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THEORETICAL INVESTIGATION OF THE VIBRATIONS OF ACETYLSALICYCLIC ACID

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Theoretical investigation, using high speed computers are very effective and sensitive tools for the qualitative and quantitative analysis of compounds. Present paper reports the vibrational spectra of Aspirin and its comparison with experimental results.

KEY WORDS: Vibrational spectra, aspirin.

INTRODUCTION

Acetyl salicyclic acid also called Aspirin is an aromatic compound containing carboxyl group and ester functional group bounded directly to benzene ring. Boezar *et al* (2002) calculated normal modes of aspirin, and proposed the assignment of the observed Raman and IR spectra. Vibrational spectra analysis of aspirin was carried by V. Renganayaki *et al* (2012).

With the advent of DFT and using high speed computers, determination of the structure and dynamics of system containing large number of atoms are made easy. Spectroscopic techniques are very effective and sensitive tools for the qualitative and quantitative analysis of many compounds and results of analysis can be directly put to a help to pharmaceutical labs [1-6].

The present investigation was taken to study the vibrational spectra of aspirin and compare the experimentally obtained vibrational wavenumbers with the theoretically calculated wavenumbers.

Computational details

For the analysis of the molecule, calculations were carried with Gaussian software programme using the Beckes three parameter hybrid model and lee-Yang-parr correlation functional [3, 4], *i.e.* B3LYP methods and 6-31G*basis set.

RESULTS AND DISCUSSIONS

The vibrational spectrum of a compound is the superposition of the absorption bands of specific functional groups present in the compound. The functional groups were identified and vibrational band assignment of the compound was made by comparing the spectra of similar compounds.

In a non-linear polyatomic molecule, having N atom, the total number of normal modes of vibrations are given by 3N-6 [1, 2]. Aspirin has 21 atomic non-linear molecules therefore it has 57 normal modes of vibrations as shown in table.

Table : Experimental & Calculated Frequency in Aspirin by DFT

Assignment	Experimental Frequency (cm^{-1})	DFT Calculated Frequency (cm^{-1})	HF Calculated Frequency (cm^{-1})
1		2252	3301
2	3200	2226	3224
3		3216	3283
4		3209	3273
5		3193	3253
6	2900	2981	2925
7		2938	2900
8	2846	2872	2813
9		1966	2046
10	1753	1712	1700
11	1693	1662	1611
12	1560	1593	1578
13		1528	1558
14	1453	1450	1522
15		1488	1504
16		1483	1500
17		1405	1447
18	1312	1394	1424
19		1354	1416
20		1293	1286
21	1238	1245	1256
22		1233	1238
23	1195	1122	1224
24	1138	1100	1208

25		1135	1215
26		1113	1197
27		1063	1170
28	1039	1061	1040
29		1022	1130
30	942	997	999
31	922	980	935
32		931	936
33		993	905
34	842	841	823
35		802	800
36	750	755	798
37	732	749	799
38		720	788
39	700	669	725
40	630	637	693
41	643	613	660
42		592	640
43		541	589
44	540	542	589
45		516	567
46		438	475
47		408	438
48		360	389
49		309	332
50		275	303
51	246	230	248

52		138	156
53		108	118
54		101	110
55		78	86
56		74	83
57		25	24

Conclusions

The results indicate that DFT calculated vibration frequencies are close to experimental values. Thus DFT can be considered as good tool for simulation of vibrational spectra.

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