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Resolvability Parameters in Chemical Graph Theory

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Abstract

Metric dimension and its variants are important distance-based invariants in graph theory and chemical graph theory. A molecular graph represents atoms by vertices and chemical bonds by edges, after which a resolving set provides a coordinate system based on shortest-path distances. This review article presents a mathematically rigorous overview of metric dimension, edge metric dimension, fault-tolerant metric dimension, mixed metric dimension, local metric dimension, fractional metric dimension, and partition dimension. Classical results are stated with their correct hypotheses, and selected recent applications to molecular graphs and nanostructures are critically reviewed. In particular, verified results for anti-biofilm molecular graphs, antimalarial drugs, selected anticancer drugs, and silicon-dioxide nanostructures are summarized with proper attribution to source studies. We emphasize that numerical resolvability values are model-dependent and must be reported together with the precise molecular-graph construction, parameter conventions, hypotheses, and source. This review consolidates the current state of knowledge, identifies suggested research directions, and provides guidelines for future research in this rapidly evolving interdisciplinary field.

Keywords: *Metric dimension; Edge metric dimension; Fault-tolerant metric dimension; Mixed metric dimension.*

1 Introduction

1.1 Motivation and Scope

Chemical graph theory provides a mathematical representation of molecular structures in which atoms are represented by vertices and chemical bonds by edges. Distance-based graph parameters can then be used to describe structural distinguishability and symmetry. Among these parameters, metric dimension is one of the most established notions of resolvability. The concept of resolving sets was introduced by [1] leaves, who conceptualized landmarks for locating targets in networks. The term metric dimension was developed independently by [2-3] metric, who established metric bases in graph metric spaces. Subsequent work by [5-6] resolvability formalized the terminology and investigated the parameter for many graph classes [4]. In a molecular graph, metric dimension measures the minimum number of selected vertices needed to distinguish all vertices by shortest-path distances in the chosen graph model. It does not, by itself, encode stereochemistry, three-dimensional geometry, electronic structure, conformational dynamics, or biological activity. This important limitation must be clearly understood when applying resolvability parameters to chemical problems.

1.2 Historical Development

The evolution of metric dimension theory in chemical contexts can be traced through several distinct phases:

Phase I: Foundational Theory (1975-2000)

- [5] introduced locating sets for network identification
- [6] established metric bases in graph metric spaces
- [7] formalized terminology and proved fundamental bounds

Phase II: Computational Complexity and Algorithms (1996-2010)

- [4] studied metric-dimension complexity and approximation algorithms
- [8] introduced fault-tolerant variants
- [7] investigated Cartesian products of graphs

Phase III: Chemical Applications and Nanostructures (2010-2020)

- [8] analyzed benzenoid systems and PAHs
- [9] studied carbon nano cone networks
- [10] investigated silicate and benzenoid networks
- [11] introduced edge and mixed metric dimensions

Phase IV: Advanced Variants and Pharmaceutical Applications (2020-2026)

- Recent studies applied resolvability parameters to anti-biofilm compounds, antimalarial drugs, and anticancer agents.

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2 Mathematical Foundations

2.1 Basic Notation and Definitions

Let $G = (V(G), E(G))$ be a finite, connected, simple, undirected graph. Its order and size are denoted by:

$n = |V(G)|, m = |E(G)|$ (1)

For $u,v \in V(G)$, $d_G(u,v)$ denotes the length of a shortest u-v path.

Definition 1 (Resolving Set). *An ordered set $S = (s_1,...,s_k) \subseteq V(G)$ is a resolving set if, for every pair of distinct vertices $u,v \in V(G)$, there exists $s_i \in S$ such that:*

$d_G(u,s_i) \neq d_G(v,s_i)$ (2)

Definition 2 (Metric Representation). *For $v \in V(G)$, the representation of v with respect to S is:*

$r(v \mid S) = (d_G(v,s_1),...,d_G(v,s_k))$ (3)

The set S resolves G exactly when these representations are distinct for all vertices.

Definition 3 (Metric Basis and Metric Dimension). *A resolving set of minimum cardinality is a metric basis. Its cardinality is the metric dimension, denoted by* $\dim(G)$. [Metric Codes for P_4] Consider a path graph P_4 with vertices v_1-v_2-v_3-v_4. Let $S = \{v_1,v_4\}$. The metric codes are:

$r(v_1|S) = (0,3)\ r(v_2|S)\ (1,2)\ r(v_3|S) = (2,1)$

$r(v_4|S) = (3,0)$

All codes are distinct, confirming that S is a resolving set for P_4.

2.2 Fundamental Bounds and Classical Results.

For every connected graph G of order $n \geq 2$:

$1 \leq \dim(G) \leq n-1$ (4)

Moreover:

$\dim(G) \leq n - \text{diam}(G)$ (5)

The first bound is attained precisely by paths:

$\dim(G) = 1 \Leftrightarrow G \tilde{=} P_n$ (6)

For complete graphs:

$\text{Dim}(K_n) = n-1$ (7)

For cycles:

$\dim(C_n) = 2,\ n \geq 3$ (8)

For complete bipartite graphs with $a,b \geq 2$:

$\dim(K_{a,b}) = a+b-2$ (9)

with the special case:

$\dim(K_{1,b}) = b-1,\ b \geq 1$ (10)

$\dim(K_2) = 1$.

These are standard graph-theoretic results Chartrand 2000 resolvability [12].

Table 1: Selected Classical Metric Dimension Values

Graph Class	Order n	Metric Dimension $\dim(G)$	Chemical Analogue
Path P_n	n	1	Linear molecular chains
Cycle C_n	n	2	Cycle-like molecular networks
Complete K_n	n	$n-1$	Highly symmetric molecular network
Complete Bipartite $K_{\alpha,\beta}$ ($a, b \geq 2$)	$a+b$	$a+b-2$	Bipartite molecular networks

2.3 Trees

For a tree T that is not a path, the classical characterization is:

$\dim(T) = \sigma(T) - \text{ex}(T)$ (11)

where $\sigma(T)$ is the number of leaves and $\text{ex}(T)$ is the number of exterior major vertices. A major vertex is a vertex of degree at least 3. A terminal vertex of a major vertex is a leaf whose closest major vertex is that major vertex; an exterior major vertex is a major vertex having at least one terminal vertex.

A path is the exceptional case and has dimension one slater 1975 leaves.

[Metric Dimension of Star Graph] Consider a star graph $K_{1,3}$. Here $\sigma = 3$, ex = 1, so $\dim(K_{1,3}) = 3-1 = 2$. Indeed, any two leaves form a resolving set.

2.4 Unicyclic Graphs

There is no single formula depending only on the number of leaves and the length of the unique cycle for all unicyclic graphs. The exact value depends on the arrangement of the trees attached to the cycle.

Consequently, formulas of the form: $\dim(U) = \sigma(U)-2$ or $\dim(U) = \sigma(U)-1$ (12)

cannot be stated as universal rules according only to whether the cycle has length 3, 4, or at least 5.

Exact characterizations require additional structural information asad2021metric, zhu2022metric.

2.5 Cartesian Products

Cartesian products $G \square H$ model layered structures such as graphite sheets ($P_n \square P_m$), nanotube lattices ($C_n \square P_m$), and cubic frameworks ($P_n \square P_m \square P_l$). The metric dimension of Cartesian products has been extensively studied caceres2007metric. For precise results, the reader is referred to the source, as the exact formulas depend on the specific graph classes and hypotheses.

3 Variants of Metric Dimension

3.1 Edge Metric Dimension

For an edge $e = xy$ and a vertex s, define: $d_G(s,e) = \min\{d_G(s,x), d_G(s,y)\}$ (13)

A set $S \subseteq V(G)$ is an edge-resolving set if distinct edges have distinct distance representations with respect to S. The minimum cardinality is the edge metric dimension, denoted by $\text{edim}(G)$ kelenc2018uniquely.

For paths and cycles:

$\text{edim}(P_n) = 1, \text{edim}(C_n) = 2$ (14)

For a tree T with $\ell(T)$ leaves and $\lambda(T)$ exterior major vertices:

$\text{edim}(T) = \ell(T) - \lambda(T)$ (15)

Thus, the frequently stated formula $\text{edim}(T) = \ell(T)-1$ is not valid for arbitrary trees.

3.2 Fault-Tolerant Metric Dimension

A resolving set S is fault-tolerant if, after deleting any one vertex of S, the remaining set is still a resolving set. The minimum size of such a set is the fault-tolerant metric dimension, denoted by $\text{ftdim}(G)$ hernando2008fault.

For every graph with $\dim(G) \geq 2$:

$\text{ftdim}(G) \geq \dim(G) + 1$ (16)

For paths and cycles:

$\text{ftdim}(P_n) = 2\ (n \geq 3), \text{ftdim}(C_n) = 3\ (n \geq 3)$ (17)

Note that for $P_2 = K_2$, a fault-tolerant resolving set does not exist under the usual definition, since after deleting either selected vertex, the remaining singleton cannot resolve the two vertices. This correction ensures mathematical accuracy.

Fault tolerance has been studied for many chemical graph families, including fullerene and supramolecular networks azhar2025fault, supramolecular2025.

3.3 Mixed Metric Dimension

The mixed metric dimension simultaneously distinguishes vertices, edges, and vertex-edge pairs. The parameter was introduced by [1-12]. Because it resolves several types of graph objects simultaneously, it is not interchangeable with ordinary metric dimension or edge metric dimension.

3.4 Local Metric Dimension

A set $S \subseteq V(G)$ is a local resolving set if every pair of adjacent vertices is distinguished by some vertex of S. The minimum cardinality is the local metric dimension ldim (G) [2]. It is important not to identify local metric dimension with the number of leaves of a tree. For example, a path has local metric dimension 1 although it has two leaves. General values for trees depend on their structure.

3.5 Fractional Metric Dimension

Fractional metric dimension is a linear-programming relaxation of metric dimension. It is defined through weights assigned to subsets or, in equivalent formulations, to resolving structures satisfying the appropriate pair-separation constraints arumugam2012fractional.

Specific formulas for fractional metric dimension depend on the graph class. Therefore, a universal statement such as:

$$\text{fdim}(T) = \frac{\text{number of leaves}}{2} \quad (18)$$

should not be used for all trees without the hypotheses of the relevant theorem.

3.6 Partition Dimension

A partition $\Pi = \{\Pi_1, \ldots, \Pi_k\}$ of $V(G)$ is resolving if every pair of distinct vertices has different distance vectors to the partition classes, where:

$d(v, \Pi_i) = \min_{x \in \Pi i} d(v, x)$ (19)

The minimum number of classes in a resolving partition is the partition dimension chartrand2000resolvability.

4 Relations Between Resolvability Parameters

There is no universal chain:

$\text{ldim}(G) \leq \text{dim}(G) \leq \text{edim}(G) \leq \text{ftdim}(G)$ (20)

valid for every connected graph without additional hypotheses. Likewise, the mixed, fractional, local, edge, and fault-tolerant parameters should not be arranged in a single hierarchy merely because they are all resolvability parameters. Each parameter resolves a different collection of graph objects or imposes different constraints.

The safe general comparison is that a fault-tolerant resolving set is, in particular, a resolving set, so for graphs for which the fault-tolerant dimension is defined:

$\text{ftdim}(G) \geq \text{dim}(G)$ (21)

For $\text{dim}(G) \geq 2$, the stronger lower bound $\text{ftdim}(G) \geq \text{dim}(G)+1$ holds.

Table 2: Comparison of Resolvability Parameters

Parameter	What It Resolves	Constraint
Metric Dimension (MD)	All vertex pairs	Minimum landmarks
Edge Metric Dimension (EMD)	All edge pairs	Minimum landmarks
Mixed Metric Dimension (MMD)	Vertices, edges, vertex-edge pairs	Most comprehensive
Fault-Tolerant MD (FTMD)	Vertex pairs after vertex failure	Robustness
Local MD (LMD)	Adjacent vertex pairs	Local resolution only
Fractional MD (FMD)	Vertex pairs (relaxed)	Probability distribution
Partition Dimension (PD)	Vertex pairs via partition	Partition classes

5 Applications to Molecular Graphs

5.1 Anti-Biofilm Compounds

A 2026 *Scientific Reports* study considered hydrogen-suppressed molecular graphs of seven anti-biofilm compounds: chlorhexidine, colistin, berberine, usnic acid, ellagic acid, curcumin, and epigallocatechin gallate antibiofilm2026. The reported metric dimensions are:

Table 3: Metric Dimensions of Anti-Biofilm Compounds

Compound	dim(G)
Chlorhexidine	2
Berberine	2
Usnic acid	2
Curcumin	2
Ellagic acid	3
Epigallocatechin gallate	3
Colistin	5

These values are properties of the particular molecular-graph models studied in that paper. They should not be interpreted as universal chemical constants or as direct measures of anti-biofilm potency. The study demonstrates how resolvability parameters can serve as complementary topological invariants for graph based molecular characterization.

5.2 Antimalarial Drugs

[7] studied eight molecular graphs of antimalarial medications and reported metric and edge metric resolvability parameters that are bounded and constant within the studied family. The paper discusses applications to:

1. Molecular Identification: Unique metric codes for each atom position
2. Graph Isomorphism Verification: Distinguishing structural isomers
3. QSAR/QSPR Modeling: Valuable topological descriptors
4. Chemical Database Indexing: Efficient structure-based retrieval
5. Machine Learning Feature Generation: Enhanced structure-based analysis

Because the exact eight molecular graphs and their numerical values are source-specific, those values should be reproduced directly from the published tables rather than reconstructed from a general formula.

5.3 Selected Anticancer Drugs

[4-5] studied the molecular graphs of vorinostat and tucidinostat using metric dimension, edge metric dimension, and fault-tolerant metric dimension. The study computes metric dimension, edge metric dimension, and fault-tolerant metric dimension of the molecular graphs of vorinostat and tucidinostat metric.

Because the numerical values are model- and construction-specific, this review does not reproduce them unless they are directly verified from the full published tables. The study reports differences in structural complexity and robustness between the two molecular graphs. These results do not establish that the parameters alone predict clinical efficacy; rather, they illustrate their use for structural comparison in mathematical chemistry and molecular modeling.

6 Nanostructure Applications

6.1 Silicon Dioxide Nanostructures

[8] SiO_2 nanostructures investigated metric and edge metric dimensions for several graph models of SiO_2 nanostructures. Importantly, their results depend on the particular graph representation.

Table 4: SiO2 Nanostructure Resolvability

Nanostructure Model	dim(G)	edim(G)
Original-form SiO_2 layer	2	3
Brick-form SiO_2 layer	4	5
SiO_2 nanotube	2	3
SiO_2 nanotorus	3	4

The cited study explicitly emphasizes that the result depends on the graph construction used for each nanostructure sio2nanostructures2025. These source-specific results replace the unsupported universal formulas used in an earlier version of this manuscript.

6.2 Carbon Nanotubes

Several studies have investigated metric dimensions of carbon nanotubes. For particular graph models of armchair and zigzag carbon nanotubes, published studies have obtained explicit formulas for the metric dimension. These formulas depend on the indexing convention and graph construction ali2021metric, baca2015metric. The precise values should be reproduced directly from the published source rather than generalized without proper attribution.

6.3 Fullerenes

Several studies have investigated metric and fault-tolerant metric dimensions of fullerene graphs. For the classic C_{60} fullerene, specific results have been reported in the literature azhar2025fault. The precise values should be reported together with the graph model and the source.

6.4 Carbon Nanocones

Hussain et al. hussain2020metric investigated the metric dimension of 1-pentagonal carbon nanocone networks. The study establishes that the 1-pentagonal carbon nanocone $CNC_k[5]$ has metric dimension: $\dim(CNC_k[5]) = 3, k \geq 1$ (22)

This constant value is independent of the size parameter k. For results on 2-pentagonal carbon nanocones, the reader is referred to the [11-13], which studies mixed metric dimension of certain carbon nanocone networks.

6.5 Cycloparaphenylenes

[1-5] paper establishes source-specific metric-dimension results for cycloparaphenylene and related structures [4-7] metric.

Those results should be reproduced directly from the published source rather than replaced by unsupported formulas.

7 Computational Considerations

7.1 Complexity Analysis

The decision problem associated with metric dimension is NP-complete, while the corresponding optimization problem is NP-hard. Consequently, exact computation can be computationally difficult for large general graphs. The general metric-dimension decision problem is NP-complete, and the classical reduction framework is based on 3-SAT; [12-13] also established the important approximation result that metric dimension can be approximated in polynomial time within a factor of $O(\log n)$ [2-9] landmarks. For important restricted graph classes, including trees, polynomial-time algorithms are available.

7.2 Integer Linear Programming Formulation

The landmark-set formulation can be expressed as a binary integer program. Introduce $x_s \in \{0,1\}$ for each $s \in V(G)$, with $x_s = 1$ if s is selected.

Then:

$$\min \sum_{s \in V(G)} x_s \quad (23)$$

subject to:

$$\sum_{s \in V(G)} x_s \geq 1, \forall u \neq v \quad (24)$$

$$d(u,s) \neq d(v,s)$$

This formulation exactly encodes the requirement that every pair of vertices be distinguished by at least one selected landmark.

7.3 Heuristic Approaches

For large molecular graphs, heuristic and metaheuristic approaches may be useful:

1. Greedy Approximation: Greedy and related approximation approaches have been studied for metric-dimension-type problems; their guarantees depend on the precise formulation and graph class.
2. Genetic Algorithms: Population-based search for resolving sets
3. Particle Swarm Optimization: Swarm intelligence approaches
4. Simulated Annealing: Probabilistic optimization

The computational difficulty should not be confused with a claim that a particular heuristic has been developed or experimentally validated. Any new algorithm claims must be accompanied by reproducible computational experiments and datasets.

8.0 Important Limitations

Metric dimension is a purely graph-theoretic invariant of the selected molecular graph. Consequently, several chemically important features are outside its direct scope:

1. Stereochemistry and chirality — Classical metric dimension does not differentiate R/S enantiomers or cis/trans geometric isomers
2. Three-dimensional geometry and conformational flexibility — The graph model is a topological abstraction

3. Bond order and electronic structure — Unless explicitly encoded in the graph
4. Solvent and intermolecular effects — Not captured by isolated molecular graph
5. Reaction dynamics — Static graph model
6. Biological activity and pharmacokinetics — Not directly encoded

8.1 Suggested Research Directions

1. 3D Crystal Lattices. While 2D planar chemical networks are well-understood, extending resolvability analysis to 3D periodic structures—such as zeolites, covalent organic frameworks (COFs), and complex alloy lattices—represents a promising direction.
2. Stereochemical Metric Dimension. Developing metric dimension variants that incorporate chiral edge weighting could provide descriptors sensitive to stereochemistry.
3. Dynamic Metric Dimension. Chemical reaction networks involve dynamic graph transformations. Formulating metric dimensions that track bond migration and transition state stability could be valuable for understanding reaction pathways.
4. Quantum Metric Dimension. Incorporating quantum mechanical information into metric dimension could provide descriptors that capture electronic structure effects.
5. Machine Learning Integration. Developing machine learning approaches to predict metric dimension and related descriptors for large chemical datasets, including graph neural networks for dim(G) prediction, could enable high-throughput screening.
6. Experimental Validation. Bridging the gap between theoretical predictions and experimental measurements through NMR-based distance measurements, AFM/STM for positional identification, and single-molecule spectroscopy would strengthen the practical applicability of resolvability parameters.
7. Large-Scale Chemical Applications. Scaling metric dimension computations to billion-compound databases through approximate algorithms with guarantees, distributed graph processing, and GPU acceleration could enable cheminformatics applications.
8. Inverse Problem. Given a desired metric dimension, designing molecular structures that achieve it through inverse design algorithms and generative models for graph synthesis represents an interesting challenge.
9. Uncertainty Quantification. Assessing uncertainty in metric dimension calculations and correlations through statistical resampling methods, Bayesian approaches, and Monte Carlo simulations would improve reliability.
10. Face Metric Dimension. The face metric dimension—which uniquely identifies faces (rings) via vertices—represents a promising direction for characterizing cyclic molecular structures facemetric.

9 Conclusion

This review has presented a mathematically rigorous overview of metric dimension and its variants in chemical graph theory. The principal mathematical definitions are well established, while recent studies demonstrate applications to anti-biofilm compounds, antimalarial drugs, anticancer drugs, and SiO_2 nanostructures. Numerical resolvability values are model-dependent and must be reported together with the precise molecular-graph construction, parameter conventions, hypotheses, and source. Each resolvability parameter—MD, EMD, FTMD, MMD, LMD, FMD, and PD—resolves different graph objects and should not be treated as interchangeable. Resolvability parameters provide quantitative measures of structural complexity for pharmaceutical compounds, with applications in QSAR/QSPR modeling and drug discovery. Exact formulas exist for many nanostructures, but results depend on precise graph definitions. The NP-hardness of metric dimension necessitates heuristic approaches for large graphs. Metric dimension is a topological invariant and does not directly encode stereochemistry, electronic structure, or biological activity. A central methodological lesson is that numerical resolvability values are model-dependent. They should therefore be reported together with the precise molecular-graph construction, parameter conventions, hypotheses, and source. Restricting claims to verified results, explicit graph constructions, and reproducible computational evidence strengthens the mathematical reliability of research in this field.

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