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Cluster Behavior of Barbituric Acid Based on Hartree-Fock (HF) Theoretic Calculations

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Abstract: ***Barbiturates, a class of aromatic hydrocarbons, were discovered during the first decade of the twentieth century. They act as central nervous system depressants. This article discuss the cluster behavior of barbituric acid based on Hartree-Fock (HF) theoretic calculations for (BA)n, n =1-7***

Keywords Barbiturates, Hartree-Fock (HF)

I. INTRODUCTION

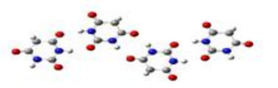
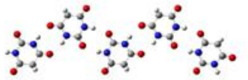
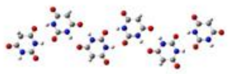
Barbiturates, a class of aromatic hydrocarbons, were discovered during the first decade of the twentieth century. The primary compound/substance familiar with the market from the gathering of barbiturates is diethyl-barbituric destructive and is generally called barbital, malonal, or gardenal. One of the barbital straightforward prescriptions named as phenobarbital opened up the course to the therapeutic utilization of barbiturates in the treatment of epilepsy. [1],[3],[5]

The pharmacologically active barbiturates are based on barbituric acid i.e., 2,4,6-(1H,3H,5H)-pyrimidinetrione. The frequent lethal effect of barbital compounds by overdose gave a therapeutic margin of all these substances (Wilson et al 1971, Foye et al 1974). Recently, Oakley et al have reported how barbiturates are recognized by their protein targets and revealed the role of polar and hydrophobic elements (Oakley et al 2012). The and their activity/toxicity raised the importance of QSTR studies of barbiturates for screening novel anesthetic candidates (Doroteia et al 2009). In the present investigation N–H…O=C bonded cluster of barbituric acid (BA)n, are reported and discussed . [7],[9] ,[11]

II RESULTS AND DISCUSSION

Geometries of different bunches of barbituric corrosive (BA)n, n= 1-7, have been enhanced without geometrical imperatives at various degrees of hypothesis utilizing the G03W suite of projects. Every one of them are observed to be steady with respect to the isolated monomers (Table1).

Table1 **Optimized structures of** (BA)*n*, *n* =4-7 using HF/6-31G**

Vertical view	Horizontal view
	
	
	
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The adjustment energies (SE)/restricting energies(B.E) of the considerable number of groups have been determined utilizing the supermolecule approach: and amended for premise set superposition mistake (BSSE) following the methodology received by Boys and Bernardi..Hartree-Fock(HF) theoretic calculations using 6-31G* basis set for (BA)n, n =1-7given in table2 showed that the geometry optimization results were distinguishable. [20],[22], [24]

Sl.No	No of H-B	H…..A	D…A	BSSE energy	B.E
Dimer	2	1.99648	2.98241	1.620767628	- -9.416780925
Trimer	4	2.00219	2.98668	3.317399848	-18.33087968
Tetramer	6	2.00027	2.82098	4.982685249	-27.48387381
Pentamer	8	2.00228	2.98655	6.67557064	-36.39701749
Hexamer	10	2.00117	2.98553	8.290471485	-45.77997816
Septaumer	12	2.00136	2.98550	9.994076647	-54.68712599

TABLE 2:GEOMETRY OPTIMIZATION

Table 2Structural geometry and binding enery calculation of (BA)n, n =2-7 using HF/6-31G**

In this calculation , an effort has been put forth to analyze

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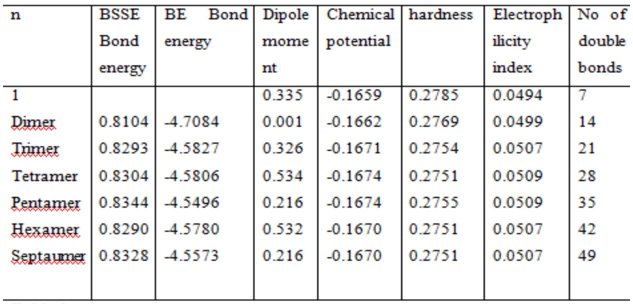
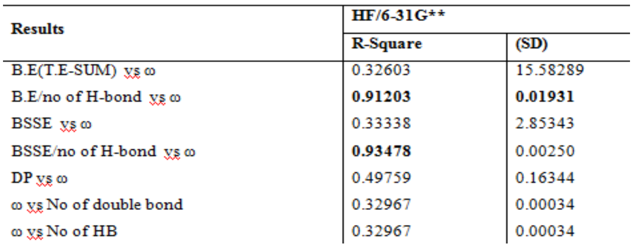
the (BA)n, n =2-7 using

and to develop new QSAR models using the DFT based descriptors. Various descriptors such as Dipole moment , no of H-bond were calculated. Their inter dependency were calculated using multiple regression analysis and are given in table 3a and 3b [32],[34],[36]

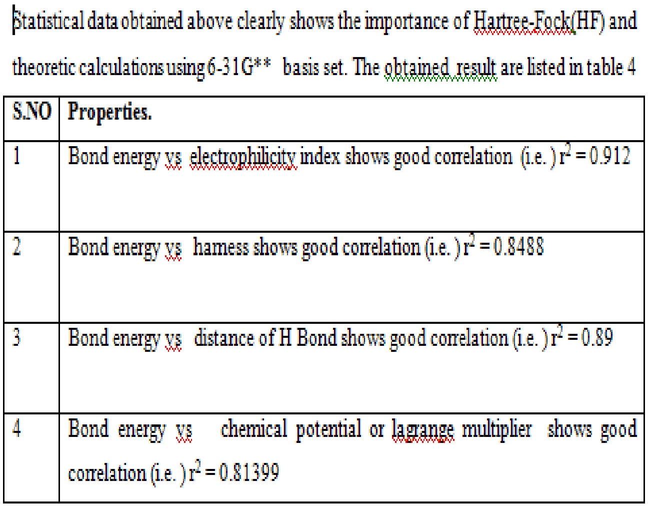


n	BSSE Bond energy	BE Bond energy	Dipole moment	Chemical potential	hardness	Electrophilicity index	No of double bonds
1			0.335	-0.1659	0.2785	0.0494	7
Dimer	0.8104	-4.7084	0.001	-0.1662	0.2769	0.0499	14
Trimer	0.8293	-4.5827	0.326	-0.1671	0.2754	0.0507	21
Tetramer	0.8304	-4.5806	0.534	-0.1674	0.2751	0.0509	28
Pentamer	0.8344	-4.5496	0.216	-0.1674	0.2755	0.0509	35
Hexamer	0.8290	-4.5780	0.532	-0.1670	0.2751	0.0507	42
Septaumer	0.8328	-4.5573	0.216	-0.1670	0.2751	0.0507	49

Table 3a



Results	**HF/6-31G****	
	R-Square	**(SD)**
B.E(T.E-SUM) vs ω	0.32603	15.58289
B.E/no of H-bond vs ω	**0.91203**	**0.01931**
BSSE vs ω	0.33338	2.85343
BSSE/no of H-bond vs ω	**0.93478**	0.00250
DP vs ω	0.49759	0.16344
ω vs No of double bond	0.32967	0.00034
ω vs No of HB	0.32967	0.00034



Statistical data obtained above clearly shows the importance of Hartree-Fock(HF) and theoretic calculations using 6-31G** basis set. The obtained result are listed in table 4

S.NO	Properties.
1	Bond energy vs electrophilicity index shows good correlation (i.e.) $r^2 = 0.912$
2	Bond energy vs harness shows good correlation (i.e.) $r^2 = 0.8488$
3	Bond energy vs distance of H Bond shows good correlation (i.e.) $r^2 = 0.89$
4	Bond energy vs chemical potential or lagrange multiplier shows good correlation (i.e.) $r^2 = 0.81399$

III CONCLUSION

Barbiturates form strong, specific hydrogen bonds within its cluster . The linear extension of barbituric acid from monomer to septaumer is **in planor form showing the rigidity** of the compound with more stability.—Solid form.

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