

# Energy Value Of Benzoxepine Derivatives

Mrs.G.Jenitha ,Dr.I. Paulraj Jayasimman ,Dr.A.Kumaravel

**Abstract:** In this article, Minimum Domination energy value and Minimum neighborhood energy value of Benzoxepine derivatives has studied. By using these derivatives are useful intermediates for the synthesis of many natural products and biologically active molecules. These molecules are an essential objective in modern organic synthesis. AMS Subject Classification (2010): 05C69

**Key Words:** Minimum Domination energy value and Minimum neighborhood energy value

## 1. INTRODUCTION:

The concept of a energy graph was studied by Ivan Gutman . But the motivation for this concept started in the 1930s by Erich Huckel. Huckel Molecular Orbital theory enables us to approximate  $\pi$ -electronic energies. This chemical concept has been modeled as a graph which represents the carbon skeleton of a molecule. This concept is closely related to solving the Eigenvalue problem. It follows that solving the Eigenvalue problem for H is equivalent to solving the Eigenvalue problem for A. It is noted that most frequently an orbital contains two  $\pi$ -electrons exactly when the corresponding E value is positive, and no  $\pi$ -electrons when E is harmful.

Let  $G$  be a graph with  $n$  vertices and  $m$  edges and let  $A = (a_{ij})$  be the adjacency matrix of the graph. The Eigen values  $\lambda_1, \lambda_2, \dots, \lambda_n$  of  $A$ , assumed in non increasing order, are the Eigen values of the graph  $G$ . As  $A$  is real symmetric, the Eigen values of  $G$  are real with sum equal to zero. The energy  $E(G)$  of  $G$  is defined to be the sum of the absolute values of the Eigen values of  $G$ .

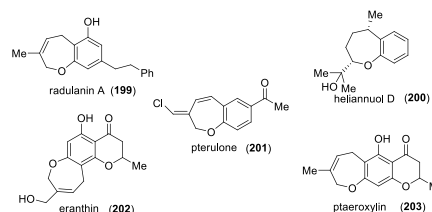
$$\text{i.e, } E(G) = \sum_{i=1}^n |\lambda_i|$$

## 2. SYNTHESIS OF BENZOXEPINES DERIVATIVES:

The Baylis-Hillman adducts and their derivatives are useful intermediates for the synthesis of many natural products and biologically active molecules. Benzoxepine is an important benzo-fused medium-sized heterocycle, because there are numerous biologically active natural products and synthetic molecules, which contain this structural framework. Thus synthesis of benzoxepine derivatives constitutes an important objective in modern organic synthesis.

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The benzoxepine ring system occurs in number of biologically active natural products isolated mainly from plant sources. Some of the examples which contain benzoxepine moiety are radulanin A, heliannuol D, pterulone, eranthin and ptaeroxylin .



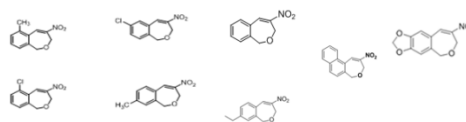
Natural products

containing

benzoxepine skeleton

The 2-benzoxepine moiety is an important structural unit present in many biologically important molecules such as doxaminol (vasodilator and  $\beta$ -sympathomimetic agent), isoxepac (antiinflammatory agent), oxepinac (antiinflammatory, analgesic, antipyretic agent), and pinoxepin (neuroleptic agent, tranquilliser used for treatment of schizophrenia). Natural products such as cassialactone, psorolactone, secofuranoeremophilane have also possessing benzoxepine core structure. Also synthetic 2-benzoxepine derivatives are found to possess oral hypotensive and antiulcer activities.[6][15]

**Benzoxepine derivatives:**



## 3. ENERGY VALUE OF BENZOXEPINE DERIVATIVES:

**Domination parameter:**

**DERIVATIVE: 1**

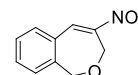


Figure 1- Minimum Dominating Energy value



$$\lambda^{15} - 4\lambda^{14} - 11\lambda^{13} + 53\lambda^{12} + 44\lambda^{11} - 271\lambda^{10} - 82\lambda^9 + 673\lambda^8 + 87\lambda^7 - 833\lambda^6 - 83\lambda^5 + 464\lambda^4 + 63\lambda^3 - 80\lambda^2 - 11\lambda = 0$$

The Eigen value of the matrix Minimum Dominating Matrix are

$$\lambda_1 \approx 2.82713, \lambda_2 \approx 2.50594, \lambda_3 \approx 2.21209, \lambda_4 \approx 1.69984, \lambda_5 \approx 1.31645, \lambda_6 \approx 1.17119, \lambda_7 \approx 0.524884, \lambda_8 \approx 0.073936, \lambda_9 \approx -0.137554, \lambda_{10} \approx -0.84577, \lambda_{11} \approx -1.2807, \lambda_{12} \approx 1.56531, \lambda_{13} \approx -1.73864, \lambda_{14} \approx -2.08647, \lambda_{15} \approx 0.$$

Energy value of Minimum Dominating Matrix is

$$E_{MD}(G) = \sum_{i=1}^n |\lambda_i| = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6 + \lambda_7 + \lambda_8 + \lambda_9 + \lambda_{10} + \lambda_{11} + \lambda_{12} + \lambda_{13} + \lambda_{14} + \lambda_{15} \approx 19.911968$$

**DERIVATIVE :5**

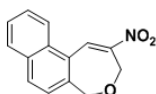


Figure 5- Minimum Dominating Energy value

Characteristic equation

$$f_n(G, \lambda) = \det [\lambda I - A_D(G)]$$

The characteristics equation of  $f_n(G, \lambda)$  is

$$\lambda^{16} - 5\lambda^{15} - 8\lambda^{14} + 68\lambda^{13} + \lambda^{12} - 362\lambda^{11} + 146\lambda^{10} + 972\lambda^9 - 473\lambda^8 - 1404\lambda^7 + 552\lambda^6 + 1067\lambda^5 - 208\lambda^4 - 373\lambda^3 - 3\lambda^2 + 33\lambda + 1 = 0$$

The Eigen value of Minimum Dominating Matrix are

$$\lambda_1 \approx -2.15912, \lambda_2 \approx -1.68024, \lambda_3 \approx -1.62622, \lambda_4 \approx -1.28339, \lambda_5 \approx -0.74236, \lambda_6 \approx -0.634319, \lambda_7 \approx -0.475706, \lambda_8 \approx -0.0305337, \lambda_9 \approx 0.329328, \lambda_{10} \approx 0.934231, \lambda_{11} \approx 1.24518, \lambda_{12} \approx 1.70176, \lambda_{13} \approx 1.92482, \lambda_{14} \approx 2.23729, \lambda_{15} \approx 2.43666, \lambda_{16} \approx 2.82262.$$

Energy value of Minimum Dominating Matrix is

$$E_{MD}(G) = \sum_{i=1}^n |\lambda_i| = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6 + \lambda_7 + \lambda_8 + \lambda_9 + \lambda_{10} + \lambda_{11} + \lambda_{12} + \lambda_{13} + \lambda_{14} + \lambda_{15} + \lambda_{16} \approx 22.2637777$$

Neighborhood Parameter:

**DERIVATIVE: 1**

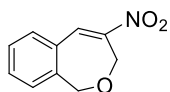


Figure 2- Minimum neighborhood Energy value

The characteristics equation of  $f_n(G, \lambda)$

$$\lambda^{12} - 6\lambda^{11} + 2\lambda^{10} + 43\lambda^9 - 46\lambda^8 - 115\lambda^7 + 131\lambda^6 + 150\lambda^5 - 116\lambda^4 - 98\lambda^3 + 13\lambda^2 + 13\lambda + 1 = 0$$

Energy value of Minimum Dominating Matrix is

$$E_{MD}(G) = \sum_{i=1}^n |\lambda_i| = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6 + \lambda_7 + \lambda_8 + \lambda_9 + \lambda_{10} + \lambda_{11} + \lambda_{12} \approx 16.549138$$

**DERIVATIVE :2**

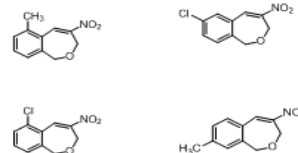


Figure 2- Minimum Neighborhood Energy value

Therefore Minimum Neighborhood Matrix of

$$A_D(G) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}$$

Characteristic equation

$$f_n(G, \lambda) = \det [\lambda I - A_D(G)]$$

$$f_n(G, \lambda) = \begin{bmatrix} \lambda & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & \lambda-1 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & \lambda-1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & \lambda & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & \lambda-1 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & \lambda-1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & -1 & \lambda & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & \lambda & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & \lambda-1 & -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & \lambda & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & \lambda & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & \lambda-1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & \lambda-1 & -1 \end{bmatrix}$$

The characteristics equation of  $f_n(G, \lambda)$  is

$$\lambda^{13} - 6\lambda^{12} + \lambda^{11} + 48\lambda^{10} - 45\lambda^9 - 147\lambda^8 + 146\lambda^7 + 223\lambda^6 - 151\lambda^5 - 167\lambda^4 + 30\lambda^3 + 37\lambda^2 + 5\lambda = 0$$

The Eigen value of Minimum Neighborhood Matrix are

$$\lambda_1 \approx 3.01367, \lambda_2 \approx 2.53082, \lambda_3 \approx 2.17235, \lambda_4 \approx 1.97678, \lambda_5 \approx 1.43725, \lambda_6 \approx 0.626918, \lambda_7 \approx -0.186537, \lambda_8 \approx -0.370762, \lambda_9 \approx -0.860543, \lambda_{10} \approx -1.06677, \lambda_{11} \approx -1.53741, \lambda_{12} \approx 1.73576, \lambda_{13} \approx 0.$$

Energy value of Minimum Neighborhood Matrix is

$$E_{MN}(G) = \sum_{i=1}^n |\lambda_i| = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6 + \lambda_7 + \lambda_8 + \lambda_9 + \lambda_{10} + \lambda_{11} + \lambda_{12} + \lambda_{13} \approx 17.51557$$

**DERIVATIVE :3**

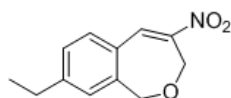


Figure 3- Minimum Neighborhood Energy value

Characteristic equation

$$f_n(G, \lambda) = \det [\lambda I - A_D(G)]$$

The characteristics equation of  $f_n(G, \lambda)$  is

$$\lambda^{14} - 7\lambda^{13} + 6\lambda^{12} + 54\lambda^{11} - 100\lambda^{10} - 144\lambda^9 + 364\lambda^8 + 173\lambda^7 - 549\lambda^6 - 135\lambda^5 + 348\lambda^4 + 97\lambda^3 - 62\lambda^2 - 22\lambda - 1 = 0$$

The Eigen value of Minimum Neighborhood Matrix are

$$\lambda_1 \approx 2.93044, \lambda_2 \approx 2.5099, \lambda_3 \approx 2.19724, \lambda_4 \approx 2.06288, \lambda_5 \approx 1.58914,$$

$$\lambda_6 \approx 1.405, \lambda_7 \approx 0.565132, \lambda_8 \approx -0.0543452, \lambda_9 \approx -0.321594,$$

$$\lambda_{10} \approx -0.500642, \lambda_{11} \approx -0.788475, \lambda_{12} \approx -1.23305, \lambda_{13} \approx -1.50571, \lambda_{14} \approx -1.85594.$$

Energy value of Minimum Neighborhood Matrix is

$$E_{MN}(G) = \sum_{i=1}^n |\lambda_i| = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6 + \lambda_7 + \lambda_8 + \lambda_9 + \lambda_{10} + \lambda_{11} + \lambda_{12} + \lambda_{13} + \lambda_{14} \approx 19.5194882$$

#### DERIVATIVE:4

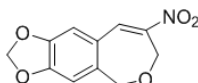


Figure 4- Minimum Neighborhood Energy value

Characteristic equation

$$f_n(G, \lambda) = \det [\lambda I - A_D(G)]$$

The characteristics equation of  $f_n(G, \lambda)$  is

$$\lambda^{15} - 7\lambda^{14} + 4\lambda^{13} + 65\lambda^{12} - 98\lambda^{11} - 239\lambda^{10} + 441\lambda^9 + 468\lambda^8 - 853\lambda^7 - 564\lambda^6 + 735\lambda^5 + 415\lambda^4 - 201\lambda^3 - 125\lambda^2 - 11\lambda = 0$$

The Eigen value of Minimum Neighborhood Matrix is

$$\lambda_1 \approx 3.09624, \lambda_2 \approx 2.69805, \lambda_3 \approx 2.26469, \lambda_4 \approx 1.98663,$$

$$\lambda_5 \approx 1.64531, \lambda_6 \approx 1.55586, \lambda_7 \approx 0.797435, \lambda_8 \approx -0.111718,$$

$$\lambda_9 \approx -0.428568, \lambda_{10} \approx -0.72537, \lambda_{11} \approx -1.15781, \lambda_{12} \approx 1.30024,$$

$$\lambda_{13} \approx -1.54114, \lambda_{14} \approx -1.77936, \lambda_{15} \approx 0.$$

value of Minimum Neighborhood Matrix is

$$E_{MD}(G) = \sum_{i=1}^n |\lambda_i| = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6 + \lambda_7 + \lambda_8 + \lambda_9 + \lambda_{10} + \lambda_{11} + \lambda_{12} + \lambda_{13} + \lambda_{14} + \lambda_{15} \approx 21.088421$$

#### DERIVATIVE :5

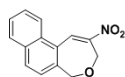


Figure 5- Minimum Neighborhood Energy value

Characteristic equation

$$f_n(G, \lambda) = \det [\lambda I - A_D(G)]$$

The characteristics equation of  $f_n(G, \lambda)$  is

$$\lambda^{16} - 8\lambda^{15} + 10\lambda^{14} + 69\lambda^{13} - 174\lambda^{12} - 194\lambda^{11} + 799\lambda^{10} + 178\lambda^9 - 1720\lambda^8 - 6\lambda^7 + 1926\lambda^6 + 69\lambda^5 - 1054\lambda^4 - 209\lambda^3 - 179\lambda^2 + 61\lambda + 4 = 0$$

The Eigen value of Minimum Neighborhood Matrix are

$$\lambda_1 \approx 2.61906, \lambda_2 \approx 2.2626, \lambda_3 \approx 2.10971, \lambda_4 \approx 1.93026,$$

$$\lambda_5 \approx 1.59538, \lambda_6 \approx 1.40494, \lambda_7 \approx 0.577944, \lambda_8 \approx -0.0916545,$$

$$\lambda_9 \approx -0.296547, \lambda_{10} \approx -0.513619, \lambda_{11} \approx -0.749902, \lambda_{12} \approx -0.984379,$$

$$\lambda_{13} \approx -1.40015, \lambda_{14} \approx -1.50318, \lambda_{15} \approx -1.96412, \lambda_{16} \approx 3.00368.$$

Energy value of Minimum Neighborhood Matrix is

$$E_{MN}(G) = \sum_{i=1}^n |\lambda_i| = \lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6 + \lambda_7 + \lambda_8 + \lambda_9 + \lambda_{10} + \lambda_{11} + \lambda_{12} + \lambda_{13} + \lambda_{14} + \lambda_{15} + \lambda_{16} \approx 23.0071$$

TABLE:

SL.NO	BENZOXEPINE DERIVATIVES	DOMINATION PARAMETER	NEIGHBORHOOD PARAMETER
1		$E_{MD}(G) \approx 16.249138$	$E_{MN}(G) \approx 16.549138$
2		$E_{MD}(G) \approx 17.346846$	$E_{MN}(G) \approx 17.51557$
3		$E_{MD}(G) \approx 19.071409$	$E_{MN}(G) \approx 19.5194882$
4		$E_{MD}(G) \approx 19.911968$	$E_{MN}(G) \approx 21.088421$
5		$E_{MD}(G) \approx 22.2637777$	$E_{MN}(G) \approx 23.0071$

#### 5. CONCLUSION:

The author Investigate the Minimum dominating energy value and Minimum neighborhood energy value for Benzoxipine derivatives. Further the author will Investigate the energy value through the other parameter in domination for this Chemical graphs.

#### 6. ACKNOWLEDGEMENT:

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