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NOTE

Parametric Method-3 for the Geometry Optimization of Bis-coumarin

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In the present work, the author described the full geometry optimization of bis-coumarin extracted from *Colvillea racemosa* (Leguminosae).

Recently Sreenath and Rao[1] extracted a new compound bis-coumarin from *Colvillea racemosa* (Leguminosae) which is found in Madagascar. This compound is isolated and identified as 6-methoxy-7-hydroxy-biscoumarin. This compound has been of great interest because of the *in-vivo* antineoplastic activity shown against the Ehrlich ascites carcinoma in mice[2, 3].

In the present work the full geometry optimization of this compound, by using Parametric Method 3 (PM3)[4], have been done. For any medicinal drug, for its efficacy, it is of paramount importance, to have stabilization energy, besides other physical parameters like dipole moment, hardness and electronegativity.

Calculations

The stabilization energy of this new compound has been calculated and the results are shown in Table-1. Since this compound is made of 7-OH coumarin and 6-methoxy-7-hydroxy coumarin minus H-atom, so the relative stability is calculated by using simple Hess's law of first law of thermodynamics. Since experimental values are not available for stabilization energy for this new compound as yet, so comparison cannot be made at this stage. Furthermore, the activity of bis-coumarin is evident from the fact that its hardness value is minimum in comparison to its fragments (Table-2). According to the definition of hardness (η), higher value of 'η' leads to more rigidity of the molecule and lower value makes the molecule much softer and reactive. Hence, bis-coumarin is found to be more reactive than its fragments. The stabilization energy is calculated by subtracting the E_T of all fragments of bis-coumarin from the $6CH_3O$–7OH-bis-coumarin (Table-1). The other parameters are shown in Table-2. The bond angles and bond distances are given in Table-3. Sreenath and Rao[1] have shown the angle between C—O—C in the structure as 180° but actually it is a non-linear joint and both molecules connected through O-atom are not in a plane (see figure).

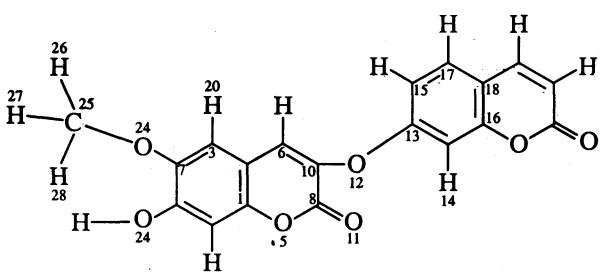

TABLE-1
CALCULATED TOTAL ENERGY OF BIS-COUMARIN AND ITS FRAGMENTS

System	E_T (ev)	Stabilization energy (ev)
Coumarin (I)	-1745.2	
7-OH coumarin (II)	-2039.1	
6-CH_3O coumarin (III)	-2188.1	
6-CH_3O-7-OH coumarin (IV)	-2481.7	
6-CH_3O-7-OH bis-coumarin	-4489.4	
S.E. = V - (IV + I)		-262.5

TABLE-2
CALCULATED VALUES OF HARDNESS (η), DIPOLE MOMENT (μ), HEAT OF FORMATION (ΔH) AND ELECTRONEGATIVITY (χ) FOR BIS-COUMARIN FRAGMENTS

System	ΔH (kcal)	μ(D)	η	χ
Coumarin	-37.9	4.42	4.24	5.24
7-OH	-83.5	5.63	4.15	5.96
6-CH_3O	-75.2	4.41	4.56	5.68
6CH_3O-7-OH	-114.6	5.70	4.03	4.99
Bis-coumarin	-178.7	5.76	3.93	5.32

TABLE-3
CALCULATED GEOMETRY OF 6 METHOXY-7-OH BIS-COUMARIN

Atom	Symbol	Bond length NA : I (Å)	Bond angle NB : NA : I (degree)	NA	NB
1.	C				
2.	C	1.405			
3.	C	1.402	121.5	1	2
4.	C	1.400	119.4	2	1
5.	O	1.878	122.7	1	2
6.	C	1.446	119.2	2	1
7.	C	1.391	118.5	3	1
8.	C	1.377	118.6	5	1
9.	C	1.394	119.8	4	2
10.	C	1.353	118.7	6	2
11.	O	1.210	108.7	8	5
12.	O	1.386	119.8	10	6
13.	C	1.394	115.3	12	10
14.	C	1.393	114.9	13	12
15.	C	1.404	123.3	13	12
16.	C	1.400	118.7	14	13
17.	C	1.383	119.8	15	13

Atom	Symbol	Bond length NA : I (Å)	Bond angle NB : NA : I (degree)	NA	NB
18.	C	1.405	119.5	16	14
19.	C	1.449	121.6	16	14
20.	O	1.376	122.7	18	16
21.	C	1.343	119.5	16	14
22.	C	1.380	117.9	20	18
23.	O	1.211	108.6	22	20
24.	O	1.391	117.1	7	3
25.	C	1.411	114.3	24	7
26.	H	1.092	102.8	25	24
27.	H	1.094	112.8	25	24
28.	H	1.099	110.9	25	24
29.	O	1.368	115.5	9	4
30.	H	0.952	108.1	29	9
31.	H	1.098	120.6	3	1
32.	H	1.097	119.8	4	2
33.	H	1.097	118.9	6	2
34.	H	1.097	121.1	14	13
35.	H	1.096	120.0	15	13
36.	H	1.096	120.6	17	15
37.	H	1.096	118.3	19	16
38.	H	1.095	123.1	21	19

The molecular orbital calculations are extremely useful in establishing the stability of the molecule and its reaction *in-vivo* for drug activity.

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