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Professional paper

ABSORPTION OF UV RAYS BY CAFFEINE SOLUTION IN VARIOUS SOLVENTS

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Abstract

Pure caffeine is dissolved in various solvents such as: water, ethyl alcohol, acetone, chloroform, ethyl acetate, at a temperature of 25ºC, and prepared solutions of the same concentrations, after which we proceeded to measure the absorption of UV rays with different wavelengths:190,200,210,220,230,240, 250, 260, 270, 280, 290, 300 nm. We found that some solvents affect the absorption of UV rays.

Keywords: Caffeine, UV ray, solvents, absorption

1. Introduction

Caffeine is a sapid molecule found in coffee, tea, chocolate, and some medications [1]. Caffeine (3,7-dihydro-1,3,7- trimethyl-1-H-purine—2,6-dione) has complex hydration because of the simultaneous presence of $–CH_3$ groups and C=O groups on its structure [1]. The structure of caffeine molecules limits the solubility in water because of the self-association of caffeine molecules by hydrophobic ineraction [1-8], and it is also responsible for interactions and complexation with a lot of molecules.
Molecular modeling and NMR studies suggest that caffeine dimerization in solution may occur through stacking, with many possible distinct caffeine-caffeine orientations. Previous work by the same author also pointed out, using FT-IR studies, the tendency of caffeine to associate to form dimers and higher order clusters, but, however, could not quantify the average size of the aggregates, generically indicated as “polymers” [5].

Table 1: The solubility of Caffein in different solvents at 25ºC[2]

Solvent	Dipole moment (μ)	Solubility (% w/w)
Water	μ=1.84 D	2.2
Ethyl Alcohol	μ=1.66 D	1.2
Diethyl Ether	μ=1.18 D	0.3
Ethyl acetate	μ=1.78 D	2.5
Chloroform	μ=1.15 D	18.0
Acetone	μ=2.98 D	2.0

Considering the above, we dissolved caffeine in several solvents with different molecular structures at room temperature in where the solubility of caffeine is different, and measured the absorption of UV rays of different wavelengths.

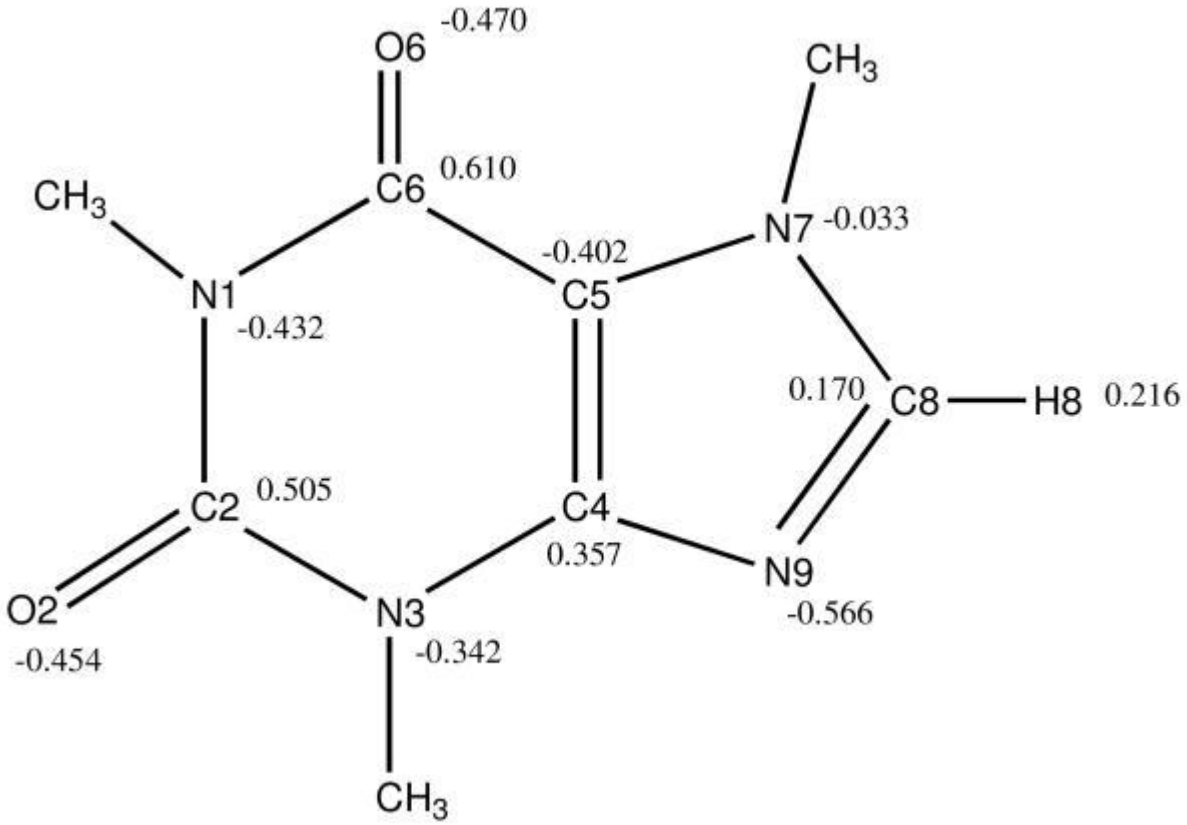

Figure:1. The covalent structure and atomic numbering of caffeine (1,3,7-trimethyl xanthine). The atomic partial charges for all atoms except those of the methyl groups [5].

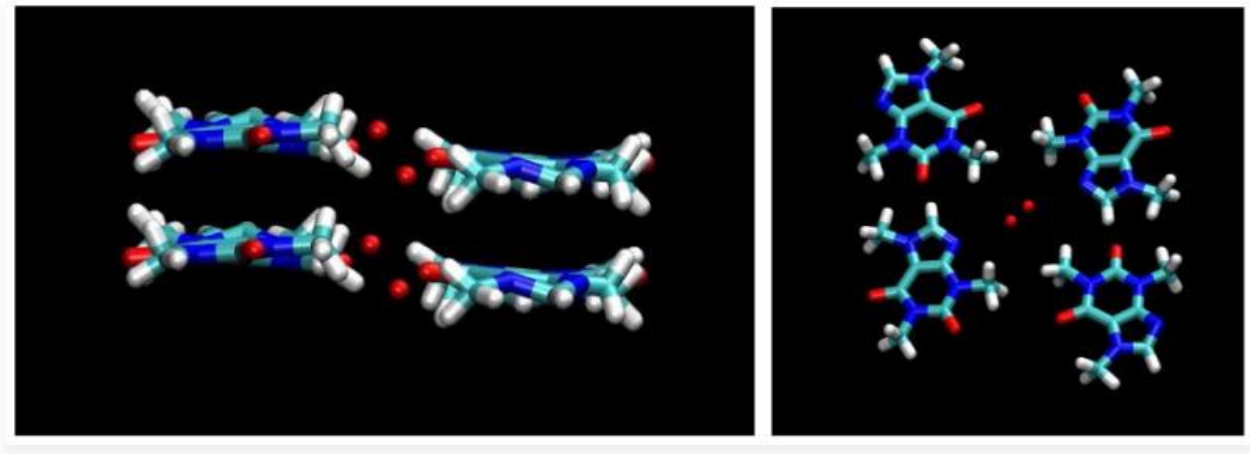

Figure 2. Two views of the monohydrate crystal structure of caffeine, illustrating the position of the water molecule (shown as red spheres on the oxygen atom), hydrogen-bonded to the N9 atom of the caffeine molecule and making a second bond to another symmetry-related water molecule [5].

2. Experimental

We dissolved 0.1 g of caffeine in each solvent at room temperature and obtained 50 ml of solution. We measured the absorbance of UV rays of different wavelengths on the device:
and obtained these results:

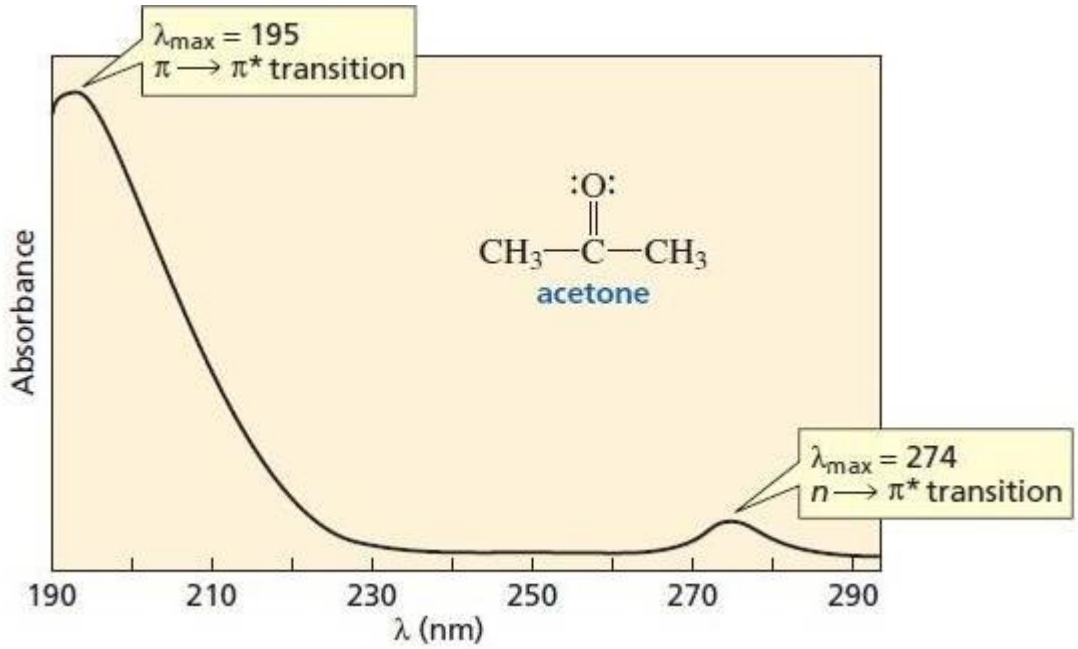

Figure 3. Absorption of acetone [6]

Table 1. Absorbance of a solution of caffeine in acetone

λ(nm)	A	nm	A	nm	A	nm	A
200,0	0,049	234,0	0,007	269,0	-0,208	300,0	0,346
201,0	0,109	235,0	0,112	270,0	0,086	301,0	0,008
202,0	2,786	236,0	0,376	271,0	-0,079	302,0	0,110
203,0	-0,022	237,0	0,026	272,0	-0,016		
204,0	-0,025	238,0	-0,086	273,0	-0,043		
205,0	0,022	239,0	-0,136	274,0	-0,151		
206,0	0,111	240,0	0,004	275,0	-0,066		
207,0	0,282	241,0	-0,086	276,0	0,007		
208,0	0,288	242,0	0,245	277,0	-0,136		
209,0	-0,027	243,0	0,246	278,0	-0,233		
210,0	0,077	244,0	0,004	279,0	0,230		
211,0	-0,250	245,0	0,089	280,0	-0,209		
212,0	0,036	246,0	0,103	281,0	0,077		
213,0	0,169	247,0	-0,060	282,0	0,145		
214,0	0,012	248,0	-0,177	283,0	-0,123		
215,0	-0,268	249,0	-0,002	284,0	0,103		
216,0	0,022	250,0	-0,038	285,0	0,056		
217,0	0,070	251,0	-0,015	286,0	0,688		
218,0	-0,012	252,0	-0,124	287,0	0,922		
219,0	0,117	253,0	-0,032	288,0	-0,306		

220,0	0,025	254,0	-0,041	289,0	0,455
221,0	0,001	255,0	0,016	290,0	-0,105
222,0	-0,178	256,0	-0,043	291,0	-0,136
223,0	-0,229	257,0	0,092	292,0	-0,057
224,0	0,324	258,0	-0,121	293,0	0,475
225,0	0,094	259,0	-0,030	294,0	-0,216
226,0	-0,044	260,0	-0,024	295,0	2,462
227,0	0,209	261,0	0,021	296,0	0,920
228,0	0,237	262,0	-0,035	297,0	0,217
229,0	-0,044	263,0	0,112	298,0	0,501
230,0	0,154	264,0	-0,002	299,0	0,478
231,0	0,069	265,0	-0,035		
232,0	0,014	266,0	-0,089		
233,0	0,271	267,0	-0,140		
		268,0	0,261		

A solution of caffeine in acetone of the same concentration as a solution of caffeine in water shows the greatest changes. It absorbs strongly at 202nm, while it absorbs at 227, 228, 230, 233, 243nm. It absorbs best at 286,287nm and 295-299nm.

Absorption of UV rays 286-287 nm is attributed to molecules containing the C=O group (n $\rightarrow \pi^*$). This group also contains acetone and caffeine. In this case, the absorption of shorter wavelengths 202 nm corresponding to the approach $\pi \rightarrow \pi^*$ is very strong.

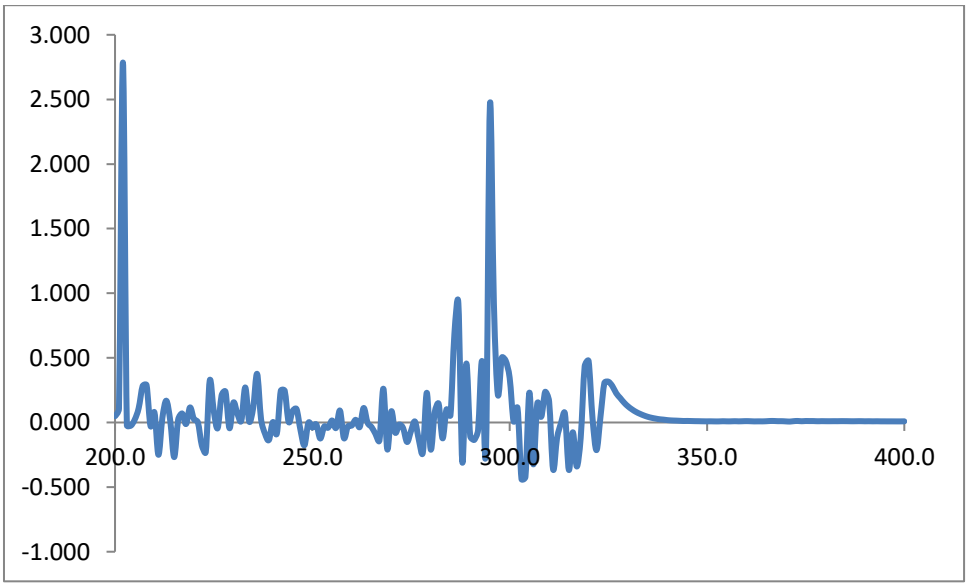

Figure 4. Absorbance of a solution of caffeine in acetone

Table 2. Absorbance of a solution of caffeine in methanol

λ(nm)	A	nm	A	nm	A	nm	A
200,0	0,290	225,0	-0,078	258,0	0,037	301,0	0,211
201,0	0,851	226,0	-0,127	259,0	0,033	302,0	0,143
202,0	-0,138	227,0	-0,055	260,0	0,006	303,0	0,095
203,0	-0,033	228,0	0,200	261,0	0,064	304,0	0,063
204,0	0,405	229,0	0,167	262,0	0,128	305,0	0,040
205,0	-0,185	230,0	0,062	263,0	0,108		
206,0	-0,182	231,0	0,015	264,0	0,066		
207,0	0,026	232,0	-0,048	265,0	0,109		
208,0	-0,058	233,0	0,003	266,0	0,270		
209,0	-0,079	234,0	0,129	267,0	0,322		
210,0	0,056	235,0	0,175	268,0	0,457		
211,0	-0,264	236,0	-0,007	269,0	0,671		
212,0	-0,058	237,0	-0,036	270,0	0,891		
213,0	0,067	238,0	0,045	271,0	1,108		
214,0	-0,085	239,0	0,055	272,0	1,258		
215,0	0,157	240,0	0,095	273,0	1,445		
216,0	0,145	241,0	0,106	274,0	1,639		
217,0	-0,083	242,0	0,126	275,0	1,795		
218,0	-0,058	243,0	0,124	276,0	1,921		
219,0	0,248	244,0	0,149	277,0	1,888		
220,0	0,175	245,0	0,123	278,0	2,084		
221,0	0,050	246,0	0,114	279,0	2,195		
222,0	0,015	247,0	0,036	280,0	2,186		
223,0	-0,114	248,0	-0,026	281,0	2,332		
224,0	-0,081	249,0	0,130	282,0	2,426		
		250,0	0,066	283,0	2,538		
		251,0	0,051	284,0	2,633		
		252,0	-0,032	285,0	2,699		
		253,0	-0,051	286,0	2,763		
		254,0	0,008	287,0	2,648		
		255,0	0,053	288,0	2,745		
		256,0	0,186	289,0	2,881		
		257,0	0,050	290,0	2,661		
				291,0	2,699		
				292,0	2,729		
				293,0	2,483		
				294,0	1,988		
				295,0	1,575		
				296,0	1,171		
				297,0	0,861		
				298,0	0,622		
				299,0	0,436		
				300,0	0,305		

A solution of caffeine in methanol of the same concentration as a solution of caffeine in water absorbs at 200 and 201 nm, then at 228 and 229 nm. Also, absorption in the interval from 256 to 302 nm is present, the highest at 0d 280-295nm.

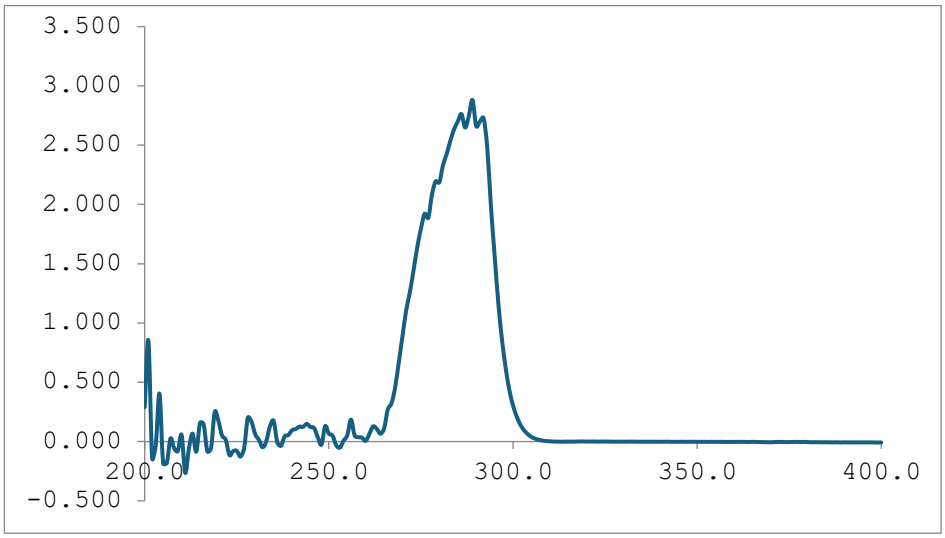

Figure5. Absorbance of a solution of caffeine in methanol

Table 3: Absorbance of a solution of caffeine in water

λ(nm)	A	nm	A	nm	A	nm	A
200,0	2,683	226,0	0,306	251,0	0,026	276,0	1,875
201,0	0,211	227,0	0,191	252,0	0,159	277,0	1,977
202,0	0,036	228,0	0,047	253,0	0,139	278,0	2,167
203,0	0,519	229,0	0,273	254,0	0,031	279,0	2,308
204,0	0,598	230,0	0,129	255,0	0,039	280,0	2,286
205,0	0,239	231,0	0,157	256,0	0,023	281,0	2,308
206,0	0,154	232,0	0,085	257,0	0,072	282,0	2,468
207,0	0,379	233,0	0,175	258,0	0,022	283,0	2,528
208,0	0,292	234,0	0,130	259,0	0,120	284,0	2,518
209,0	0,001	235,0	0,077	260,0	0,138	285,0	2,494
210,0	0,227	236,0	0,057	261,0	0,099	286,0	2,450
211,0	0,117	237,0	0,029	262,0	0,098	287,0	2,220
212,0	-0,039	238,0	-0,025	263,0	0,198	288,0	2,057
213,0	0,424	239,0	0,269	264,0	0,169	289,0	1,797
214,0	-0,131	240,0	0,173	265,0	0,143	290,0	1,513
215,0	0,205	241,0	0,119	266,0	0,151	291,0	1,244
216,0	0,148	242,0	0,108	267,0	0,412	292,0	1,025
217,0	-0,032	243,0	0,021	268,0	0,610	293,0	0,813
218,0	0,073	244,0	0,184	269,0	0,720	294,0	0,618
219,0	0,152	245,0	0,002	270,0	0,964	295,0	0,475
220,0	0,022	246,0	0,099	271,0	1,189	296,0	0,354
221,0	-0,016	247,0	0,016	272,0	1,318	297,0	0,260
222,0	0,075	248,0	0,023	273,0	1,450	298,0	0,188
223,0	0,169	249,0	0,133	274,0	1,707		
224,0	0,088	250,0	0,069	275,0	1,811		
225,0	0,053						

The absorption at 200nm is very strong, while at 201-211nm it is also significant. A solution of caffeine in water absorbs both 226-234 nm and 274-299nm. It should be noted that the highest absorption is shown at 229nm. and 283 nm.

For pure water, the small absorption peak is reported around 275 nm [6]

Absorption at 190 – 220 nm of bond C = O, electron transition $\pi \rightarrow \pi^*$

Absorption at 270-290 nm of bond C = O, electron transition $n \rightarrow \pi^*$

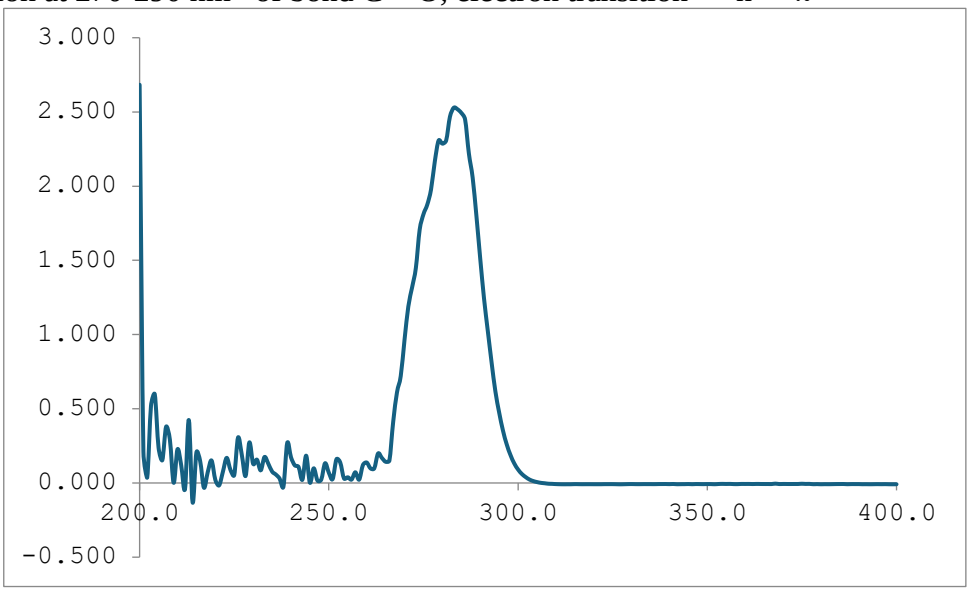

Figure 6. . Absorbance of solution of caffeine in water

Table 4. Absorbance of solution of caffeine in acetic acid

λ(nm)	A	nm	A	nm	A	nm	A
200,0	-0,240	231,0	0,057	264,0	0,068	297,0	0,490
201,0	0,006	232,0	0,017	265,0	0,124	298,0	0,359
202,0	-0,019	233,0	0,000	266,0	0,131	299,0	0,255
203,0	0,060	234,0	-0,060	267,0	0,330	300,0	0,180
204,0	0,010	235,0	-0,062	268,0	0,521	301,0	0,126
205,0	0,080	236,0	-0,078	269,0	0,649	302,0	0,086
206,0	-0,104	237,0	-0,095	270,0	0,934	303,0	0,057
207,0	0,177	238,0	-0,106	271,0	1,129	304,0	0,037
208,0	-0,098	239,0	0,005	272,0	1,283	305,0	0,022
209,0	0,121	240,0	0,024	273,0	1,546		
210,0	-0,002	241,0	0,082	274,0	1,774		
211,0	0,269	242,0	0,166	275,0	1,840		
212,0	-0,088	243,0	0,068	276,0	2,020		
213,0	-0,243	244,0	-0,095	277,0	2,023		
214,0	0,076	245,0	-0,070	278,0	2,121		
215,0	-0,078	246,0	0,075	279,0	2,148		
216,0	0,091	247,0	0,130	280,0	2,249		
217,0	-0,174	248,0	0,023	281,0	2,372		
218,0	0,363	249,0	-0,068	282,0	2,612		
219,0	0,353	250,0	-0,018	283,0	2,514		
220,0	-0,119	251,0	-0,026	284,0	2,502		
221,0	-0,058	252,0	-0,005	285,0	3,004		

222,0	-0,061	253,0	0,090	286,0	2,776
223,0	0,063	254,0	0,057	287,0	2,649
224,0	-0,095	255,0	-0,029	288,0	2,605
225,0	-0,012	256,0	0,113	289,0	2,638
226,0	0,086	257,0	0,097	290,0	2,443
227,0	0,040	258,0	0,056	291,0	2,182
228,0	-0,004	259,0	0,062	292,0	1,838
229,0	0,102	260,0	0,132	293,0	1,480
230,0	0,193	261,0	0,124	294,0	1,133
		262,0	0,081	295,0	0,881
		263,0	0,116	296,0	0,661

A solution of caffeine in acetic acid of the same concentration as a solution of caffeine in water absorbs at 207, 209 and 211 nm, in the interval from 225 nm to 264 nm it does not show absorption. While 265 - 300 nm, absorption is obvious and its maximum is at 285 nm.

Absorption at 190 – 220 nm of bond C = O, electron transition $\pi \rightarrow \pi^*$

Absorption at 265-295 nm of bond C = O, electron transition $n \rightarrow \pi^*$

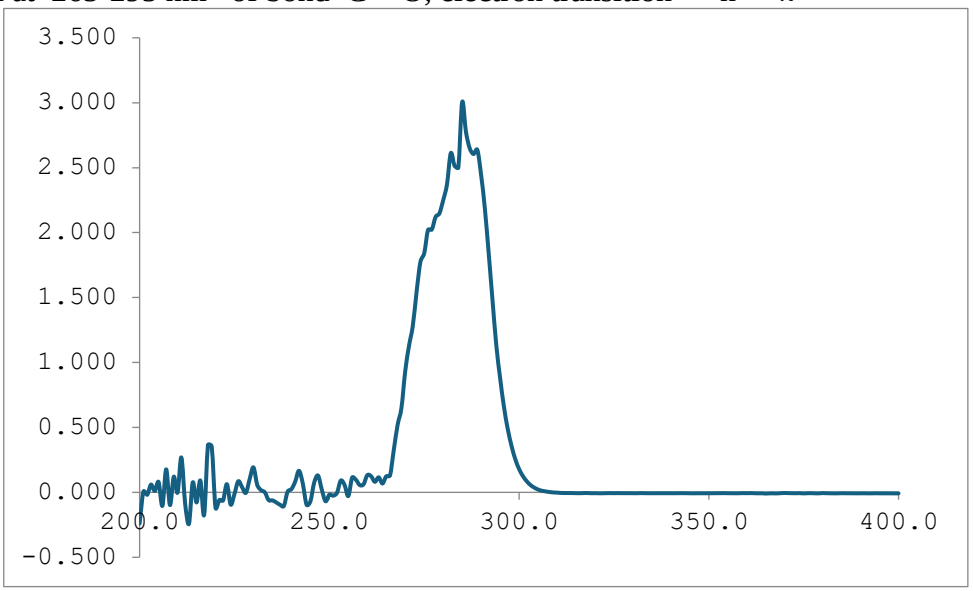

Figure 7. Absorbance of solution of caffeine in acetic acid

Table 5. Absorbance of solution of caffeine in ethyl alcohol

λ(nm)	A	nm	A	nm	A
200,0	-0,219	234,0	0,159	272,0	0,058
201,0	-0,081	235,0	0,182	273,0	0,101
202,0	0,162	236,0	0,091	274,0	0,004
203,0	0,646	237,0	-0,036	275,0	0,202
204,0	0,382	238,0	0,030	276,0	0,269
205,0	0,110	239,0	-0,004	277,0	0,442
206,0	-0,106	240,0	0,038	278,0	0,392
207,0	0,466	241,0	-0,019	279,0	0,509
208,0	-0,012	242,0	-0,071	280,0	0,654
209,0	0,383	243,0	0,076	281,0	0,793
210,0	0,001	244,0	-0,102	282,0	1,012

211,0	0,139	245,0	-0,042	283,0	1,067
212,0	-0,212	246,0	0,019	284,0	1,381
213,0	0,122	247,0	0,089	285,0	1,413
214,0	-0,022	248,0	-0,049	286,0	1,519
215,0	0,043	249,0	0,049	287,0	1,613
216,0	-0,039	250,0	-0,121	288,0	1,734
217,0	0,199	251,0	-0,038	289,0	1,803
218,0	0,378	252,0	-0,092	290,0	1,719
219,0	0,131	253,0	-0,015	291,0	1,424
220,0	-0,095	254,0	0,078	292,0	1,170
221,0	-0,019	255,0	-0,047	293,0	0,902
222,0	0,069	256,0	-0,108	294,0	0,668
223,0	-0,055	257,0	0,123	295,0	0,504
224,0	-0,149	258,0	0,087	296,0	0,367
225,0	0,085	259,0	0,141	297,0	0,265
226,0	0,018	260,0	-0,059	298,0	0,190
227,0	-0,060	261,0	-0,058	299,0	0,132
228,0	-0,100	262,0	0,008	300,0	0,091
229,0	0,139	263,0	-0,041	301,0	0,063
230,0	-0,040	264,0	-0,024	302,0	0,042
231,0	0,179	265,0	0,056	303,0	0,028
232,0	0,060	266,0	0,065		
233,0	0,220	267,0	0,039		
		268,0	0,083		
		269,0	0,067		
		270,0	0,034		
		271,0	0,031		

A solution of caffeine in ethanol of the same concentration as a solution of caffeine in water shows changes in absorption at 202-204 nm, but weaker than the aqueous solution. Absorbs at 217,218,219 nm. Absorbs at 233,234,235 nm. Absorption at 275-299 nm is also present. It absorbs best at 289 nm.

Absorption at 202 – 204 nm of bond C = O, electron transition $\pi \rightarrow \pi^*$

Absorption at 275-299 nm of bond C = O, electron transition $n \rightarrow \pi^*$

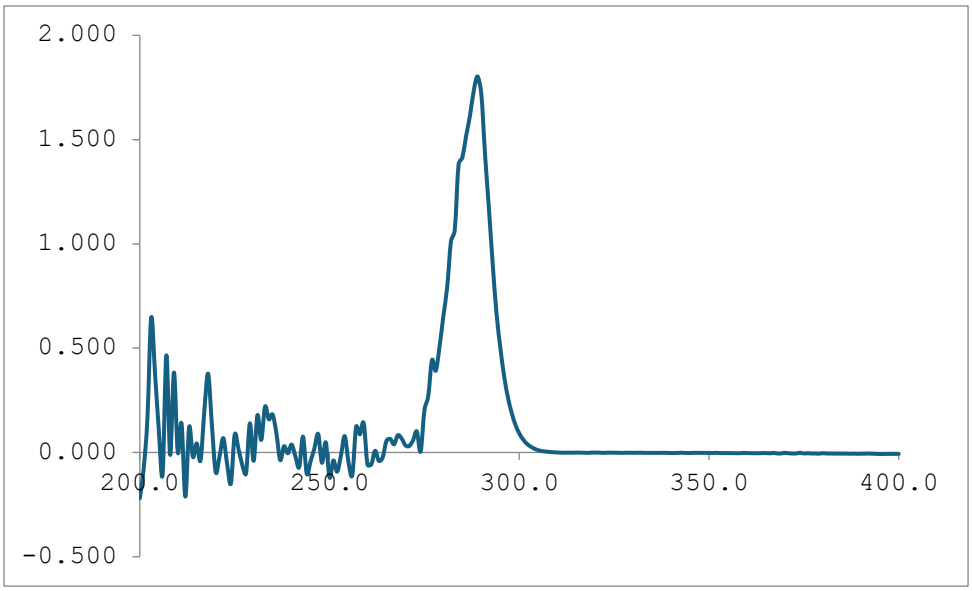

Figure 8. Absorbance of solution of caffeine in ethyl alcohol

Table 7. Absorbance of solution of caffeine in chloroform

λ (nm)	A	nm	A	nm	A
200,0	0,940	234,0	0,083	270,0	0,929
201,0	0,332	235,0	0,067	271,0	1,069
202,0	0,201	236,0	0,252	272,0	1,294
203,0	0,225	237,0	0,150	273,0	1,371
204,0	0,117	238,0	0,172	274,0	1,582
205,0	0,260	239,0	0,066	275,0	1,776
206,0	-0,279	240,0	0,228	276,0	1,929
207,0	0,280	241,0	0,194	277,0	2,142
208,0	0,266	242,0	0,125	278,0	2,150
209,0	-0,059	243,0	0,133	279,0	2,350
210,0	0,446	244,0	-0,007	280,0	2,376
211,0	-0,334	245,0	0,117	281,0	2,423
212,0	-0,012	246,0	0,013	282,0	2,311
213,0	0,293	247,0	-0,066	283,0	2,497
214,0	0,514	248,0	0,134	284,0	2,971
215,0	0,007	249,0	0,099	285,0	2,816
216,0	0,198	250,0	0,003	286,0	2,730
217,0	-0,136	251,0	0,048	287,0	2,616
218,0	0,227	252,0	0,043	288,0	3,265
219,0	-0,017	253,0	-0,037	289,0	2,765
220,0	-0,052	254,0	0,167	290,0	2,716
221,0	0,099	255,0	0,141	291,0	2,843
222,0	0,076	256,0	0,046	292,0	2,645
223,0	0,059	257,0	0,080	293,0	2,527
224,0	-0,048	258,0	0,145	294,0	2,101
225,0	-0,111	259,0	0,082	295,0	1,632
226,0	0,089	260,0	0,151	296,0	1,176

227,0	0,303	261,0	0,125	297,0	0,826
228,0	0,095	262,0	-0,060	298,0	0,570
229,0	-0,026	263,0	0,040	299,0	0,378
230,0	0,054	264,0	0,080	300,0	0,248
231,0	0,281	265,0	0,174	301,0	0,162
232,0	0,130	266,0	0,404	302,0	0,102
233,0	-0,035	267,0	0,336	303,0	0,064
		268,0	0,479		
		269,0	0,617		

A solution of caffeine in chloroform of the same concentration as a solution of caffeine in water absorbs less at 200 nm, while at 227, 231, 236-240 it is present, as well as at 265-302 nm, with the remark that it absorbs best at 284-300 nm

Absorption at 200 – 240 nm of bond C = O, electron transition $\pi \rightarrow \pi^*$

Absorption at 265-300 nm of bond C = O, electron transition $n \rightarrow \pi^*$

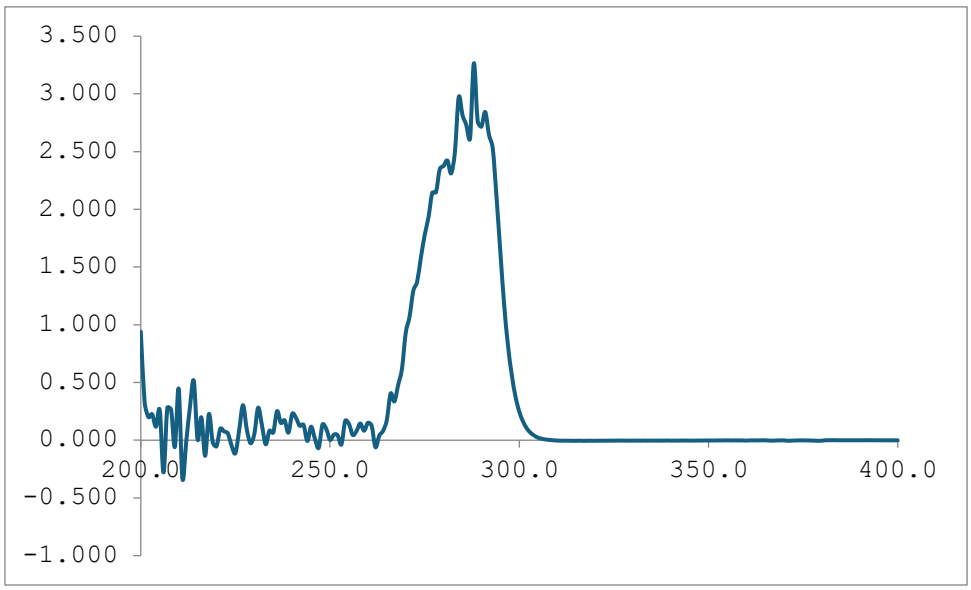

Figure 9. Absorbance of solution of caffeine in chloroform

Table 8. Absorbance of solution of caffeine in ethyl acetate

λ(nm)	**A**	**nm**	**A**	**nm**	**A**
200,0	0,246	237,0	0,007	273,0	1,519
201,0	-0,091	238,0	0,085	274,0	1,685
202,0	-0,003	239,0	0,241	275,0	1,930
203,0	0,039	240,0	0,160	276,0	1,915
204,0	0,026	241,0	0,062	277,0	2,125
205,0	-0,043	242,0	0,023	278,0	2,205
206,0	0,077	243,0	-0,036	279,0	2,354
207,0	0,133	244,0	-0,062	280,0	2,231
208,0	0,059	245,0	-0,005	281,0	2,338
209,0	0,369	246,0	0,161	282,0	2,352
210,0	0,014	247,0	0,007	283,0	2,434
211,0	-0,089	248,0	0,090	284,0	2,616

212,0	0,023	249,0	-0,023	285,0	2,545
213,0	0,025	250,0	-0,057	286,0	2,632
214,0	0,270	251,0	-0,087	287,0	2,654
215,0	0,228	252,0	0,051	288,0	2,660
216,0	0,076	253,0	0,123	289,0	2,524
217,0	0,344	254,0	0,079	290,0	2,206
218,0	-0,031	255,0	-0,023	291,0	1,705
219,0	-0,065	256,0	0,039	292,0	1,297
220,0	0,055	257,0	0,123	293,0	0,905
221,0	0,278	258,0	0,138	294,0	0,594
222,0	0,145	259,0	0,167	295,0	0,396
223,0	0,150	260,0	0,027	296,0	0,252
224,0	0,035	261,0	-0,010	297,0	0,155
225,0	0,006	262,0	0,052	298,0	0,092
226,0	0,205	263,0	0,048	299,0	0,049
227,0	0,068	264,0	0,055	300,0	0,023
228,0	0,122	265,0	0,134	301,0	0,005
229,0	0,037	266,0	0,186	302,0	-0,006
230,0	0,082	267,0	0,258		
231,0	0,122	268,0	0,503		
232,0	-0,011	269,0	0,675		
233,0	-0,111	270,0	0,891		
234,0	0,067	271,0	1,130		
235,0	0,153	272,0	1,328		
236,0	0,093				

A solution of caffeine in ethyl acetate of the same concentration as a solution of caffeine in water absorbs less at 200 nm, weaker than the solution in chloroform, while at 227, 231, 236-240 it is present, as well as at 265-302 nm, with the remark that it absorbs best at 288 nm.

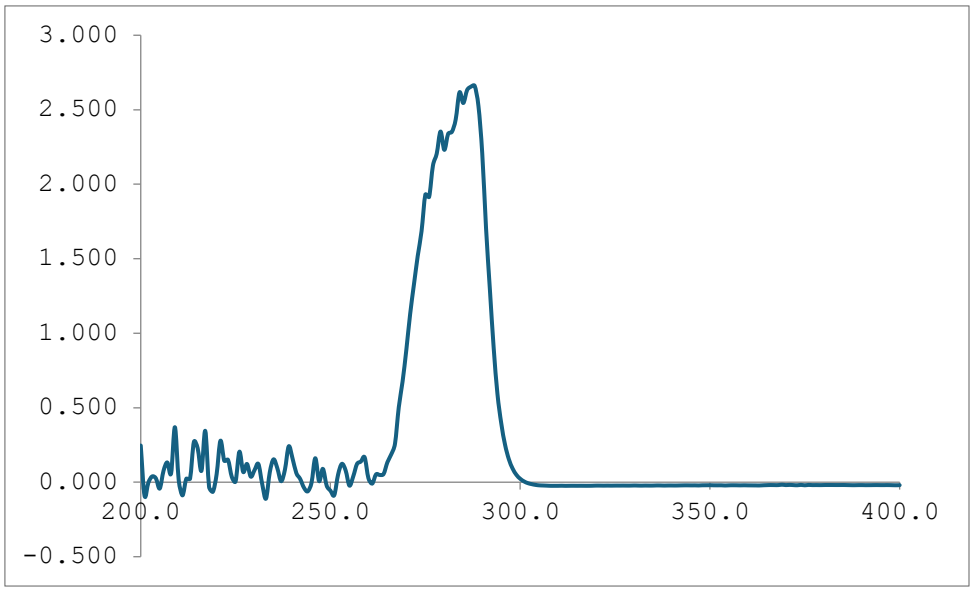

Figure10. Absorbance of a solution of caffeine in ethyl acetate

Conclusion

In an aqueous solution, absorption at 200 nm is very strong, then we have moderate absorption at 203-208 nm, from 268-283 nm it increases permanently, and then starts to decrease from 284-298 nm.
In the methanol solution, the absorption at 200 nm is significantly weaker compared to the aqueous solution. While at 203-208nm, it absorbs only at 204nm it absorbs. In the interval 265-292nm, the absorption increases, and then begins to decrease, but not linearly.
In contrast to the aqueous solution, in the acetone solution, the absorption is strongest at 202 nm. While at 205-208 nm, there is a weaker absorption. While in the interval 263-283 nm, there is no similarity with the absorption of an aqueous solution. It shows strong absorbance at 295 nm.
The acetic acid solution also differs from the aqueous solution, namely, this solution does not absorb at 200nm; it shows weak absorption at 207, 209, and 2011 nm. In the interval from 265-285nm, the absorption increases, after which it begins to decrease and is lowest at 305nm.
The ethanol solution does not absorb at 200nm; it absorbs at 202-205nm, 209, and 2011nm. From 275nm to 289nm, the absorption increases and then starts to decrease and reaching its lowest point at 303nm.
A solution of caffeine in chloroform absorbs at 200nm, but less than an aqueous solution, it also absorbs at 201,202,203,204,205, 207,208, 2010 nm. From 265-284 nm, the absorption increases, and then begins to decrease, reaching its lowest at 303nm.
The caffeine solution in ethyl acetate absorbs 200 nm, but much weaker than the aqueous solution, as well as at 207 and 209 nm. In the range of 268-288 nm, the absorbance increases constantly and then starts to decrease in the range of 288-301 nm.
We can say that acetone has the greatest influence on the UV absorption spectrum of caffeine.

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