



Article **Properties and Recognition of Atom Graphs**

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Abstract: The atom graph of a connected graph is a graph whose vertices are the atoms obtained by clique minimal separator decomposition of this graph, and whose edges are the edges of all its atom trees. A graph *G* is an atom graph if there is a graph whose atom graph is isomorphic to *G*. We study the class of atom graphs, which is also the class of atom graphs of chordal graphs, and the associated recognition problem. We prove that each atom graph is a perfect graph and give a characterization of atom graphs in terms of a spanning tree, inspired by the characterization of clique graphs of chordal graphs as expanded trees. We also characterize the chordal graphs having the same atom and clique graph, and solve the recognition problem of atom graphs of two graph classes.

Keywords: clique minimal separator decomposition; atom tree; atom graph; clique graph of a chordal graph; atom graph recognition

1. Introduction

Decomposition by clique separators was introduced by Tarjan [1] in 1985 to help the resolution of hard problems. This decomposition of a graph *G* can be represented by a binary tree whose nodes are vertex subsets of *G*. Its root is the vertex set of *G*, and for each node *V'*, if G(V') has a clique separator then the node *V'* has two children $A \cup S$ and $B \cup S$, where $\{A, B, S\}$ is a partition of *V'* and *S* is a clique *AB*-separator, otherwise, *V'* is a leaf of the tree and is called an *atom*. However, the set of atoms depends on the choice of the clique separators. Leimer [2] proved that the set of atoms is uniquely defined if the set *S* is a clique *minimal AB*-separator in the definition above, leading to the notion of *clique minimal separator decomposition*.

Clique minimal separator decomposition has been studied in different contexts. A general survey is given in [3], and the complexity of its computation is improved in [4]. This decomposition is investigated in some particular graph classes [5–10] and is used in the domains of databases [11], text mining [12], and biology [13,14].

The atoms of a chordal graph are its maximal cliques. Several graphs are defined from a connected chordal graph G, whose nodes are the maximal cliques of G: its *clique trees* [15,16], its *clique graph* [17], which is the intersection graph of its maximal cliques, and the union of its clique trees, which is a subgraph of its clique graph and is shown to better capture the structure of G than its clique graph [18,19].

These graphs, defined from a connected chordal graph, can be generalized to any connected graph G, whose nodes are the atoms of G: its *atom trees* [20] and its *atom graph*, which is the union of its atom trees and a subgraph of the intersection graph of its atoms, which better captures the structure of G than the intersection graph of its atoms. Hence, the atom trees of a connected chordal graph are its clique trees, and its atom graph is a subgraph of its clique graph.

The notion of atom graph was introduced in 2007 in [14] to visualize biological clusters. Several algorithms computing the atom graph of a graph are presented in [21] and extended to the computation of the union join tree of an α -acyclic hypergraph.



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Copyright: © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). In this paper, we focus on the class of atom graphs. A graph *G* is an atom graph if there is a graph whose atom graph is isomorphic to *G*. First of all, we deduce from known results that the atom graphs are exactly the atom graphs of chordal graphs, which is not the case for clique graphs. We prove that each atom graph is a *perfect* graph, i.e., a graph such that each induced subgraph has the same chromatic and clique number, or equivalently (Strong Perfect Graph Theorem), a graph having no induced odd hole nor induced odd anti-hole. We give a characterization of an atom graph in terms of a spanning tree, leading to an algorithm recognizing an atom graph in $O(m^{n-1}n^5)$ time. We also define two graph classes such that the atom graphs of the graphs of these classes can be recognized in linear time.

The paper is organized as follows. Section 2 provides some preliminaries. Section 3 characterizes an atom graph as an atom graph of a chordal graph. Section 4 proves that each atom graph is perfect. Section 5 characterizes the chordal graphs having the same atom and clique graph. Sections 6 and 7 provide characterizations of an atom graph in terms of a hypergraph and a spanning tree, respectively. Section 8 investigates the atom graphs of two graph classes. We conclude in Section 9.

2. Preliminaries

The preliminaries of this paper are similar to those of [21]. In order to avoid useless repetition, we only recall here the main definitions, results and notations, and add some results from [21], the new notions appearing in this paper and the results that are explicitly referred to in this paper. We invite the reader to have a look at the preliminaries section of [21] for more detail and an example.

We consider here finite and undirected graphs. For a graph G = (V, E), n = |V| (order of G) and m = |E|. For any subset X of V, G(X) denotes the subgraph of G induced by S. For any vertex v of G, $N_G(v)$ denotes the neighborhood of v in G, i.e., $N_G(v) = \{w \in V | vw \in E\}$, and $N_G[v]$ denotes its closed neighborhood in G, i.e., $N_G[v] = \{v\} \cup N_G(v)$. For any subset X of V, $N_G(X) = (\bigcup_{v \in X} N_G(v)) \setminus X$ and $N_G[X] = X \cup N_G(X)$.

For each graph *G*, $\mathcal{K}(G)$ denotes the set of maximal cliques of *G* and the *clique graph* of *G*, denoted by CG(G), is the intersection graph of $\mathcal{K}(G)$. If *X* and *Y* are nodes of a tree *T*, $P_T(X, Y)$ denotes the path in *T* between *X* and *Y*.

For each integer $k \ge 3$, a C_k is a graph which is a cycle of length k and a k-sun is a graph obtained from a C_k by adding for each edge xy of this C_k a vertex adjacent to x and y and adding all edges that are necessary to make this C_k into a clique. A *hole* is a C_k with $k \ge 5$, and an *anti-hole* is its complement graph. A hole or anti-hole is *odd* if its number of vertices is odd. *G* is (*odd-*)(*anti-*)*hole-free* if no induced subgraph of *G* is an (odd)(anti-)hole. We do not use the definition of a *perfect* graph in this paper, but we use its well-known characterization as an odd-hole-free and odd-anti-hole-free graph (Strong Perfect Graph Theorem).

Separation. Let G = (V, E) be a connected graph and let S be a subset of V. S is a separator of G if $G(V \setminus S)$ is disconnected. The connected components of $G(V \setminus S)$ are called the *components of* S in G. For any pair $\{a, b\}$ of $V \setminus S$, S is an *ab-separator* of G if a and b are in different components of S in G. S is a *minimal ab-separator* if it is an inclusion-minimal *ab-separator*, and a *minimal separator* if there is some pair $\{a, b\}$ of V such that S is a minimal *ab-separator*. A *full component* of S in G is a component C of S in G such that $N_G(C) = S$. Sis a minimal separator if S has at least two full components, and S is a minimal *ab-separator* if a and b lie in two different full components of S. Let A and B be two subsets of V. S is a (minimal) AB-separator of G if it is a (minimal) *ab*-separator of G for each $a \in A$ and each $b \in B$.

If *G* is disconnected, then a (minimal) (*ab*-)separator of *G* is a (minimal) (*ab*-)separator of one of its connected components.

Chordal graph. A graph is *chordal*, or *triangulated*, if it has no chordless cycle of length at least 4. A graph is chordal if and only if all its minimal separators are cliques [22]. A connected graph is chordal if and only if it has a *clique tree* [16,23].

Definition 1. Let G = (V, E) be a connected chordal graph. A clique tree of G is a tree $T = (\mathcal{K}(G), E_T)$ such that for each vertex x of G, the set \mathcal{K}_x of nodes of T containing x induces a subtree of T.

Characterization 1 ([15]). Let G = (V, E) be a connected chordal graph, let T be a clique tree of G, and let $S \subseteq V$; then S is a minimal separator of G if and only if there is an edge XY of T such that $S = X \cap Y$.

Property 1 ([24]). Let G = (V, E) be a connected chordal graph, let T be a clique tree of G, and let S be a minimal separator of G. The number of edges XY of T such that $S = X \cap Y$ is equal to the number of full components of S in G minus 1.

If *G* is a disconnected chordal graph, we associate with *G* a forest whose connected components are clique trees of the connected components of *G*. A clique tree (forest) can be computed in linear time [15].

A *block graph* is a (necessarily chordal) graph whose minimal separators are of size 1. *Atom.* In this paper, we do not use the definition of atoms as the vertex sets produced by clique minimal separator decomposition, but their following characterization.

Characterization 2 ([2]). Let G = (V, E) be a graph and let A be a subset of V. A is an atom of G if and only if A is an inclusion-maximal subset of V inducing a connected subgraph of G with no clique separator.

We denote the set of atoms of *G* by A(G). A graph has at most *n* atoms.

Atom tree.

Definition 2 ([20]). Let G = (V, E) be a connected graph. An atom tree of G is a tree $T = (\mathcal{A}(G), E_T)$ such that for each vertex x of G, the set \mathcal{A}_x of nodes of T containing x induces a subtree of T.

Characterization 3 ([20]). Let G = (V, E) be a connected graph, let T be an atom tree of G, and let $S \subseteq V$; then S is a clique minimal separator of G if and only if there is an edge AB of T such that $S = A \cap B$.

Atom graph.

Definition 3 ([21]). The atom graph of a graph G, denoted by AG(G), is the graph $(\mathcal{A}(G), E')$, where $\mathcal{A}(G)$ is the set of atoms and E' the set of pairs $\{A, B\}$ of $\mathcal{A}(G)$ such that $A \cap B$ is a clique minimal $(A \setminus B)(B \setminus A)$ -separator of G.

Property 2 ([21]). *Let A and B be distinct atoms of a graph G. Then,* $G(A \setminus B)$ *is connected and* $A \cap B \subseteq N_G(A \setminus B)$.

Property 3 ([2,21]). Let G = (V, E) be a connected graph, and let G^+ be the graph obtained from *G* by adding all the edges that are necessary to make each atom of *G* into a clique. Then G^+ is chordal, its clique trees are the atom trees of *G*, its atom graph is the atom graph of *G* and for each clique *S* of *G*, the full components of *S* in G^+ are the full components of *S* in *G*.

Characterization 4 ([21]). *The atom graph of a connected graph G is the union of all the atom trees of G.*

Characterization 5 ([21]). Let *G* be a connected graph, let *A* and *B* be distinct atoms of *G* and let *T* be an atom tree of *G*. Then, *AB* is an edge of AG(G) if and only if there is an edge A'B' on the path $P_T(A, B)$ from *A* to *B* in the tree *T* such that $A \cap B = A' \cap B'$.

By definition of an atom tree, for each pair $\{A, B\}$ of nodes of an atom tree *T* and each edge A'B' of $P_T(A, B)$, $A \cap B \subseteq A' \cap B'$. It follows that in Characterization 5, the equality $A \cap B = A' \cap B'$ can be replaced by $A' \cap B' \subseteq A \cap B$, $|A' \cap B'| = |A \cap B|$ or $|A' \cap B'| \leq |A \cap B|$. We associate with each edge *AB* of an atom tree or an atom graph the set $A \cap B$ of weight $|A \cap B|$.

Clique graph of a chordal graph. A graph G is a *clique graph of a chordal graph* if there is a chordal graph G' such that G is isomorphic to the clique graph of G'.

Characterization 6 ([25]). *A graph G is a clique graph of a chordal graph if and only if it has a spanning tree T such that each maximal clique of G induces a subtree of T.*

a-acyclic hypergraphs. A *simple hypergraph*, or *hypergraph* for short, is a structure $H = (V, \mathcal{E})$, where *V* is its vertex set and \mathcal{E} is a set of non-empty subsets of *V*, called the *hyperedges* of *H*, whose union is equal to *V*. A hypergraph is a *clutter* if the elements of \mathcal{E} are pairwise non-inclusive. Its *line graph*, denoted by L(H), is the intersection graph of \mathcal{E} . Its 2-section graph, denoted by 2SEC(H), is the graph whose vertex set is *V* and whose edges are the pairs of *V* that are contained in a hyperedge of *H*. *H* is *connected* if L(H) is connected, or equivalently if 2SEC(H) is connected.

A *join tree* of *H* is a tree *T* whose node set is \mathcal{E} and such that for each vertex *x* of *H*, the set \mathcal{E}_x of nodes of *T* containing *x* induces a subtree of *T*, or equivalently, such that for each pair $\{X, Y\}$ of $\mathcal{E}, X \cap Y$ is a subset of each node of $P_T(X, Y)$. *H* is *α*-*acyclic* if it has a join tree.

Definition 4 ([21]). *The* union join graph of an α -acyclic hypergraph H, denoted by UJ(H), is the union of its join trees.

Definition 5 ([21]). Let G = (V, E) be a graph. The atom hypergraph of G is the hypergraph $H = (V, \mathcal{A}(G))$.

Property 4 ([21]). *Let G be a connected graph and let H be its atom hypergraph. Then, H is a connected* α *-acyclic hypergraph and the atom graph of G is the union join graph of H*.

Property 5. *Let H be an* α *-acyclic hypergraph, and let G be the* 2*-section graph* 2SEC(*H*)*. Then, G is chordal and if H is a clutter then it is the atom hypergraph of G.*

A non-clutter α -acyclic hypergraph can be turned into a clutter by adding a specific element to each non-inclusion-maximal hyperedge, so any connected α -acyclic hypergraph is an atom hypergraph up to some isomorphism as stated in Property 6.

Property 6 ([21]). *Let* H *be a connected* α *-acyclic hypergraph. Then, there is a connected chordal graph G such that the atom graph of G is isomorphic to the union join graph of H.*

Characterization 5 can be rewritten in terms of α -acyclic hypergraph as follows (*tuj* stands for *to union join*).

Definition 6 ([21]). For each join tree $T = (\mathcal{E}, E_T)$ of a hypergraph, tuj(T) is the graph whose node set is \mathcal{E} and whose edges are the pairs $\{X, Y\}$ of \mathcal{E} such that there is an edge X'Y' of $P_T(X, Y)$ such that $X \cap Y = X' \cap Y'$ (or equivalently $X' \cap Y' \subseteq X \cap Y$).

Characterization 7 ([21]). *For each* α *-acyclic hypergraph H and each join tree T of H,* UJ(H) = tuj(T).

We associate with each edge *AB* of a join tree or an union join graph the set $A \cap B$ of weight $|A \cap B|$.

3. Atom Graphs Are Atom Graphs of Chordal Graphs

A graph is an atom graph if it is isomorphic to the atom graph of some graph. Similarly, for a given graph class C, a graph is an atom graph of a graph of C if it is isomorphic to the atom graph of some graph of C. The atom graph recognition problem consists of determining whether a given graph is an atom graph. According to Definition 3, the connected components of the atom graph of a graph are the atom graphs of the connected components of this graph. It follows that a graph is an atom graph if and only if each one of its connected components is, so we may, without loss of generality, assume that the given graph is connected. We obtain similar definitions by replacing 'atom graph' with 'clique graph' for which we may also assume that the given graph is connected.

We immediately deduce from Property 3 the following characterization.

Characterization 8. A graph is an atom graph if and only if it is an atom graph of a chordal graph.

Thus, the atom graph recognition problem can be reduced to an atom graph of a chordal graph recognition problem. It is not the case for clique graph recognition, which is NP-complete [26], whereas clique graph of a chordal graph recognition is polynomial [17]. As far as we know, the complexity of recognizing an atom graph (or equivalently an atom graph of a chordal graph) is an open question.

4. Atom Graphs Are Perfect

The clique graph of a chordal graph is not necessarily chordal, and not even perfect. For instance, the clique graph of the 5-sun is non-perfect, but its atom graph is chordal (see Figure 1), which follows from Characterization 14 below since the minimal separators of the 5-sun are pairwise non-inclusive. Introducing inclusion-comparable minimal separators, we can build a graph whose atom graph is non-chordal, as shown in Figure 2. This non-chordal atom graph is perfect though.



Figure 1. A chordal graph, its non-perfect clique graph and its chordal atom graph.



Figure 2. A chordal graph, its chordal clique graph and its non-chordal (but perfect) atom graph.

We will show that each atom graph is perfect, and more accurately, that it is odd-hole-free and anti-hole-free.

Notation 1. Let G = (V, E) be a graph. For each atom A and each clique S of G distinct from A, $C_S(A)$ denotes the connected component of $G(V \setminus S)$ containing $A \setminus S$.

This definition is correct since by definition of an atom, for each atom *A* and each clique *S* of *G* distinct from $A G(A \setminus S)$ is necessarily non-empty and connected. In particular

 $C_S(A)$ is defined if *S* is in the form $X \cap Y$ where *X* and *Y* are distinct atoms of *G*. Note that in that case, by Property 2, *XY* is an edge of AG(G) if and only if $C_S(X) \neq C_S(Y)$.

Lemma 1. Let A be an atom and S a clique of a graph G such that $S \subset A$. Then $S = N_G(C_S(A))$.

Proof. $N_G(C_S(A))$ is clearly a subset of *S*, and it cannot be a strict subset of *S* since in that case it would be a clique *ab*-separator of G(A) for any *a* in $A \setminus S$ and any *b* in $S \setminus N_G(C_S(A))$. \Box

Lemma 2. Let G be a graph, let μ be a cycle of AG(G), let AB be an edge of μ and let $S = A \cap B$; then there is an edge A'B' of μ such that $C_S(B) = C_S(B')$ and $A' \cap B' \subseteq S$, with A, B, B', A' in this order on μ (with possibly B = B' or A' = A).

Proof. As *AB* is an edge of AG(G), $C_S(A) \neq C_S(B)$. Let *A'* be the first node *X* of the path $\mu - \{AB\}$ from *B* such that $C_S(X) \neq C_S(B)$, and let *B'* be the node preceding *A'* on this path from *B*. $C_S(B) = C_S(B')$ with *A*, *B*, *B'*, *A'* in this order on μ , and as $C_S(A') \neq C_S(B)$, it follows that $C_S(A') \neq C_S(B')$, and therefore $A' \cap B' \subseteq S$. \Box

We deduce from Lemma 2 the following properties of atom graphs. Property 8 is proved in [18] for chordal graphs.

Property 7. Let *G* be a graph, let μ be a cycle of AG(G) and let *S* be an inclusion-minimal set among the sets associated with the edges of μ ; then *S* is associated with at least two edges of μ .

Property 8. *Let G be a graph and let* μ *be a* C_3 *of* AG(G)*; then two of the clique minimal separators associated with the edges of* μ *are equal and included in the third one.*

Lemma 3. Let G be a connected graph, let X, X' and Y be atoms and let S be the intersection of two distinct atoms of G.

(a) If $S \subseteq X$ and $C_S(X) \neq C_S(Y)$ then (XY is an edge of $AG(G) \Leftrightarrow N(C_S(Y)) \subseteq Y$),

(b) If $S \subseteq X \cap Y$ and $C_S(X) \neq C_S(Y)$ then XY is an edge of AG(G),

(c) If $S \subseteq X \cap X'$, $C_S(X) = C_S(X')$ and Y is adjacent to X but not to X' in AG(G) then $C_S(X) = C_S(Y)$.

Proof. (a) Let G = (V, E). We assume that $S \subseteq X$ and $C_S(X) \neq C_S(Y)$. Let us show that *XY* is an edge of $AG(G) \Leftrightarrow N(C_S(Y)) \subseteq Y$.

XY is an edge of AG(G) if $C_{X\cap Y}(X) \neq C_{X\cap Y}(Y)$, which is still equivalent to $C_{X\cap Y}(Y) \cap (X \setminus Y) = \emptyset$. Let $C = C_{X\cap Y}(Y)$. It is sufficient to show that $N(C_S(Y)) \subseteq Y \Leftrightarrow C \cap (X \setminus Y) = \emptyset$.

First, note that as $N(C_S(Y)) \subseteq S \subseteq X$, we have $N(C_S(Y)) \subseteq X$, and that as $C_S(X) \neq C_S(Y)$, we have $X \cap Y \subseteq S$, and therefore $C_S(Y) \subseteq C \subseteq V \setminus (X \cap Y)$.

⇒: We assume that $N(C_S(Y)) \subseteq Y$. Then, $N(C_S(Y)) \subseteq X \cap Y$, with $C_S(Y)$ being a connected subset of $V \setminus (X \cap Y)$, so $C = C_S(Y)$ and therefore $C \cap (X \setminus Y) \subseteq C_S(Y) \cap X = \emptyset$.

⇐: We now assume that $N(C_S(Y)) \not\subseteq Y$. Let $x \in N(C_S(Y)) \setminus Y$. $x \in X \setminus Y$, and as $x \notin X \cap Y$ and x has a neighbor in $C_S(Y)$ with $C_S(Y) \subseteq C$, $x \in C$. Hence, $x \in C \cap (X \setminus Y)$, and therefore $C \cap (X \setminus Y) \neq \emptyset$.

(b) As $N(C_S(Y)) \subseteq S \subseteq Y$, by a) XY is an edge of AG(G).

(c) We assume for contradiction that $S \subseteq X \cap X'$, $C_S(X) = C_S(X')$, Y is adjacent to X but not to X' in AG(G) and $C_S(X) \neq C_S(Y)$. By (a) on X and Y, $N(C_S(Y)) \subseteq Y$, and by (a) on X' and Y, $N(C_S(Y)) \not\subseteq Y$, a contradiction. \Box

Property 9. Let G be a graph and let μ be a chordless cycle of AG(G) of length at least 4; then either μ is of length 4 and its four edges are associated with the same clique minimal separator or there is an integer $k \ge 2$ such that μ is of length 2k, there are exactly k distinct clique minimal separators associated with the edges of μ which are pairwise non-inclusive and each such separator is associated with two consecutive edges of μ .

In both cases, for each set of consecutive edges XY and YZ of μ associated with the same clique minimal separator S, $C_S(X) = C_S(Z)$.

Proof. Let *AB* be an edge of μ such that $A \cap B$ is inclusion-minimal among the clique minimal separators associated with the edges of μ and let $S = A \cap B$. Let us first prove the following property P_1 .

*P*₁: for each pair {*X*, *Y*} of nodes of μ such that $C_S(X) \neq C_S(Y)$, the following propositions are equivalent:

(1) *XY* is an edge of μ ,

(2) $X \cap Y = S$,

(3) $S \subseteq X \cap Y$.

 $1 \Rightarrow 2$: as $C_S(X) \neq C_S(Y) \ X \cap Y \subseteq S$, and by the minimality of $S \ X \cap Y \not\subset S$, so $X \cap Y = S$.

 $2 \Rightarrow 3$ is evident.

 $3 \Rightarrow 1$: by Lemma 3 (b) *XY* is an edge of AG(G), and therefore of μ since μ is chordless. By Lemma 2, there is an edge A'B' of μ such that $C_S(B) = C_S(B')$ and $A' \cap B' \subseteq S$, with *A*, *B*, *B'*, *A'* in this order on μ . By the minimality of *S*, $A' \cap B' = S$. As *AB* is an edge of AG(G), $C_S(A) \neq C_S(B)$, and therefore $C_S(A) \neq C_S(B')$. As $S \subseteq A \cap B'$, by $P_1 AB'$ is an edge of μ . It follows that B = B' or A = A'. We assume, without loss of generality, that B = B'. By P_1 again, as $S \subseteq A \cap A'$ and AA' is not an edge of μ , $C_S(A) = C_S(A')$. Let *D* be the neighbor of *A* on μ different from *B*.

First case : $C_S(D) = C_S(B)$

As $C_S(A) \neq C_S(D)$ and AD is an edge of μ , by $P_1 A \cap D = S$. Hence, as $C_S(D) \neq C_S(A')$ and $S \subseteq D \cap A'$, by $P_1 DA'$ is an edge of μ and $D \cap A' = S$. Thus, μ satisfies the first alternative of Property 9 and for each set of consecutive edges XY and YZ of μ associated with the same clique minimal separator S, $C_S(X) = C_S(Z)$.

Second case : $C_S(D) \neq C_S(B)$

Let us show that for each node *X* of $\mu - \{A, B, A'\}$, $S \not\subseteq X$. Let *X* be a node of $\mu - \{A, B, A'\}$, and let *Y* be a node of $\{A, B\}$ such that $C_S(X) \neq C_S(Y)$ and *XY* is not an edge of μ (if X = D then Y = B otherwise *Y* exists since neither *XA* nor *XB* is an edge of μ and $C_S(A) \neq C_S(B)$). By $P_1 S \not\subseteq X \cap Y$, so as $S \subseteq Y, S \not\subseteq X$. It follows that for each edge *XY* of $\mu - \{B\}$, $S \not\subseteq X \cap Y$. Hence, *S* is associated with no other edge than the two consecutive edges *AB* and *A'B* of μ . It also follows that *S* is a strict subset of no other clique minimal separator associated with an edge of μ , the clique minimal separators associated with an edge of μ , the clique minimal separators associated with the edges of μ are pairwise non-inclusive and therefore all inclusion-minimal. Hence, μ satisfies the second alternative of Property 9, and for each set of consecutive edges *XY* and *YZ* of μ associated with the same clique minimal separator *S*, $C_S(X) = C_S(Z)$.

Example 1. A graph and its atom graph having an induced C_4 satisfying the first alternative of Property 9 is shown in Figure 3 (the cycle (A, D, C, F) is such a C_4). A graph and its atom graph having an induced C_4 satisfying the second alternative of Property 9 is shown in Figure 4 (the cycle (A, B, E, D) is such a C_4). Note that in both cases, the graph is chordal and has a clique tree which is a path: the path (A, B, C, D, E, F), for instance, in the first case, and (A, B, C, D, E), for instance, in the second case. This contradicts the claim from [18] that any path of a clique tree of a chordal graph induces a chordal subgraph of its atom graph.

For each $k \ge 3$, the atom graph of the graph obtained from a k-sun by adding a vertex of degree 1 adjacent to x for each vertex x of the clique of size k has an induced C_{2k} satisfying the second alternative of Property 9 (see Figure 2 for k = 3).



Figure 3. A graph and its atom graph having an induced C_4 whose edges are associated with the same clique minimal separator *S*.



Figure 4. A graph and its atom graph having an induced C_4 whose edges are associated with two distinct clique minimal separators ({2} and {7}).

Corollary 1. *Each atom graph is odd-hole-free.*

Property 10. Each atom graph is anti-hole-free.

Proof. We assume for contradiction that some induced subgraph of some atom graph *G* is an anti-hole and let k be its length. $k \ge 6$ by Corollary 1 since an anti-hole of length 5 is a hole. Let G' be a graph such that G is isomorphic to AG(G'), let μ be a chordless cycle of AG(G') of length k, and let (A', A, D_1, B_1, B_2) be a sequence of consecutive nodes of μ . As $k \ge 6$ {A', A, B_1 , B_2 } induces a C_4 of AG(G'), so by Property 9 $A \cap B_1$ is equal to $A' \cap B_1$ or to $A \cap B_2$. We assume without loss of generality that $A \cap B_1 = A' \cap B_1$. Let $(A', A, D_1, B_1, \ldots, B_p, D_p)$ be the full sequence of consecutive vertices of μ , and for each $i \in [1, p]$, let $S_i = A \cap B_i$ and let P(i) be the predicate $S_i = A' \cap B_i$. As P(1) holds and for each $i \in [1, p-1], P(i) \Rightarrow P(i+1)$ holds by Property 9, it follows by induction that $\forall i \in [1, p] P(i)$. Let $Y \in \{D_1, D_p\}$ and let $i \in \{1, p\}$. As AB_i is an edge of $AG(G') C_{S_i}(A) \neq i$ $C_{S_i}(B_i)$, and by Property 9 $C_{S_i}(A) = C_{S_i}(A')$. By Lemma 3 c) with $\{X, X'\} = \{A, A'\}$, $C_{S_i}(A) = C_{S_i}(Y)$. It follows that $C_{S_i}(B_i) \neq C_{S_i}(Y)$, so by Lemma 3 a) ($B_i Y$ is an edge of $AG(G') \Leftrightarrow N_{G'}(C_{S_i}(Y)) \subseteq Y$. By Lemma 1 $S_i = N_{G'}(C_{S_i}(A))$, so $S_i = N_{G'}(C_{S_i}(Y))$, and therefore we have the equivalence ($B_i Y$ is an edge of $AG(G') \Leftrightarrow S_i \subseteq Y$). Hence $S_1 \not\subseteq D_1$, $S_p \subseteq D_1, S_1 \subseteq D_p \text{ and } S_p \not\subseteq D_p.$ Let $x \in S_1 \setminus D_1$ and let $y \in S_p \setminus D_p$. $x \in D_p \setminus D_1$, $y \in D_1 \setminus D_p$ and $\{x, y\} \subseteq A \setminus (D_1 \cap D_p) \subseteq C_{D_1 \cap D_p}(A)$. Hence $D_1 D_p$ is not an edge of AG(G'), a contradiction. \Box

Corollary 2. *Each atom graph is perfect.*

5. Atom Graph and Clique Graph of a Chordal Graph

The atom graph of a chordal graph *G* is a subgraph of its clique graph with the same node set. These two graphs may be equal. It is the case if *G* is a block graph by Lemma 6 below, or the graph obtained from a C_4 by adding a chord, which is not a block graph. We have the following characterization.

Characterization 9. *Let G be a connected chordal graph. The following propositions are equivalent* $(C_S(A) \text{ is defined in Notation 1})$:

- 1. AG(G) = CG(G),
- 2. for each minimal separator S of G and each maximal clique A of G, $S \cap A = \emptyset$ or $N(C_S(A)) \subseteq A$,
- 3. each cycle of CG(G) has two edges that are of minimum weight among the edges of this cycle and are associated with the same set,
- 4. each cycle of CG(G) has two edges that are of minimum weight among the edges of this cycle.

Proof. Let *T* be a clique tree of *G*.

1 ⇒ 2: let *S* be a minimal separator of *G* and let *A* be a maximal clique of *G* such that $S \cap A \neq \emptyset$. Let us show that $N(C_S(A)) \subseteq A$. Let *XY* be an edge of *T* associated with *S*. As $C_S(X) \neq C_S(Y)$, at least one of them, say $C_S(X)$ is different from $C_S(A)$. Moreover, as $S \subseteq X$ and $S \cap A \neq \emptyset$, it follows that $X \cap A \neq \emptyset$. Hence, *XA* is an edge of CG(G), i.e., of AG(G), so by item (a) of Lemma 3, $N(C_S(A)) \subseteq A$.

 $2 \Rightarrow 1$: as AG(G) is a subgraph of CG(G) with the same node set, it is sufficient to show that each edge of CG(G) is an edge of AG(G). Let XY be an edge of CG(G), and let us show that it is an edge of AG(G). Let Y' be the neighbor of X on $P_T(X, Y)$ and let $S = X \cap Y'$. As XY is an edge of CG(G) and $X \cap Y \subseteq S \cap Y$, it follows that $S \cap Y \neq \emptyset$, and therefore $N(C_S(Y)) \subseteq Y$. As X and Y are in different connected components of $T - \{XY'\}$, $C_S(X) \neq C_S(Y)$ [15], so by item a) of Lemma 3 again XY is an edge of AG(G).

 $1 \Rightarrow 3$ immediately follows from Property 7.

 $3 \Rightarrow 4$ is evident.

 $4 \Rightarrow 1$: we assume for contradiction that $AG(G) \neq CG(G)$. Let *XY* be an edge of CG(G) that is not an edge of AG(G). Then, by Characterization 5 for each edge *X'Y'* of $P_T(X, Y) X \cap Y \subset X' \cap Y'$. Hence, *XY* is the unique edge of minimum weight of the cycle of CG(G) formed by *XY* and $P_T(X, Y)$, a contradiction. \Box

We immediately refind from Characterization 9 that a block graph has the same atom and clique graph since it satisfies item 2. If *G* is not chordal then its atom graph is necessarily different from its clique graph since its atoms are not its maximal cliques (a chordless cycle of length at least 4 is connected and has no clique separator, and therefore is a subset of some atom). However, Characterization 9 extends to each connected graph, replacing 'CG(G)' by 'the intersection graph of the set of atoms of *G*', 'minimal separator' by 'clique minimal separator' and 'maximal clique' by 'atom' by Property 3.

These classes are inclusion-uncomparable. The 3-sun is an atom graph (it is the atom graph of the graph shown in Figure 5).



Figure 5. The 3-sun is an atom graph.

However, by Characterization 6 it is not a clique graph of a chordal graph (if it had a spanning tree *T* such that each maximal clique induces a subtree of *T* then each one of the three external triangles of the 3-sun would induce a subtree of *T*, and therefore *T* would have a cycle). Conversely, the non-perfect clique graph of a chordal graph shown in Figure 1 is not an atom graph since atom graphs are perfect. It follows that no necessary (resp. sufficient) condition for a graph to be a clique graph of a chordal graph immediately extends to atom graphs. We will go further into the comparison of these two classes in Section 7.

6. Atom Graph and Union Join Graph

We immediately deduce from Properties 4 and 6 and from Characterization 7 the following result, which will be useful to prove the characterization of an atom graph as an AG-expanded tree in Section 7.

Characterization 10. A connected graph. *G* is an atom graph if and only if there is a join tree T of a connected α -acyclic hypergraph such that *G* is isomorphic to tuj(T).

Let *H* be a connected α -acyclic hypergraph. By Property 6 there is a connected chordal graph *G* such that UJ(H) = AG(G) and L(H) = CG(G) up to some isomorphism. It follows that UJ(H) is a subgraph of L(H) with the same node set and that we can deduce from Characterization 9 the following characterizations of a connected α -acyclic hypergraph having the same union join graph and line graph.

Characterization 11. *Let H be a connected* α *-acyclic hypergraph. The following propositions are equivalent:*

- 1. UJ(H) = L(H),
- 2. each cycle of L(H) has two edges that are of minimum weight among the edges of this cycle and are associated with the same set,
- 3. each cycle of L(H) has two edges that are of minimum weight among the edges of this cycle.

7. Characterizations in Terms of Spanning Trees

The polynomial complexity of recognizing a clique graph of a chordal graph is proved using a characterization of this graph as an *expanded tree* [17]. We recall this characterization, which will give inspiration for a characterization of an atom graph.

Definition 7. A graph G is an expanded tree if there is a spanning tree T of G such that for each edge xy of G, the set of vertices of $P_T(x, y)$ is a clique of G.

The clique graph of a chordal graph *G* is an expanded tree since any clique tree of *G* satisfies the condition. The converse holds by the following characterization.

Characterization 12 ([17]). *A connected graph is a clique graph of a chordal graph if and only if it is an expanded tree.*

For instance, trees and complete graphs are clearly expanded trees, and therefore clique graphs of chordal graphs, which also follows from Characterization 14.

We now come to a characterization of an atom graph in terms of a spanning tree.

Definition 8. An AG-structure of a graph G = (V, E) is a triple (T, S_e, S_V) where T is a spanning tree of G, S_e is an ordering (e_1, \ldots, e_p) of the edges of T and S_V is a sequence (V_1, \ldots, V_p) of subsets of V such that for each $i, j \in [1, p]$, $T(V_i)$ is a subtree of T containing the edge e_i and if e_j is an edge of $T(V_i)$ then $j \ge i$ and $V_j \subseteq V_i$, and for each pair $\{x, y\}$ of V, xy is an edge of G if and only if $\{x, y\} \subseteq V_i$, where $i = \min\{j \in [1, p], e_j$ is an edge of $P_T(x, y)\}$. *G* is an AG-expanded tree if it has an AG-structure.

Example 2. Figure 6 shows a graph G and an AG-structure (T, S_e, S_V) of G: the edges of T are represented by full lines, $S_e = (e_1 = \{2,5\}, e_2 = \{4,5\}, e_3 = \{1,5\}, e_4 = \{3,5\})$ and $S_V = (V_1 = \{1,2,3,5\}, V_2 = \{1,3,4,5\}, V_3 = e_3, V_4 = e_4)$. Underlining e_i means that $V_i = e_i$. It follows that G is an AG-expanded tree, and it is an atom graph since it is isomorphic to the atom graph of the graph shown in Figure 4.



Figure 6. An AG-expanded tree G and one of its AG-expanded structures.

As for expanded trees, each tree *T* is an AG-expanded tree (with the AG-structure (T, S, S) where *S* is an arbitrary ordering of the edges of *T*) and each complete graph *G* is an AG-expanded tree (with the AG-structure (P, S_e, S_V) where *P* is a spanning path of *G*, S_e is a natural ordering (e_1, \ldots, e_p) of the edges of *P* and S_V is the sequence (V_1, \ldots, V_p) such that for each *i* from 1 to *p* V_i is the union of the edges e_j , $j \ge i$. Hence, according to Characterization 13 below, trees and complete graphs are atom graphs, which also follows from Characterization 14.

Characterization 13. A connected graph is an atom graph if and only if it is an AG-expanded tree.

To prove Characterization 13, we will use the following Lemma.

Lemma 4. Let *T* be a join tree of a connected hypergraph, let *X*, *Y* be distinct nodes of *T* and let $X_m Y_m$ be an edge of $P_T(X, Y)$ whose associated set is inclusion-minimal among the sets associated with the edges of $P_T(X, Y)$. Then, *XY* is an edge of tuj(T) if and only if $X \cap Y = X_m \cap Y_m$ (or equivalently $X_m \cap Y_m \subseteq X \cap Y$).

Proof. We assume that *XY* is an edge of tuj(T). Let *X'Y'* be an edge of $P_T(X, Y)$ such that $X \cap Y = X' \cap Y'$. As $X \cap Y \subseteq X_m \cap Y_m$ and $X \cap Y = X' \cap Y' \not\subset X_m \cap Y_m$, $X \cap Y = X_m \cap Y_m$. The converse implication is evident \Box

Proof. (of Characterization 13) By Characterization 10 it is sufficient to show that there is a join tree *T* of a connected α -acyclic hypergraph such that *G* is isomorphic to tuj(T) if and only if *G* is an AG-expanded tree.

⇒: let *T* be a join tree of a connected hypergraph such that *G* is isomorphic to tuj(T). It is sufficient to show that tuj(T) is an AG-expanded tree. Let $S_e = (e_1 = X_1Y_1, \ldots, e_p = X_pY_p)$ be an ordering of the edges of *T* ordered by increasing weight, and let $S_V = (V_1, \ldots, V_p)$ where V_i is the connected component of $T(\mathcal{E}_{S_i}) - \{e_j, 1 \le j < i\}$ containing e_i, \mathcal{E}_{S_i} being the set of nodes of *T* containing $S_i = X_i \cap Y_i$, for each $i \in [1, p]$. Let us show that (T, S_e, S_V) is an AG-structure of tuj(T). *T* is a spanning tree of tuj(T). Let $i, j \in [1, p]$. By definition of $V_i, T(V_i)$ is a subtree of *T* containing the edge e_i and if e_j is an edge of $T(V_i)$ then $j \ge i$ and $V_j \subseteq V_i$ (as $e_j \subseteq V_i, S_i \subseteq X_j \cap Y_j = S_j$). Let $\{X, Y\}$ be a pair of nodes of *T* and let $i = min\{j \in [1, p], e_j \text{ is an edge of } P_T(X, Y)\}$. Let us show that XY is an edge of tuj(T) if and only if $\{X, Y\} \subseteq V_i$. By Lemma 4 and the definition of i, XY is an edge of tuj(T) if and only if $S_i \subseteq X \cap Y$, which is still equivalent to $\{X, Y\} \subseteq V_i$ since $T(\mathcal{E}_{S_i})$ is connected and for each edge e_j of $P_T(X, Y), j \ge i$. Hence, (T, S_e, S_v) is an AG-structure of tuj(T), which implies that tuj(T) it is an AG-expanded tree.

⇐: let G = (V, E) and let (T, S_e, S_V) be an AG-structure of G, with $S_e = (e_1 = x_1y_1, ..., e_p = x_py_p)$ and $S_V = (V_1, ..., V_p)$. Let H be the hypergraph (V', \mathcal{E}) where $V' = V + \{v_1, ..., v_p\}$ and $\mathcal{E} = \{A_x, x \in V\}$, with $A_x = \{x\} + \{v_i, i \in [1, p] \land x \in V_i\}$. Let f map each vertex x of G to the hyperedge A_x of H, and let T' = f(T). As $T(V_i)$ is a subtree of T for each $i \in [1, p], T'$ is a join tree of H, and as no edge of T' is associated with

the empty set (the set associated with $f(e_i)$ contains at least v_i since e_i is an edge of $T(V_i)$), H is connected.

Let us show that *G* is isomorphic to tuj(T'). Let $\{x,y\} \subseteq V$. Let us show that xy is an edge of *G* if and only if $A_x A_y$ is an edge of tuj(T'). Let $i = min\{j \in [1, p], e_j \text{ is an edge} of P_T(x, y)\}$. As xy is an edge of *G* if and only if $\{x, y\} \subseteq V_i$, it is sufficient to show that $\{x, y\} \subseteq V_i$ if and only if $A_x A_y$ is an edge of tuj(T'). We assume that $\{x, y\} \subseteq V_i$. Let us show that $A_x A_y$ is an edge of tuj(T'). It is sufficient to show that $A_{x_i} \cap A_{y_i} \subseteq A_x \cap A_y$. Let $v \in A_{x_i} \cap A_{y_i}$, and let $j \in [1, p]$ such that $v = v_j$. As e_i is an edge of $T(V_j)$, $V_i \subseteq V_j$, so $\{x, y\} \subseteq V_j$, i.e., $v_j \in A_x \cap A_y$, and therefore $v \in A_x \cap A_y$. Hence, $A_{x_i} \cap A_{y_i} \subseteq A_x \cap A_y$. Conversely, we assume that $A_x A_y$ is an edge of tuj(T'). Let us show that $\{x, y\} \subseteq V_i$. Let $j \in [1, p]$ such that e_j is an edge of $P_T(x, y)$ and $A_x \cap A_y = A_{x_j} \cap A_{y_j}$. As e_j is an edge of $T(V_j)$, $v_j \in A_{x_j} \cap A_{y_j}$, and therefore $v_j \in A_x \cap A_y$, i.e., $\{x, y\} \subseteq V_j$. As $T(V_j)$ is a subtree of T, e_i is an edge of $T(V_j)$ and therefore $i \ge j$. As $i \le j$ by definition of i, i = j and therefore $\{x, y\} \subseteq V_i$. Hence, *G* is isomorphic to tuj(T').

The proof of the implication from right to left of Characterization 13 describes how to define a chordal graph G' such that G is isomorphic to AG(G') from an AG-structure $(T, S_e = (e_1, \ldots, e_p), S_V = (V_1, \ldots, V_p))$ of G. As the hyperedges A_x of the hypergraph H defined in the proof are pairwise non-inclusive (because of the presence of x in A_x) H is a clutter. It follows by Property 5 that G is isomorphic to the atom graph of the chordal graph G' = 2SEC(H) having T' as a clique tree. Note that G' can be defined from the set $\{V_1, \ldots, V_p\}$ alone: G' = (V', E'), with $V' = V + \{v_1, \ldots, v_p\}$ and $E' = \{xv_i, x \in V \land i \in [1, p] \land x \in V_i\} + \{v_iv_j, \{i, j\} \subseteq [1, p] \land V_i \cap V_j \neq \emptyset\}$.

Example 3. We recall in Figure 7 the graph G and its AG-structure shown in Figure 6, and we add the join tree T' as defined in the proof of Characterization 13 and the chordal graph G' such that G is isomorphic to AG(G') as defined above. The edges incident to vertex 5 in G' are dashed because vertex 5 may be removed (it is not necessary in A_5 to turn H into a clutter). We refind the graph shown in Figure 4 whose atom graph is G (up to isomorphism).

Characterization 13 can be used to show that a graph is or is not an atom graph, and to deduce some properties of atom graphs. We leave as an open question whether it can be used to determine the complexity of atom graph recognition, as was the case for the characterization as an expanded tree for clique graph of a chordal graph recognition. We first define a superclass of both the classes of expanded and AG-expanded trees.

Definition 9. A join-path spanning tree of a graph G is a spanning tree T of G such that for each edge xy of G, there is an edge x'y' of $P_T(x, y)$, with x, x', y', y in this order on this path, such that each vertex of $P_T(x, x')$ is adjacent to each vertex of $P_T(y', y)$ in G (i.e., the join of the subgraphs of G induced by the paths $P_T(x, x')$ and $P_T(y', y)$ is a subgraph of G). G is an join-path-expanded tree if it has a join-path spanning tree.

Note that if *T* is a join-path spanning tree of *G* then for each edge *xy* of *G*, each vertex of $P_T(x, y)$ is adjacent to *x* or *y* in *G*).

We immediately deduce from the characterizations of a clique graph of a chordal graph and an atom graph as an expanded tree and an AG-expanded tree, respectively, the following property.



Figure 7. Construction of a graph G' such that G is isomorphic to AG(G') from an AG-structure of G.

Property 11. Each connected atom graph (resp. clique graph of a chordal) is a join-path-expanded tree.

As the classes of clique graphs of chordal graphs and atom graphs are inclusionuncomparable, they are necessarily strict subclasses of the class of join-path-expanded trees, so having a join-path spanning tree is a necessary, but non-sufficient, condition for a connected graph to be an atom graph (or a clique graph of a chordal graph).

Property 12. *No cycle of length at least 4 is an atom graph.*

Proof. We assume for contradiction that some cycle *G* of length at least 4 is an atom graph. Then by Property 11 *G* has a join-path spanning tree *T*, which is necessarily a path whose extremities *x* and *y* are adjacent in *G*. As *T* is a join-path spanning tree of *G*, each vertex of *G* is adjacent to *x* or *y* in *G*, a contradiction. \Box

Though a C_4 is not an atom graph, the graph obtained from a C_4 by adding a universal vertex is an atom graph, as is shown in Figure 7. We have the following result.

Corollary 3. The class of atom graphs is not hereditary.

Note that these results also hold for clique graphs of chordal graphs. No cycle of length at least 4 is a clique graph of a chordal graph for the same reason as for atom graphs. As any graph having a universal vertex is a clique graph of a chordal graph (by Characterization 6, considering the spanning tree whose edges are the edges incident to a universal vertex) the class of clique graphs of chordal graphs also fails to be hereditary.

We deduce from the proof of Characterization 13 the following property.

Property 13. Each connected atom graph of order *n* is isomorphic to the atom graph of some chordal graph of order 2n - 1 whose minimal separators have exactly 2 full components.

Proof. In the proof of Characterization 13 we define from an AG-structure of a connected graph *G* of order *n* a clique tree *T'* of a chordal graph *G'* such that *G* is isomorphic to AG(G'). *G'* has n + p vertices, where *p* is the number of edges of a spanning tree of *G*, so *G'* is of order 2n - 1. Let us show that the sets associated with the edges of *T'* are pairwise distinct. Let $i, j \in [1, p]$ such that . $A_{x_i} \cap A_{y_i} = A_{x_j} \cap A_{y_j}$. Let us show that i = j. As e_i is an edge of $T(V_i)$, $v_i \in A_{x_i} \cap A_{y_i}$, so $v_i \in A_{x_j} \cap A_{y_j}$, i.e., e_j is an edge of $T(V_i)$, and therefore $j \ge i$. Symetrically $i \ge j$, so i = j. Hence, the sets associated with the edges of *T'* are pairwise distinct, so by Property 1 each minimal separator of *G'* has exactly 2 full components. \Box

Property 13 provides a polynomial certificate for atom graph recognition. Given a graph *G* of order *n*, the certificate is composed of a graph *G*' of order 2n - 1, its atom graph *G*'' and an isomorphism *f* from *G* to *G*''. We can check in polynomial time that *G*'' is the atom graph of *G*' and that *f* is an isomorphism from *G* to *G*''.

Corollary 4. Atom graph recognition is in NP.

Property 13 also provides a brute force algorithm recognizing an atom graph: computing all the graphs having 2n - 1 given vertices, and for each one of these graphs satisfying the conditions of Property 13, computing its atom graph and determining whether it is isomorphic to the input graph. We deduce from Characterization 13 another brute force algorithm which is (relatively !) more efficient since it runs in $O(m^{n-1}n^5)$ time. Whereas the number of graphs having 2n - 1 given vertices is $2^{(2n-1)(2n-2)/2}$, i.e., $(2^{2n-1})^{n-1}$. Note that this algorithm is still quite intractable except for very small graphs.

Theorem 1. An atom graph can be recognized in $O(m^{n-1}n^5)$ time.

Proof. We assume without loss of generality that *G* is connected. The idea is to consider each spanning tree of *G* and each ordering of its edges. For that, we associate each edge of *G* with an integer from 1 to *m*. A subset of n - 1 edges (potential set of edges of a spanning tree) is represented by the sequence of their associated integers in increasing order. There are $\binom{m}{n-1}$ such sequences that we process in lexicographic order. As finding the next sequence in lexicographic order and checking that it defines a spanning tree (connected and covering all vertices) take O(n) time, this process is in $O(n\binom{m}{n-1})$ time, and therefore in $O(nm^{n-1}/(n-1)!)$ time.

An ordering of the edges is represented by the sequence of their associated integers. There are (n - 1)! such sequences that we process in lexicographic order. As finding the next sequence in this order takes O(n) time, this process is in O(n(n - 1)!) time.

Now, given a spanning tree *T* and an ordering (e_1, \ldots, e_p) , for each *i* from 1 to *p*, V_i is necessarily the set defined as follows. Let $e_i = x_i y_i$, and V_{x_i} (resp. V_{y_i}) be the connected component of $T - \{e_j, j \in [1, i]\}$ containing x_i (resp. y_i). V_i is the union of the set of neighbors of x_i in V_{y_i} and the set of neighbors of y_i in V_{x_i} . Computing V_i and checking its connexity takes O(n) time, and therefore $O(n^2)$ time for all *i*. If e_j is an edge of $T(V_i)$ then necessarily $j \ge i$, and checking that $V_j \subseteq V_i$ takes O(n) time, and therefore $O(n^3)$ time for all *i*, *j*. It is sufficient to check the equivalence "xy is an edge of *G* if and only if $\{x, y\} \subseteq V_i$ " for each pair $\{x, y\}$ such that x is in V_{x_i} and y is in V_{y_i} defined as above), since these pairs are exactly the pairs $\{x, y\}$ such that $i = \min\{j \in [1, p], e_j$ is an edge of $P_T(x, y)\}$. This process adds a time complexity in $O(n^2)$ for all *i*, since the sets V_{x_i} and V_{y_i} have already been computed and each pair $\{x, y\}$ is checked exactly once. Hence, the algorithm is in $O(nm^{n-1}/(n-1)! * n(n-1)!) * n^3)$ time , i.e., in $O(m^{n-1}n^5)$ time. \Box

We use Characterization 13 to show that the *k*-sun is not an atom graph if $k \ge 4$. We recall that the 3-sun is an atom graph (it is the atom graph of the graph shown in Figure 5).

Property 14. *There is no integer* $k \ge 4$ *such that the k-sun is an atom graph.*

Proof. We assume for contradiction that there is an integer $k \ge 4$ such that the *k*-sun is an atom graph, and therefore an AG-expanded tree. Let G = (V, E) be a *k*-sun and let $(T, (e_1, \ldots, e_p), (V_1, \ldots, V_p))$ be an AG-structure of *G*. Let *C* be the clique of *G* of size *k*, let $D = V \setminus C$, let D_1 (resp. D_2) be the set of vertices of *D* of degree 1 (resp. 2) in *T*, and let $C_2 = C \cup D_2$. $T(C_2)$ is a subtree of *T*. Let $i_0 = min\{i \in [1, p], e_i \text{ is an edge of } T(C_2)\}$, let $e_{i_0} = x_1x_2$, and for each $i \in \{1, 2\}$ let X_i be the connected component of T- $\{e_{i_0}\}$ containing x_i and let y_i be equal to x_i if $x_i \in C$ and to the neighbor of x_i in X_i otherwise, so that in both cases $y_i \in C \cap X_i$. Let us show that $C_2 \subseteq V_{i_0}$.

Let us first show that $C \subseteq V_{i_0}$. Let $x \in C$, and let i, j such that $x \in X_i$ and $\{i, j\} = \{1, 2\}$. As $T(C_2)$ is a subtree of T, $P_T(x, y_j)$ is a path in $T(C_2)$, so $i_0 = min\{i \in [1, p], e_i \text{ is an edge of } P_T(x, y_j)\}$. As xy_j is an edge of G, $x \in V_{i_0}$. Hence, $C \subseteq V_{i_0}$. As $T(V_{i_0})$ is connected and each vertex of D_2 is on the path in T between its two neighbors which belong to C and therefore to V_{i_0} , $C_2 \subseteq V_{i_0}$.

Let us show that for any triangle (c, c', d) in G such that $d \in D_1 \setminus V_{i_0}$, there is an integer j in [1, p] such that $V_j = e_j = cc'$. Let (c, c', d) be such a triangle. We assume w.l.o.g. that c is the neighbor of d in T. Let $i = min\{r \in [1, p], e_r \text{ is an edge of } P_T(c', d)\}$. As c'd is an edge of G, $\{c', d\} \subseteq V_i$. It follows that $e_i = cd$ (otherwise e_i would be a subset of C_2 , and therefore an edge of $T(V_{i_0})$, so V_i would be a subset of V_{i_0} and would not contain d). Hence, d is adjacent to each vertex of $V_i \setminus \{d\}$, so $V_i = \{c, c', d\}$ and cc' is an edge of T. Let j be the integer such that $cc' = e_j$. As e_j is an edge of $T(V_i)$, $V_j \subseteq V_i$ and as V_j contains the edge e_j , but not the edge e_i since i < j, $V_j = e_j$.

Now, as the vertices of D are pairwise non-adjacent in G, there is some $i \in \{1, 2\}$ such that $D \cap V_{i_0} \subseteq X_i$. We assume without loss of generality that i = 1. Then, $D \cap V_{i_0} \subseteq V_{i_0} \cap X_1 \subseteq N_G(y_2)$. As G is a k-sun with $k \ge 4$, there are 2 triangles (c, c_1, d_1) and (c, c_2, d_2) such that for each $i \in \{1, 2\}$, d_i is in $D \setminus N_G(y_2)$, and therefore in $D \setminus V_{i_0}$, which is equal to $D_1 \setminus V_{i_0}$ since $D_2 \subseteq V_{i_0}$. So by the preceding argument, for each $i \in \{1, 2\}$ there is an integer j_i in [1, p] such that $V_{j_i} = e_{j_i} = cc_i$. Hence, there is no integer r such that e_r is an edge of $P_T(c_1, c_2)$ and $\{c_1, c_2\} \subseteq V_r$, and therefore c_1c_2 is not an edge of G, a contradiction. \Box

We showed in Section 5 that by Characterization 6 the 3-sun is not a clique graph of a chordal graph. The same argument holds for each $k \ge 3$: there is no integer k such that the k-sun is a clique graph of a chordal graph. However, the k-sun is a join-path-expanded tree for each $k \ge 3$: it is easy to check that any spanning tree T of the k-sun which is a spanning tree of the union of its external triangles such that each vertex of degree 2 in the k-sun is of degree 1 in T is a join-path spanning tree of the k-sun. A join-path spanning tree of the 4-sun is shown in Figure 8 (its edges are represented by full lines). It follows that the union of the classes of atom graphs and clique graphs of chordal graphs is a strict subclass of the class of join-path-expanded graphs.



Figure 8. The 4-sun is a join-path-expanded tree.

8. Atom Graph Subclasses

8.1. Atom Graphs of \mathcal{G}_{ninc}

Notation 2. G_{ninc} denotes the class of graphs whose clique minimal separators are pairwise noninclusive (ninc stands for non-inclusive). Equivalently, \mathcal{G}_{ninc} is the class of graphs whose clique minimal separators have only full components (since the minimal separators that are subsets of a minimal separator *S* in a connected graph *G* are the neighborhoods of the connected components of $G(V \setminus S)$). We recall that a block graph is a chordal graph whose minimal separators are of size 1. Each block graph is in \mathcal{G}_{ninc} . As announced in Section 4, the atom graph of a graph of \mathcal{G}_{ninc} is necessarily chordal. Moreover, it is a block graph and is an atom graph of a block graph.

Characterization 14. *Let G be a connected graph. The following propositions are equivalent.*

- 1. *G* is an atom graph of a graph of \mathcal{G}_{ninc} ,
- 2. *G* is a block graph,
- 3. *G* is an atom graph of a block graph,
- 4. *G* is a clique graph of a block graph,

To prove Characterization 14 we will use the following results. We first recall a characterization of the edges of the atom graph that are associated with a given clique minimal separator.

Characterization 15 ([21]). Let G be a connected graph, let T be an atom tree of G and let S be a minimal separator of G. Then the edges of AG(G) associated with S are the pairs of nodes of T whose endpoints are in different connected components of $T(A_S) - E_S$, where A_S is the set of nodes of T containing S and E_S is the set of edges of T associated with S.

Lemma 5. Let G be a connected graph of \mathcal{G}_{ninc} . Then AG(G) is a block graph, and if G has at least two atoms then the maximal cliques of AG(G) are the sets \mathcal{A}_S of atoms of G containing S for each clique minimal separator S of G, and each edge in the clique \mathcal{A}_S is associated with S.

Proof. If *G* has a unique atom then AG(G) is clearly a block graph.

We assume now that *G* has at least two atoms. Let *S* be a clique minimal separator of *G*, let *T* be an atom tree of *G*, and let \mathcal{A}_S and E_S be defined as in Characterization 15. As the edges of $T(\mathcal{A}_S)$ are associated with clique minimal separators containing *S* and $G \in \mathcal{G}_{ninc}$, all the edges of $T(\mathcal{A}_S)$ are in E_S . It follows from Characterization 15 that \mathcal{A}_S is a clique of AG(G) and each edge in \mathcal{A}_S is associated with *S*. Hence, to show that the maximal cliques of AG(G) are the sets \mathcal{A}_S , it is sufficient to show that each element of $\mathcal{K}(AG(G))$ is a subset of \mathcal{A}_S for some clique minimal separator *S*. Let $\mathcal{K} \in \mathcal{K}(AG(G))$. As *G* has at least two atoms $|\mathcal{K}| \ge 2$. Let $\{X, Y\} \subseteq \mathcal{K}$ and let $S = X \cap Y$. Let us show that $\mathcal{K} \subseteq \mathcal{A}_S$. Let $Z \in \mathcal{K}$. Let us show that $Z \in \mathcal{A}_S$. It is evident if $Z \in \{X, Y\}$. Otherwise by Property 8 and the fact that $G \in \mathcal{G}_{ninc}$, the three edges of the triangle (X, Y, Z) are associated with *S*, and therefore $Z \in \mathcal{A}_S$. Hence, the maximal cliques of AG(G) are the sets \mathcal{A}_S for each clique minimal separator *S*.

Let us show that AG(G) is chordal. Let μ be a cycle in AG(G) of length ≥ 4 . By Property 7 two edges of μ are associated with the same set *S*, which are contained in the clique \mathcal{A}_S of AG(G). Hence, μ has a chord, and therefore AG(G) is chordal. It follows that each minimal separator of AG(G) is the intersection of two maximal cliques of AG(G), and therefore is of size 1 since otherwise, there would be a pair $\{S, S'\}$ of clique minimal separators of *G* and an edge of AG(G) in $\mathcal{A}_S \cap \mathcal{A}_{S'}$ which would be associated with both *S* and *S'*. It follows that AG(G) is a block graph. \Box

Lemma 6. For each connected block graph G, AG(G) = CG(G).

Proof. As *G* is chordal, AG(G) is a subgraph of CG(G) with the same node set. Let us show that each edge of CG(G) is an edge of AG(G). Let *XY* be an edge of CG(G), let *T* be an atom tree of *G* and let X'Y' be an edge of $P_T(X, Y)$. As $1 \le |X \cap Y| \le |X' \cap Y'| = 1$ with $X \cap Y \subseteq X' \cap Y'$, it follows that $X \cap Y = X' \cap Y'$, and therefore *XY* is an edge of AG(G) by Characterization 5. \Box

To prove that a block graph is an atom graph of a block graph, or equivalently by Lemma 6, a clique graph of a block graph, we will use a well-known technique allowing to compute a chordal graph whose clique graph is isomorphic to a given graph.

Notation 3. For each graph G = (V, E), RetroCG(G) denotes the intesection graph of the set $\mathcal{K}(G) \cup \{\{x\}, x \in V\}$.

Lemma 7. Let G = (V, E) be a connected graph, and let $G' = \operatorname{RetroCG}(G)$. If CG(G) is chordal and for each maximal clique \mathcal{K} of CG(G), the elements of \mathcal{K} have a non-empty intersection then G'is chordal, G is isomorphic to CG(G') and the maximal cliques of G' are the sets $N_{G'}[\{x\}]$ for each element x of V.

Proof. We recall the following properties of RetroCG(G), which are easy to check:

(1) For each $x \in V$, $N_{G'}[\{x\}]$ is a maximal clique of G',

(2) For each $\{x, y\} \subseteq V$ *xy* is an edge of *G* if and only if $N_{G'}[\{x\}] \cap N_{G'}[\{y\}] \neq \emptyset$,

(3) If for each maximal clique \mathcal{K} of CG(G), the elements of \mathcal{K} have a non-empty intersection then the maximal cliques of G' are the sets $N_{G'}[\{x\}]$ for each element x of V,

(4) CG(G) is chordal if and only if G' is chordal.

It follows from these properties that under the hypothesis of the lemma, G' is chordal, and the mapping associating each vertex x of G with $N_{G'}[\{x\}]$ is an isomorphism from G to CG(G'). \Box

Lemma 8. Let G = (V, E) be a connected block graph, and let G' = RetroCG(G). Then G' is a block graph and G is isomorphic to CG(G').

Proof. By Lemma 6 CG(G) = AG(G), so by Lemma 5 CG(G) is chordal. Let \mathcal{K} be a maximal clique of CG(G), let us show that the elements of \mathcal{K} have a non-empty intersection. If G has a unique atom then it is trivial, otherwise by Lemma 5 again it is the case since all the elements of \mathcal{K} contain a given clique minimal separator S of G. Hence, by Lemma 7 G' is chordal, G is isomorphic to CG(G') and the maximal cliques of G' are the sets $N_{G'}[\{x\}]$ for each element x of V. Let us show that each minimal separator of G' is of size 1. We assume for contradiction that it is not the case. Then, there is a pair $\{x, y\}$ of V and a pair $\{K, L\}$ of $\mathcal{K}(G)$ in $N_{G'}[\{x\}] \cap N_{G'}[\{y\}]$, i.e., such that $\{x, y\} \subseteq K \cap L$. It follows that KL is an edge of CG(G), i.e., of AG(G), and therefore is associated with a minimal separator of G is a block graph. \Box

Proof. (of Characterization 14) $1 \Rightarrow 2$ follows from Lemma 5, $2 \Rightarrow 4$ follows from Lemma 8, $4 \Rightarrow 3$ follows from Lemma 6, and $3 \Rightarrow 1$ is evident. \Box

Example 4. The 5-sun shown in Figure 1 is a graph of \mathcal{G}_{ninc} and its atom graph is a block graph, with $\{F\}$ as unique minimal separator. Let G be this atom graph and let $G' = \operatorname{RetroCG}(G)$. The 5-sun, G and G' are shown in Figure 9. G' is a block graph whose atom graph is isomorphic to G. Note that G is also isomorphic to the atom graph of $G' - \{F\}$, as the presence in G' of the node $\{F\}$ is not necessary since $N_{G'}(\{F\})$ is already a maximal clique of G'.

The graph shown in Figure 2 is not a graph of \mathcal{G}_{ninc} . Its atom graph is not a block graph, and is isomorphic to the atom graph of no graph of \mathcal{G}_{ninc} by Characterization 14.



Figure 9. A graph of \mathcal{G}_{ninc} , its atom graph *G*, which is a block graph, and the block graph G' = RetroCG(G) whose atom graph is isomorphic to *G*.

It follows that block graphs, and in particular trees and complete graphs, are atom graphs. We have the following complexity results.

Lemma 9. Let G be a connected block graph. Then RetroCG(G) can be computed on $O(n^2)$ time.

Proof. Let G' = RetroCG(G). Its node set is computed in linear time since *G* is chordal. The edges of *G'* that are incident to a node of size 1 are computed in linear time too by scanning the maximal cliques of *G*, as the sum of their sizes is bounded by n + m. The other edges are computed by making $N_{G'}(\{v\})$ into a clique for each vertex v of *G*. Each edge is added only once by this process since two distinct non-disjoint maximal cliques of *G* have exactly one vertex in common since, by Lemma 6, their intersection is a minimal separator of *G* and *G* is a block graph. So this process takes $O(n^2)$ time, as *G* has at most *n* maximal cliques, and therefore *G'* is computed in $O(n^2)$ time. \Box

Theorem 2. Recognition of an atom graph of a graph of \mathcal{G}_{ninc} takes linear time, and if it is the case then a block graph whose atom graph is isomorphic to the input graph can be computed on $O(n^2)$ time.

Proof. The first result results from Characterization 14 and the fact that recognizing a block tree takes linear time. The second one results from Lemmas 6, 8 and 9. \Box

A block graph can be the atom graph of a graph not belonging to \mathcal{G}_{ninc} . For instance, if *G* is the chordal graph whose maximal cliques are $\{1, 2, 3\}$, $\{1, 2, 4\}$, and $\{1, 5\}$, its minimal separators are $\{1, 2\}$, and $\{1\}$, so *G* is not in \mathcal{G}_{ninc} but its atom graph is a block graph since it is a complete graph.

8.2. Atom Graphs of \mathcal{G}_{ninc}^2

Notation 4. \mathcal{G}_{ninc}^2 denotes the class of graphs whose clique minimal separators have exactly 2 components.

 $\mathcal{G}_{ninc}^2 \subseteq \mathcal{G}_{ninc}$ since a minimal separator has at least two full components. Thus, \mathcal{G}_{ninc}^2 is the set of graphs of \mathcal{G}_{ninc} whose clique minimal separators have exactly two full components.

The equivalence between items 1 and 3 of Characterization 16 is proved in [24] for chordal graphs.

Characterization 16. *Let G be a connected graph. The following propositions are equivalent.*

- 1. *G* is a graph of \mathcal{G}_{ninc}^2 ;
- 2. AG(G) is a tree;
- 3. *G* has a unique atom tree;
- 4. The sets associated with the edges of AG(G) are pairwise distinct;
- 5. Each minimal separator of *G* is a subset of exactly 2 atoms of *G*.

Proof. Let *S* be a clique minimal separator of *G*, let A_S be the set of atoms of *G* containing *S*, let *T* be a clique tree of *G*, and let E_S (resp. E'_S) be the set of edges of *T* (resp. AG(G)) associated with *S*. By Properties 1 and 3 the number of full components of *S* in *G* is equal to $|E_S| + 1$.

 $1 \Rightarrow 5$: as $G \in \mathcal{G}_{ninc}$, each edge of $T(\mathcal{A}_S)$ is in E_S , and as S has exactly two full components, $|E_S| = 1$. Hence $T(\mathcal{A}_S)$ has a unique edge, and therefore two nodes.

 $5 \Rightarrow 4$: each edge of E'_S is a subset of \mathcal{A}_S .

 $4 \Rightarrow 3$: As *T* is a subgraph of AG(G) by Characterization 4, $E_S \subseteq E'_S$ with $1 \le |E_S| \le |E'_S| = 1$. Hence, $E_S = E'_S$ for each *S*, and therefore T = AG(G).

 $3 \Rightarrow 2$: it follows from Characterization 4.

 $2 \Rightarrow 1$: there is no clique minimal separator *S'* stricly containing *S*, otherwise by Characterization 15 there would be a triangle in AG(G) whose edges are associated with *S'*, *S* and *S*, respectively, and $|E_S| = 1$, otherwise by Characterization 15 again there would be a triangle in AG(G) whose edges are associated with *S*. As this holds for each *S*, $G \in \mathcal{G}_{ninc}$ and each clique minimal separator has exactly 2 full components, i.e., $G \in \mathcal{G}_{ninc}^2$.

Characterization 17. A connected graph is an atom graph of a graph of \mathcal{G}_{ninc}^2 if and only if it is *a tree.*

Proof. The implication from left to right follows from Characterization 16. The converse implication follows from the fact that by Characterization 14, a tree is an atom graph, and from Characterization 16. \Box

We deduce from Theorem 2 and Characterizations 16 and 17 the following corollary.

Corollary 5. Recognition of an atom graph of a graph of \mathcal{G}_{ninc}^2 takes linear time, and if it is the case then a block graph of \mathcal{G}_{ninc}^2 whose atom graph is isomorphic to the input graph can be computed on $O(n^2)$ time.

Contrary to the block graphs which are the atom graphs of block graphs, the trees are not the atom graphs of trees. As a non-path tree has a vertex of degree at least 3, its atom graph has a clique of size at least 3 and therefore is not a tree. It follows that conversely, a non-path tree is not an atom graph of a tree since it is an atom graph of neither a path nor a non-path tree. We easily check that the paths are the atom graphs of paths (though a path may be the atom graph of a non-path graph) and that the paths are the trees of \mathcal{G}_{ninc}^2 . Still contrary to blocks graphs which can be atom graphs of graphs not belonging to \mathcal{G}_{ninc} , a tree can only be an atom graph of a graph of \mathcal{G}_{ninc}^2 by Characterization 16.

9. Conclusions

We have studied several aspects of atom graphs and atom graph recognition. We proved that each atom graph is perfect, presented characterizations of atom graphs and investigated the relationship between atom graphs, or equivalently atom graphs of chordal graphs, and clique graphs of chordal graphs. We also proved that the atom graphs of the graphs of two graph classes can be recognized in linear time. However, we leave as an open question the complexity of atom graph recognition. We only proved that it is in NP with a complexity in $O(m^{n-1}n^5)$ time. This result follows from the characterization of an atom graph as an AG-expanded tree, which is inspired by the characterization of a clique graph of a chordal graph as an expanded tree. As this characterization of a clique graph of a chordal graph leads to a polynomial recognition algorithm, this polynomial algorithm may be a source of inspiration for polynomial atom graph recognition. On the other side, as the definition of an AG-expanded tree is significantly more complex than that of an expanded tree, it is also possible that atom graph recognition is NP-complete.

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