contains the basic definitions and background of the current topic. In section 2, we show the chemical applicability of c-dominating energy for molecular graphs G. The section 3, contains the mathematical properties of c-dominating energy. In the last section, we have characterized, trees, unicyclic graphs and cubic graphs and block graphs with equal minimum dominating energy and c-dominating energy. Finally, we conclude this paper by posing an open problem.

2 Chemical Applicability of $E_{D_{cc}}(G)$

We have used the doubly-dominating energy for modeling eight representative physical properties like boiling points(bp), molar volumes(mv) at $20°C$, molar refractions(mr) at $20°C$, heats of vaporization (hv) at $25°C$, critical temperatures(ct), critical pressure(cp) and surface tension (st) at $20°C$ of the 74 alkanes from ethane to nonanes. Values for these properties were taken from http://www.moleculardescriptors.eu/dataset.htm. The doubly-dominating energy $E_{D_{cc}}(G)$ was correlated with each of these properties and surprisingly, we can see that the $E_{D_{cc}}$ has a good correlation with the critical temperature of alkanes with correlation coefficient $r = 0.896$.

The following structure-property relationship model has been developed for the doubly connected-dominating energy $E_{D_{cc}}(G)$.

$$ct = 135.128 + [E(D_{cc})(G)]4.317 \quad (1)$$

$$ct = 10.791[E(D_{cc})(G)]^2 - 0.0101[E(D_{cc})(G)] + 70.999 \quad (2)$$

$$ct = -53.591 + \ln[E(D_{cc})(G)]100.568 \quad (3)$$

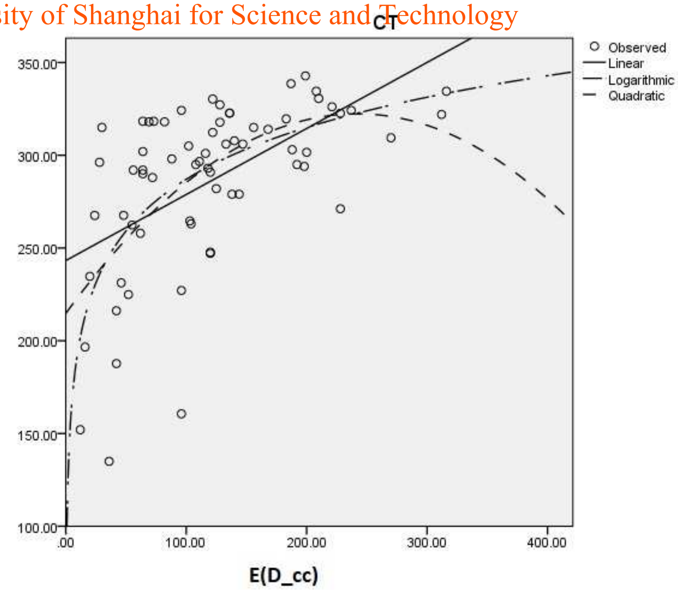

Figure 3: Correlation of $E_{D_{cc}}(G)$ with critical temperature of alkanes.

3 Mathematical Properties of Doubly Connected-Dominating Energy of Graph

We begin with the following straightforward observations.

Observation 1. *Note that the trace of* $A_{D_cc}(G) = \gamma_c c(G)$.

Observation 2. *Let* $G = (V, E)$ *be a graph with* $\gamma_c c$*-set* $D_c c$. *Let* $f_n(G, \lambda) = c_0\lambda^n + c_1\lambda^{n-1} + \cdots + c_n$ *be the characteristic polynomial of* G. *Then*

1. $c_0 = 1$,
2. $c_1 = -|D_c c| = -\gamma_c c(G)$.

Theorem 3. *If* $\lambda_1, \lambda_2, \cdots, \lambda_n$ *are the eigenvalues of* $A_{D_cc}(G)$, *then*

1. $\sum\limits_{i=1}^{n} \lambda_i = \gamma_c c(G)$
2. $\sum\limits_{i=1}^{n} \lambda_i^2 = 2m + \gamma_c c(G)$.

Proof.

1. Follows from Observation 1.

2. The sum of squares of the eigenvalues of $A_{D_{cc}}(G)$ is just the trace of $A_{D_{cc}}(G)^2$.

Therefore

$$\begin{aligned}\sum_{i=1}^{n}\lambda_i^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n}a_{ij}a_{ji}\\ &= 2\sum_{i<j}(a_{ij})^2+\sum_{i=1}^{n}(a_{ii})^2\\ &= 2m+\gamma_c c(G).\end{aligned}$$

□

We now obtain bounds for $E_{D_{cc}}(G)$ of G, similar to McClelland's inequalities [21] for graph energy.

Theorem 4. *Let G be a graph of order n and size m with $\gamma_{cc}(G)=k$. Then*

$$E_{D_{cc}}(G) \;\leq\; \sqrt{n(2m+k)}. \tag{4}$$

Proof. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of $A_{D_{cc}}(G)$. Bearing in mind the Cauchy-Schwarz inequality,

$$\left(\sum_{i=1}^{n}a_ib_i\right)^2 \leq \left(\sum_{i=1}^{n}a_i\right)^2\left(\sum_{i=1}^{n}b_i\right)^2$$

we choose $a_i=1$ and $b_i=|\lambda_i|$, which by Theorem 3 implies

$$\begin{aligned}E_{D_{cc}}^2 &= \left(\sum_{i=1}^{n}|\lambda_i|\right)^2\\ &\leq n\left(\sum_{i=1}^{n}|\lambda_i|^2\right)\\ &= n\sum_{i=1}^{n}\lambda_i^2\\ &= 2(2m+k).\end{aligned}$$

□

Theorem 5. *Let G be a graph of order n and size m with $\gamma_c c(G)=k$. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be a non-increasing arrangement of eigenvalues of $A_{D_{cc}}(G)$. Then*

$$E_{D_{cc}}(G) \;\geq\; \sqrt{2mn+nk-\alpha(n)(|\lambda_1|-|\lambda_n|)^2} \tag{5}$$

where $\alpha(n)=n[\frac{n}{2}](1-\frac{1}{n}[\frac{n}{2}])$, where $[x]$ denotes the integer part of a real number k.

Proof. Let $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$ be real numbers for which there exist real constants a, b, A and B, so that for each i, $i = 1, 2, \cdots, n, a \leq a_i \leq A$ and $b \leq b_i \leq B$. Then the following inequality is valid (see [6]).

$$| \, n \sum_{i=1}^{n} a_i b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \, | \;\; \leq \;\; \alpha(n)(A-a)(B-b), \tag{6}$$

where $\alpha(n) = n[\frac{n}{2}](1 - \frac{1}{n}[\frac{n}{2}])$. Equality holds if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$.

We choose $a_i := |\lambda_i|, b_i := |\lambda_i|, a = b := |\lambda_n|$ and $A = B := |\lambda_1|, i = 1, 2, \cdots, n$, inequality (4) becomes

$$|n \sum_{i=1}^{n} |\lambda_i|^2 - \left(\sum_{i=1}^{n} |\lambda_i| \right)^2 | \;\; \leq \;\; \alpha(n)(|\lambda_1| - |\lambda_n|)^2. \tag{7}$$

Since $E_{G_c c}(G) = \sum_{i=1}^{n} |\lambda_i|$, $\sum_{i=1}^{n} |\lambda_i|^2 = \sum_{i=1}^{n} |\lambda_i|^2 = 2m + k$ and $E_{D_c c}(G) \leq \sqrt{n(2m+k)}$, the inequality (5) becomes

$$\begin{aligned} n(2m+k) - (E_{D_c c})^2 &\leq \alpha(n)(|\lambda_1| - |\lambda_n|)^2 \\ (E_{D_c c})^2 &\geq 2mn + nk - \alpha(n)(|\lambda_1| - |\lambda_n|)^2. \end{aligned}$$

Hence equality holds if and only if $\lambda_1 = \lambda_2 = \cdots = \lambda_n$. □

Corollary 6. *Let G be a graph of order n and size m with $\gamma_c c(G) = k$. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be a non-increasing arrangement of eigenvalues of $A_{D_c c}(G)$. Then*

$$E_{D_c c}(G) \;\; \geq \;\; \sqrt{2mn + nk - \frac{n^2}{4}(|\lambda_1| - |\lambda_n|)^2}. \tag{8}$$

Proof. Since $\alpha(n) = n[\frac{n}{2}](1 - \frac{1}{n}[\frac{n}{2}]) \leq \frac{n^2}{4}$, therefore by (3), result follows. □

Theorem 7. *Let G be a graph of order n and size m with $\gamma_c(G) = k$. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be a non-increasing arrangement of eigenvalues of $A_{D_c c}(G)$. Then*

$$E_{G_c c}(G) \;\; \geq \;\; \frac{|\lambda_1||\lambda_2|n + 2m + k}{|\lambda_1| + |\lambda_n|}. \tag{9}$$

Proof. Let $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$ be real numbers for which there exist real constants r and R so that for each i, $i = 1, 2, \cdots, n$ holds $ra_i \leq b_i \leq Ra_i$. Then the following inequality is valid (see [11]).

$$\sum_{i=1}^{n} b_i^2 + rR \sum_{i=1}^{n} a_i^2 \;\; \leq \;\; (r+R) \sum_{i=1}^{n} a_i b_i. \tag{10}$$

Equality of (8) holds if and only if, for at least one i, $1 \leq i \leq n$ holds $ra_i = b_i = Ra_i$.

For $b_i := |\lambda_i|$, $a_i := 1$ $r := |\lambda_n|$ and $R := |\lambda_1|$, $i = 1, 2, \cdots, n$ inequality (8) becomes

$$\sum_{i=n}^{n} |\lambda_i|^2 + |\lambda_1||\lambda_n| \sum_{i=1}^{n} 1 \leq (|\lambda_1| + |\lambda_n|) \sum_{i=1}^{n} |\lambda_i|. \quad (11)$$

Since $\sum_{i=1}^{n} |\lambda_i|^2 = \sum_{i=1}^{n} \lambda_i^2 = 2m + k$, $\sum_{i=1}^{n} |\lambda_i| = E_{D_cc}(G)$, from inequality (9),

$$2m + k + |\lambda_1||\lambda_n|n \leq (\lambda_1 + \lambda_n)E_{D_cc}(G)$$

Hence the result. □

Theorem 8. *Let G be a graph of order n and size m with $\gamma_{cc}(G) = k$. If $\xi = |detA_{D_c}(G)|$, then*

$$E_{D_cc}(G) \geq \sqrt{2m + k + n(n-1)\xi^{\frac{2}{n}}}. \quad (12)$$

Proof.

$$\begin{aligned} (E_{D_cc}(G))^2 &= \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \\ &= \sum_{i=1}^{n} |\lambda_i|^2 + \sum_{i \neq j} |\lambda_i||\lambda_j|. \end{aligned}$$

Employing the inequality between the arithmetic and geometric means, we obtain

$$\frac{1}{n(n-1)} \sum_{i \neq j} |\lambda_i||\lambda_j| \geq \left(\prod_{i \neq j} |\lambda_i||\lambda_j|\right)^{\frac{1}{n(n-1)}}.$$

Thus,

$$\begin{aligned} (E_{D_cc})^2 &\geq \sum_{i=1}^{n} |\lambda_i|^2 + n(n-1)\left(\prod_{i \neq j} |\lambda_i||\lambda_j|\right)^{\frac{1}{n(n-1)}} \\ &\geq \sum_{i=1}^{n} |\lambda_i|^2 + n(n-1)\left(\prod_{i \neq j} |\lambda_i|^{2(n-1)}\right)^{\frac{1}{n(n-1)}} \\ &= 2m + k + n(n-1)\xi^{\frac{2}{n}}. \end{aligned}$$

□

Lemma 9. *If $\lambda_1(G)$ is the largest minimum doubly-connected dominating eigenvalue of $A_{D_cc}(G)$, then $\lambda_1 \geq \frac{2m+\gamma_cc(G)}{n}$.*

Proof. Let X be any nonzero vector. Then we have $\lambda_1(A) = max_{X\neq 0}\{\frac{X'AX}{X'X}\}$, see [16]. Therefore, $\lambda_1(A_{D_c}(G)) \geq \frac{J'AJ}{J'J} = \frac{2m+\gamma_c c(G)}{n}$. □

Next, we obtain Koolen and Moulton's [19] type inequality for $E_{D_cc}(G)$.

Theorem 10. *If G is a graph of order n and size m and $2m + \gamma_c c(G) \geq n$, then*

$$E_{D_cc}(G) \leq \frac{2m+\gamma_c c(G)}{n} + \sqrt{(n-1)\left[(2m+\gamma_c c(G)) - \left(\frac{2m+\gamma_c c(G)}{n}\right)^2\right]}. \quad (13)$$

Proof. Bearing in mind the Cauchy-Schwarz inequality,

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} a_i\right)^2 \left(\sum_{i=1}^{n} b_i\right)^2.$$

Put $a_i = 1$ and $b_i = |\lambda_i|$ then

$$\begin{aligned} \left(\sum_{i=2}^{n} a_i b_i\right)^2 &\leq (n-1)\left(\sum_{i=2}^{n} b_i\right)^2 \\ (E_{D_cc}(G) - \lambda_1)^2 &\leq (n-1)(2m+\gamma_c(G) - \lambda_1^2) \\ E_{D_cc}(G) &\leq \lambda_1 + \sqrt{(n-1)(2m+\gamma_c(G)-\lambda_1^2)}. \end{aligned}$$

Let

$$f(x) = x + \sqrt{(n-1)(2m+\gamma_c c(G) - x^2)}. \quad (14)$$

For decreasing function

$$\begin{aligned} f'(x) &\leq 0 \\ \Rightarrow 1 - \frac{x(n-1)}{\sqrt{(n-1)(2m+\gamma_c c(G)-x^2)}} &\leq 0 \\ x &\geq \sqrt{\frac{2m+\gamma_c c(G)}{n}}. \end{aligned}$$

Since $(2m+k) \geq n$, we have $\sqrt{\frac{2m+\gamma_c c(G)}{n}} \leq \frac{2m+\gamma_c c(G)}{n} \leq \lambda_1$. Also $f(\lambda_1) \leq f\left(\frac{2m+\gamma_c c(G)}{n}\right)$.

$$\text{i.e } E_{D_cc}(G) \leq f(\lambda_1) \leq f\left(\frac{2m+\gamma_c c(G)}{n}\right).$$

$$\text{i.e } E_{D_cc}(G) \leq f\left(\frac{2m+\gamma_c c(G)}{n}\right)$$

Hence by (12), the result follows. □

We conclude this paper by posing the following open problem for the researchers:

Open Problem: Construct non- cospectral graphs with unequal dominating, connected dominating and total dominating energy with respect to doubly-connected dominating energy.

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