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Molecular Directed, Bidirected, and Multidirected Graphs

Takaaki Fujita[*]

Independent Researcher, Tokyo, Japan; Takaaki.fujita060@gmail.com.

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Abstract

A *directed graph* (or *digraph*) consists of a finite vertex set V and a set of ordered edges $E \subseteq V \times V$, each edge (u, v) indicating a one-way connection from u (source) to v (target). A bidirected graph is a generalization of an undirected graph where each edge is assigned a direction at each of its endpoints independently, allowing more expressive edge orientation. A multidirected graph is a structure with vertices and edges, where edges may repeat, sources and targets are assigned, and multiplicities recorded. A molecular graph models a molecule with atoms as vertices and bonds as edges, representing its structural connectivity. In this paper, we examine definitions such as molecular bidirected graphs and multidirected graphs. These are concepts that extend molecular graphs by incorporating directional information.

Keywords: Directed graph, Bidirected graph, Multidirected graph, Molecular graph.

1 | Preliminaries

This section provides an overview of the fundamental concepts and definitions essential for the discussions in this paper. Throughout this work, all graphs are assumed to be finite and without loops.

Corresponding Author: Takaaki.fujita060@gmail.com

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1.1 | Bidirected and Multidirected Graphs

Graph theory studies vertices and edges, modeling pairwise relationships, enabling analysis of networks, connectivity, paths, cycles, and structures [1]. A *directed graph* (or *digraph*) consists of a finite vertex set V and a set of ordered edges $E \subseteq V \times V$, each edge (u, v) indicating a one-way connection from u (source) to v (target) [2, 3]. A bidirected graph is a generalization of an undirected graph where each edge is assigned a direction at each of its endpoints independently, allowing more expressive edge orientation [4, 5].

Definition 1 (Directed Graph)**.** [1] A *directed graph* (or *digraph*) is a pair

$$G = (V, E),$$

where

- V is a finite set of vertices, and
- $E \subseteq V \times V$ is a set of ordered pairs called *directed edges* (or *arcs*).

Each edge $(u, v) \in E$ represents a connection directed from vertex u (the *tail*) to vertex v (the *head*).

Example 1 (Directed Graph example: Hydrogen chloride polarity (H→Cl))**.** (cf.[6]) Consider the molecule HCl. Take the vertex set $V = \{H, Cl\}$ and define the directed edge set

$$E = \{(H, Cl)\} \ \subseteq V \times V.$$

Thus $G = (V, E)$ is a directed graph (digraph) whose single arc (H, Cl) encodes the orientation of the polar covalent bond from hydrogen (tail) to chlorine (head).

Definition 2 (Bidirected Graph)**.** [4] A *bidirected graph* $B = (G, \tau)$ is given by

$$G = (V, E), \quad \tau : V \times E \to \{-1, 0, 1\},$$

where:

- G is a simple undirected graph on vertex set V and edge set E.
- For each vertex-edge pair (v, e),

$$\tau(v, e) = \begin{cases} +1, & \text{if } e \text{ is directed toward } v, \\ -1, & \text{if } e \text{ is directed away from } v, \\ 0, & \text{if } v \text{ is not incident to } e. \end{cases}$$

We call G the *underlying graph* and τ the *bidirection function.*

Example 2 (Bidirected Graph example: Ammonia–borane dative bond $NH_3 \to BH_3$)**.** (cf.[7]) Let the underlying simple undirected graph be $G = (V, E)$ with

$$V = \{N, B\}, \qquad E = \big\{\{N, B\}\big\} = \{e\}.$$

Define the bidirection function $\tau : V \times E \to \{-1, 0, 1\}$ by

$$\tau(N, e) = -1 \quad \text{and} \quad \tau(B, e) = +1,$$

with $\tau(v, e) = 0$ for any nonincident pair (none here). Then $B = (G, \tau)$ is a bidirected graph in which the edge is locally oriented "away from" N and "toward" B, encoding the donor $(N) \to$ acceptor (B) dative interaction.

A multidirected graph is a structure with vertices and edges, where edges may repeat, sources and targets are assigned, and multiplicities recorded[8, 9, 10].

Definition 3 (Multidirected Graph)**.** [8, 9, 10] A *multidirected graph* is a tuple

$$G = (V, E, s, t, m),$$

where

- V is a finite set of vertices,
- E is a finite set of edges,
- $s, t : E \to V$ assign to each edge its source and target,
- $m : V \times V \to \mathbb{N}_0$ gives the multiplicity of edges from one vertex to another.

Example 3 (Multidirected Graph example: Carbon monoxide triple bond as multiplicity)**.** (cf.[11]) Model CO with a multidirected graph $G = (V, E, s, t, m)$ where

$$V = \{C, O\}, \quad E = \{e_1, e_2, e_3\}, \quad s(e_i) = C, \ t(e_i) = O \ \ (i = 1, 2, 3).$$

Define the multiplicity map $m : V \times V \to \mathbb{N}_0$ by

$$m(C, O) = \big|\{e \in E : \ s(e) = C, \ t(e) = O\}\big| = 3, \qquad m(u, v) = 0 \text{ for all } (u, v) \neq (C, O).$$

Thus G encodes the C≡O triple bond as three parallel directed edges from C to O with consistent multiplicity.

1.2 | Molecular Graph

A molecular graph models a molecule with atoms as vertices and bonds as edges, representing its structural connectivity [12, 13, 14, 15, 16, 17]. Related concepts include molecular hypergraphs [18, 19, 20, 21], which extend this framework to capture higher-order interactions among multiple atoms simultaneously.

Definition 4 (Molecular Graph)**.** [12, 13] A *molecular graph* is a finite, simple, undirected graph $G = (V, E)$ in which each vertex $v \in V$ represents an atom and each edge $e = \{u, v\} \in E$ represents a chemical bond between atoms u and v. (Optionally, vertex/edge labels may encode atom types and bond types or orders.)

Example 4 (Molecular Graph example: Methane (CH_4) connectivity)**.** (cf.[22]) A molecular graph is a finite simple undirected graph whose vertices are atoms and edges are chemical bonds. For methane, let

$$V = \{C, H_1, H_2, H_3, H_4\}, \qquad E = \big\{\{C, H_1\}, \{C, H_2\}, \{C, H_3\}, \{C, H_4\}\big\}.$$

Then $G = (V, E)$ captures the tetrahedral connectivity of CH_4 without imposing any edge orientation.

2 | Main Results

As the main outcome of this paper, we introduce definitions of new graph classes and examine their properties.

2.1 | Molecular Directed Graph

A molecular directed graph represents atoms as labeled vertices and chemical bonds as directed edges, capturing oriented molecular interactions.

Definition 5 (Molecular Directed Graph (MDG))**.** Fix finite attribute sets Σ_V (vertex/atom attributes, e.g., element, charge, isotope) and Σ_E (edge/bond attributes, e.g., bond order, stereo). A *molecular directed graph* is a tuple

$$\mathcal{M}_D = (V, E, s, t, \lambda_V, \lambda_E),$$

where

- V is a finite set of vertices (atoms),
- E is a finite set of edges (bonds),
- $s, t : E \to V$ assign to each edge $e \in E$ its source $s(e)$ and target $t(e)$,
- $\lambda_V : V \to \Sigma_V$ labels each vertex with its atomic attributes,
- $\lambda_E : E \to \Sigma_E$ labels each edge with its bond attributes.

We write the underlying directed edge set of $\mathcal{M}_D$ as

$$E^{\rightarrow} \;:=\; \{\,(s(e), t(e)) \mid e \in E\,\} \;\subseteq\; V \times V.$$

Example 5 (Ammonia ($\mathrm{NH_3}$): three polar N–H bonds oriented $H_i \to N$)**.** (cf.[23]) Let $\Sigma_V = \{\mathrm{N}, \mathrm{H}\}$ and $\Sigma_E = \{\text{single}\}$. Define the MDG

$$\mathcal{M}_D = (V, E, s, t, \lambda_V, \lambda_E)$$

by

$$V = \{N, H_1, H_2, H_3\}, \qquad E = \{e_1, e_2, e_3\},$$
$$s(e_i) = H_i, \quad t(e_i) = N \quad (i = 1, 2, 3).$$

Label vertices and edges as

$$\lambda_V(N) = \mathrm{N}, \quad \lambda_V(H_i) = \mathrm{H}\ (i = 1, 2, 3), \qquad \lambda_E(e_i) = \text{single}\ (i = 1, 2, 3).$$

The underlying directed edge set is

$$E^{\rightarrow} = \{(H_1, N), (H_2, N), (H_3, N)\},$$

encoding the polarity of each N–H bond from hydrogen (source) to nitrogen (target).

Example 6 (Carbon dioxide ($\mathrm{CO_2}$): two polar C=O bonds oriented $C \to O_i$)**.** Let $\Sigma_V = \{\mathrm{C}, \mathrm{O}\}$ and $\Sigma_E = \{\text{double}\}$. Define

$$\mathcal{M}_D = (V, E, s, t, \lambda_V, \lambda_E)$$

with

$$V = \{C, O_1, O_2\}, \qquad E = \{e_1, e_2\},$$
$$s(e_1) = C,\ t(e_1) = O_1, \qquad s(e_2) = C,\ t(e_2) = O_2.$$

Vertex and edge labels are

$$\lambda_V(C) = \mathrm{C}, \quad \lambda_V(O_i) = \mathrm{O}\ (i = 1, 2), \qquad \lambda_E(e_1) = \lambda_E(e_2) = \text{double}.$$

Thus

$$E^{\rightarrow} = \{(C, O_1), (C, O_2)\},$$

representing both C=O bonds by directed edges from carbon to oxygen (one per oxygen). Multiplicity information (double bonds) is carried here only as an edge label.

Example 7 (Sodium chloride (NaCl): ionic interaction oriented $Na \to Cl$)**.** (cf.[24]) Let $\Sigma_V = \{\mathrm{Na}, \mathrm{Cl}\}$ and $\Sigma_E = \{\text{ionic}\}$. Define

$$\mathcal{M}_D = (V, E, s, t, \lambda_V, \lambda_E)$$

by

$$V = \{Na, Cl\}, \qquad E = \{e\}, \qquad s(e) = Na,\ t(e) = Cl.$$

Set the labels

$$\lambda_V(Na) = \mathrm{Na}, \quad \lambda_V(Cl) = \mathrm{Cl}, \qquad \lambda_E(e) = \text{ionic}.$$

Then

$$E^{\rightarrow} = \{(Na, Cl)\},$$

capturing the ionic character by a single directed edge pointing from sodium (donor/source) to chlorine (acceptor/target).

Example 8 (Water (polar O–H bonds as oriented edges))**.** (cf.[25]) Let $\Sigma_V = \{\mathrm{H}, \mathrm{O}\}$ and $\Sigma_E = \{\text{single}\}$. Define the MDG

$$\mathcal{M}_D = (V, E, s, t, \lambda_V, \lambda_E)$$

by

$$V = \{O, H_1, H_2\}, \quad E = \{e_1, e_2\},$$
$$s(e_1) = H_1,\ t(e_1) = O, \qquad s(e_2) = H_2,\ t(e_2) = O,$$
$$\lambda_V(O) = \mathrm{O},\ \lambda_V(H_i) = \mathrm{H}\ (i = 1, 2), \qquad \lambda_E(e_j) = \text{single}\ (j = 1, 2).$$

Thus $E^{\rightarrow} = \{(H_1, O), (H_2, O)\}$ captures the polarity (hydrogen → oxygen).

Example 9 (Hydrogen chloride (H→Cl bond polarity)). (cf.[26]) Let $\Sigma_V = \{\mathrm{H}, \mathrm{Cl}\}$ and $\Sigma_E = \{\mathrm{single}\}$. Define

$$\mathcal{M}_D = (V, E, s, t, \lambda_V, \lambda_E)$$

with

$$V = \{H, Cl\}, \quad E = \{e\}, \quad s(e) = H,\ t(e) = Cl,$$

$$\lambda_V(H) = \mathrm{H},\ \lambda_V(Cl) = \mathrm{Cl}, \qquad \lambda_E(e) = \mathrm{single}.$$

Then $E^{\to} = \{(H, Cl)\}$ represents the oriented H–Cl bond.

Theorem 1 (MDG generalizes a directed graph). *Let* $\mathbf{Dig}$ *denote the class of finite directed graphs* $G = (V, E^{\to})$ *with* $E^{\to} \subseteq V \times V$. *There exist maps*

$$U_D :\ \mathcal{M}_D \mapsto (V, E^{\to}) \in \mathbf{Dig}, \qquad I_D :\ (V, E^{\to}) \mapsto \mathcal{M}_D$$

such that $U_D \circ I_D = \mathrm{id}_{\mathbf{Dig}}$. *Hence every directed graph is (canonically) a special case of a molecular directed graph.*

Proof: Define the *forgetful map*

$$U_D(V, E, s, t, \lambda_V, \lambda_E) \ :=\ (V,\ \{(s(e), t(e)) :\ e \in E\}) \in \mathbf{Dig}.$$

Given any $G = (V, E^{\to}) \in \mathbf{Dig}$, define the *trivial-label embedding*

$$I_D(G) \ :=\ (V, E, s, t, \lambda_V, \lambda_E),$$

by taking $E := E^{\to}$, $s(u, v) := u$, $t(u, v) := v$ for each $(u, v) \in E^{\to}$, and choosing fixed elements $v_* \in \Sigma_V$, $e_* \in \Sigma_E$ with

$$\lambda_V(v) := v_* \ \text{ for all } v \in V, \qquad \lambda_E(e) := e_* \ \text{ for all } e \in E.$$

Then

$$U_D\big(I_D(G)\big) \ =\ (V,\ \{(s(u, v), t(u, v)) : (u, v) \in E^{\to}\}) \ =\ (V, E^{\to}) \ =\ G,$$

so $U_D \circ I_D = \mathrm{id}_{\mathbf{Dig}}$. Therefore every directed graph is realized as an MDG with constant labels, and every MDG forgets to a directed graph via U_D. □

2.2 | Molecular BiDirected Graph

A molecular bidirected graph models atoms as labeled vertices with edges independently directed at endpoints, encoding bidirectional or asymmetric bond orientations.

Definition 6 (Molecular BiDirected Graph (MBDG)). Fix finite attribute sets Σ_V and Σ_E. A *molecular bidirected graph* is a quintuple

$$\mathcal{M}_B = (V, E, \tau, \lambda_V, \lambda_E),$$

where

- V is a finite set of vertices and E a finite set of (undirected) edges,
- $\tau : V \times E \to \{-1, 0, 1\}$ is a bidirection function satisfying:

$$\tau(v, e) = 0 \text{ if } v \text{ is not incident to } e;$$

$$\tau(v, e) = +1 \text{ if } e \text{ is directed toward } v \text{ at } v;$$

$$\tau(v, e) = -1 \text{ if } e \text{ is directed away from } v \text{ at } v;$$

- $\lambda_V : V \to \Sigma_V$ and $\lambda_E : E \to \Sigma_E$ assign molecular attributes to vertices/edges.

The *underlying bidirected graph* is (G, τ) with $G = (V, E)$.

Example 10 (Ammonia–borane dative bond: $\mathrm{NH_3} \to \mathrm{BH_3}$). (cf.[7]) Let $\Sigma_V = \{\mathrm{N}, \mathrm{B}\}$, $\Sigma_E = \{\text{dative}\}$. Consider the MBDG

$$\mathcal{M}_B = (V, E, \tau, \lambda_V, \lambda_E), \quad V = \{N, B\},\ E = \{e\},$$

with bidirection function $\tau : V \times E \to \{-1, 0, 1\}$ given by

$$\tau(N, e) = -1, \qquad \tau(B, e) = +1,$$

and vertex/edge labels

$$\lambda_V(N) = \mathrm{N},\ \lambda_V(B) = \mathrm{B}, \qquad \lambda_E(e) = \text{dative}.$$

Nonincident pairs map to 0 by definition. Endpoint signs encode "away from N" and "toward B".

Example 11 (Diammine copper(II): two N→Cu donations). (cf.[27]) Let $\Sigma_V = \{\mathrm{Cu}, \mathrm{N}\}$, $\Sigma_E = \{\text{dative}\}$ and define

$$\mathcal{M}_B = (V, E, \tau, \lambda_V, \lambda_E), \quad V = \{Cu, N_1, N_2\},\ E = \{e_1, e_2\},$$

with

$$\tau(N_1, e_1) = -1,\ \tau(Cu, e_1) = +1, \qquad \tau(N_2, e_2) = -1,\ \tau(Cu, e_2) = +1,$$

(all other $\tau(\cdot, \cdot) = 0$), and labels

$$\lambda_V(Cu) = \mathrm{Cu},\ \lambda_V(N_i) = \mathrm{N}, \quad \lambda_E(e_i) = \text{dative } (i = 1, 2).$$

Each edge is oriented locally from N (donor) to Cu (acceptor) via τ.

Example 12 (Acetone–boron trifluoride adduct: O→B donation). (cf.[28]) Let $\Sigma_V = \{\mathrm{O}, \mathrm{B}\}$ and $\Sigma_E = \{\text{dative}\}$. Define the MBDG

$$\mathcal{M}_B = (V, E, \tau, \lambda_V, \lambda_E), \quad V = \{O_{\mathrm{ac}}, B\}, \quad E = \{e\}.$$

The bidirection function $\tau : V \times E \to \{-1, 0, 1\}$ is

$$\tau(O_{\mathrm{ac}}, e) = -1, \qquad \tau(B, e) = +1,$$

and $\tau(v, e') = 0$ for any nonincident pair (none here). Vertex/edge labels are

$$\lambda_V(O_{\mathrm{ac}}) = \mathrm{O}, \quad \lambda_V(B) = \mathrm{B}, \qquad \lambda_E(e) = \text{dative}.$$

At the oxygen endpoint the edge is locally "away" (-1), and at boron it is "toward" $(+1)$, encoding the coordinate bond donation from the carbonyl oxygen of acetone to $\mathrm{BF_3}$.

Example 13 (Iron–carbonyl unit: σ donation and π backbonding (two bidirected edges)). (cf.[29]) Let $\Sigma_V = \{\mathrm{Fe}, \mathrm{CO}\}$ and $\Sigma_E = \{\sigma\text{-donation},\ \pi\text{-backbonding}\}$. Consider

$$\mathcal{M}_B = (V, E, \tau, \lambda_V, \lambda_E), \quad V = \{Fe, CO\}, \quad E = \{e_\sigma, e_\pi\}.$$

Define τ on incident pairs by

$$\tau(CO, e_\sigma) = -1, \quad \tau(Fe, e_\sigma) = +1 \quad (\mathrm{CO} \to \mathrm{Fe}\ \sigma\text{-donation}),$$

$$\tau(Fe, e_\pi) = -1, \quad \tau(CO, e_\pi) = +1 \quad (\mathrm{Fe} \to \mathrm{CO}\ \pi\text{-backbonding}),$$

and set $\tau(\cdot, \cdot) = 0$ for all nonincident pairs. Labels are

$$\lambda_V(Fe) = \mathrm{Fe}, \quad \lambda_V(CO) = \mathrm{CO}, \qquad \lambda_E(e_\sigma) = \sigma\text{-donation}, \quad \lambda_E(e_\pi) = \pi\text{-backbonding}.$$

Thus the σ edge is locally oriented away from CO and toward Fe, while the π edge is locally oriented away from Fe and toward CO, capturing the classical synergic bonding picture of metal–carbonyl complexes within the bidirected framework.

Theorem 2 (MBDG generalizes a bidirected graph). *Let* **BiDig** *denote the class of finite bidirected graphs $B = (G, \tau)$ with $G = (V, E)$. There exist maps*

$$U_B :\ \mathcal{M}_B \mapsto (G, \tau) \in \mathbf{BiDig}, \qquad I_B :\ (G, \tau) \mapsto \mathcal{M}_B$$

such that $U_B \circ I_B = \mathrm{id}_{\mathbf{BiDig}}$.

Proof: Define the forgetful map $U_B(V, E, \tau, \lambda_V, \lambda_E) := ((V, E), \tau)$. Given $B = ((V, E), \tau) \in \mathbf{BiDig}$, fix $v_* \in \Sigma_V$, $e_* \in \Sigma_E$ and define

$$I_B(B) := (V, E, \tau, \lambda_V, \lambda_E), \quad \lambda_V(v) := v_* \ \forall v \in V, \quad \lambda_E(e) := e_* \ \forall e \in E.$$

Then $U_B(I_B(B)) = ((V, E), \tau) = B$, hence $U_B \circ I_B = \mathrm{id}_{\mathbf{BiDig}}$. Thus every bidirected graph appears as an MBDG with constant labels, and every MBDG forgets to a bidirected graph. □

2.3 | Molecular MultiDirected Graph

A molecular multidirected graph extends directed models by allowing multiple labeled directed edges between atoms, capturing multiplicities and parallel chemical interactions.

Definition 7 (Molecular MultiDirected Graph (MMDG))**.** Fix finite attribute sets Σ_V and Σ_E. A *molecular multidirected graph* is a septuple

$$\mathcal{M}_M = (V, E, s, t, m, \lambda_V, \lambda_E),$$

where

- V is a finite set of vertices, E a finite set of edges,
- $s, t : E \to V$ assign the source and target of each edge,
- $m : V \times V \to \mathbb{N}_0$ records multiplicities and is required to satisfy the consistency constraint

$$m(u, v) \;=\; \big|\{\, e \in E \;:\; s(e) = u,\ t(e) = v \,\}\big| \quad \text{for all } (u, v) \in V \times V,$$

- $\lambda_V : V \to \Sigma_V$ and $\lambda_E : E \to \Sigma_E$ assign molecular attributes.

The *underlying multidirected graph* is (V, E, s, t, m).

Example 14 (Dimethyl sulfoxide S=O double bond as parallel directed edges)**.** Let $\Sigma_V = \{\mathrm{S}, \mathrm{O}\}$, $\Sigma_E = \{\sigma, \pi\}$ and define

$$\mathcal{M}_M = (V, E, s, t, m, \lambda_V, \lambda_E)$$

by

$$V = \{S, O\}, \quad E = \{e_\sigma, e_\pi\}, \quad s(e_\sigma) = s(e_\pi) = S, \quad t(e_\sigma) = t(e_\pi) = O,$$

$$\lambda_V(S) = \mathrm{S},\ \lambda_V(O) = \mathrm{O}, \qquad \lambda_E(e_\sigma) = \sigma,\ \lambda_E(e_\pi) = \pi.$$

Then the multiplicity function satisfies

$$m(S, O) = \big|\{e \in E : s(e) = S,\ t(e) = O\}\big| = 2, \quad m(u, v) = 0 \text{ otherwise.}$$

Thus the S=O double bond is modeled by two parallel directed edges $S \to O$.

Example 15 (Carbon monoxide C≡O triple bond as three parallel directed edges)**.** Let $\Sigma_V = \{\mathrm{C}, \mathrm{O}\}$, $\Sigma_E = \{\sigma, \pi_1, \pi_2\}$ and define

$$\mathcal{M}_M = (V, E, s, t, m, \lambda_V, \lambda_E)$$

with

$$V = \{C, O\}, \quad E = \{e_\sigma, e_{\pi_1}, e_{\pi_2}\},$$

$$s(e) = C,\ t(e) = O \text{ for all } e \in E, \qquad \lambda_V(C) = \mathrm{C},\ \lambda_V(O) = \mathrm{O},$$

$$\lambda_E(e_\sigma) = \sigma,\ \lambda_E(e_{\pi_1}) = \pi_1,\ \lambda_E(e_{\pi_2}) = \pi_2.$$

Hence

$$m(C, O) = 3, \qquad m(u, v) = 0 \text{ otherwise,}$$

capturing a triple bond as three parallel directed edges in the same orientation $C \to O$.

Example 16 (Carbon dioxide: two C=O double bonds as four parallel directed edges)**.** (cf.[30, 31]) Let $\Sigma_V = \{\mathrm{C}, \mathrm{O}\}$ and $\Sigma_E = \{\sigma, \pi\}$. Define the MMDG

$$\mathcal{M}_M = (V, E, s, t, m, \lambda_V, \lambda_E)$$

by

$$V = \{C, O_1, O_2\}, \qquad E = \{e_{\sigma,1}, e_{\pi,1}, e_{\sigma,2}, e_{\pi,2}\}.$$

Assign sources and targets

$$s(e_{\sigma,i}) = C, \quad t(e_{\sigma,i}) = O_i, \qquad s(e_{\pi,i}) = C, \quad t(e_{\pi,i}) = O_i \quad (i = 1, 2),$$

so each C–O bond is represented by two parallel directed edges $C \to O_i$. Label vertices and edges by

$$\lambda_V(C) = \mathrm{C}, \quad \lambda_V(O_i) = \mathrm{O}\ (i = 1, 2), \qquad \lambda_E(e_{\sigma,i}) = \sigma,\ \lambda_E(e_{\pi,i}) = \pi.$$

The multiplicity function $m : V \times V \to \mathbb{N}_0$ satisfies

$$m(C, O_1) = \big|\{e \in E : s(e) = C,\ t(e) = O_1\}\big| = 2, \quad m(C, O_2) = 2, \quad m(u, v) = 0 \text{ otherwise.}$$

Thus the linear O=C=O structure is captured as two C=O double bonds, each modeled by a σ and a π edge in the same orientation $C \to O_i$.

Example 17 (Metal–carbonyl synergy: CO→Ni σ donation and Ni→CO π backbonding)**.** (cf.[32]) Let $\Sigma_V = \{\mathrm{Ni}, \mathrm{CO}\}$ and $\Sigma_E = \{\sigma\text{-donation},\ \pi\text{-backbonding}\}$. Consider

$$\mathcal{M}_M = (V, E, s, t, m, \lambda_V, \lambda_E), \qquad V = \{Ni, CO\}, \quad E = \{e_\sigma, e_\pi\}.$$

Assign directions to encode the synergic interaction:

$$s(e_\sigma) = CO,\ t(e_\sigma) = Ni \quad (\sigma \text{ donation } CO \to Ni), \qquad s(e_\pi) = Ni,\ t(e_\pi) = CO \quad (\pi \text{ backbonding } Ni \to CO).$$

Set labels

$$\lambda_V(Ni) = \mathrm{Ni}, \quad \lambda_V(CO) = \mathrm{CO}, \qquad \lambda_E(e_\sigma) = \sigma\text{-donation}, \quad \lambda_E(e_\pi) = \pi\text{-backbonding}.$$

The multiplicity map is then

$$m(CO, Ni) = \big|\{e \in E : s(e) = CO,\ t(e) = Ni\}\big| = 1, \qquad m(Ni, CO) = \big|\{e \in E : s(e) = Ni,\ t(e) = CO\}\big| = 1,$$

$$m(u, v) = 0 \text{ for all other ordered pairs } (u, v).$$

Hence this MMDG simultaneously represents two directed interactions between the same pair of vertices with opposite orientations and distinct edge labels, reflecting the classical σ/π synergy in metal–carbonyl bonding.

Theorem 3 (MMDG generalizes a multidirected graph)**.** *Let* **MultiDig** *denote the class of finite multidirected graphs* $G = (V, E, s, t, m)$ *satisfying* $m(u, v) = |\{e \in E : s(e) = u, t(e) = v\}|$. *There exist maps*

$$U_M : \ \mathcal{M}_M \mapsto (V, E, s, t, m) \in \mathbf{MultiDig}, \qquad I_M : \ (V, E, s, t, m) \mapsto \mathcal{M}_M$$

such that $U_M \circ I_M = \mathrm{id}_{\mathbf{MultiDig}}$.

Proof: Define the forgetful map

$$U_M(V, E, s, t, m, \lambda_V, \lambda_E) \ := \ (V, E, s, t, m).$$

Given $(V, E, s, t, m) \in \mathbf{MultiDig}$, choose fixed $v_* \in \Sigma_V$, $e_* \in \Sigma_E$ and put

$$I_M(V, E, s, t, m) \ := \ (V, E, s, t, m, \lambda_V, \lambda_E), \quad \lambda_V(v) := v_* \ \forall v \in V, \quad \lambda_E(e) := e_* \ \forall e \in E.$$

Then $U_M(I_M(V, E, s, t, m)) = (V, E, s, t, m)$, so $U_M \circ I_M = \mathrm{id}_{\mathbf{MultiDig}}$. Hence every multidirected graph is a special case of an MMDG with constant labels, and every MMDG forgets to a multidirected graph. □

Lemma 1 (Conservative extension)**.** *In each of the three settings (MDG, MBDG, MMDG), taking* Σ_V *and* Σ_E *to be singletons yields exactly the corresponding classical structure (directed, bidirected, multidirected) on the same carrier sets.*

Proof: Let $\Sigma_V = \{*\}$ and $\Sigma_E = \{\diamond\}$. Then all label maps λ_V, λ_E are uniquely determined and carry no additional information. The defining tuples reduce, under U_D, U_B, U_M, to the classical data $(V, E^{\rightarrow})$, $((V, E), \tau)$, and (V, E, s, t, m) respectively, with no loss or addition beyond the classical structures. Thus the molecular variants are conservative extensions. □

Lemma 2 (Exact retrieval via forgetful maps)**.** *For each molecular structure* $\mathcal{M} \in \{\mathcal{M}_D, \mathcal{M}_B, \mathcal{M}_M\}$*, the corresponding forgetful map* $U \in \{U_D, U_B, U_M\}$ *returns the exact classical object obtained by discarding labels and keeping only the incidence/orientation data.*

Proof: Immediate from the definitions of U_D, U_B, U_M, which simply erase λ_V, λ_E and retain the structural maps (either (s, t), or τ, together with E and V). The equalities

$$U_D(\mathcal{M}_D) = (V, E^{\rightarrow}), \quad U_B(\mathcal{M}_B) = ((V, E), \tau), \quad U_M(\mathcal{M}_M) = (V, E, s, t, m)$$

hold by construction. □

3 | Conclusion

In this paper, we examined definitions such as molecular bidirected graphs and multidirected graphs. In future work, we aim to conduct quantitative analyses of the proposed concepts through computational experiments. We also plan to explore possible extensions employing Fuzzy Graphs [33], Intuitionistic Fuzzy Graphs [34, 35], HyperFuzzy Sets[36], HyperGraphs[37, 38], SuperHyperGraph[39, 40], Neutrosophic Graphs [41], and Plithogenic Graphs [42].

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Data Availability

This manuscript presents purely conceptual work without empirical data. Scholars interested in these ideas are invited to undertake experimental or case-study research to substantiate and extend the proposed frameworks.

Ethical Approval

This paper involves no human or animal subjects and thus did not require ethics committee review or approval.

Use of Generative AI and AI-Assisted Tools

We use generative AI and AI-assisted tools for tasks such as English grammar checking, and We do not employ them in any way that violates ethical standards.

Conflicts of Interest

The authors declare that there are no competing interests concerning the content or publication of this article.

Disclaimer

The theoretical models and propositions herein have not yet been subjected to practical validation. Readers should independently verify all citations and be aware that inadvertent inaccuracies may remain. The opinions expressed are those of the authors and do not necessarily represent the views of affiliated organizations.

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