

Computational studies of solvent effects on structure and Vibrational Spectra of isoflavonoid 5,7-Dihydroxy-3-(4-hydroxyphenyl)chromen-4-one(Genistein) by *ab initio* HF and DFT methods

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ABSTRACT

*The structural, Vibrational and Raman frequencies of 5,7-Dihydroxy-3-(4-hydroxyphenyl)chromen-4-one (genistein) has been studied in different solvents (toluene, ethanol, and water) using by *ab initio* Hartree–Fock (HF) and at the Becke-3-Lee-Yang-Parr (B3LYP) density functional theory (DFT) PCM method at the 6-311G basis set. The influence of these solvents on the optimized geometry, frequency, Mullikan charge distribution scheme and were studied. The thermodynamic functions of the titled compound have been computed at HF/6-311G and B3LYP/6-311G levels of theory.*

Key words: genistein, HF, DFT, vibrational and Raman frequencies, Mullikan charge, thermodynamic properties.

INTRODUCTION

Almost all flavone derivatives have been identified from botanical sources[1]. They are commonly found in vascular plants as phenyl-benzopyrones with different basic structures. Many of the flavonoids found in plants exist as sugar derivatives (glycosides)[2]. Owing to their active role in photo sensitization, energy transport and cellular metabolism, many of flavone derivatives are ingredients for biochemical and pharmacological products used as human diet supplements[3]. Flavones and flavonols found in plants are yellow compounds and are the main components of a number of natural dyes used in textile dyeing since antiquity. Fustic, young fustic, quercitron, Persian berries, weld, dyer's broom and saw wort, which are important yellow dyes, all contain flavonoids such as quercetin, luteolin, fisetin, rhamnetin, genistein and morin[4].

Genistein, the principal soy isoflavone, is a molecule of great interest as a lead compound in anticancer drug design or as an innovative chemotherapeutic agent. Early works showed that genistein acted as an inhibitor of the tyrosine-specific protein kinases of the epidermal growth factor (EGF) receptor [5], and also inhibited the activity of topoisomerases [6]. Recent studies suggest that genistein potentially inhibits proliferation of various cancer cells [7] and induces cell differentiation [8] and apoptosis [9,10]. Meanwhile, genistein also exhibits antiangiogenic [11] and antioxidant activities [12] that are important for cancer prevention. One of the most important advantages of genistein is its low toxicity in comparison with many current chemotherapeutic drugs [13]. However, the clinical utility of genistein is hindered by some of its disadvantages, including poor solubility in water, insufficient targeting of cancer cells, rapid *in vivo* metabolism and excretion, and low serum level after oral administration [14]. One obvious strategy to overcome these problems is to synthesize structurally modified genistein derivatives. A large amount of synthetic genistein analogues have been prepared in the last decade but yet meet the requirements for practical applications [14, 15]. An alternative strategy to the labor intensive organic synthesis is to design

appropriate drug delivery system that may overcome the shortcoming of genistein and greatly improve its performance in anticancer therapy [16, 17].

A number of papers have recently appeared in the literature concerning the calculation of vibrational assignments by quantum-chemistry methods [18]. These papers indicate that geometry optimization is a crucial factor in an accurate determination of computed vibrational frequencies. Moreover, it is known that the density functional theory (DFT) adequately takes into account electron correlation contributions, which are especially important in systems containing extensive electron conjugation and/or electron lone pairs. However, considering that as molecular size increases, computing-time also increases. To optimize computing-time the DFT level was used. It was proposed that the single-point calculation of magnetic shielding by DFT methods was combined with a fast and reliable geometry-optimization procedure at the molecular mechanics level. In most cases, in order to take into account correlation effects, post-Hartree-Fock calculations of organic molecules have been performed using (i) Møller-Plesset perturbation methods, which are very time consuming and hence applicable only to small molecular systems, and (ii) density functional theory (DFT) methods, which usually provide significant results at a relatively low computational cost. *ab initio* calculations were performed as an aid in assigning the normal modes to which the spectral lines correspond. DFT has proven to be the best theoretical approach for the study of flavone and derivatives [19,20], and for that reason we chose to use it here. Furthermore, good normal mode assignments are useful in extrapolating possible spectral changes to other flavone derivatives.

Literature survey reveals that to the best of our knowledge, no *ab initio* HF/DFT frequency calculations of genistein in different solvents have been reported so far. In this study, we have investigated the structural and electronic properties of genistein molecule theoretically, by performing *ab initio* calculations because of biological and medical importance of title compound.

MATERIALS AND METHODS

Computational Details:

The entire calculations performed at HF and DFT (B3LYP) levels on personal computer using Gaussian 09 W Revision B.01, program package [21]. Initial geometry generated from standard geometrical parameters minimized without any constraint in the potential energy surface at HF level, adopting the standard 6-31G basis set. The optimized structural parameters used in the vibrational wave number calculation at the HF and DFT levels to characterize all stationary points as minima, i.e. the geometry optimization resulted in a planar geometry and no imaginary frequencies were observed in the calculated spectrum. In addition the effects of three solvents, toluene, ethanol and water were studied by means of the self-consistent reaction-field (SCRF) method based on PCM developed by Tomasi and coworkers [18]. It is one of the most widely used approaches. In this model, a solute is considered inside a cavity and the solvent as a structure less medium characterized by some parameters such as its dielectric constant, molar volume and polarizability. This consideration can substantially improve the simulation results for the electronic or vibrational spectroscopy of real molecular systems [19,20]. Finally, the calculated normal mode vibrational wave numbers provide thermodynamic properties also through the principle of statistical mechanics. Vibrational frequencies were computed on the optimized geometries in all media. By combining the results of the Gauss View (5.0) program with symmetry considerations, vibrational frequency assignments are made with a high degree of accuracy. No scale factor was used in the calculated frequencies.

RESULTS AND DISCUSSION

The Genistein assumed as C_s point group of symmetry and the optimized geometrical parameters of the title compound are calculated by *ab initio* HF and DFT(B3LYP) levels with the 6-311G basis set. The labeling of atoms in genistein is given in Figure 1. We designate the benzo ring in the chromone system as Ring A, the phenyl ring as Ring B and the pyrone ring as Ring C. The most optimized bond lengths and bond angles of this compound were calculated in gas phase and in toluene, ethanol and water, in order of increasing dielectric constants (1.0, 2.379, 24.55 and 78.39, respectively) and shown in Table 1. Comparing bond lengths of B3LYP with those of HF as a whole, the formers are on higher side than the later; because of it is well known that the DFT(B3LYP) method adequately takes into account electron correlation contributions which are especially important in systems containing extensive electron conjugation and/or electron lone pairs. As the result of solvent effect, the calculated geometries of genistein in solutions have some differences, but ethanol and water are almost same values, because of both solvents are polarities.

Table 1 Interatomic bond distances (Å) and bond angles(°) for the genistein molecule

S.No	Å	In gas phase		In toluene		In alcohol		In water	
		HF 6-311G	DFT 6-311G	HF 6-311G	DFT 6-311G	HF 6-311G	DFT 6-311G	HF 6-311G	DFT 6-311G
1	C1-C2	1.3332	1.3567	1.3337	1.3572	1.3346	1.3577	1.3347	1.3578
2	C1-O13	1.3605	1.3788	1.3597	1.3782	1.3579	1.3767	1.3577	1.3765
3	C1-H21	1.065	1.0768	1.0649	1.0767	1.0648	1.0765	1.0647	1.0765
4	C2-C3	1.4688	1.4696	1.4662	1.4674	1.4625	1.4642	1.4621	1.4638
5	C2-C14	1.4841	1.4825	1.4848	1.483	1.4857	1.4837	1.4857	1.4838
6	C3-O4	1.2396	1.2762	1.2427	1.2788	1.2471	1.2825	1.2476	1.2829
7	C3-C5	1.4528	1.4504	1.4521	1.4496	1.4506	1.4483	1.4504	1.4482
8	O4-H22	1.8591	1.7194	1.8515	1.7098	1.8415	1.6998	1.8401	1.6986
9	C5-C6	1.4136	1.4288	1.4131	1.4282	1.4124	1.4272	1.4123	1.4271
10	C5-C12	1.3919	1.406	1.3922	1.4064	1.3925	1.407	1.3925	1.4071
11	C6-O7	1.349	1.3641	1.3522	1.3675	1.3558	1.3716	1.3561	1.372
12	C6-C8	1.3768	1.3894	1.3757	1.3884	1.3743	1.387	1.3741	1.3868
13	O7-H22	0.9555	0.9979	0.956	0.9991	0.9566	1.0002	0.9566	1.0004
14	C8-C9	1.3864	1.3973	1.3883	1.3992	1.3906	1.4014	1.3908	1.4017
15	C8-H23	1.0659	1.0777	1.0662	1.078	1.0666	1.0783	1.0666	1.0784
16	C9-O10	1.3629	1.385	1.3619	1.3834	1.3609	1.3816	1.3608	1.3814
17	C9-C11	1.3859	1.3993	1.3851	1.3988	1.3841	1.3982	1.384	1.3982
18	O10-H24	0.946	0.9719	0.9469	0.9724	0.9479	0.9729	0.948	0.9729
19	C11-C12	1.3774	1.3872	1.3778	1.3872	1.3783	1.3873	1.3783	1.3873
20	C11-H25	1.0682	1.08	1.0679	1.0796	1.0675	1.0792	1.0675	1.0792
21	C12-O13	1.3673	1.3942	1.3669	1.3937	1.366	1.393	1.3658	1.3929
22	C14-C15	1.3888	1.4053	1.3891	1.4055	1.3898	1.4057	1.3899	1.4057
23	C14-C20	1.3975	1.4096	1.3969	1.4093	1.3964	1.4089	1.3964	1.4089
24	C15-C16	1.3883	1.3951	1.3886	1.3954	1.389	1.3958	1.389	1.3959
25	C15-H26	1.071	1.0822	1.0707	1.082	1.0704	1.0817	1.0703	1.0816
26	C16-C17	1.381	1.3961	1.3814	1.3964	1.382	1.3969	1.3821	1.397
27	C16-H27	1.0718	1.0835	1.0713	1.0829	1.0708	1.0822	1.0707	1.0821
28	C17-O18	1.3747	1.3929	1.3756	1.393	1.3763	1.3931	1.3764	1.3931
29	C17-C19	1.3864	1.3969	1.3868	1.3975	1.3873	1.3984	1.3873	1.3985
30	O18-H28	0.9457	0.9717	0.9465	0.9722	0.9472	0.9725	0.9473	0.9726
31	C19-C20	1.379	1.3901	1.3798	1.3907	1.381	1.3916	1.3811	1.3917
32	C19-H29	1.0685	1.08	1.0687	1.0801	1.069	1.0804	1.0691	1.0805
33	C20-H30	1.0677	1.0778	1.0683	1.078	1.069	1.0786	1.069	1.0787
Bond angles(°)									
1	C2-C1-O13	124.35	124.77	124.21	124.64	124.02	124.46	124.00	124.44
2	C2-C1-H21	124.58	124.79	124.61	124.84	124.67	124.89	124.67	124.89
3	O13-C1-H21	111.08	110.43	111.19	110.52	111.31	110.66	111.33	110.67
4	C1-C2-C3	118.21	118.13	118.31	118.21	118.41	118.34	118.42	118.35
5	C1-C2-C14	120.90	120.25	120.79	120.17	120.79	120.11	120.80	120.10
6	C3-C2-C14	120.89	121.62	120.89	121.62	120.79	121.55	120.76	121.54
7	C2-C3-O4	121.90	122.08	121.96	122.10	122.00	122.12	122.00	122.13
8	C2-C3-C5	116.63	116.92	116.67	116.98	116.75	117.02	116.76	117.02
9	O4-C3-C5	121.47	121.00	121.37	120.92	121.25	120.86	121.24	120.85
10	C3-C5-C6	122.44	121.77	122.57	121.88	122.72	122.02	122.73	122.03
11	C3-C5-C12	120.32	121.02	120.29	121.00	120.23	120.96	120.23	120.95
12	C6-C5-C12	117.24	117.21	117.14	117.12	117.05	117.02	117.04	117.01
13	C5-C6-O7	121.73	120.73	121.56	120.52	121.38	120.29	121.36	120.27
14	C5-C6-C8	120.68	120.51	120.78	120.61	120.86	120.71	120.87	120.72
15	O7-C6-C8	117.59	118.76	117.66	118.87	117.76	119.00	117.77	119.01
16	C6-O7-H22	113.63	109.29	113.29	108.94	112.85	108.54	112.80	108.50
17	C6-C8-C9	119.51	119.62	119.51	119.61	119.53	119.62	119.53	119.62
18	C6-C8-H23	120.08	120.08	120.15	120.15	120.22	120.23	120.22	120.24
19	C9-C8-H23	120.41	120.31	120.34	120.24	120.26	120.15	120.25	120.14
20	C8-C9-O10	116.54	116.26	116.49	116.22	116.34	116.10	116.32	116.09
21	C8-C9-C11	121.83	121.89	121.76	121.82	121.69	121.73	121.69	121.73
22	O10-C9-C11	121.63	121.85	121.74	121.96	121.97	122.16	121.99	122.19
23	C9-O10-H24	115.15	112.46	115.30	112.74	115.47	113.06	115.48	113.09
24	C9-C11-C12	117.51	117.46	117.51	117.47	117.50	117.46	117.49	117.46
25	C9-C11-H25	122.71	122.69	122.59	122.57	122.49	122.46	122.48	122.45
26	C12-C11-H25	119.78	119.84	119.90	119.96	120.02	120.08	120.03	120.09
27	C5-C12-C11	123.23	123.31	123.30	123.37	123.38	123.45	123.38	123.46

28	C5-C12-O13	119.55	119.54	119.50	119.47	119.43	119.40	119.42	119.39
29	C11-C12-O13	117.22	117.14	117.20	117.15	117.19	117.15	117.20	117.15
30	C1-C13-C12	120.92	119.57	121.01	119.68	121.15	119.82	121.17	119.83
31	C2-C14-C15	120.52	120.37	120.57	120.40	120.69	120.47	120.70	120.48
32	C2-C14-C20	121.34	121.56	121.23	121.49	121.06	121.37	121.04	121.35
33	C15-C14-C20	118.14	118.07	118.19	118.10	118.24	118.15	118.24	118.16
34	C14-C15-C16	121.26	121.27	121.23	121.27	121.21	121.26	121.21	121.26
35	C14-C15-H26	119.81	119.77	119.81	119.80	119.81	119.80	119.81	119.80
36	C16-C15-H26	118.92	118.93	118.95	118.91	118.97	118.93	118.98	118.94
37	C15-C16-C17	119.47	119.53	119.46	119.52	119.43	119.50	119.43	119.50
38	C15-C16-H27	120.03	120.03	120.06	120.06	120.11	120.07	120.11	120.07
39	C17-C16-H27	120.50	120.44	120.48	120.41	120.45	120.42	120.45	120.42
40	C16-C17-O18	122.70	122.89	122.60	122.83	122.57	122.83	122.57	122.84
41	C16-C17-C19	120.30	120.21	120.33	120.22	120.37	120.24	120.38	120.24
42	O18-C17-C19	117.01	116.90	117.07	116.95	117.06	116.93	117.06	116.92
43	C17-O18-H28	114.71	112.09	114.68	112.22	114.67	112.39	114.68	112.40
44	C17-C19-C20	119.82	119.96	119.76	119.92	119.72	119.89	119.72	119.88
45	C17-C19-H29	118.80	118.74	118.97	118.89	119.16	119.05	119.18	119.06
46	C20-C19-H29	121.38	121.30	121.26	121.19	121.12	121.06	121.10	121.05
47	C14-C20-C19	121.01	120.96	121.02	120.97	121.02	120.96	121.02	120.96
48	C14-C20-H30	119.68	119.50	119.72	119.59	119.76	119.65	119.77	119.65
49	C19-C20-H30	119.30	119.54	119.26	119.44	119.22	119.39	119.21	119.39

2. Table. Vibrational frequencies (cm^{-1}), IR intensities and Raman intensities of genistein in various solvents, the frequency shifts (Δ) in different solvents with respect to gas phase and their assignments HF/6-311G method.

mode NO	Assignments	In gas phase			In toluene			In ethanol			In water		
		Fre	IR	R	Δ	IR	R	Δ	IR	R	Δ	IR	R
1	-----	37	0	1	0	1	14	-1	0	5	-1	1	7
2	-----	48	0	9	9	0	2	5	1	19	6	1	18
3	-----	67	0	2	0	0	3	2	1	4	2	1	5
4	-----	113	0	0	0	0	1	0	1	1	1	1	1
5	-----	139	0	1	1	0	1	-3	0	1	-3	0	1
6	-----	202	1	0	1	1	0	3	1	0	3	1	0
7	-----	231	0	0	0	1	0	1	1	1	1	1	1
8	-----	239	0	3	1	0	4	2	1	5	2	1	5
9	Ring A,B,C ip stretch	266	4	1	0	4	2	1	5	3	1	5	3
10	Ring A,B,C, C-OH deformation	306	9	1	-2	2	3	-2	7	6	-2	8	6
11	Ring A,C-OH deformation	322	136	2	-5	22	1	-5	1	3	-5	2	4
12	Ring A,B,C, deformation ,O-H out of plane	326	49	3	-3	199	6	-11	268	4	-10	274	4
13	O18-H28 out of plane	373	2	1	-2	5	1	0	10	1	0	10	1
14	O-H out of plane	391	180	3	-5	31	1	-6	34	1	-7	35	1
15	O10-H24 out of plane bend	394	31	1	-17	215	4	-9	266	4	-7	273	4
16	Ring B,O18-H28,C=O out of plane	427	2	5	0	1	7	1	1	8	1	2	8
17	Ring A,B,C deformation	442	5	2	0	7	3	0	9	5	0	9	5
18	Ring B C-C ,O18-H28 stretch	459	9	1	-1	10	2	0	14	3	0	14	3
19	Ring B C-C In plane stretch	478	1	1	1	2	1	-1	2	2	-1	2	2
20	Ring B, O-H out of plane bend	523	3	1	-3	4	1	-7	14	2	-8	18	3
21	Ring A,B out of plane deformation	535	29	3	1	36	4	1	37	5	1	35	5
22	Ring A,B,C,C-C deformation	561	23	1	0	29	1	0	37	1	0	38	1
23	Ring A,B,C, C-C deformation	591	33	1	2	42	2	2	54	3	2	55	4
24	Ring A,B,C deformation	621	40	4	-1	48	6	-2	51	9	-2	51	9
25	Ring A,B, C-C In plane bend	635	1	19	0	2	30	0	2	46	0	2	47
26	Ring A breathing	672	6	2	0	9	2	1	13	3	1	14	3
27	Ring A,B,C deformation	693	0	0	0	1	0	2	64	1	3	119	1
28	Ring A,B rock	696	16	3	-1	19	6	-1	25	9	0	33	9
29	Ring a,B,C C-C,C-H out of plane	714	17	4	1	38	7	14	167	6	16	125	5
30	Ring A,B deformation	721	4	5	1	7	6	3	23	14	3	20	16
31	Ring B deformation	760	42	2	18	167	1	38	21	0	39	12	0
32	Ring B,C-H out of plane, C-H bend	768	127	0	3	7	2	1	3	3	1	3	4
33	Ring B C-H out of plane, C=C stretch	811	4	2	0	5	3	-1	6	6	-1	6	6
34	Ring A ip, C=C stretch	852	20	20	0	29	28	0	46	37	0	48	38
35	C11-H25 out of plane bend	889	47	4	-1	63	6	-2	110	8	-1	118	8
36	C16-H27,C15-H26 out of plane bend	895	10	16	2	12	22	3	16	32	3	16	33
37	Ring B breathing	915	123	0	0	134	0	4	135	1	5	133	2
38	O7-H22, C8-H30 out of plane bend	935	30	3	-2	28	4	-6	1	0	-5	1	0

39	C19-H29, C20-H30 out of plane bend	947	2	0	2	1	0	6	17	3	5	14	3
40	C-H,O-H out of plane bend	953	39	11	2	54	15	3	84	21	3	89	22
41	Ring B,CC bend,COC strip	964	48	5	1	51	9	3	53	18	3	54	19
42	Ring B C-H out of plane ben, C1-H21, bend	1059	9	9	0	15	25	1	33	38	1	36	40
43	C16-H27,C15-H26 out of plane bend	1061	6	14	-3	8	8	-11	10	12	-12	10	13
44	Ring a Trigonal stretch	1079	1	6	-2	2	8	-7	2	10	-8	2	10
45	Ring B CH out of plane bend	1112	0	0	0	0	0	-2	237	8	-2	248	9
46	Ring A,B Trigonal stretch	1120	72	2	2	141	4	3	1	0	3	1	0
47	Ring B trigonal stretch	1125	44	2	1	36	2	3	29	2	3	29	2
48	Ring A B C quinoid stretch, C12-O13 St	1152	12	5	0	14	10	-1	14	18	-1	14	19
49	Ring B CH bend(out of phase),OH bend	1220	22	1	0	20	1	1	23	2	1	23	2
50	Ring B CH In plane bend ,O18-H28,O10-H24 bend	1237	220	6	2	242	14	5	269	32	6	272	35
51	O18-H28 bend	1245	101	6	0	136	10	1	181	13	1	186	13
52	Ring A b C CH,O18-H28 In plane bend	1274	107	11	-1	147	19	-2	194	28	-2	198	29
53	O18-H24,C11-H25 In plane bend	1304	169	18	0	253	21	2	342	22	2	350	22
54	Ring B CH In plane bend	1309	39	5	1	24	6	3	20	9	3	21	9
55	O7-H22,O10-H24,C8—H23 in plane bend	1337	647	3	1	767	3	4	861	5	4	868	5
56	Ring B CH In plane bend, C2-C14 St	1351	3	1	1	2	4	4	11	14	5	12	15
57	Ring B CH In plane ben, C17-O18 stretch	1360	27	2	0	29	3	1	29	5	2	29	5
58	O7-H22 bend,CH In plane bend	1387	34	13	2	28	19	4	23	26	4	23	27
59	Ring B CH, C1-H21, In plane bend, CC stretch	1405	25	25	0	42	29	1	77	25	1	82	25
60	C6-O7 stretch,O7-H22 bend,C11-H25 bend	1440	85	53	2	94	93	4	99	159	4	100	166
61	C1-H21 ip bend, Ring B CH in plane bend	1475	212	18	0	252	29	0	352	68	1	363	74
62	O18-H28 bend, Ring B CH in plane bend	1484	25	22	0	44	46	1	38	66	1	37	69
63	OH,CH ip ben, Ring A B C ,CC bend	1503	34	11	3	46	13	5	56	20	5	57	21
64	O7-H22 O10-H24 in plane bend	1537	116	19	2	155	36	3	193	66	3	197	69
65	O18-H28 bend Ring B CH in plane bend	1579	5	1	1	6	2	3	6	4	3	6	4
66	O7-H22,O10-H24, CH in plane bend,C=O stretch	1617	131	24	4	163	45	9	220	91	10	230	98
67	C=O st,O7-H22 bend, Ring A CC stretch	1654	103	11	2	142	20	7	212	38	7	222	40
68	Ring B CH in plane bend	1688	114	8	2	132	9	4	150	12	4	150	12
69	C=O St,O7-H22 bend ip bend, C1=C2 stretch	1745	126	26	7	86	38	22	215	47	24	234	48
70	C=O,C1=c2 st,O7-H22 ,O10-H24 bend	1760	95	3	7	334	14	14	421	59	14	422	65
71	Ring A B quinoid stretch	1766	146	3	3	95	6	5	93	13	5	95	14
72	C1=C2 stretch, Ring A B ,CCC stretch	1799	72	37	5	113	59	12	171	106	13	178	111
73	C1=C2 stretch	1807	213	143	3	231	190	7	247	221	7	249	222
74	O7-H22 bend, Ring A quinoid stretch	1836	709	198	9	874	310	19	1047	448	19	1063	462
75	C16-H27 , C15-H26) asymmetric stretch	3325	24	72	-8	22	84	-15	21	109	-15	21	111
76	C16-H27 ,C15-H26 stretch	3349	17	90	-5	21	142	-10	26	197	-10	23	136
77	C19-H29 , C20-H30 asymmetric stretch	3373	7	72	6	10	89	12	12	123	13	16	192
78	C11-H25 ,O7-H22 stretch	3379	2	96	-6	2	139	-1	17	322	0	18	341
79	C19-H29 ,C20-H30 stretch	3393	5	113	7	9	187	4	1	198	3	1	204
80	C8-H23, stretch	3415	0	118	5	0	163	12	1	227	12	2	235
81	C1-H21 stretch	3425	8	71	-1	7	108	-5	5	160	-5	5	166
82	O7-H22 stretch	3883	223	37	14	290	54	31	371	74	33	379	76
83	O18-H28 stretch	4086	112	129	13	151	169	28	197	214	30	202	218
84	O10-H24 stretch	4089	83	141	8	112	166	20	143	190	22	146	193

According to molecular structure of genistein have mainly three different bond lengths between different atom such as C-C, C-O, and O-H .Fig.2 shows the bond lengths between C-C. The bond length between C1-C2 has low value, when compared to other C-C bonds in the molecule, i.e the C1-C2 represent double bond in the molecule. The bonds C2-C3, C2-C14 and C3-C5 are showing higher values comparison of other all C-C bonds, because of these bonds represents C-C single bonds in the molecule. The other aromatic C=C bonds are showing different values depending upon the substituents. C5-C6 bond length is higher than other the aromatic C=C bonds, due to the reason C5 and C6 attached to carbonyl carbon (C3=O4) and hydroxyl group (O7-H22) respectively and C6-O7-H22 involve in hydrogen bond with O14 atom.

Fig.3. shows the calculated bond lengths between O-H in different solvents and HF and DFT methods. An O---H separation that is less than the sum of O and H vanderwaals radii (0.14 and 0.12 nm ,respectively) is assigned to the inteamolecular hydrogen bonding[22].One intramolecular hydrogen bond is observed: the oxygen of the carbonyl group and the hydrogen of the 7- OH; the distance is show in table 1 in different media and different methods. The

O7-H22 bond length is have higher value than the O8-H28 and O18-H22 bond lengths in both methods and all solvents, because of the O7-H22 bond is involve in intramolecular hydrogen bond with O4 atom shown in fig.1. The bond angles between C6-O7-H22 is less than the other bond angles between C17-O10-H28 and C9-O10-H24 .

3. Table. Vibrational frequencies (cm^{-1}), IR intensities and Raman intensities of genistein in various solvents , the frequency shifts(Δ) in different solvents with respect to gas phase and their assignments DFT(B3LYP) /6-311G method.

mode NO	Assignments	In gas phase			In toluene			In ethanol			In water		
		Fre	IR	R	Δ	IR	R	Δ	IR	R	Δ	IR	R
1	-----	35	0	1	-2	0	2	0	1	3	0	1	3
2	-----	51	0	11	0	1	18	6	1	29	6	1	30
3	-----	67	0	3	1	0	4	3	1	5	3	1	5
4	-----	112	0	1	-1	0	1	1	0	2	1	0	2
5	-----	132	0	2	-2	0	3	0	0	4	1	0	4
6	-----	191	0	0	1	0	0	3	0	0	3	0	0
7	-----	216	0	0	0	0	0	1	0	1	1	0	1
8	-----	227	0	3	1	0	3	2	1	3	3	1	4
9	Ring A,B,C ip stretch	245	2	1	0	2	2	0	3	3	1	3	3
10	Ring A,B,C, C-OH deformation	285	1	1	-1	1	1	-2	2	3	-2	2	3
11	Ring A,C-OH deformation	298	0	2	-1	1	3	0	1	5	0	1	5
12	Ring A,B,C, deformation ,O-H out of plane	345	0	1	-2	2	1	-2	3	2	-2	3	2
13	O18-H28 out of plane	360	150	4	-2	165	5	-3	224	5	-6	230	5
14	O-H out of plane	375	35	1	-2	51	1	-1	42	2	0	43	2
15	O10-H24 out of plane bend	392	144	4	-11	4	9	-10	6	12	-9	6	12
16	Ring B,O18-H28,C=O out of plane	403	6	7	-10	12	5	-10	30	7	-10	46	7
17	Ring A,B,C deformation	412	4	3	-6	162	4	-4	187	4	-3	177	5
18	Ring B C-C ,O18-H28 stretch	429	7	3	-2	7	6	-2	14	7	-1	15	6
19	Ring B C-C In plane stretch	435	2	5	-1	7	7	0	8	12	0	7	12
20	Ring B, O-H out of plane bend	476	4	2	-3	6	3	-6	6	4	-6	7	4
21	Ring A,B out of plane deformation	498	27	4	0	35	6	1	46	8	1	47	8
22	Ring A,B,C,C-C deformation	523	16	0	0	21	0	0	28	1	0	28	1
23	Ring A,B,C, C-C deformation	543	18	1	0	23	1	1	30	1	1	31	1
24	Ring A,B,C deformation	571	53	5	0	66	9	-1	78	15	-1	79	16
25	Ring A,B, C-C In plane bend	591	4	24	0	5	38	0	6	62	0	6	65
26	Ring A breathing	617	2	0	-1	1	0	-1	1	0	-1	1	0
27	Ring A,B,C deformation	626	6	4	0	8	5	1	12	6	1	13	6
28	Ring A,B rock	638	10	0	-1	11	1	-2	12	2	-2	13	2
29	Ring a,B,C C-C,C-H out of plane	646	8	4	-1	11	8	-1	14	15	-1	14	16
30	Ring A,B deformation	664	0	7	0	1	11	-1	2	17	-1	2	18
31	Ring B deformation	675	3	3	0	4	4	-1	3	6	-1	3	6
32	Ring B,C-H out of plane, C-H bend	735	5	1	-1	7	2	-1	8	4	-1	8	4
33	Ring B C-H out of plane, C=C stretch	785	10	3	-1	12	6	-2	20	22	-2	22	27
34	Ring A ip, C=C stretch	791	14	67	0	18	103	0	21	140	0	21	140
35	C11-H25 out of plane bend	813	85	0	-5	123	1	-1	310	1	1	317	1
36	C16-H27,C15-H26 out of plane bend	831	18	7	-1	14	13	5	1	2	5	5	2
37	Ring B breathing	832	12	11	-2	12	13	2	16	21	2	16	21
38	O7-H22, C8-H30 out of plane bend	848	109	1	10	127	1	11	22	16	10	20	16
39	C19-H29, C20-H30 out of plane bend	861	41	1	3	49	1	7	1	0	7	1	0
40	C-H,O-H out of plane bend	865	35	0	6	22	0	10	82	3	10	86	3
41	Ring B,CC bend,COC strip	891	20	24	0	25	38	1	29	58	1	29	60
42	Ring B C-H out of plane ben, C1-H21, bend	917	9	5	-5	12	8	-10	15	14	-11	15	14
43	C16-H27,C15-H26 out of plane bend	958	0	1	-5	1	1	-9	3	2	-9	3	2
44	Ring a Trigonal stretch	985	14	32	1	21	44	2	32	57	2	34	58
45	Ring B CH out of plane bend	990	1	0	1	2	1	-1	2	4	-1	2	5
46	Ring A,B Trigonal stretch	1039	72	4	2	126	8	5	203	15	6	211	16
47	Ring B trigonal stretch	1044	16	3	0	12	4	2	10	4	2	10	4
48	Ring A B C quinoid stretch, C12-O13 St	1063	23	5	-1	30	9	-2	39	16	-2	40	17
49	Ring B CH bend(out of phase),OH bend	1138	141	5	0	192	22	4	270	50	5	284	53
50	Ring B CH In plane bend ,O18-H28,O10-H24 bend	1145	49	13	-1	30	12	3	26	19	4	25	22
51	O18-H28 bend	1179	590	53	1	749	90	3	881	132	3	886	135
52	Ring A b C CH,O18-H28 In plane bend	1188	13	4	0	23	7	1	61	12	1	70	13
53	O18-H24,C11-H25 In plane bend	1211	13	30	-2	15	39	-2	20	50	-2	21	51
54	Ring B CH In plane bend	1223	23	12	0	32	21	2	25	26	3	22	26
55	O7-H22,O10-H24,C8—H23 in plane bend	1256	250	6	-1	337	7	1	390	2	2	388	2
56	Ring B CH In plane bend, C2-C14 St	1273	70	47	0	61	71	0	85	109	1	92	113

57	Ring B CH In plane ben, C17-O18 stretch	1289	14	5	2	12	9	5	9	16	5	8	17
58	O7-H22 bend,CH In plane bend	1328	126	90	1	165	118	3	229	143	3	237	145
59	Ring B CH, C1-H21, In plane bend, CC stretch	1332	14	86	0	23	183	2	36	318	2	37	332
60	C6-O7 stretch,O7-H22 bend,C11-H25 bend	1347	55	28	3	64	44	5	82	65	6	84	67
61	C1-H21 ip bend, Ring B CH in plane bend	1382	34	5	1	47	9	2	64	17	3	66	18
62	O18-H28 bend, Ring B CH in plane bend	1387	32	2	-2	34	4	-1	33	4	0	32	4
63	OH,CH ip ben, Ring A B C ,CC bend	1422	21	6	-1	30	13	-1	59	28	-1	66	33
64	O7-H22 O10-H24 in plane bend	1434	227	94	1	331	205	3	464	419	3	474	443
65	O18-H28 bend Ring B CH in plane bend	1465	2	22	0	5	56	4	15	123	4	16	129
66	O7-H22,O10-H24, CH in plane bend,C=O stretch	1476	87	39	3	99	53	6	96	64	7	95	67
67	C=O st,O7-H22 bend, Ring A CC stretch	1517	100	12	3	134	20	6	186	31	7	192	32
68	Ring B CH in plane bend	1558	75	29	0	84	38	3	95	41	3	97	40
69	C=O St,O7-H22 bend ip bend, C1=C2 stretch	1583	120	80	4	168	103	10	236	119	11	243	119
70	C=O,C1=c2 st,O7-H22 ,O10-H24 bend	1613	32	27	2	29	56	6	25	110	7	25	116
71	Ring A B quinoid stretch	1620	81	11	1	123	37	4	190	98	4	197	105
72	C1=C2 stretch, Ring A B ,CCC stretch	1634	136	497	2	157	764	4	175	995	5	176	1002
73	C1=C2 stretch	1655	55	294	2	64	483	6	70	741	6	71	768
74	O7-H22 bend, Ring A quinoid stretch	1695	503	192	5	667	334	11	866	533	12	885	553
75	C16-H27 , C15-H26) asymmetric stretch	3156	26	97	-7	29	117	8	536	201	12	549	209
76	C16-H27 ,C15-H26 stretch	3180	15	86	4	400	129	9	23	142	8	23	146
77	O7-H22 stretch	3202	277	51	18	18	140	13	22	212	13	22	218
78	C19-H29 , C20-H30 asymmetric stretch	3204	2	113	3	8	164	7	13	240	8	14	248
79	C11-H25 ,O7-H22 stretch	3206	24	147	-6	4	169	-11	3	242	-12	2	250
80	C19-H29 ,C20-H30 stretch	3232	3	74	4	5	122	11	10	229	12	11	245
81	C8-H23, stretch	3238	0	147	4	1	209	9	2	301	10	3	311
82	C1-H21 stretch	3245	7	79	-3	7	121	-6	5	193	-6	5	201
83	O18-H28 stretch	3700	62	220	4	90	283	8	159	387	9	162	401
84	O10-H24 stretch	3701	66	226	4	100	315	8	103	383	8	106	384

Fig.4. represents the calculated bond lengths between O-H in different solvents and HF and DFT methods. The C-O bond lengths are different values due to the chemical environment, the C3-O4 bond length is very low value, it is represented by carbonyl group(C3=O4), C6-O7(C-O-H) is low value compared of other C9-O10(C-O-H) and C17-O18(C-O-H) bond lengths due to C6-O7 involve in the intramolecular hydrogen bond. In all solvents the bond angles are approximately the same in all the media, while the size of C2-C3-C5 and C1-C13-C12 increase with increasing solvent polarity. This is large variation is due to the intramolecular hydrogen bonding and the electrostatic interaction of the solute with the solvent.

Vibrational Assignments:

According to the theoretical calculations, genistein has a structure of Cs point group symmetry. The molecule has 30 atoms and 84 modes of fundamental vibrations. All the 84 fundamental vibrations are active in both IR absorption and Raman scattering. The vibrational wave numbers were calculated using the ab initio HF/6-311G and DFT(B3LYP)/6-311G level of theory to get the optimized geometry(Fig.1) under different media. The absence of imaginary values of wave numbers as the calculated vibrational spectrum confirms that the structure deduced corresponds to minimum energy.No scale factor was used in the calculated frequencies. Gauss view molecular visualization program was used to assign the calculated harmonic frequencies. The resulting vibrational wave numbers, IR intensities, Raman intensities for the optimized geometry of title compound and the proposed assignments, and also the frequency shifts in different solvents with respect to gas phase are given in table 2 and 3.The calculated IR spectra and Raman spectra plotted using Lorentzian band shape with a bandwidth of (FWHM) of 20 cm⁻¹ as shown fig (6 -9) in different solvents.

The results shows that the frequency values at HF level are higher than the DFT method; the DFT partitions the electronic energy $E = E_t + E_v + E_j + E_{xc}$, where E_t , E_v , and E_j are electronic kinetic energy, electron nuclear attraction and electron-electron repulsion terms respectively. The electron correlation is taken into account in the DFT via the exchange-correlation term E_{xc} , which includes exchange energy arising from the antisymmetry of quantum mechanical wave function and dynamic correlation in the motion of individual electrons, and it makes DFT dominant over the conventional Hartree-Fock(HF) producer[23].

Genistein molecule contains three O-H groups, two are (O7-H22 & O10-H24) benzo ring in the chromone system and one is(O18-H28) phenyl ring system. In both IR and Raman, vibrations 84 and 83 assigned for O10-H24 and O18-H28 (3701, 3700 cm⁻¹) respectively and Vibration 77 assigned for O7-H22 (3202 cm⁻¹) at B3LYP level. The

O7-H22 bond vibration wave number is lower than other –OH groups, which explained the electronic behavior of the molecule and confirmed that the hydroxyl group forms a strong hydrogen bond between the phenolic hydrogen atom and the negatively charged carbonyl oxygen atom.

Table 4. Atomic charges (e) and dipole moments (Debye) of genistein in various solvents.

Atom Name	HF/6-311G				DFT/6-311G			
	Gas	Toluene	Ethanol	Water	Gas	Toluene	Ethanol	Water
C1	0.2774	0.2922	0.9312	0.3173	0.1598	0.1689	0.1845	0.1866
C2	-0.2817	-0.2912	-0.4471	-0.3005	-0.1860	-0.1885	-0.1917	-0.1923
C3	0.6038	0.6187	1.6681	0.6398	0.3759	0.3831	0.3926	0.3937
O4	-0.5949	-0.6163	-1.3654	-0.6503	-0.4735	-0.4902	-0.5129	-0.5155
C5	-0.2954	-0.2951	-0.8358	-0.2945	-0.2028	-0.2032	-0.2026	-0.2026
C6	0.4862	0.4850	1.0508	0.4840	0.3343	0.3331	0.3313	0.3312
O7	-0.7742	-0.7886	-1.0613	-0.8059	-0.6052	-0.6208	-0.6382	-0.6398
C8	-0.2432	-0.2510	-0.5860	-0.2634	-0.1658	-0.1724	-0.1822	-0.1832
C9	0.4760	0.4760	1.3161	0.4762	0.3073	0.3071	0.3070	0.3071
O10	-0.7499	-0.7665	-1.1240	-0.7863	-0.6067	-0.6212	-0.6369	-0.6383
C11	-0.2666	-0.2637	-0.7315	-0.2556	-0.1828	-0.1799	-0.1728	-0.1718
C12	0.3970	0.4011	1.1288	0.4092	0.2643	0.2677	0.2730	0.2737
O13	-0.6858	-0.6880	-1.3212	-0.6884	-0.5048	-0.5067	-0.5066	-0.5064
C14	-0.0115	-0.0197	-0.0472	-0.0383	-0.0440	-0.0501	-0.0637	-0.0656
C15	-0.1370	-0.1353	0.0685	-0.1309	-0.1090	-0.1112	-0.1115	-0.1112
C16	-0.2118	-0.2149	-0.2620	-0.2156	-0.1855	-0.1894	-0.1910	-0.1909
C17	0.3800	0.3801	0.8164	0.3787	0.2645	0.2653	0.2654	0.2653
O18	-0.7607	-0.7798	-1.0576	-0.8021	-0.6156	-0.6329	-0.6515	-0.6532
C19	-0.2032	-0.2111	-0.2078	-0.2244	-0.1802	-0.1880	-0.1995	-0.2008
C20	-0.0671	-0.0787	0.1066	-0.0980	-0.0533	-0.0632	-0.0764	-0.0778
H21	0.2235	0.2356	0.1024	0.2497	0.2075	0.2196	0.2330	0.2343
H22	0.4638	0.4646	0.5676	0.4646	0.3973	0.3964	0.3944	0.3942
H23	0.2202	0.2194	0.1035	0.2157	0.1969	0.1966	0.1940	0.1937
H24	0.4141	0.4314	0.4428	0.4514	0.3792	0.3969	0.4159	0.4176
H25	0.2032	0.2165	0.1046	0.2330	0.1816	0.1956	0.2116	0.2132
H26	0.1769	0.1867	0.0564	0.2001	0.1626	0.1725	0.1853	0.1866
H27	0.1722	0.1869	0.0486	0.2062	0.1544	0.1694	0.1872	0.1890
H28	0.4036	0.4192	0.4125	0.4379	0.3707	0.3868	0.4044	0.4060
H29	0.1929	0.1952	0.0591	0.1969	0.1749	0.1771	0.1785	0.1786
H30	0.1920	0.1910	0.0627	0.1931	0.1840	0.1816	0.1791	0.1789
μ	6.4509	7.4205	8.7344	8.8741	6.2589	7.2870	8.6611	8.8051

Table 5. Calculated energies (a.u), zero-point vibrational energies (ZPVE) (kcal mol⁻¹), Thermal Enthalpy (ΔH)(a.u) Thermal Free Energy (ΔG)(a.u), Entropies (cal mol⁻¹k⁻¹) and Cv (Cal/Mol-Kelvin) for Genistein in different solvents.

Parameters	Method	Gas	Toluene	Ethanol	water
Total Energy	HF/6-311G	-947.9858	-947.9858	-948.0094	-948.0106
	DFT/6-311G	-953.6987	-953.7081	-953.7189	-953.7200
ZPVE	HF/6-311G	149.3189	149.1888	148.9809	148.9412
	DFT/6-311G	138.2946	138.2867	138.0956	138.0699
Enthalpy	HF/6-311G	-947.7323	-947.7434	-947.7565	-947.7578
	DFT/6-311G	-953.4619	-953.4713	-953.4824	-953.4835
Free energy	HF/6-311G	-947.7902	-947.7434	-947.7565	-947.7578
	DFT/6-311G	-953.5212	-953.5306	-953.5419	-953.5430
Entropy	HF/6-311G	121.814	122.179	121.940	122.082
	DFT/6-311G	124.978	124.757	125.261	125.309
Cv	HF/6-311G	58.553	58.541	58.611	58.633
	DFT/6-311G	62.911	62.822	62.890	62.898

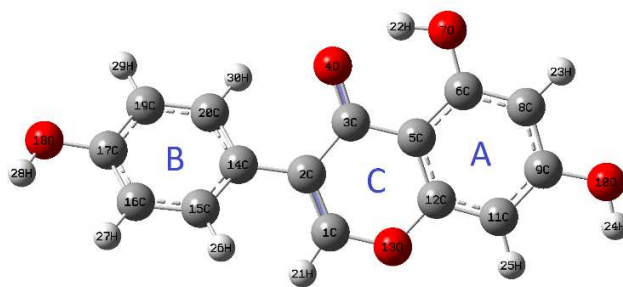


Fig .1. Molecular structure of the genistein molecule calculated with the DFT(B3LYP)/6-311G level.

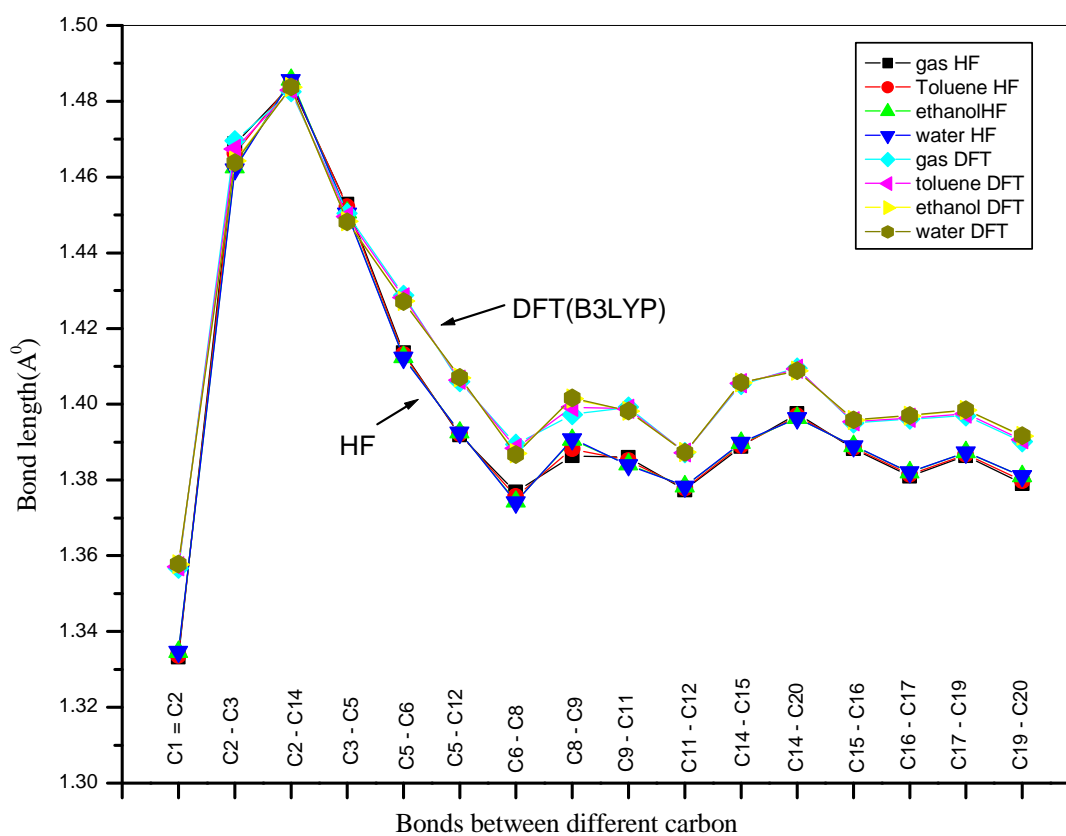


Fig.2. Theoretical calculated bond lengths between different carbon - carbon atoms at HF and B3LYP/6-311G level in different solvents

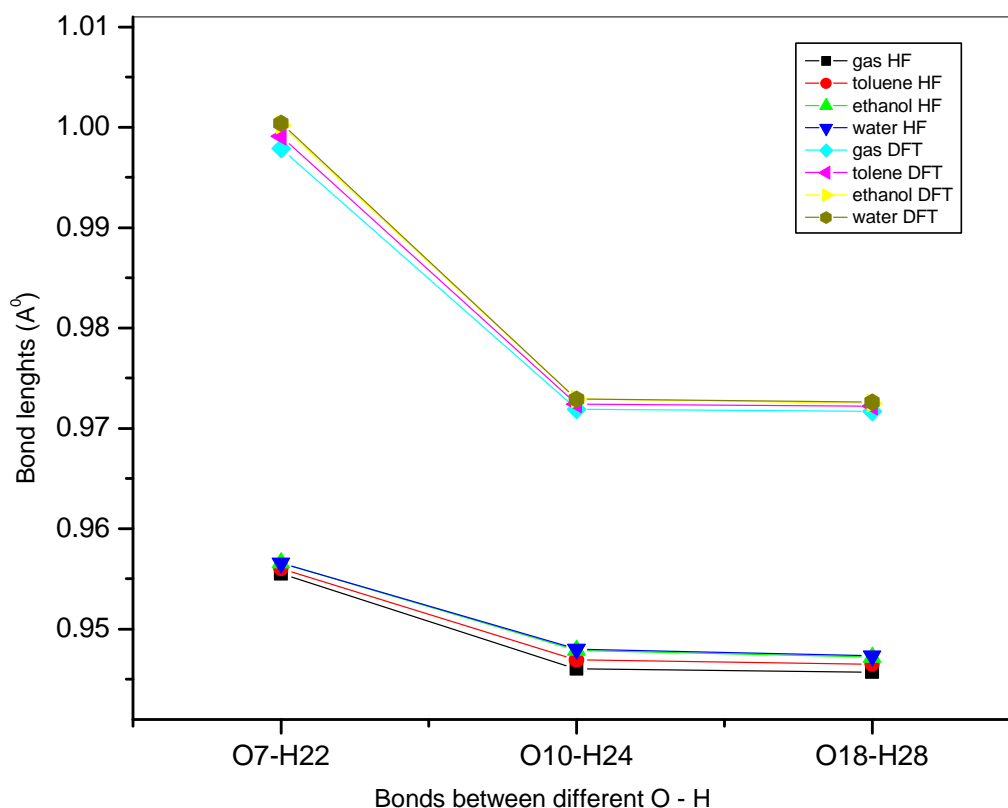


Fig.3. Theoretical calculated bond lengths between different oxygen - hydrogen atoms at HF and B3LYP/6-311G level in different solvents

The vibration modes 84,83 and 82 assigned for O10-H24, O18-H28 and O7-H22 (4089, 4086, 3883 cm^{-1}) respectively at HF level. The Raman intensities are higher than IR intensities in all cases. The C-H stretching vibration modes are assigned 81-75 and 81-75 (expect 77) in the range of 3425-3325 cm^{-1} and 3245-3156 cm^{-1} at HF and DFT levels respectively. The C-H stretching modes usually appear with strong Raman intensity and are highly polarized. The band predicted by DFT to be at 1613 cm^{-1} (v70), attributed to the C=O stretch is either too weak or blended with the more intense 1583 cm^{-1} (v69) peak to be observed. Both intense bands 1634 and 1695 cm^{-1} involve ring quinoid-like stretches in addition to C=O stretches. The weaker band at 1476 cm^{-1} (v66) also involves considerable OH inplane bending. In all the previously studied flavones the most intense lines were those near 1600 cm^{-1} , which represented the C=O and C2=C3 stretching region. The vibrations modes at 1434 and 1328 cm^{-1} assigned for O-H in-plane bending and CH bending vibrations. The most intensive lines at 1695 cm^{-1} (v74) is assigned O7-H22 bend and Ring a quinoid stretching and at 1179 cm^{-1} (v51) is assigned for O18-H28 bending vibration. The prominent band at 392 cm^{-1} (v15) and 360 cm^{-1} (v13) involves mostly O-H out of plane bends. The range of 523 to 675 cm^{-1} is assigned for Rings deformations. The bands in the region from 1400 to 1600 cm^{-1} are associated with aromatic in-plane skeletal vibrations, double bond character of the carbonyl group and the aromatic character of the pyrone ring, i.e. the overlapping of C=O with C=C. Note also that, except for the band at 1558 cm^{-1} (v68), all the bands between 1476 and 1613 cm^{-1} involve the C=O stretch and the C2=C3 stretch, with some degree of O-H bend.

Solvent effect

The results in Table 2 and 3 indicate that solvents have effects on the peak locations of Vibrational modes shift higher and lower values. In general the more polar the solvent is, the larger effect it has. But some modes, the difference between the frequency shifts in different solvents are maximum 12 cm^{-1} indicating that these solvents have essentially the same effect on these Vibrational modes of genistein. From the comparison of the frequency

intensities in solutions with these in gas phase, it can be seen that the intensities of IR and Raman intensities are increase.

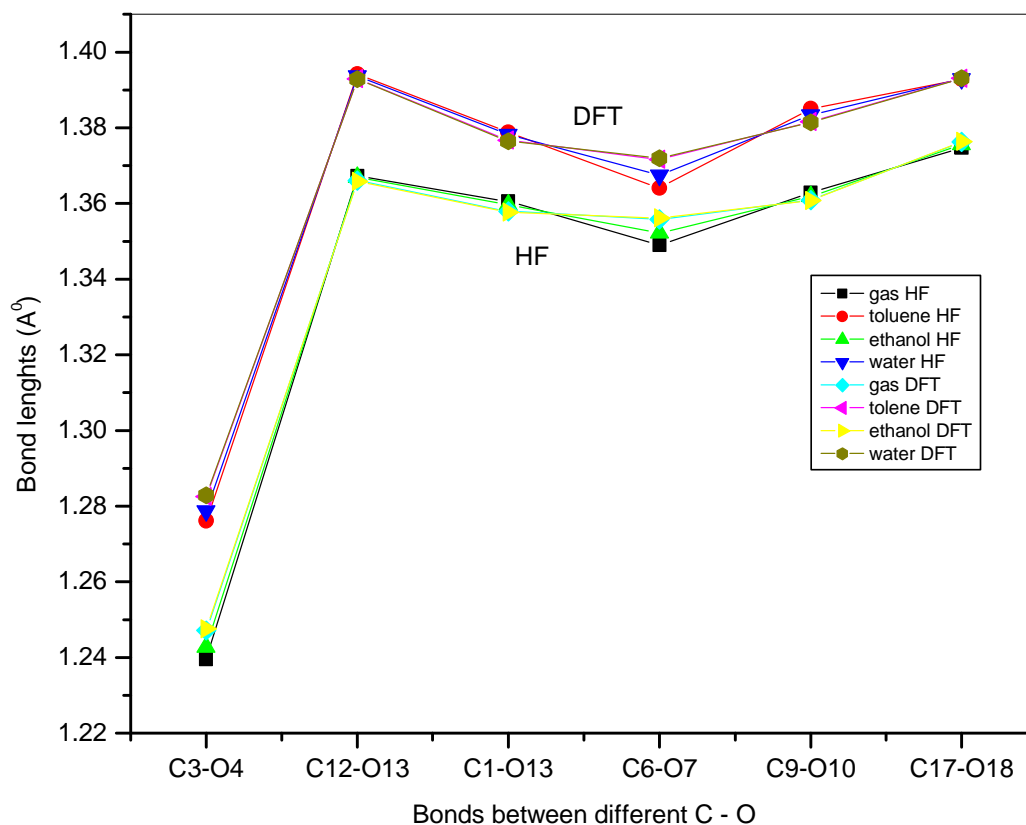


Fig.4. Theoretical calculated bond lengths between different carbon - oxygen atoms at HF and B3LYP/6-311G level in different solvents

Other molecular properties

Mulliken charges

The calculation of effective atomic charges plays an important role in the application of quantum mechanical calculations to molecular systems. The net atomic charges of Gensitien in various solvents by using Mulliken population Analysis (MPA) method[24], finding the evidence of charge transfer and polarization. The Mulliken charges calculated different levels and in media listed in table 3. The results can, however, better be represented in graphical form as has been given in figure 5. The significant influences of the solvents on the atomic charges are observed from the calculation. The atomic charges are increase with increasing solvent polarity from toluene to ethanol to water, the values of atomic charges in ethanol are large variation in HF method but not in DFT. All carbon atoms making bond with oxygen atom have positive excess charge, the rest of the carbon atoms have negative excess charges accumulation. The C14 atom have very low value in all cases, because of it is a tertiary carbon.

The dipole moment of Gensitien computed at HF and DFT(B3LYP)/6-311G level, increases as the dielectric constant of the medium increases as shown in table 3. the dipole moment is related to the hydrogen bonding iteration. When the solute interacts with solvent, the high electrostatic interaction and large polarization can be induced by the stronger hydrogen bonding interaction between solute and solvent.

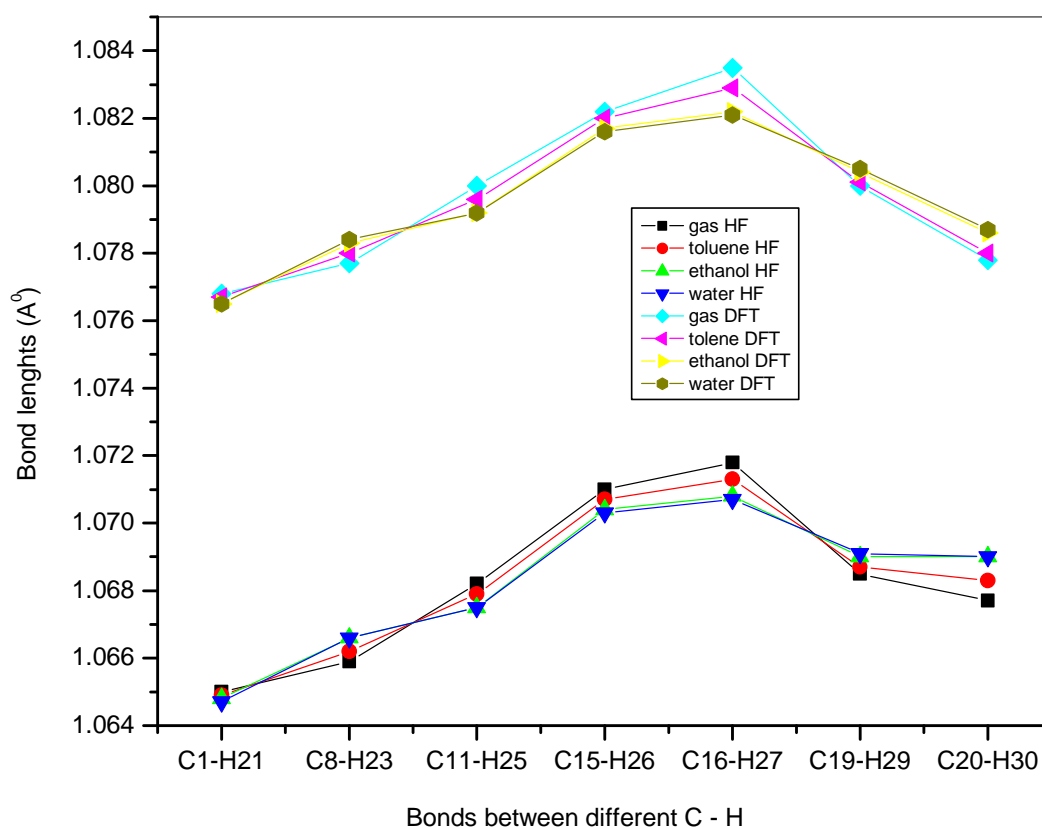


Fig.5. Theoretical calculated bond lengths between different carbon - hydrogen atoms at HF and B3LYP/6-311G level in different solvents

Thermodynamic parameters

Tables 4 summarize energies of the optimized structures of the title compounds obtained by HF and DFT/B3LYP method in the gas phase, in toluene, ethanol and water. Further, some calculated thermodynamic parameters are presented in Table (4). The total energies obtained at the B3LYP level is the lowest for each solvent and that obtained at HF level is the highest. Analyzing the results of the thermodynamic functions we see that the total energies and ZPVE decrease with increase solvent polarity other hand enthalpies and entropies are increase with increase solvent polarity.

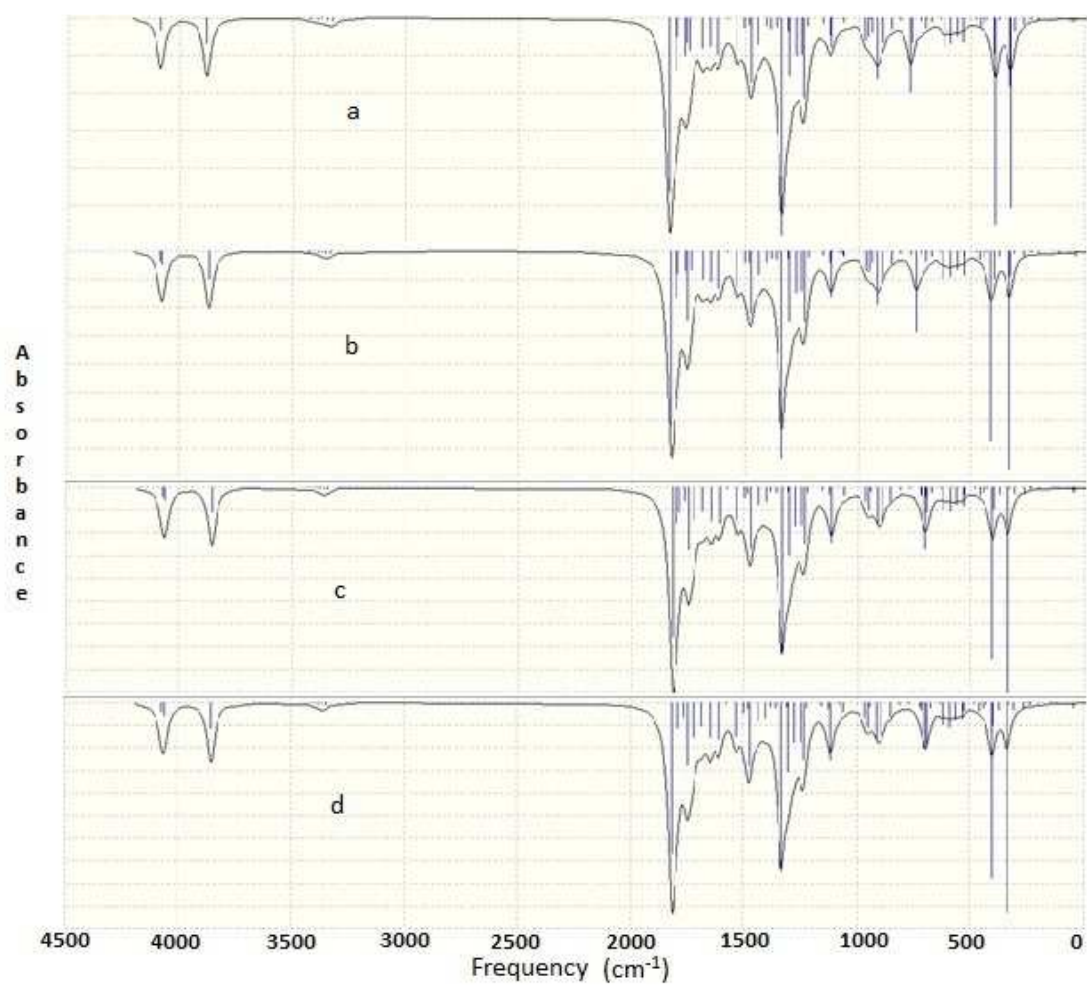


Fig.6. Calculated Vibrational spectra of genistein in gas phase (a),toluene(b),ethanol(c) and water(d) at HF/6-311G level.

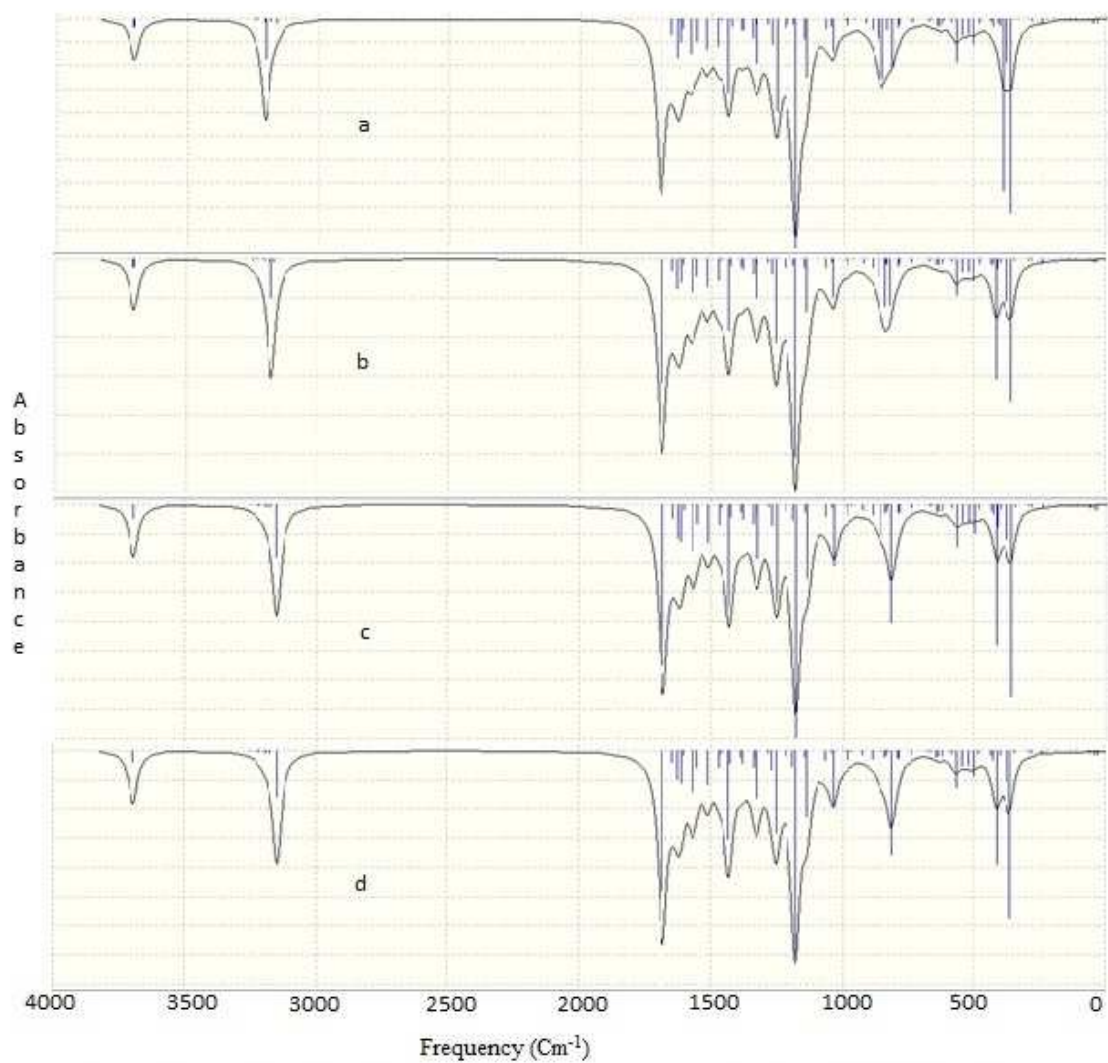


Fig.7. Calculated Vibrational spectra of genistein in gas phase (a), toluene (b), ethanol (c) and water (d) at DFT (B3LYP)/6-311G level.

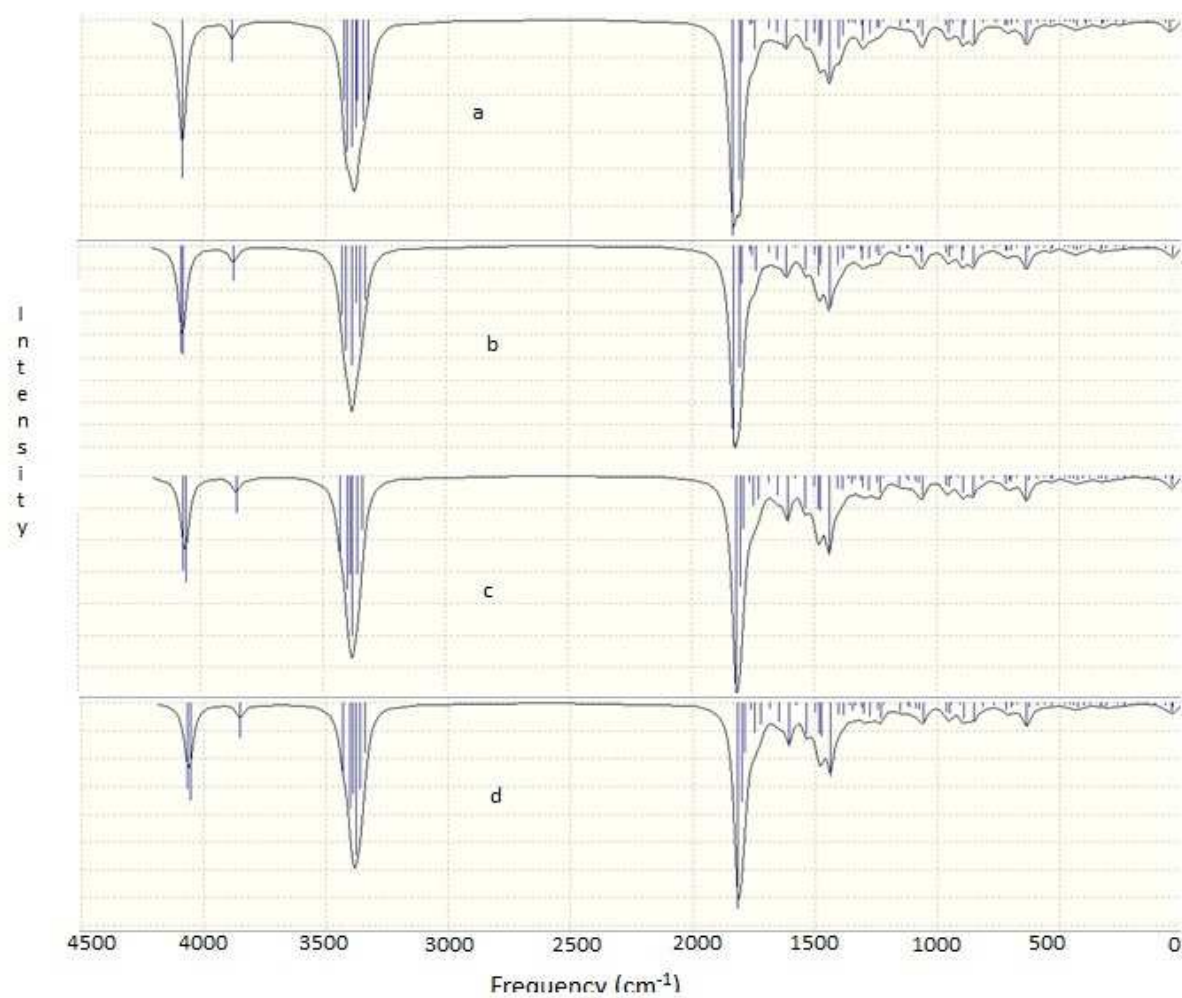


Fig.8. Calculated Raman spectra of genistein in gas phase (a),toluene(b),ethanol(c) and d water(d) at HF/6-311G level.

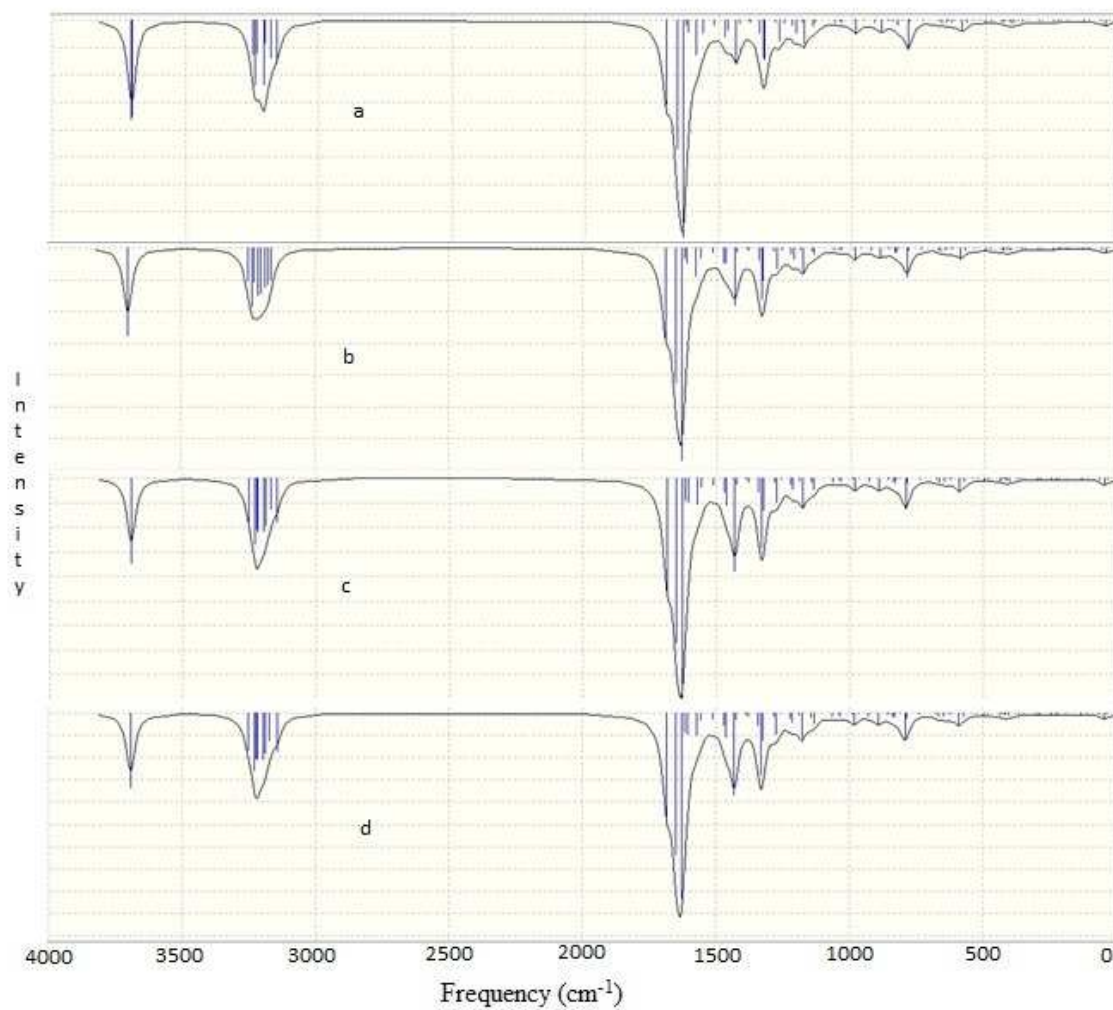


Fig.9. Calculated Raman spectra of genistein in gas phase (a), toluene (b), ethanol(c) and water (d) at DFT (B3LYP)/6-311G level.

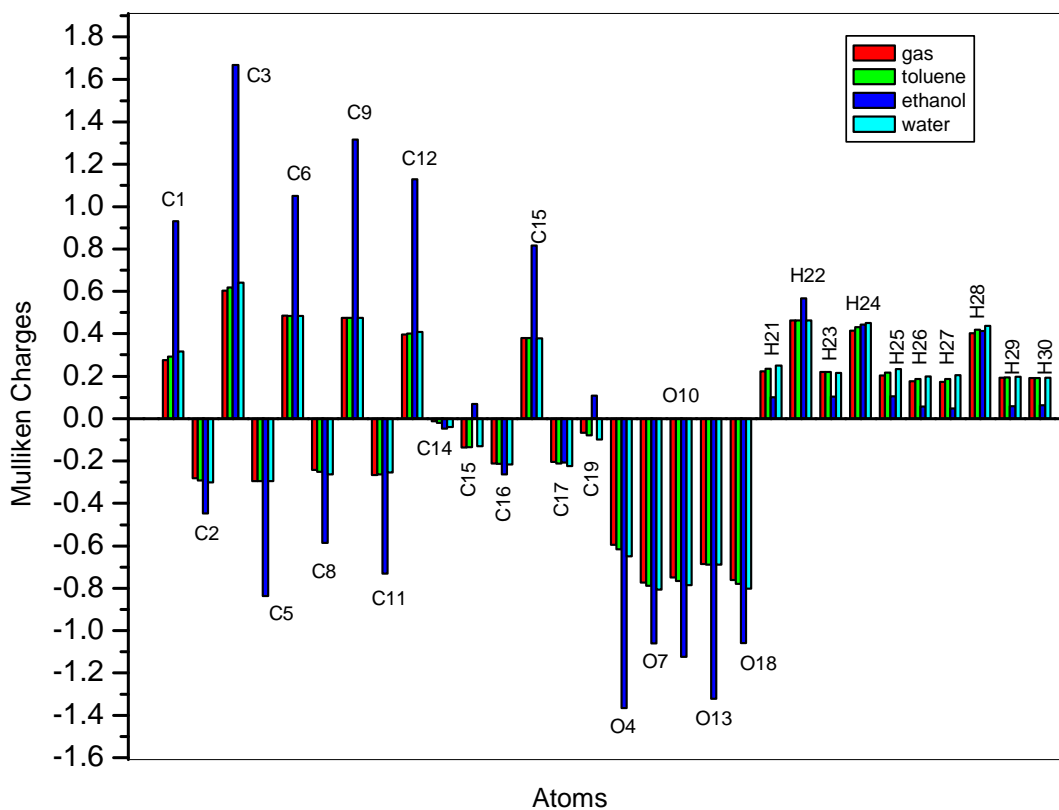


Fig.10. Comparison of different calculated atomic charges in different solvents at HF/6-311G methods.

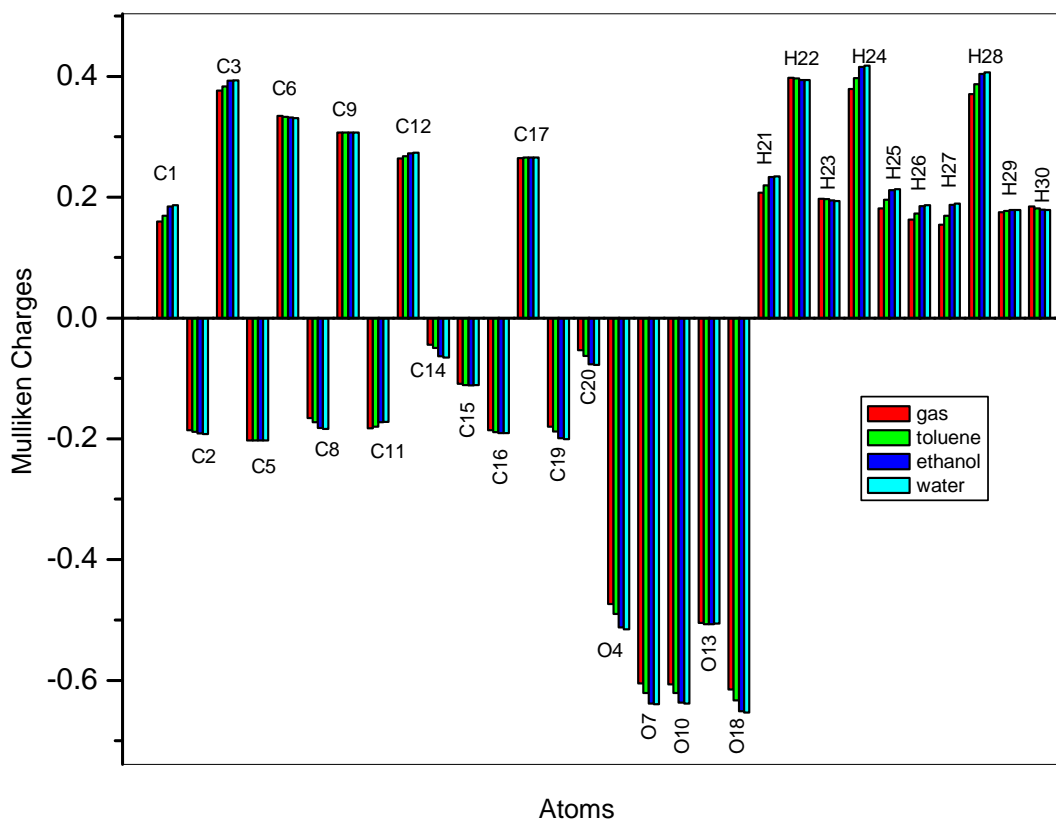


Fig.11. Comparison of different calculated atomic charges in different solvents at DFT(B3LYP)/6-311G methods.

CONCLUSION

The equilibrium geometry of genistein has been obtained at HF and B3LYP levels of theory using the 6-311G basis set in different solvents. Comparing bond lengths of B3LYP with those of HF as a whole, the former are on higher side than the latter and both the methods have performed nearly to the same level across the bond angles sets. Attempts have been made for the proper frequency assignments for the compound genistein in different solvents. The results show that the frequency values at HF level are higher than the DFT method. The solvents have effects on the peak locations of vibrational modes shift higher and lower values, the difference between the frequency shifts in different solvents are maximum 12 cm^{-1} indicating that these solvents have essentially the same effect on these vibrational modes of genistein. In addition Mulliken charges and dipole moments of the titled compound at different levels were calculated in different solvents and discussed.

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