Theoretical Study of Chalcones Compounds by using Semi-Empirical Method

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Abstract: New compounds of (E-(1, 3-bis)3-bromophenyl)prop-2-en-1-one], [E-(1-(3-Nitrophenyl-(3-(1H-pyrrol-2-yl)prop-2-en-1-one], [E-(1-(3-Nitrophenyl-(3-(1-H-pyrrol-2-yl)prop-2-en-1-one],(E-(1-(3-Nitrophenyl-(3-(1-h-pyrrol-2-yl)prop-2-en-1-one] and [(E)-N, N-1, 3-bis)3-Nitrophenyl)propan-3-yl-1-ylidene) dimethan amine] were synthesized. These prepared compounds were synthesized from chalcone and characterized through using FT-IR, ultraviolet/visible and H-NMR spectroscopy. The newly prepared compounds were studied theatrically in gas phase through using HyperChem.8 program for the molecular mechanics, semi-empirical calculations. Binding Energy ($\bullet$Eb) the Heat formation ($\bullet$H°f) and Total Energy ($\bullet$ET) for chalcones were calculated measured by the semi-empirical (PM3). Semi-empirical method was used to assess the infrared spectra and ultraviolet/visible spectra for the chalcones and the wave numbers which were theoretically calculated, then were was a comparison with the experimented values. There was an agreement between theoretically obtained frequencies and with frequencies found experimentally, furthermore, calculations assisted in assigning unambiguously the most diagnostic bands.

Key words: HyperChem.8, chalcone, semi-empirical method, PM3 method, ultraviolet, visible spectra

INTRODUCTION

Chalcones are famous and good intermediates to synthesize several heterocyclic compounds. The compounds that have chalcones as the backbone have been reported to have various biological activities such as anti-microbial (Nowakowska *et al.*, 2008; Narender and Reddy, 2007; Mishra *et al.*, 2008) anti-inflammatory (Li *et al.*, 2002), anti-malaria (Karthikeyan *et al.*, 2007; Rateb, 2008), antilies-hmanial (Dhar, 1981), antioxidant (Go *et al.*, 2005) and anti-tubercular (Azarifar and Ghasemn, 2003). Chalcones consist of an enone and aromatic ketone that form the central core for many significant biological compounds which are known as chalcones. Aldol condensation represents a vital class of carbon-double bond carbon natural formation reactions as well as in synthetic Chemistry. Compounds known as chalcones (Hanna *et al.*, 2010) can be synthesized by aldol condensation of an aromatic ketone along with aldehyde. Computational chemistry is a novel discipline. Its beginning and popularity have paralleled improvements in computing power for the last several decades (Christopher, 2004). Computational Chemistry can be defined as an application of theoretical and mathematical principles to give solutions to chemical problems. Molecular modelling, a subset of computational Chemistry, focuses on predicting the behaviour of an individual molecule within a chemical system. Doresstt (1998) types of possible predictions for molecules and reactions consist of (Lipkowitz and Boyd, 1996):

- Heat formation
- Structures and energies molecules
- Bond and reaction energies
- Structures and energies and of transition states (activation energies)
- Reaction paths, mechanisms and kinetics
- Distributing charge in molecule (reactive sites)
- Alternative effects
- Ionization potentials and electron affinities
- Vibrational frequency (IR and Raman Spectra)
- Magnetic shielding effects (NMR spectra)
- Electronic transition (ultraviolet and visible spectrum)

Semi-empirical quantum chemistry methods are depends on the Hartree-Fock modal but make many approximations and obtain some variable from experimental data. They are very valuable in computational chemistry for treatment large molecules where the full Hartree-Fock method without the approximations is too exorbitant. The use of empirical variable appears to allow some inclusion of electron correlation effects into the methods (Cook, 1998).

MATERIALS AND METHODS

Preparation of chalcones compounds: Chalcones compounds [3-(2-substitutedphenyl) 1-(3-nitrophenyl) prop-2-en-1-one (1-5)] were prepared according to the literature (Mahmoud, 2014) (Fig. 1).
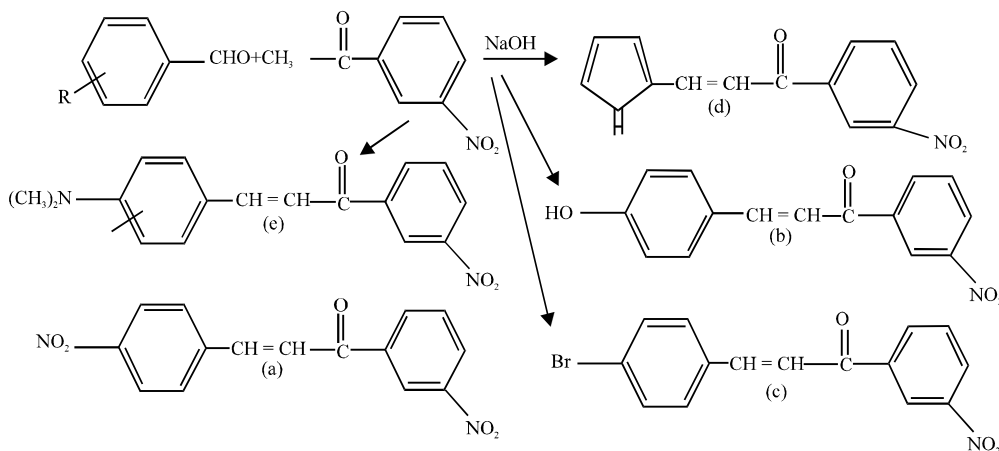
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Fig. 1: Preparation of chalcones compounds

Program used in theoretical calculations: HyperChem-8.0 program is the most powerful and sophisticated molecular modeling environment that is known because it is flexible, easy to use and has a good quality, it presents 10 semi-empirical methods (Muellr, 2001; Young, 2001). Three dimension visualization and animation are united with chemical quantum calculations, molecular dynamic and mechanics. Hyperchem.8 puts more molecular modeling tools at use than any other windows program (Anonymous, 2007). The parameters for PM3 were made a comparison of a much larger number and wider variation of experimental against properties of computed molecular. PM3 is semi-empirical method that has been developed recently hand may contain as yet undiscovered defects (Clark, 1985). Using PM3 method of HyperChem 8.0 was used for the calculation of Heat formation •H°f, binding Energy •Eb, total energy WET, IR and (UV-Vis) spectroscopy for all prepared Chalcones.

RESULTS AND DISCUSSION

Some analytical data and sine physical properties of the chalcones compounds were shown in literature (Mahmoud, 2014).

Theoretical studies
Optimized energies: The HyperChem.8 program was used to calculate thermochemical stability (Lipkowitz *et al.*, 2007; Alias *et al.*, 2013). The Heat Formation (•H°f), binding Energy (•Eb) and total Energy (•ET) for the chalcons compounds were measure by using semi empirical (PM3) method as displayed in Table 1.

Table 1: Configuration energetic in (kJ.mol⁻¹) for the chalcons compounds

Compounds	PM3		
	•H°f	•Eb	•ET
1	59.582	-15047.08	-358879.41
2	-101.480	-14703.82	-316643.97
3	123.17	-14123.61	-320903.42
4	78.2639	-17268.35	-334279.94
5	845.78	-12331.200	-278811.64

Geometries of chalcons compounds: Calculations of geometry optimization use energy minimization algorithms to detect stable structure by using (HyperChem-8.0) program (Choinacki and Pruchnik, 2001), the geometry optimization is shown in Fig. 2.

Bond lengths and atomic charges measurements for chalcones compounds: Figure 2 and 3 show atomic charges and bond lengths and of chalcones compounds. Bond lengths and angles are calculated in angstroms and in degrees, respectively. Calculation parameters were optimized of bothe of bond lengths and atomic charges for the chalcones compounds by the use of (PM3) Method at geometry optimization (0.001 kcal.mol⁻¹) that agrees very well with the experimental data (Henryk *et al.*, 2001) (Fig. 3).

Theoretical vibration frequencies of: Theoretically infrared spectra are calculated at semi-empirical (PM3) method (Seeger *et al.*, 1991; Hassan *et al.*, 2016) and these obtained frequencies agreed with the ones experimentally found as shown in Table 2. Diagnostic calculated vibrational frequencies had been selected to assign chalcones compounds illustrated in Fig. 4 and 5.
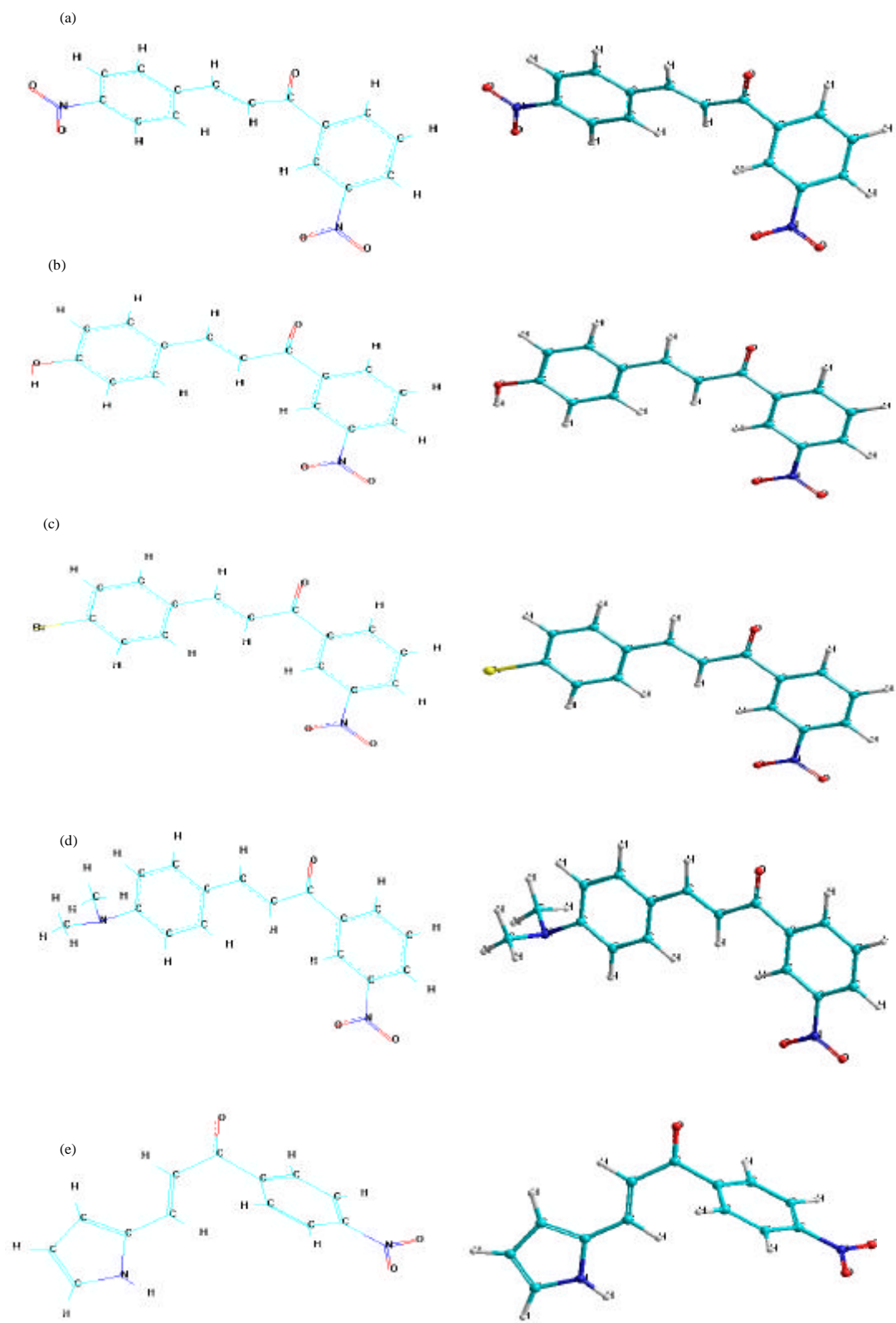
Fig. 2a-e: Conformation structure of chalcones compounds using HyperChem 8.0 program
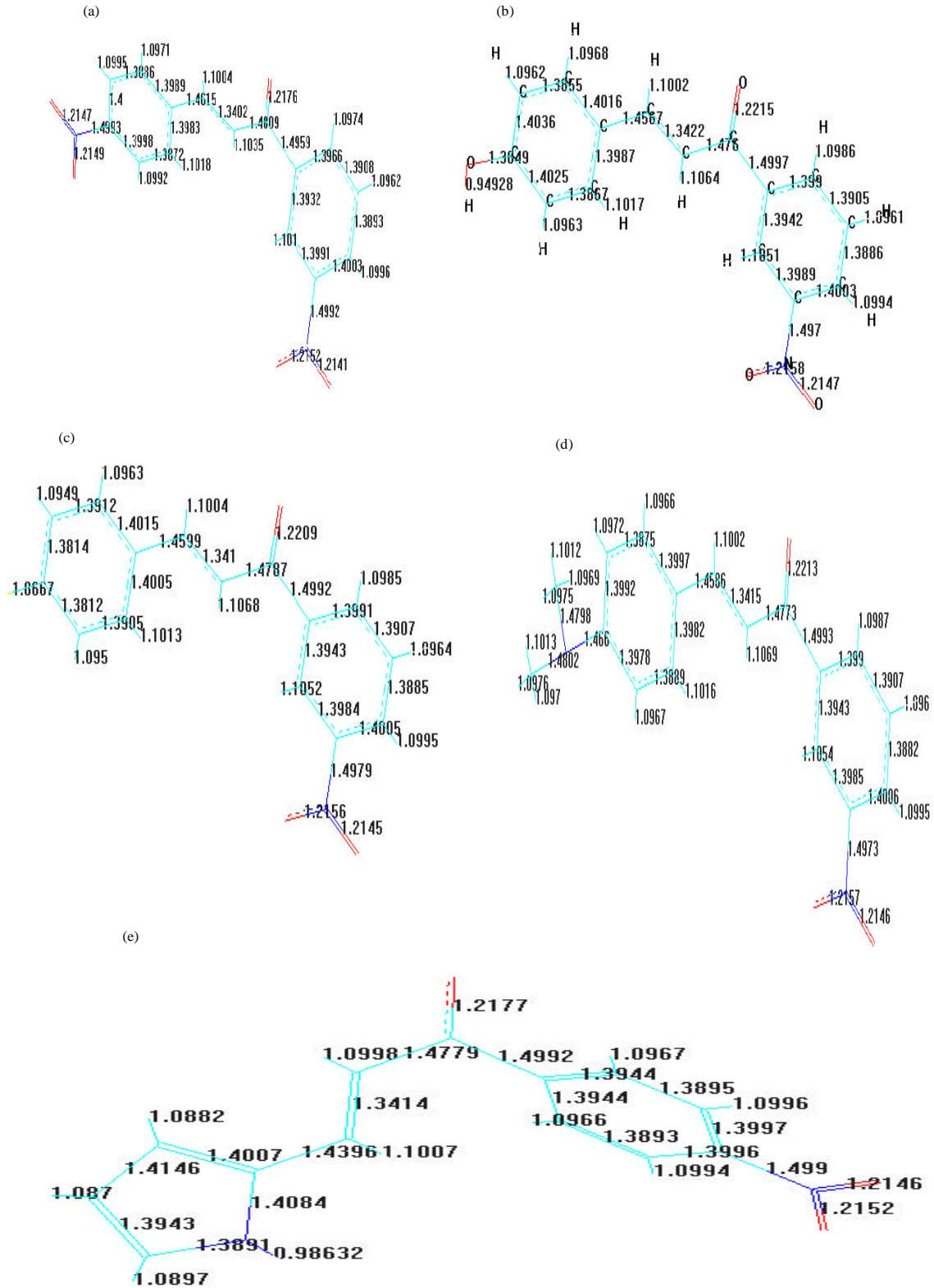
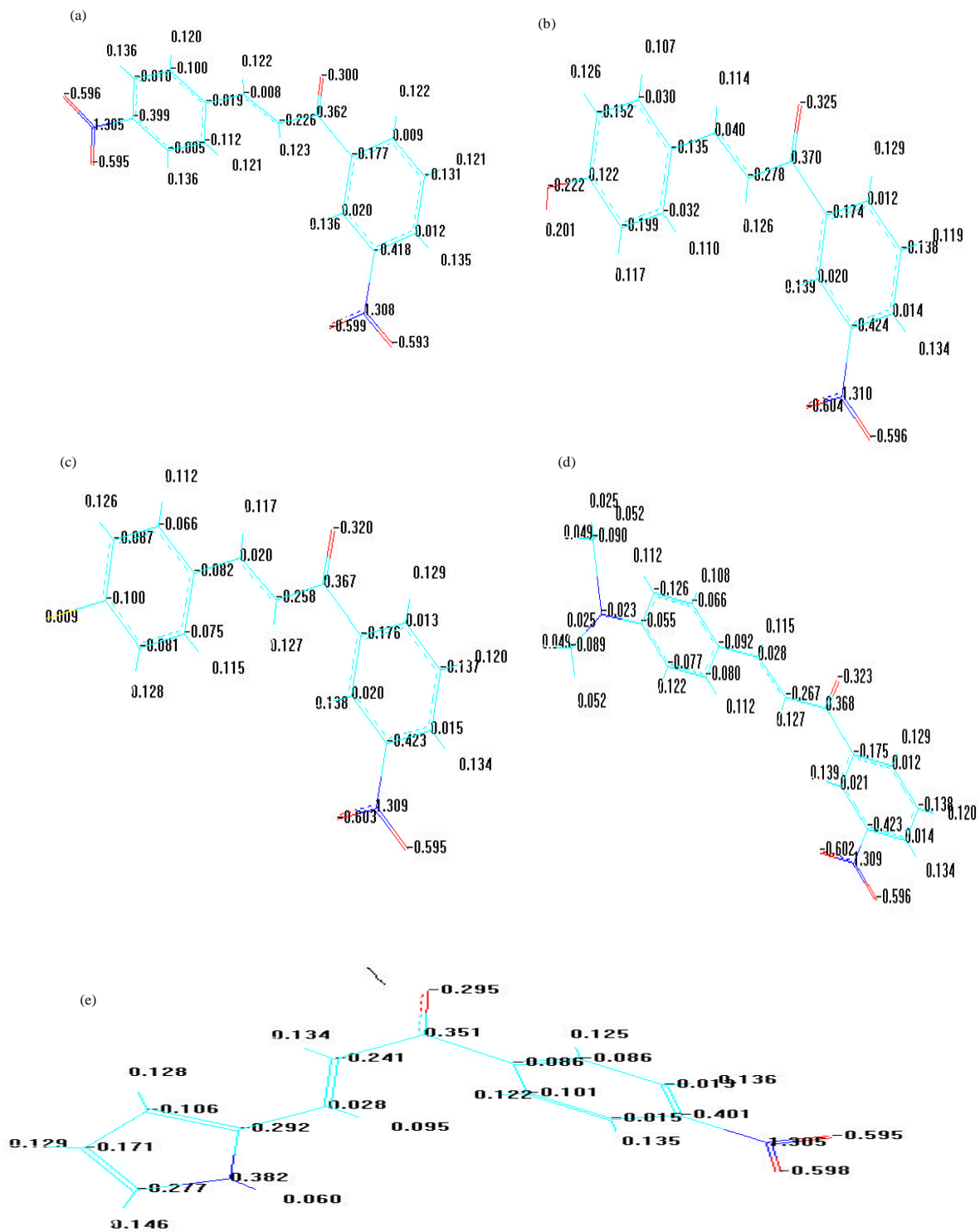Fig. 3a-e: Bond length of the chalcones compounds using (PM3) method

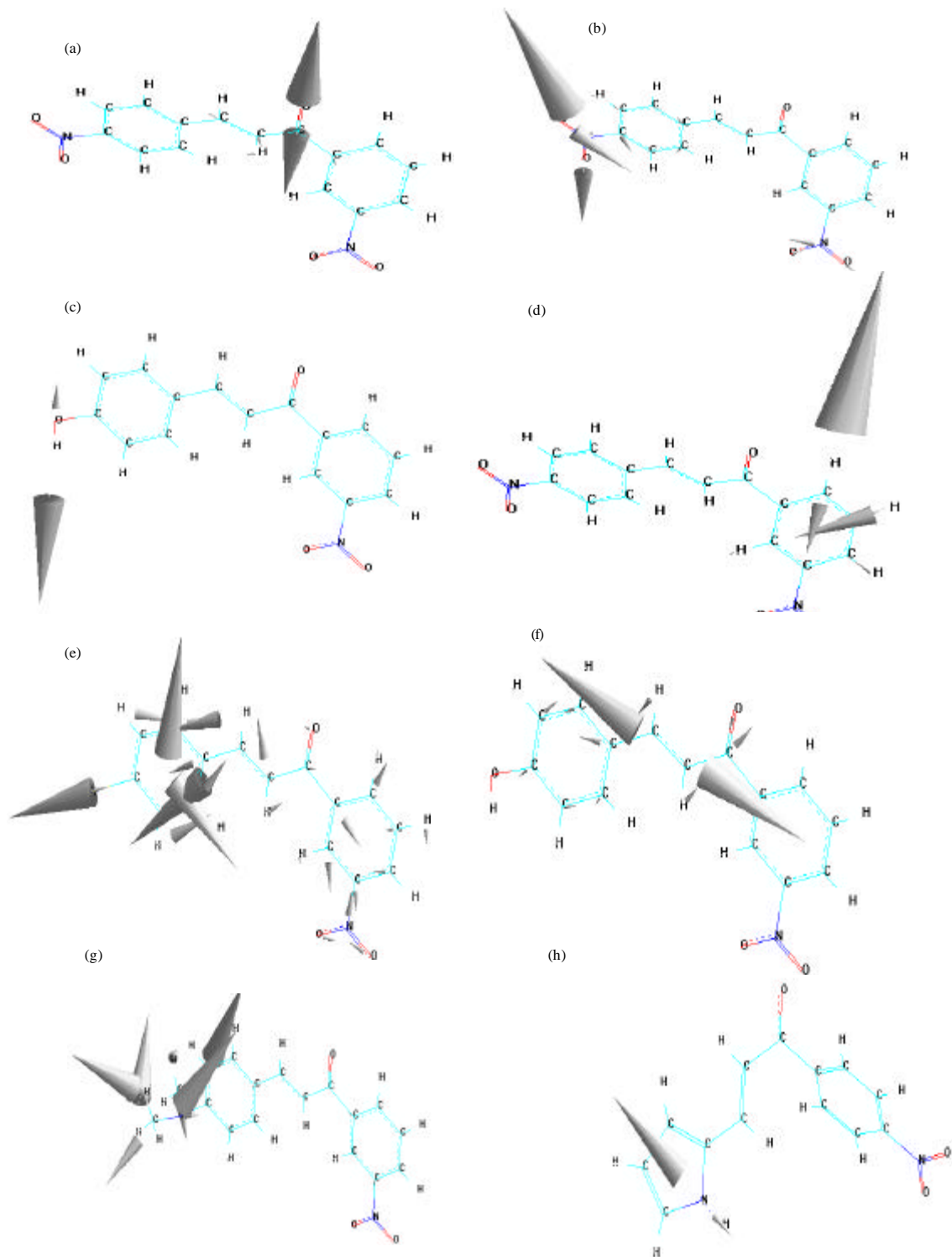Fig. 4a-e: Atomic charge the chalcones compounds using (PM3) method

Fig. 5a-e: Some theoretical vibrational modes of chalcones compounds: a) vC = O; b) vNO$_2$; c) vO-H; d) vC-HAram; e) vC-Br; f) vC = C; g) vN-Me and h) vN-H

Table 2: Theoretical and experimental vibration frequencies of chalcones compounds (cm⁻¹)

Compounds	• C-H Aliph	• C-H Arom	• C = O	• C = C	• NO2	• C-N	• C-Br	• O-H
1	2870*	3082*	1778*	1631*	1438*	1184*	-	--
	2980**	3063**	1789**	1541**	1427**	1194*		
	3.69**	-0.62	-0.61	-5.84	-0.77	*0.83		
2	2724*	3094*	1732*	1627*	1427*	1172*	-	3444*
	2764**	3068**	1770**	1641**	1391**	1143**		3486**
	1.44***	-0.84***	2.14***	0.85**	-2.58**	-2.53**		1.20
3	2730*	3091*	1797*	1593*	1454*	1176*	1089*	
	2763**	3074**	1794**	1535**	1430**	1153**	1131**	
	1.19***	-0.55***	-0.16***	-3.77***	-1.67***	-1.99***	3.71***	
4	2808*	3082*	1716*	1647*	1438*	1168*	--	
	2961**	3063**	1765**	1631**	1403**	1230**		
	5.16***	-0.62***	2.77***	-0.98***	-2.49***	5.04***		
5	2789*	3097*	1720*	1616*	1438*	1184*	--	
	3000**	3055**	1722**	1609**	1410**	1226**		
	7.03***	-1.37***	0.11***	0.43***	-1.98***	3.42***		

*Experimental frequency **Theoretical frequency ***Error percentage due to the main difference in the experimental measurements and theoretical treatment of vibrational spectrum

Table 3: Compression of experimental and theoretical electronic transition of chalcones compounds from PM3 calculation

Transition	Experimental	Theoretical (PM3)
• -• *	210	231
n-• *	313	254
n-• *	317	263
n-• *	325	288

Theoretical (Ultraviolet and Visible) spectrum of chalcones compounds: The theoretically (Ultraviolet and Visible) spectrum of chalcones compounds have been calculated at PM3 method and comparing them with the results obtained experimentally (Abbott *et al.*, 2004). It was found that the results were nearly similar between the experimental and theoretical spectrum, Table 3:

CONCLUSION

Semi-empirical methods have been calibrated to typical biological or organic complexes and tend to be inexact method to solve problems that involve hydrogen-bonding chemical transitions along nitrated compounds (Choinacki and Pruchnik, 2001).

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