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Equitable Power Domination Number of Various structure in Molecular Geometry

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ABSTRACT

The power dominating set $S \subseteq V$ in G = (V, E) is said to be equitable power dominating set when each vertex $v \in V - S$ has observed nearby vertex $u \in S$ such that difference between degree of u and the degree of v is less than or equal to 1, i.e. $|d\ (\mathrm{u}\ ) - d\ (v\ )| \leq 1$. The equitable power domination number of a graph G is the minimal cardinality of its equitable power dominating set, and it is represented by the notation $\gamma_{epd}\ (G)$. Molecular geometry is the three-dimensional arrangement of the atoms that comprise a molecule. In this research, we examine fair equitable power domination number of various structure in Molecular geometry.

Keywords: power dominating set, molecular structure, equitable power dominance, and equitable power dominance number.

1. Introduction

Molecular geometry describes how the atoms in a molecule are arranged in two or three dimensions. The most important concept in chemical science is molecular geometry. It focus with the three-dimension atom arrangement to make up a molecule. Atoms in molecules move owing to the laws of quantum physics; hence, "motion" needs to be explained in the language of quantum mechanics. Translation and rotation are examples of general (external) quantum mechanical movements that barely affect the structure of the molecule. Every atom's location is dictated by the type of chemical bonds that bind it to its nearby electrons. Based on the spatial configurations of these atoms, the molecular geometry may be defined by the bond lengths between two bonded atoms, the bond angles formed by three connected atoms, and the torsion (or dihedral) angles connected through three consecutive bonds. Three concepts can be used to describe molecular geometries: "bond lengths," "bond angles," and "torsional angles." Two atom's average distance and their nuclei is known as the bond length of a molecule. The angle that three atoms make across at least two bonds is known as a bond angle. The angle created by a chain's first three atoms and last three atoms is known as the torsional angle. In this paper the equitable power domination number of various Structure in Molecular Geometry in this research.

2. Equitable power domination in Molecular Geometry

The molecule's features, behavior, and reactivity are all impacted by its structure. Predicting the interactions between molecules and other substances turns out to be easier with an understanding of molecular structure. For instance, the bent structure of water (H2O) confers upon its certain qualities such as high surface tension and many-substance dissolution. We need to understand the Lewis electron dot structure in order to distinguish between the many kinds of molecules. Although it does not determine the morphologies of molecules, the Lewis hypothesis is the first step in anticipating their forms. The Lewis structure helps us differentiate between bond pairs and lone pairs. Next, we use the Valence Shell Electron Pair Repulsion (VSEPR) theory to compute the molecular and electron-group morphologies based on the Lewis structure. To identify and completely characterise a molecule's three-dimensional shape, we also need to know the bond angle. Lewis Electron Dot Structures are crucial for determining the geometry of molecules because they allow us to identify the valence electrons. A molecule can be trigonal planar (having three electron clouds), tetrahedral (having four electron clouds), octahedral (having six electron clouds), linear (having two "electron clouds" or zones of electron density surrounding a central atom), or trigonal bipyramid (having five). Notably, the extension of the octahedral rule around the core atom is reflected in the five and six-electron cloud forms.

3. Molecular Geometry Type

The geometric angle created by two adjacent bonds is known as a bond angle.

1. Linear:

It describes the geometry created using a center atom encircled by two additional atoms. The bond angle, or the angle between the bonds, is 180 degrees, and atoms are structured in straight line. The two bound atoms create a linear molecule by occupying the two axial places at opposite ends of an axis, while the three lone pairs occupy the less congested equatorial locations.

2. Trigonal Planar:

In the field of chemistry, the trigonal planar structure is a model of molecular geometry featuring a central atom surrounded by three atoms positioned at the vertices of an equilateral triangle, they are all located in the same plane and are known as peripheral atoms. In a perfectly trigonal planar configuration, the three ligands are the same and form bond angles of 120°.

3. Tetrahedral:

Tetra- indicates four, and hedral denotes a solid's face; the term "tetrahedral" directly translates to "having four faces." When a single core atom has four bonds and no lone electron pairs, this form is produced.

4. Trigonal Bipyramid:

A critical concept in the study of molecular structures is trigonal bipyramid geometry, which demonstrates the way atoms form bonds and organize themselves in three dimensions. Five additional atoms surround a core atom to create this geometry, which results in an individual set of bond angles and spatial configurations. Since it affects a variety of chemical behaviors and characteristics, scientists must comprehend its geometry.

5. Octahedral:

"Octahedral" literally means "having eight faces," as the prefix "octa-" denotes eight and the suffix "hedral" denotes the faces of a solid. In the same way that four electron pairs experience the least degree of repulsion when orientated towards the corners of a tetrahedron, six electron pairs want to point towards the corners of an octahedron, and all of the bond angles are 90°.

4. Main Results:

Theorem 4.1:

For $n \geq 1$, Let L be the linear molecular geometry, then γ_{epd} (L_n) =
$$\begin{cases} n & , n = 1 \\ \left\lfloor \dfrac{(n+1)}{2.5} \right\rfloor, & n \geq 2 \end{cases}$$

(If ' n ' represents number of copies in linear molecular)

Proof:

Let V= $\{v_1, v_2, \ldots\ldots.\}$ denote the vertex set E=$\{e_1, e_2, e_3, \ldots..\}$ denote the edge set. Let, S be the equitable power domination set.

γ_{epd} (L_2) = 1

From the above figure, let us choose v_3 in S. then v_3 dominates v_4, v_2. Now for v_5, v_1 are the non – observed vertex then v_4 observed v_5, v_2 observed v_1. Likewise one prove that

$$\gamma_{epd}(L_n) = \left\lfloor \frac{(n+1)}{2.5} \right\rfloor, n \geq 2$$

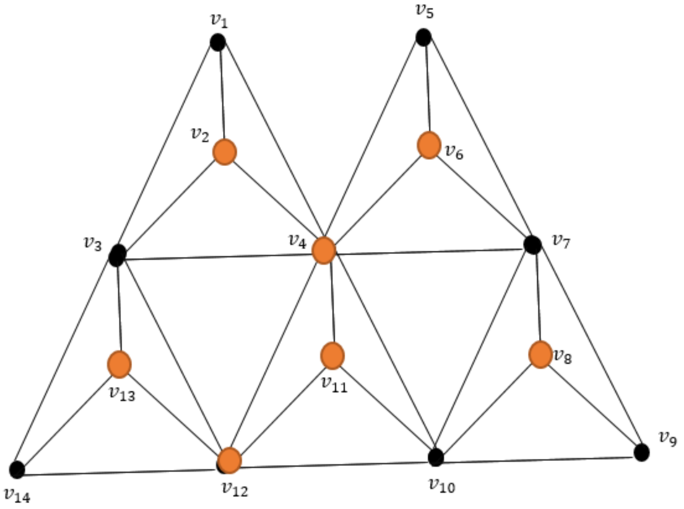
Theorem 4.2:

For n ≥ 1, Let TP be the trigonal planar molecular geometry, then $\gamma_{epd}(TP_n) = n + \left\lfloor \frac{(n+1)}{3} \right\rfloor$

(If 'n' represent number of copies in trigonal planar molecular)

Proof:

Let V= { v_1, v_2,…,} denote the vertex set E ={e_1,e_2,e_3,…,} denote the edge set. Let, S be the equitable power domination set.



$$\gamma_{epd}((TP)_5) = 7$$

From the above figure, let us choose v_4 in S then v_4 dominate itself. Then choose v_{12} in S it dominates v_3, v_{10}. Choose v_6 in S it dominates v_5. Choose v_2 in S it dominates v_1. Choose v_{13}

in S it dominates v_{14}. Choose v_8 in S it dominates v_9. choose v_{11} in S then v_{11} is dominate itself. Now v_7 is one only non- observed vertex then v_{10} observed v_7. . Likewise one prove that

$$\gamma_{epd}\,(TP_{\,n}) = n + \left\lfloor \frac{(n+1)}{3} \right\rfloor \text{, for every } n$$

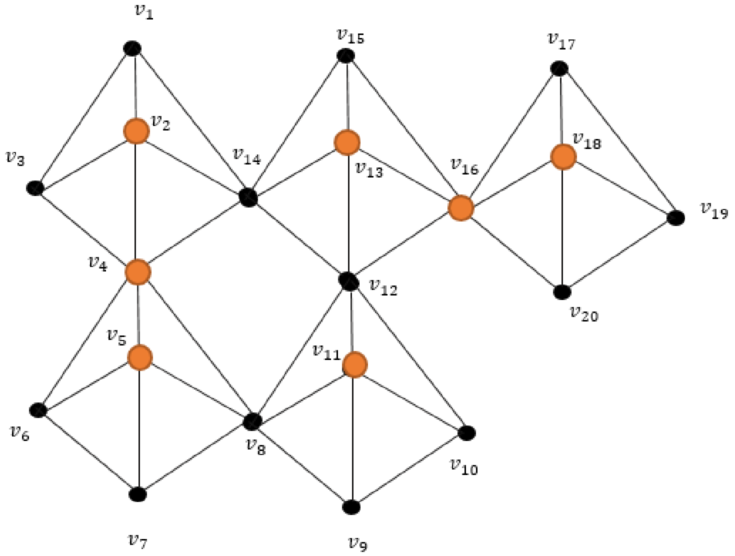
Theorem 4.3:

For n $\geq$ 1, Let T be the tetrahedral, then $\gamma_{\,epd}\,(T_{\,n}) = n + \left\lfloor \frac{(n+1)}{3} \right\rfloor$

(If n represent number of copies has tetrahedral molecule)

Proof:

Let V= { v_1, v_2,…….} denote the vertex set E={e$_1$,e$_2$,e$_3$,…..} denote the edge set. Let, S be the equitable power domination set.



γ_{epd} ((T) $_5$) = 7

From the above figure, let us choose v_4 in S. then v_4 dominates v_{14}, v_8. Then choose v_{16} in S it dominates v_{12}. Choose v_2 in S it dominates v_1, v_3. Choose v_{13} in S it dominates v_{15}. Choose v_{18} in S it dominates v_{17}, v_{19}, v_{20}. Choose v_5 in S it dominates v_6, v_7. Choose v_{11} in S it dominates v_{10}, v_9. . Likewise one prove that

$$\gamma_{epd}\ (T_n) = n + \left\lfloor \frac{(n+1)}{3} \right\rfloor, \text{for every n}$$

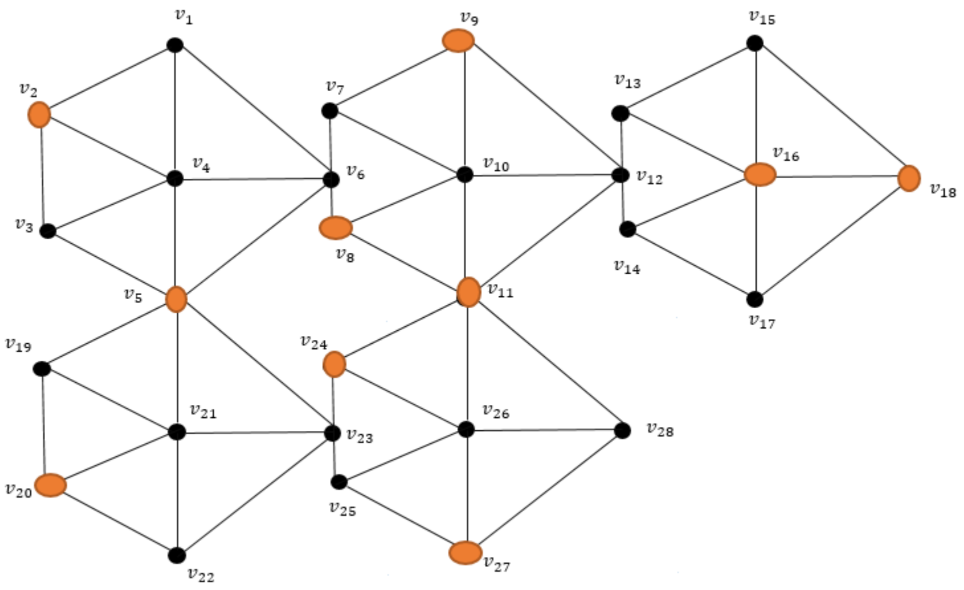
Theorem 4.4:

For $n \geq 1$, Let TB be the trigonal bipyramid molecular geometry, then γ_{epd} (TB_n) =2n

(If n represent number of copies has trigonal bipyramid)

Proof:

Let V= { $_1$, v_2,……} denote the vertex set E={e_1,e_2,e_3,…,} denote the edge set. Let S be the equitable power domination set.



$$\gamma_{epd}\ ((TB)_5) = 10$$

From the above figure, let us choose v_5 in S. then v_5 dominates v_4, v_{21}. Then choose v_{11} in S it dominates v_{10}, v_{26}. Choose v_{16} in S it dominates itself. Choose v_2 in S it dominates v_1, v_3. Choose v_9 in S it dominates v_7. Choose v_8 in S it dominates itself. Choose v_{18} in S it dominates v_{15}, v_{17}. Choose v_{20} in S is dominates v_{19}, v_{22}. Choose v_{27} in S it dominates v_{25}, v_{28}. Choose v_{24} is dominates itself. Now for v_6, v_{12}, v_{13}, v_{14}, v_{23} are the non – observed vertex then v_4 observed v_6, v_{10} observed v_{12}, v_{15} observed v_{13}, v_{17} observed v_{14}, v_{21} observed v_{23}. . Likewise one prove that

$$\gamma_{epd}\,(TB_n) = 2n, \text{for every } n.$$

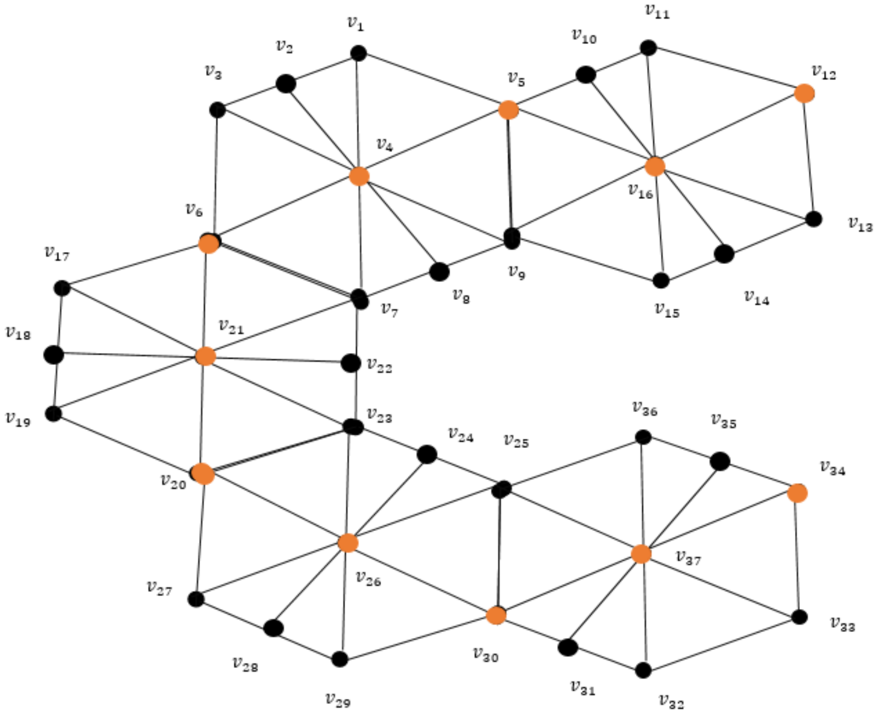
Theorem 4.5:

For n ≥ 1, Let O be the octahedral molecular geometry, then $\gamma_{epd}\,(O_n) = 2n+1$

(if n represent number of copies has octahedral)

Proof:

Let V= { v_1, v_2,…… ….} denote the vertex set E={e_1,e_2,e_3,…..} denote the edge set. Let S be the equitable power domination set.



$$\gamma_{epd}\ ((\mathrm{O})_5) = 11$$

From the above figure, let us choose v_{12} in S. then v_{12} dominates v_{11}, v_{13}. Then choose v_5 in S it dominates v_9, v_{10}, v_1. Choose v_6 in S it dominates v_3, v_7, v_{17}. Choose v_{20} in S it dominates v_{19}, v_{27}, v_{23}. Choose v_{30} in S it dominates v_{25}, v_{29}, v_{31}. Choose v_{34} in S it dominates $v_{35,}$ v_{33}. Choose v_{37}, v_{26}, v_{21}, v_4, v_{16} are the vertex dominates itself. Now for v_{14}, v_{15}, v_2, v_8, v_{18}, v_{22}, v_{28}, v_{32}, v_{36} are the non – observed vertex then v_{13} observed v_{14}, v_9 observed v_{15}, v_1 observed v_2, v_9 observed v_8, v_{17} observed v_{18}, v_7 observed v_{22}, v_{27} observed v_{28}, v_{31} observed v_{32}, v_{25} observed v_{36} . Likewise one prove that

$$\gamma_{epd}\ (\mathrm{O}_n) = 2n + 1, \text{ for every } n$$

Conclusion:

The work demonstrates that traditional domination theories may be effectively applied to molecular geometry by providing a unique explanation of equitable power dominance that is specific to molecular structures. The paper contributes to the theoretical framework of dominance in graph theory by effectively generating equitable power domination numbers for numerous types of molecular geometry, which includes trigonal planar, linear, tetrahedral, octahedral, and trigonal bipyramid. By showing how mathematical concepts may be applied to real-world problems in chemical science, this work effectively bridges the gap between graph theory and molecular research and fosters interdisciplinary collaboration and innovation. To gain a more thorough understanding of molecular architectures, future studies may look into fair power dominance in molecule classes like as oxides or carbonates compared to other areas of chemistry.

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