MCM-41 NPs were prepared by following the protocol of Ref. [7]. An aqueous solution of cetyltrimethylammonium bromide (CTAB), mixed with aqueous ammonia was left under stirring at a constant temperature of 35 °C. Then tetraethyl orthosilicate (TEOS) was added. The TEOS/CTAB/NH₄OH mixture was left at 35 °C for 2 h. Then, the system was transferred to a tightly sealed Teflon bottle placed in a drying oven at 100 °C and left under
autogenous pressure overnight. After filtration, the final step was the removal of CTAB within the pores of the MCM-41 by calcination: the solid sample was placed in a crucible in a programmable calcination oven under ambient air and the temperature was increased from 20 to 300 °C in 2 ½ h. Then the temperature was kept constant at 300 °C for 2 h. Subsequently, temperature was increased from 300 to 550 °C in 2 h. Then the temperature was kept constant at 550 °C for 12 h.

Preparation of flavonoid-doped NPs MCM-41 NPs were added to 10^{-3} M MeCN solutions of 3HF and 7HF. Samples were stirred for 5 min, centrifuged for 45 min at 4000 rpm to separate the solid (containing MCM-41 matrix with the flavonoids encapsulated). The solid was then exposed to air for 48 h in a Petri dish to let the solvent evaporate.
Fig. 8. Fluorescence spectra ($\lambda_{\text{exc}} = 300$ nm) of 7HF in an aerated MeCN solution after different period of UV light ($\lambda = 300$ nm) exposure. Spectra were recorded every 3 minutes. The $\sim 525$ nm band decreases its intensity with exposure time, the $\sim 375$ nm band increases its intensity with exposure time, as shown by the black arrows.

Fig. 9. The structure of the species mentioned in Tables 1 and 2 that exist in two forms.
Table 1
energy of the absorption and fluorescence spectra of the different species in gas phase and in acetonitrile. Energy is first given in eV, then in nm. For absorbance transitions, the third row indicates the intensity.

|                   | 3HF neutral |  | 3HF tautomer |  | 3HF anion |  | 3HF cation 1 |
|-------------------|-------------|---|--------------|---|-----------|---|-------------|
|                   | free/gas phase | in MeCN | free/gas phase | in MeCN | free/gas phase | in MeCN | free/gas phase |
| Absorbance (eV)   | 3.55 3.99 4.19 4.35 4.56 4.77 4.92 4.99 5.21 5.29 | 3.50 4.09 4.12 4.33 4.58 4.79 4.91 5.03 5.24 5.27 | 2.57 3.25 3.77 3.81 4.06 4.17 4.46 4.54 4.57 4.86 | 2.61 3.46 3.76 3.86 4.24 4.29 4.52 4.53 4.71 4.90 | 2.33 2.56 2.65 2.67 2.94 3.12 3.18 3.29 3.43 3.56 | 2.60 3.11 3.66 3.85 3.87 3.90 3.95 4.20 4.21 4.30 | 3.13 3.20 3.61 4.42 4.76 4.88 4.90 5.02 5.14 5.52 |
| (nm)              | 349 310 296 285 272 260 252 248 238 234 | 355 303 301 287 271 259 252 247 237 235 | 482 381 329 325 305 297 278 273 272 255 | 476 358 330 321 293 289 274 274 263 253 | 531 484.19 467 465 421 397 389 377 361 348 | 477 399 339 322 320 318 314 295 295 288 | 397 387 343 281 261 254 253 247 241 225 |
| Intensity         | 0.375 0.0 0.142 0.026 0.010 0.079 0.074 0.072 0.0 0.95 | 0.488 0.125 0.071 0.024 0.001 0.149 0.064 0.111 0.065 0.004 | 0.355 0.0 0.002 0.059 0.118 0.055 0.049 0.0 0.038 0.0 | 0.458 0.0 0.106 0.036 0.077 0.037 0.129 0.008 0.001 0.295 | 0.218 0.000 0.001 0.0 0.0 0.001 0.108 0.001 0.067 0.001 | 0.374 0.0 0.031 0.088 0.002 0.062 0.0 0.041 0.196 0.004 | 0.104 0.509 0.039 0.005 0.013 0.056 0.148 0.055 0.0 0.004 |
| Fluorescence (eV) | 3.1278 | 396.39 | 2.29 | 540 | 2.03 | 611 | 2.18 | 568 |

|                   | (nm) |  | (nm) |  | (nm) |  | (nm) |  |
| Fluorescence (eV) | 3.50 |  | 3.00 |  | 3.1278 |  | 396.39 |  |

(continued on next page)
### Table 1 (continued)

|          | in MeCN                                                                 |
|----------|-------------------------------------------------------------------------|
| Absorbance (eV) (nm) | 3.17 3.48 3.59 4.49 4.75 4.97 5.10 5.13 5.40 5.47                      |
| Intensity | 0.665 0.002 0.112 0.014 0.025 0.243 0.142 0.079 0.026                  |
| Fluorescence (eV) (nm) | 2.7558 449.9                                                           |

### 3HF cation 2 free/gas phase

|          | in MeCN                                                                 |
|----------|-------------------------------------------------------------------------|
| Absorbance (eV) (nm) | 3.34 3.50 3.59 4.42 4.79 5.06 5.13 5.23 5.60 5.65                      |
| Intensity | 0.398 0.007 0.115 0.023 0.020 0.118 0.019 0.013 0.034 0.083            |
| Fluorescence (eV) (nm) | 2.8227 439.23                                                           |

### 7HF neutral free/gas phase

|          | in MeCN                                                                 |
|----------|-------------------------------------------------------------------------|
| Absorbance (eV) (nm) | 3.53 4.11 4.19 4.61 4.67 4.76 4.96 5.21 5.23 5.28                      |
| Intensity | 0.001 0.305 0.079 0.216 0.035 0.0 0.050 0.003 0.009 0.086             |
| Fluorescence (eV) (nm) | 2.85 436                                                                |

### 7HF tautomer 1 free/gas phase

|          | in MeCN                                                                 |
|----------|-------------------------------------------------------------------------|
| Absorbance (eV) (nm) | 2.65 2.77 3.86 4.08 4.10 4.18 4.36 4.45 4.59 4.76                      |
| Intensity | 0.232 0.0 0.010 0.014 0.406 0.084 0.001 0.006 0.038 0.005             |
| Fluorescence (eV) (nm) | 1.74 713                                                                |

|          | in MeCN                                                                 |
|----------|-------------------------------------------------------------------------|
| Absorbance (eV) (nm) | 2.86 3.37 4.02 4.10 4.23 4.57 4.67 4.67 4.83 4.93                      |
| Intensity | 0.406 0.0 0.154 0.333 0.007 0.083 0.042 0.003 0.281 0.021             |
| Fluorescence (eV) (nm) | 2.09 594                                                               |

(continued on next page)
| 7HF tautomer 2 | free/gas phase |
|---------------|---------------|
| Absorbance (eV) | 2.59 2.70 3.75 3.98 3.99 4.07 4.14 4.14 4.50 4.65 4.66 |
| (nm) | 479 459 331 312 310 304 299 275.59 267 266 |
| Intensity | 0.215 0.0 0.015 0.008 0.134 0.039 0.330 0.008 0.080 0.002 |
| Fluorescence (eV) | 1.68 |
| (nm) | 738 |

| 7HF anion | free/gas phase |
|----------|---------------|
| Absorbance (eV) | 2.05 2.64 2.73 2.74 3.05 3.23 3.29 3.38 3.45 3.56 |
| (nm) | 605 470 454 452 406 383 377 367 359 348 |
| Intensity | 0.091 0.0 0.007 0.0 0.0 0.0 0.005 0.0 0.0 0.0 |
| Fluorescence (eV) | 2.03 |
| (nm) | 829 |

| 7HF cation 1 | free/gas phase |
|-------------|---------------|
| Absorbance (eV) | 3.35 3.42 3.82 4.31 4.81 4.85 5.02 5.33 5.44 5.51 |
| (nm) | 370 363 325 288 258 256 247 233 228 225 |
| Intensity | 0.587 0.014 0.063 0.031 0.107 0.092 0.078 0.059 0.191 0.003 |
| Fluorescence (eV) | 3.00 |
| (nm) | 413 |

| 7HF cation 2 | free/gas phase |
|-------------|---------------|
| Absorbance (eV) | 3.35 3.72 3.84 4.29 4.92 5.07 5.10 5.36 5.45 5.70 |
| (nm) | 370 334 323 289 252 244 243 231 228 217 |
| Intensity | 0.653 0.017 0.119 0.083 0.178 0.206 0.038 0.041 0.173 0.133 |
| Fluorescence (eV) | 2.94 |
| (nm) | 421 |

(continued on next page)
| Absorbance (eV) | in MeCN | Intensity | Fluorescence (eV) |
|----------------|---------|-----------|------------------|
| 3.34 3.73 3.82 4.27 4.93 5.08 5.13 5.38 5.47 5.70 | 0.607 0.037 0.138 0.094 0.169 0.248 0.019 0.042 0.148 0.117 | 2.89 | 428 |
| (nm) | 371 332 325 290 252 244 231 227 217 | |

Table 1 (continued)

Table 2
Main IR and Raman bands for 3HF and 7HF in the neutral and tautomeric forms. First column, energy in cm⁻¹; second column, IR relative intensity; third column, Raman relative intensity.

### 3HF neutral

| 3HF neutral |
|-------------|
| free/gas phase |
| 373 | 22 | – | 1375 | 84 | – |
| 678 | 50 | – | 1441 | 202 | – |
| 708 | 41 | – | 1504 | 87 | – |
| 778 | 75 | – | 1513 | 44 | – |
| 1014 | – | 162 | 1532 | 31 | – |
| 1110 | 37 | – | 1604 | 31 | 441 |
| 1156 | 98 | – | 1640 | 35 | 1569 |
| 1210 | 74 | – | 1649 | 124 | 368 |
| 1226 | 56 | – | 1656 | 178 | 321 |
| 1323 | 65 | – | 1684 | 138 | 186 |
| 1337 | 26 | 175 | 3187 | 26 | 324 |
| 1356 | 211 | 197 | 3201 | – | 283 |
| 1370 | 33 | – | 3522 | 154 | 174 |

| 3HF tautomer |
|-------------|
| free/gas phase |
| 904 | 78 | – | 1527 | 69 | 221 |
| 1012 | – | 289 | 1558 | – | 969 |
| 1177 | – | 252 | 1585 | 134 | 216 |
| 1211 | – | 258 | 1619 | 140 | – |
| 1257 | – | 371 | 1637 | – | 1504 |
| 1264 | 72 | – | 1652 | – | 844 |
| 1324 | 83 | – | 3150 | 97 | 243 |
| 1385 | 88 | – | 3173 | – | 168 |
| 1417 | 78 | 1595 | 3186 | – | 344 |
| 1446 | 490 | 762 | 3187 | – | 253 |
| 1519 | 227 | – | 3205 | – | 292 |

| in MeCN |
|---------|
| 788 | 95 | – | 1483 | 180 | – |
| 856 | 96 | – | 1519 | 352 | – |
| 1004 | – | 1031 | 1527 | 185 | – |

(continued on next page)
|   |   |   |   |   |
|---|---|---|---|---|
| 1137 | 119 | — | 1558 | 322 | 7067 |
| 1211 | — | 1287 | 1585 | 172 | 1839 |
| 1257 | 368 | 1584 | 1619 | 129 | — |
| 1324 | 355 | — | 1637 | — | 7547 |
| 1385 | 532 | — | 1652 | — | 3714 |
| 1417 | — | 1838 | 3221 | 274 | — |
| 1446 | 840 | 10211 |   |   |   |

**7HF neutral**

|   |   |   |   |   |
|---|---|---|---|---|
| 1158 | 101 | — | 3157 | — | 164 |
| 1168 | 166 | — | 3175 | — | 134 |
| 1253 | — | 105 | 3186 | — | 169 |
| 1270 | — | 267 | 3195 | — | 163 |
| 1318 | 143 | — | 3195 | — | 101 |
| 1390 | 321 | 140 | 3208 | — | 71 |
| 1487 | 195 | — | 3209 | — | 84 |
| 1606 | 46 | 263 | 3221 | — | 91 |
| 1644 | — | 550 | 3811 | 102 | 197 |
| 1651 | 96 | 386 |   |   |   |

*in MeCN*

|   |   |   |   |   |
|---|---|---|---|---|
| 612 | 132 | — | 1644 | 741 | 626 |
| 1110 | 96 | — | 1651 | — | 2862 |
| 1158 | 166 | — | 1663 | 942 | 2339 |
| 1168 | 271 | — | 1710 | 370 | — |
| 1253 | — | 308 | 3165 | — | 317 |
| 1270 | — | 1245 | 3175 | — | 313 |
| 1284 | 116 | — | 3186 | — | 370 |
| 1318 | 273 | — | 3195 | — | 539 |
| 1378 | 118 | — | 3208 | — | 298 |
| 1390 | 566 | 589 | 3209 | — | 326 |
| 1484 | 136 | — | 3221 | — | 301 |
| 1487 | 250 | — | 3811 | 240 | 403 |
| 1606 | 161 | 1455 |   |   |   |

**7HF tautomer 1**

*free/gas phase*

|   |   |   |   |   |
|---|---|---|---|---|
| 1152 | 78 | — | 1611 | 112 | — |
| 1201 | 187 | — | 1626 | 78 | 804 |
| 1469 | 163 | 583 | 1643 | — | 781 |
| 1568 | 312 | 3940 | 1680 | 207 | — |
| 1586 | 515 | 776 | 1683 | 502 | — |

*in MeCN*

|   |   |   |   |   |
|---|---|---|---|---|
| 1201 | 295 | 592 | 1626 | — | 590 |
| 1244 | — | 716 | 1643 | — | 1133 |
| 1469 | 525 | 1358 | 1680 | 305 | 477 |
| 1568 | 352 | 585 | 1683 | 776 | — |
| 1586 | 1545 | 4530 | 3188 | — | 550 |
| 1611 | 395 | 3487 |   |   |   |

**7HF tautomer 2**

*free/gas phase*

|   |   |   |   |   |
|---|---|---|---|---|
| 359 | 84 | — | 1564 | 401 | 6339 |
| 779 | 63 | — | 1587 | 291 | — |
| 1142 | 97 | — | 1642 | — | 869 |
| 1276 | 192 | — | 1682 | 616 | — |
| 1426 | 79 | — | 1691 | 98 | — |
| 1463 | 80 | — | 3812 | 68 | — |

*(continued on next page)*
UV-Vis spectra of flavonoid-doped NPs were recorded with an Agilent Cary5000 spectrophotometer. An integrating sphere was used to record reflectance; spectra were obtained through Kubelka-Munk transform.

Steady-state photoluminescence spectra of flavonoid-doped NPs were recorded with Edinburgh instruments FLS980 spectrofluorimeter. A Xenon arc lamp was used as excitation source. Photobleaching tests were performed by doing repeated emission scans of the samples in 3-minute intervals.

UV-Vis absorption spectra in MeCN solutions were carried out on a Jasco V-550 spectrophotometer or on an Agilent Cary 5000 spectrophotometer. Fluorescence spectra of MeCN solution were carried out on a Perkin Elmer LS-55 spectrofluorimeter or on an Edinburgh instruments FLS980 spectrofluorimeter. Photobleaching tests were performed by doing repeated emission scans of the samples in 3-minute intervals.

**Theoretical calculations.** Density functional theory (DFT) [8] and time-dependent DFT [9] calculations were carried out on both flavonoids in different states (neutral, tautomer, anion, cation). DFT was used to calculate the ground-state $S_0$ geometries and vibrational spectra; TD-DFT for absorption and fluorescence spectra, the latter in the first singlet state $S_1$. We employed the B3LYP [10] as the approximation in the exchange-correlation functional. The basis set cc-pVTZ in the calculation of the vibrational spectra and aug-cc-pVTZ in the calculations of TDDFT were used unless otherwise mentioned. The calculations have been performed with a free-standing molecule and using implicit solvation within the conductor-like polarisable continuum model (CPCM) [11] for MeCN.

The computer codes ORCA [1] and Gaussian09 Revision A.02 [2] were employed. We applied large integration grids and strict convergence criteria, “Grid5” and “tight SCF” in the input of ORCA and “Integral(UltraFine)” in the input of G09.

**Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships which have, or could be perceived to have, influenced the work reported in this article.

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Supplementary Materials

Supplementary material associated with this article can be found in the online version at doi: 10.1016/j.dib.2020.106630.

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