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# On Maximum Independent D–Energy of a Graph

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**Abstract.** For a simple connected graph Ω, the Maximum independent D-energy (distance energy) $DE_{Imax}$ results from the total of its absolute D-latent values. $DE_{Imax}$ has been calculated for some of the well known standard graphs. Also the basic properties of $DE_{Imax}$ are also analyzed by studying a graph's characteristic polynomial, its D-latent values and its D-energy $DE_{Imax}$. As an implementation in the field of Chemistry, $DE_{Imax}$ has been established here for Cancer medicines namely Carboplatin & Cisplatin for mathematical Comparative purposes.

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**Keywords.** Maximum independent D-latent values, Maximum independent D-energy, Maximum independent D-matrix, Maximum independent distance set.

## I.Prelude

Let Ω be a graph composed of order 's' & size 'r' but without parallel edges, loops and directions.

The D-matrix is an adjacency matrix whose each entry is the value of the distance among the considered vertices [2].

The basic Graph Energy results from its latent values as found in [3,4,6].

In 2016, K.B. Murthy et al [7] introduced Maximum independent vertex energy based on Independent set (no two members in this set constitutes an edge) and usual graph energy.

The above mentioned concepts inspired us to come up with idea of Maximum independent D-Energy of a graph $DE_{Imax}(\Omega)$ which we have computed for few standard graphs and therefore applied to molecular graphs of anti-cancer drugs Carboplatin and Cisplatin to make a comparative mathematical study.

Related studies can also be found in [8, 9 & 11].

## II.Maximum Independent D-Energy of a Graph

Let Ω be a graph composed with 's'-no. of vertices(order) and 'r'-no. of edges(size). An independent set $I_{max}$ subset of Vertex set of a graph Ω with largest number of members belonging to it is called a maximum independent set. Then the maximum independent D-matrix of Ω is the n x n matrix $A_{Imax}D(\Omega) = (g_{ij})$, where

$$g_{ij} = \begin{cases} 1 & \text{if } i=j,\ v_i \in I_{max} \\ 0 & \text{if } i=j,\ v_i \notin I_{max} \\ d_{ij} & \text{otherwise} \end{cases}$$

The characteristic polynomial of $A_{Imax}D(\Omega)$ is written as follows: $h_s(\Omega,\lambda)=det(A_{Imax}D(\Omega)-\lambda I)$.

The maximum independent D-latent values of the graph Ω are the latent values of $A_{Imax}D(\Omega)$. Since $A_{Imax}D(\Omega)$ contains real and symmetric values in them, its latent values are real and we represent them as

$\lambda_{ID_1}, \lambda_{ID_2}, \lambda_{ID_3}, ...., \lambda_{ID_r}$.

Then the maximum independent D- energy of Ω is defined as: $DE_{I_{max}}(\Omega) = \sum_{i=1}^{r} |\lambda_{ID_i}|$.

### III.Basic Theorems on $DE_{Imax}(\Omega)$

**Theorem.1** Let Ω be a simple connected graph with independence number β (Ω). If the order and size of Ω is s and r respectively with $h_s(\Omega, \lambda) = g_0\lambda^s c + g_1\lambda^{s-1}{}_c + .... + g_s$ being the characteristic polynomial obtained from I of Ω, then

1) $g_0=1$
2) $g_1 = -\beta(\Omega)$
3) $g_2 = \binom{\beta(\Omega)}{2} - \sum_{1\le i<j\le n} d^2(v_{ij})$

**Proof.** (1) It is obvious that $h_S(\Omega, \lambda) := \det(\lambda_c I - A_{Imax}D(\Omega))$ which yields $g_0=1$.

(2) As the total of the diagonal elements in $A_{Imax}D(\Omega)$ is evidently equal to independence number β(Ω) of its corresponding graph Ω, thus we get $g_1 = -\beta(\Omega)$.

(3) Since $(-1)^2 g_2$ equals total of determinants of all principal submatrices of $A_{Imax}D(\Omega)$ of order 2 × 2, it leads to

$$g_2 = \sum_{1\le i<j\le s} \begin{vmatrix} g_{ii} & g_{ij} \\ g_{ji} & g_{jj} \end{vmatrix}$$

$$= \sum_{1\le i<j\le s} (g_{ii}g_{jj} - g_{ij}g_{ji})$$

$$= \sum_{1\le i<j\le s}(g_{ii}g_{jj}) - \sum_{1\le i<j\le s}({g_{ij}}^2)$$

$$= \binom{\beta(\Omega)}{2} - \sum_{1\le i<j\le n} d^2(v_{ij})$$

**Theorem 2**. Let Ω be a graph. Let $\lambda_{ID_1}, \lambda_{ID_2}, \lambda_{ID_3}, ...., \lambda_{ID_r}$. be the latent values of maximum independent adjacency matrix $A_{Imax}D(\Omega)$. Then

(1). $\sum_{i=1}^{s} \lambda IDi = \beta(\Omega)$,

(2). $\sum_{i=1}^{s} \lambda^2 IDi = \beta(\Omega) + 2r + 2\varphi$ where $\varphi = \sum_{i<j,\ d\neq 1} d^2(v_{ij})$

**Proof**. (1) Since the total of the latent values of $A_{Imax}D(\Omega)$ equals the trace of $A_{Imax}D(\Omega)$, we get $\sum_{i=1}^{s} \lambda IDi = \sum_{i=1}^{s} g_{ii} = |I| = \beta(\Omega)$ where β (Ω) denotes the cardinality of maximum independent vertex set.

(2) Also likewise the Sum of the squares of latent values of the $A_{Imax}D(\Omega)$ matches the trace of the $(A^2{}_{Imax}D(\Omega))$.

Thus

$$\sum_{i=1}^{s} \lambda^2 IDi = \sum_{i=1}^{s}\sum_{j=1}^{s} g_{ij}g_{ji}$$

$=2\sum_{i\neq j}^{s} g_{ij}g_{ji} + \sum_{i=1}^{s}({g_{ii}}^2)$

$$= 2\sum_{i<j}^{s}({g_{ij}}^2) + \sum_{i=1}^{s}({g_{ii}}^2)$$

So $\sum_{i=1}^{s} \lambda^2$IDi= 2r + 2φ + β (Ω)

**Theorem 3**. Consider Ω to be a simple connected graph containing a maximum independent set I. If the $DE_{Imax}$(Ω)is a rational number, Then $DE_{Imax}$(Ω) ≡ |I|(mod2).

**Proof**. Let $\lambda_{ID_1}, \lambda_{ID_2}, \lambda_{ID_3}, ...., \lambda_{ID_r}$. be the maximum independent D - latent values of a graph Ω. Let (t < s) latent values be the non negative latent values and the balance being negative values, we get

$\sum_{i=1}^{s}$ |λIDi|= (λID$_1$ + λID$_2$ + λID$_3$ + ... + λID$_t$) − (λID$_{t+1}$ + λID$_{t+2}$ + λID$_{t+3}$ + .. + λID$_s$)

= 2 (λID$_1$ + λID$_2$ + λID$_3$ + .... + λID$_t$) − (λID$_1$ + λID$_2$ + λID$_3$ + .... + λID$_s$)

= 2 (λID$_1$ + $\lambda_{ID2}$ + λID$_3$ + .... + λID$_t$ ) − β (Ω)

Therefore, EIχ (Ω) = 2k − β (Ω) where k = (λID$_1$ + λID$_2$ + λID$_3$ + .... + λID$_t$)

Here the latent values λID$_1$, λID$_2$, λID$_3$, ...., λIDs are integers, so their total will also be an integer value. Then, the value of 'k' is also integer as the value of $DE_{Imax}$(Ω) is a rational.

## IV.$DE_{Imax}$ OF CERTAIN COMMON FAMILIES OF GRAPHS

**Theorem 4.** For s ≥ 2, $DE_{Imax}$ (K$_{1,s−1}$) = $(s - 2) + \sqrt{4s^2 - 8s + 5}$

**Proof.** For a Star graph K$_{1,s−1}$ with s vertices V = {v$_1$, v$_2$, ..., v$_s$}, its highest independent set $I_{max}$ = {v$_s$}

Since its independence number β (K$_{1,s−1}$) = s −1, we obtain

$$AI_{max}\,(K_{1,s-1}) = \begin{bmatrix} 0 & 1 & \cdots & 1 & 1 \\ 1 & 1 & & 2 & 2 \\ \vdots & & \ddots & \vdots & \\ 1 & 2 & \cdots & 1 & 2 \\ 1 & 2 & & 2 & 1 \end{bmatrix}_{(s \times s)}$$

Characteristic polynomial is obtained as (−1)$^s$ (λ+1)$^{s−2}$ (λ$^2$ - (2s − 3)λ − (s − 1))

Spectrum, $SpecI_{max}$ (K$_{1,s−1}$) = $\begin{pmatrix} -1 & \frac{(2s-3)\pm\sqrt{4s^2-8s+5}}{2} \\ s-2 & 1 \end{pmatrix}$

Therefore, $DE_{Imax}$(K$_{1,s−1}$) = $\sum_{i=1}^{s} |\lambda i|$

$= |-1|(s - 2) + \left|\frac{(2s-3)\pm\sqrt{4s^2-8s+5}}{2}\right| 1$

$= (s - 2) + \sqrt{4s^2 - 8s + 5}$

Thus $DE_{Imax}$(K$_{1,s−1}$) is $(s - 2) + \sqrt{4s^2 - 8s + 5}$.

**Theorem 5.** For s ≥ 2 ,$DE_{Imax}$(K$_{s,s}$) = (7s − 6).

**Proof.** Let K$_{s,s}$be a Complete Bipartite graphwith vertices V = {u$_1$, u$_2$, ..., u$_s$, v$_1$, v$_2$, ..., v$_s$}, then its $I_{max}$ = {u$_1$, v$_1$}.

Since its independence number β(K$_{s,s}$) = s, we obtain

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$$AI_{max}(K_{s,s}) = \begin{bmatrix} 0 & 2 & \cdots & 1 & 1 \\ 1 & 0 & & 1 & 1 \\ \vdots & & \ddots & & \vdots \\ 1 & 1 & \cdots & 1 & 2 \\ 1 & 1 & & 2 & 1 \end{bmatrix}_{(2s \times 2s)}$$

Characteristic polynomial of $K_{s,s}$ is found to be $(\lambda + 1)^{s-1} (\lambda + 2)^{s-1} (\lambda^2 + (4s - 3)\lambda + (3s^2 - 6s + 2))$

Its Spectrum, $SpecI_{max}(K_{s,s}) = \begin{pmatrix} -1 & -2 & \frac{(4s-3)\pm\sqrt{4s^2-1}}{2} \\ s-1 & s-1 & 1 \end{pmatrix}$

Then $DE_{Imax}(K_{s,s}) = \sum_{i=1}^{s} |\lambda i|$

$= |-1|(s-1) + |-2|(s-1) + \left|\frac{(4s-3)\pm\sqrt{4s^2-1}}{2}\right| 1$

$= (s - 1) + (2s - 2) + (4s - 3)$

$= (7s - 6)$

Thus $DE_{Imax}(K_{s,s})$ is $(7s - 6)$.

**Theorem 6.** For $s \geq 2$, $DE_{Imax}$ (Fs) is 7s - 6 .

**Proof.** For a Friendship graph $F_s$ of order (2s + 1), it assumes the maximum independent set as $I_{max} = \{v_0\}$.

Since its independence number $\beta(F_s) = s$, we obtain

$$AI_{max}(Fs) = \begin{bmatrix} 0 & 1 & \cdots & 1 & 1 \\ 1 & 1 & & 2 & 2 \\ \vdots & & \ddots & & \vdots \\ 1 & 2 & \cdots & 1 & 1 \\ 1 & 2 & & 1 & 0 \end{bmatrix}_{(2s+1 \times 2s+1)}$$

Characteristic polynomial of $F_S$ is given by $(-1)(\lambda^2 + 3\lambda + 1)^{s-1} (\lambda^3 - (4s - 1)\lambda - s)$

Spectrum, $SpecI_{max}(F_s) = \begin{pmatrix} \frac{(4s-3)}{3} & \frac{-3\pm\sqrt{5}}{2} \\ 3 & s-1 \end{pmatrix}$

Then $DE_{Imax}(F_s) = \sum_{i=1}^{s} |\lambda i|$

$= \left|\frac{-3\pm\sqrt{5}}{2}\right| (s-1) + \left|\frac{(4s-3)}{3}\right| 3$

$= 7s - 6$

Thus $DE_{Imax}$ (Fs) is $7s - 6$ .

## V. Chemical Application of Maximum Independent D Energy $DE_{Imax}(\Omega)$

Carboplatin and Cisplatin are anticancer drugs used considerably for chemotherapy treatment. $DE_{Imax}(\Omega)$ has been calculated involving the molecular graphs of these two medicines which can be utilized for future research pertaining to further development of these two medicines. Structural Formula for Carboplatin and Cisplatin are illustrated in Figure1 and its molecular graphs are involved in the below comparative study.

In Cisplatin, the maximum independent colored set is $I_{max} = \{Cl, Cl, NH_3, NH_3\}$.

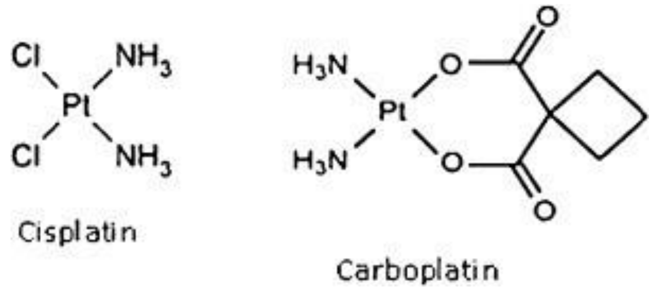
A $I_{max}$ of Cisplatin = $\begin{bmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & 2 & 2 \\ 1 & 2 & 1 & 2 & 2 \\ 1 & 2 & 2 & 1 & 2 \\ 1 & 2 & 2 & 2 & 1 \end{bmatrix}$

The Characteristic polynomial is found to $(\lambda +1)^3 (\lambda^2 - 7\lambda - 4)$

Spectrum of Cisplatin, Spec $I_{max}$ = $\begin{bmatrix} -1 & \frac{7+\sqrt{65}}{2} & \frac{7-\sqrt{65}}{2} \\ 3 & 1 & 1 \end{bmatrix}$

Thus, $DE_{I_{max}}$ of Cisplatin = 11.0623

***FIGURE1***. Cisplatin Vs Carboplatin: Structural Formula




In Carboplatin, the maximum independent colored set is $I_{max}$ = {Cl, Cl, $NH_3$, $NH_3$}.

A $I_{max}$ of Carboplatin = $\begin{bmatrix} 1 & 2 & 1 & 2 & 2 & 3 & 3 & 4 \\ 2 & 1 & 1 & 2 & 2 & 3 & 3 & 4 \\ 1 & 1 & 0 & 1 & 1 & 2 & 2 & 3 \\ 2 & 2 & 1 & 1 & 2 & 1 & 3 & 2 \\ 2 & 2 & 1 & 2 & 1 & 3 & 1 & 2 \\ 3 & 3 & 2 & 1 & 3 & 0 & 2 & 1 \\ 3 & 3 & 2 & 3 & 1 & 2 & 0 & 1 \\ 4 & 4 & 3 & 3 & 2 & 2 & 1 & 1 \end{bmatrix}$

Latent values are 15.7179, -6.0619, -3.5616, -1, -0.76632, 0.6069, 0.5616, -0.4965

Thus, $DE_{I_{max}}$ of Carboplatin = 28. 7726

Also, certain Scientific papers also suggests Carboplatin is preferred in many countries than compared to Cisplatin in various Chemotherapy treatment as found in [5 , 10]. So, Carboplatin is preferable than Cisplatin as an anticancer drug.

## VI.Conclusion

Few basic properties of $DE_{I_{max}}(\Omega)$are studied and its numerical value of certain standard graphs are calculated. Finally $DE_{I_{max}}$ is analysed for the anti-cancer drugs Cisplatin and Carboplatin and the latter is found to have more energy numerically which might be useful for scientists of medicinal field for further research.

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