Industrial Organic Chemical Use Trees

Final Report
October 1983

Prepared for:

Industrial Environmental Research Laboratory
Office of Research and Development
U.S. Environmental Protection Agency
Cincinnati, Ohio 45268

RADIAN
CORPORATION

Acknowledgements

The design of the industrial organic chemical use tree diagrams presented in this report was developed from information generated by projects conducted cooperatively by Radian Corporation and Paul W. Spaite Company for EPA's Industrial Environmental Research Laboratory, Cincinnati, Ohio. The authors wish to recognize specifically Dr. Eugene E. Berkau, former Director of IERL's Industrial Pollution Control Division, for his ongoing support and contributions to the conception and design of the study. The IERL-Cincinnati Technical Project Manager was Mark Stutsman. The report is a product of the efforts of those conducting the project and they are solely responsible for its contents.

DCN 83-211-030-09-08

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EPA Contract No. 68-03-3038-SBR09
EPA Contract No. 68-03-3171-WA61

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Background

In 1973 the U.S. Environmental Protection Agency's Industrial Environmental Research Laboratory (IERL), Research Traingle Park (RTP), undertook a series of small projects aimed at eventual development of a systematic approach to analysis of industrial pollution sources. This early work led to the establishment of a larger research program in 1977 to develop the "Industrial Process Profiles for Environmental Use" (IPPEU). The overall purpose of the IPPEU program was to develop the necessary concepts, methodology, and database to identify and define potential environmental effects of major industrial processes. Responsibility for key industries was divided between EPA's IERL-RTP and IERL-Cincinnati. Most of the complex network of industries concerned with the production and use of industrial organic chemicals was assigned to the Cincinnati laboratory, and a decision was made to apply the concepts emerging from the IPPEU work to those industries. The work was expected to: (1) provide guidance for EPA's ongoing programs that address environmental and health problems in the specified industries; and (2) provide a basis for the Agency's development of a structured approach to research and development (R&D) planning.

In 1979, shortly after the IPPEU program was initiated, IERL-Cincinnati contracted with Radian Corporation and Paul W. Spaite Company (consultant) to prepare a draft set of "Use Diagrams for Industrial Organic Chemicals." This reflected IERL's recognition of the need to create a first generation set of "chemical/use trees to establish the hierarchy and interrelationship of industries and operations." Identification of the "family" of industrial organic chemicals and their relationships was viewed as a necessary component in bounding the problem of chemical production and uses.

The Radian report, completed in November 1979, attempted to trace graphically the flow of some 400 organic chemicals (those identified in the first round of industry-specific IPPEU studies) from derivation, through processing, to end use, or consumption. Even at the time the report was completed, it was recognized that the available data on which the use

trees were based was incomplete. In addition, a more precise system for classifying end uses was needed.

This report is an extension and substantial refinement of the use trees presented in the 1979 study. It represents one of several projects started in 1981 to update the IPPEUs for the plastic and resins industries and to understand better the ways in which industrial organic chemicals are produced and used. The use tree diagrams, Figures 1 through 37, display 650 industrial organic chemicals and present information about their applications. Key concepts and definitions underpinning the development of the 37 diagrams are discussed in detail below. This is followed with a brief summary which underscores the central contributions of this effort to the current state-of-the-art.

Use Trees

The use tree diagrams are designed to show graphically the relationship between chemicals that make up the "family" of industrial organics (see below) and display qualitatively the categories of usage for each chemical. They have been developed to provide an improved perspective on chemical usage and designed so that with additional refinements, they can be expanded into a system that will quantitatively trace the flows of major chemicals through the chemical consuming industries.

Chemical Trees

The core of each complete use tree is a tree of industrial organic chemicals that was developed by analyzing the derivations and uses of individual industrial chemicals as intermediates. To qualify for inclusion on the use trees as industrial chemicals, individual chemicals met two criteria: (1) they are derived either from petroleum or natural gas feedstocks, or another industrial organic chemical; and (2) they are used in ways that require a specific chemical structure or identity that is lost when they

are consumed. Loss of structure or identity in consumption can occur in one of the three following ways:

(1) they are transformed via chemical reaction into another industrial chemical(s);

(2) they are transformed via chemical reaction into "chemical products" such as plastics and resins, organic dyes and pigments, pesticides, etc.; or

(3) they are consumed with or without chemical reaction in applications where they are valued more for some property than for their chemical structure per se (e.g., as solvents, plasticizers, antioxidants, etc.).

The individual branches of chemical trees are terminated when the last chemical is consumed as defined in (2) and (3) above and is not involved in the product of another industrial organic chemical species.

Usage Categories

Early in the development of the use diagrams it became apparent that some system of standard usage nomenclature was needed. When the analysis led to identification of major "sinks." (i.e., industries or industry uses) where organics "disappeared" as specific chemical entitites, a decision was made to make the sinks the basis for standard terminology. Ultimately, the major sinks identified were found to fall into four categories.

- **Synthetic Organic Chemical Product Industries**
  Chemicals are consumed (along with chemicai additives) in industries that manufacture products that are basically chemical in content (e.g., plastics, paints, synthetic rubber, etc.). These are shown in Table 1.

- **Non-Chemical Product Industries.**
  Chemicals are consumed in industries that manufacture products that are non-chemical in nature (e.g., as acid gas sorbents in

petroleum extraction operations, preservatives for wood, additives for refinery produced fuels, etc.). These are shown in Table 2.

- **Specialty Chemicals Industries.**
  Chemicals are used as, or converted to specialty chemicals for use in specific industries (e.g., those that are manufactured for plastic additives, paper chemicals, leather tanning chemicals, food additives, etc.). These are shown in Table 3.

- **Functional Uses.**
  Chemicals are used as, or converted to specialty chemicals that are functional in nature and used in different applications (e.g., solvents, corrosion inhibitors, surfactants, etc.). These are shown in Table 4.

The categories shown in Tables 1 through 4 were developed by analyzing the *Standard Industrial Classification Codes* (SIC) that were applicable to chemicals and comparing SIC categories with classification schemes used by other sources of information for the chemical industries. More precisely, the categories shown in Tables 1 and 2 are, as indicated, relatable to SIC codes. Those shown in Tables 3 and 4 are also to a degree relatable to SICs, but it was not possible to develop a system that was fully compatible with the codes for this effort. It is believed, however, that further analysis would permit development of a system that would allow completion of the effort to trace all flows of organics into SIC industrial categories.

Table 1. Synthetic Organic Chemical Product Industries

Industry	SIC Category(s)	No. of Industrial Organic Chemicals Consumed
Plastics and Resins & Plastic Products*	2821, 3079	152
Medicinal Chemicals and Pharmaceuticals*	2833, 2834	173
Organic Dyes and Pigments	28652-11, 28653-11	156
Synthetic Organic Agricultural Chemicals*	28694-11, 2879	148
Paint and Allied Products	2851	81
Synthetic Rubber & Rubber Products*	2822, 3011, 3021, 3041, 2069	34
Textile Fibers (Man-Made)	2823, 2824	24
Adhesives and Sealants	2891	32
Printing and Special Inks	2893, 28995-72	25

*These categories include two industries as they have been defined for IPPEU analysis. They have been combined here because of difficulty in determining in which of the two related industries some of industrial organic chemicals are used.

Table 2. Use of Industrial Organic Chemicals in Non-Chemical Product Industries

(Number of Industrial Organic Chemicals Consumed)

Industry	SIC Code
Textile Products (25)	2211, 2221, 2261, 2262, 2269, 2281, 2283, 2284
Wood Preserving (6)	2492
Inorganic Pigments (2)	2816
Soaps and Detergents (36)	2841
Polishes and Sanitation Goods (41)	2842
Perfumes, Cosmetics, & Toiletries (37)	2844
Explosives (28)	2892
Fuels (Petroleum Refining) (18)	2911
Lube Oil and Grease (23)	2992
Rubber Reclaiming (2)	3031
Leather Tanning (18)	3111
Food Products (3)	20*
Stone, Clay & Glass Products (6)	32*
Electric and Electronic Equipment (4)	36*
Instruments and Related Products (5)	38*

*Major Industry Group designation for which specific four-digit industry codes associated with consumption of industrial organics has not been identified.

Table 3. Specialty Chemicals Industries
(Number of Industrial Organic Chemicals Consumed)

Acid Gas Sorbents (9)
Anti-freeze and Automotive Chemicals (11)
Binders and Hardeners (5)
Catalysts (29)
Corrosion Inhibitors (14)
Dehydrating Agents (5)
Denaturants (9)
Embalming Fluids (1)
Flavor and Perfume Chemicals (69)
Flotation Agents (15)
Food Additives (41)
Fuel Additives (30)
Humectants (10)
Hydraulic & Related Fluids (22)
Leather Tanning Chemicals (9)
Lube Oil and Grease Additives (17)
Metal Treating Compounds (29)
Odorants (11)
Paper Chemicals (10)
Photographic Chemicals (28)
Plastic Additives (36)
Plating Compounds (14)
Plasticizers (73)
Reagent Chemicals (68)
Refrigerants (20)
Riot, Poison Gases (7)
Rocket Propellants (10)
Rubber Processing Chemicals (73)
Solvents (215)
Spray and Aerosol Compounds (17)
Surfactants (63)
Synthetic Functional Fluids (15)
Textile Chemicals (45)
Water Treatment Compounds (6)

Table 4. Functional Uses

Acid Gas Sorbents
Antioxidants
Binders and Hardeners
Catalysts
Chelating Agents
Corrosion Inhibitors
Dehydrating Agents
Denaturants
Flotation Agents
Humectants
Hydraulic and Related Fluids
Odorants
Plasticizers
Poison, Riot Gases
Refrigerants
Rocket Propellants
Solvents
Surfactants

Key Developments and Contributions

As indicated in the preceding discussion, key tasks in the development of the use tree diagrams were: (1) identification of the "family" of industrial organic chemicals; and (2) development of a logical system of nomenclature for describing the uses of industrial chemicals. The success in completing these tasks distinguishes the present use trees from earlier efforts by making this product highly comprehensive in its coverage of the building block chemicals and by organizing the trees in a way that provides a starting point for full analysis of the use of chemicals in industry.

Family of Industrial Organic Chemicals. The family of industrial organics was defined by analyzing data from many sources on the use of chemicals. The first edition of *Chemcyclopedia*, published by the American Chemical Society in the Fall of 1982, was particularly useful. Approximately 2,000 chemicals included in that volume's "General Organics" section were surveyed to identify those that met the test of industrial chemicals as defined earlier. This analysis resulted in enlargement of the family of industrial organics from about 400, as defined initially, to the present population of 650. It is believed that the list is complete.

System of Nomenclature. The system of nomenclature for uses gives order to the use diagrams, but more importantly, provides a basis for orderly, in-depth analysis of the use of chemicals in industry. This can be illustrated by considering assessment work that has been completed for the plastics and resins industry. This industry consumes 152 industrial organic chemicals and over 2,000 additives that are used as plasticizers, antioxidants, and colorants, to name only a few, whose role in the manufacture of plastic products has been documented. Success in analysis of the largest and most complex of the chemical consuming industries is believed to demonstrate the feasibility of assessment of any of the industry "sinks."

Standard Industrial Classification Codes (SIC). The work discussed here has established a system of classification that will permit association of chemical usage with specific SICs. Thus a foundation has been laid for a system that would permit relating the type and amount of chemical usage to other types of industrial information. Furthermore, development of such a system would provide a much improved basis for a full assessment of the impact of chemicals in industry on health, safety and the environment.

Figure 1. BENZENE

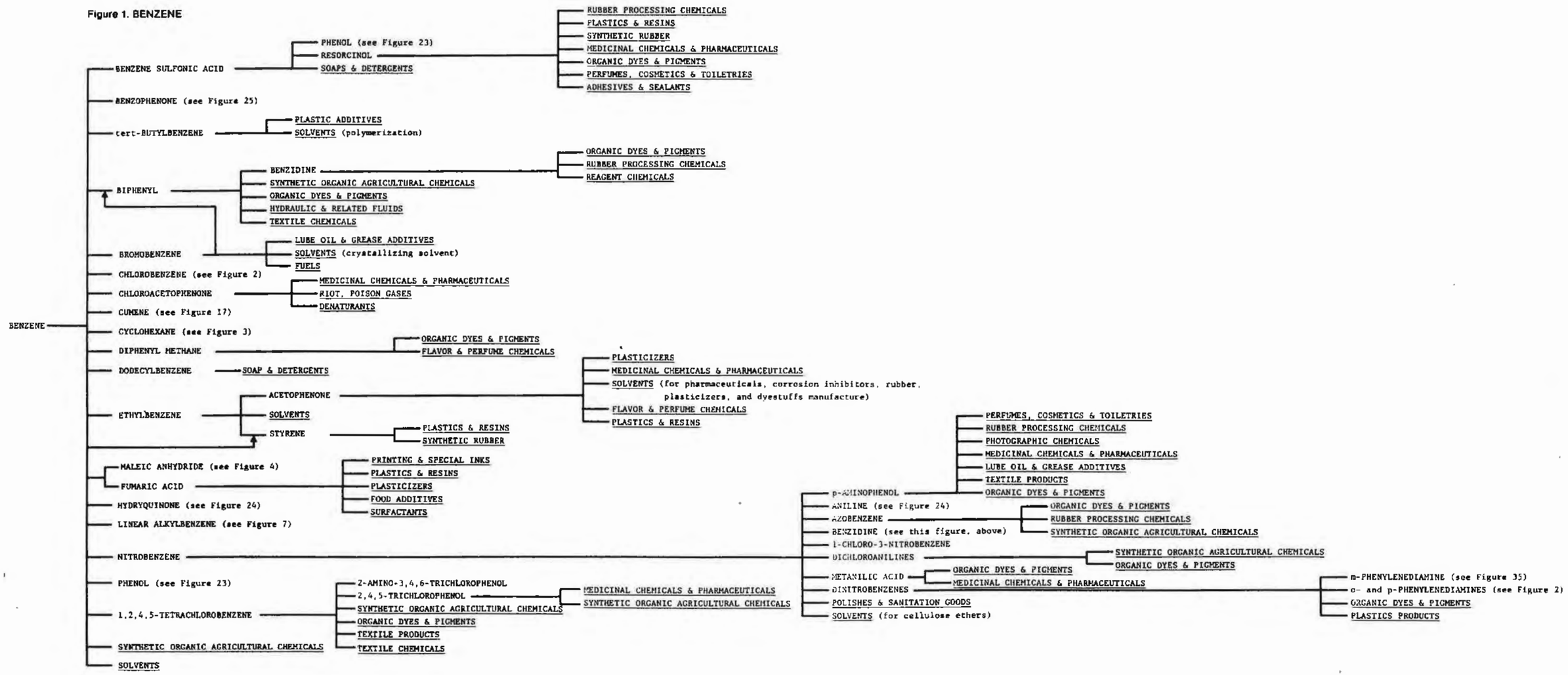


Figure 2. CHLOROBENZENE

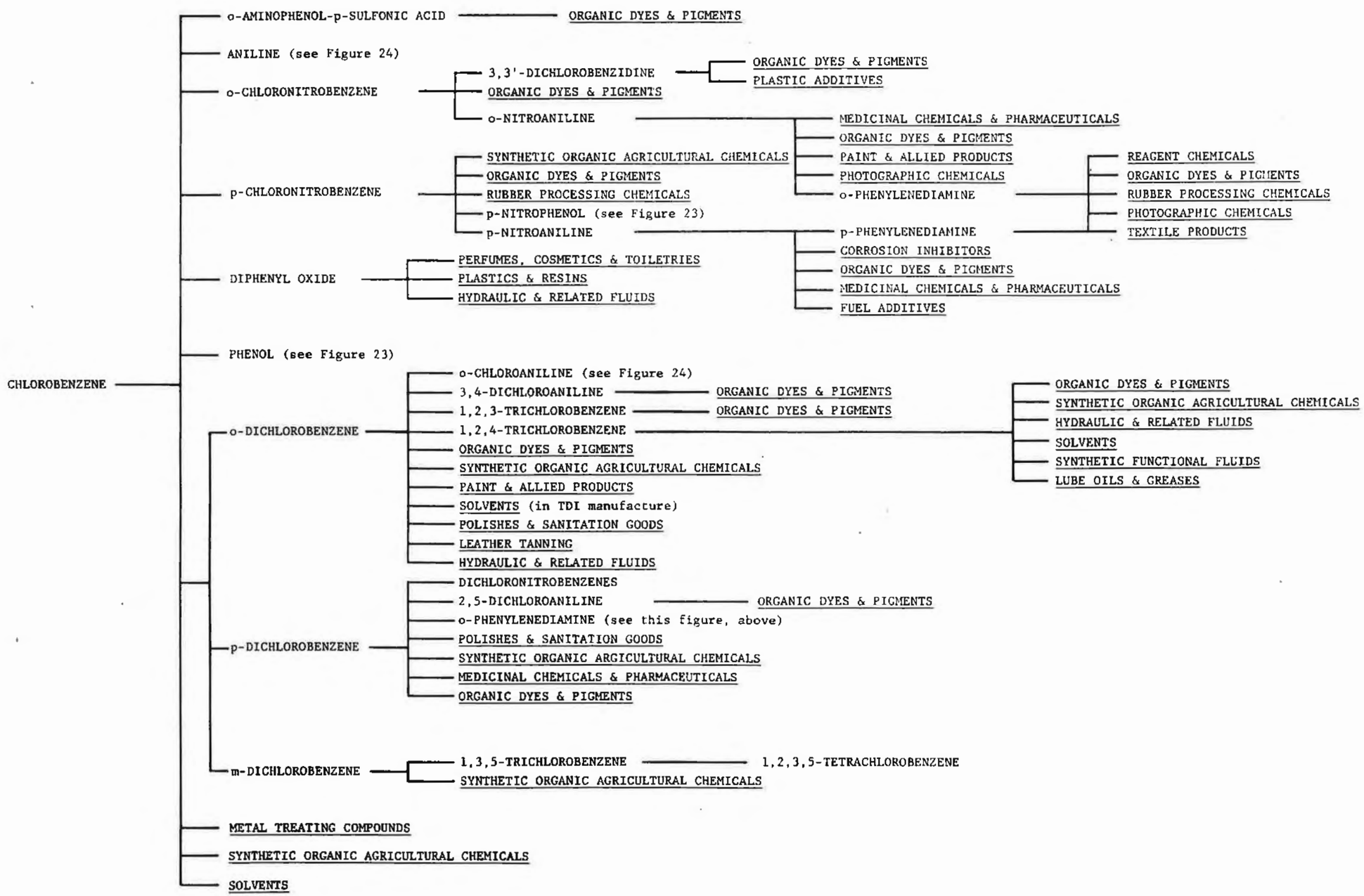


Figure 3. CYCLOHEXANE

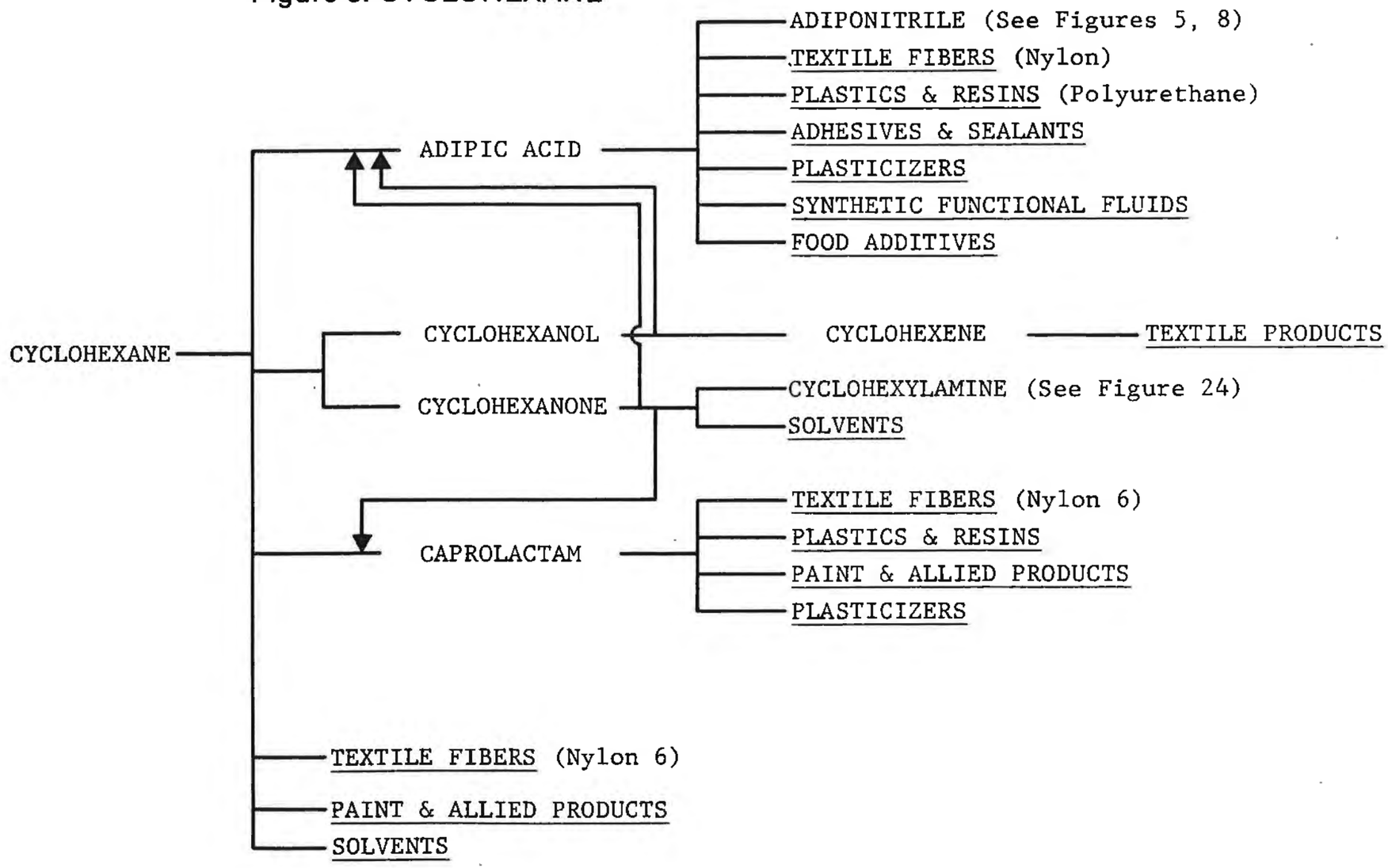


Figure 4. n-BUTYLENES

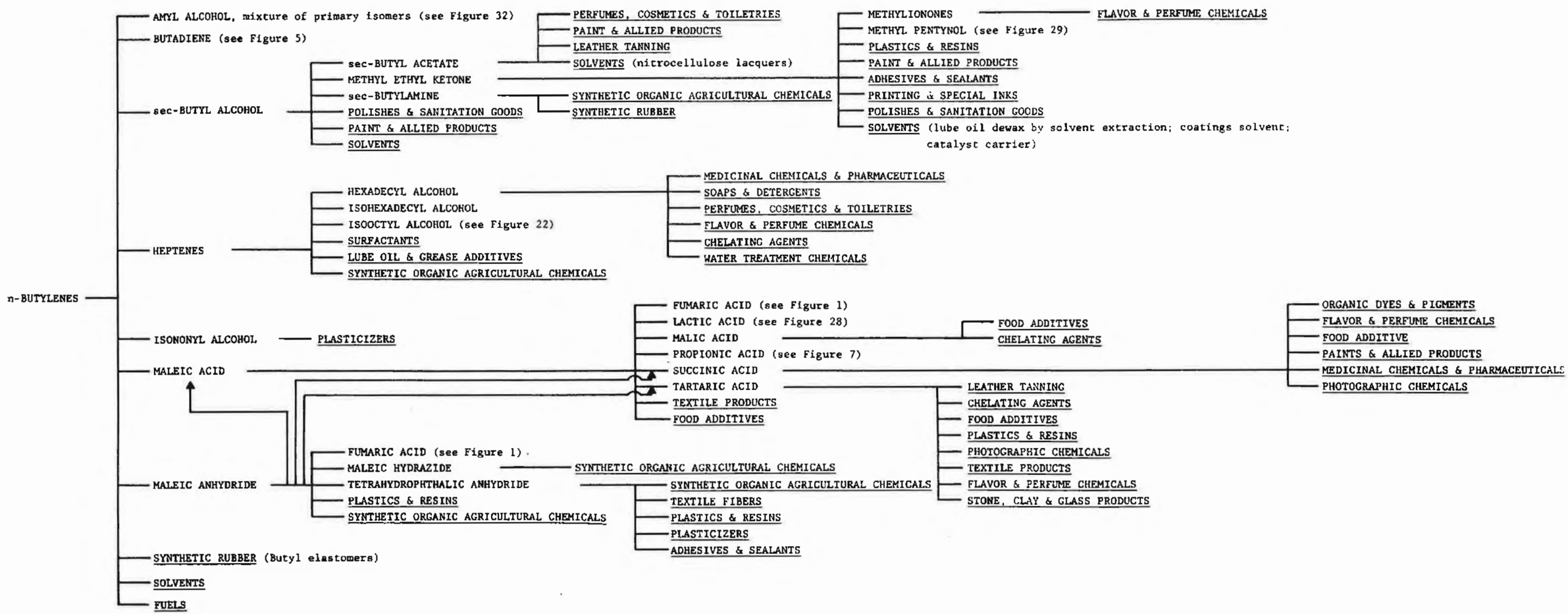


Figure 5. BUTADIENE

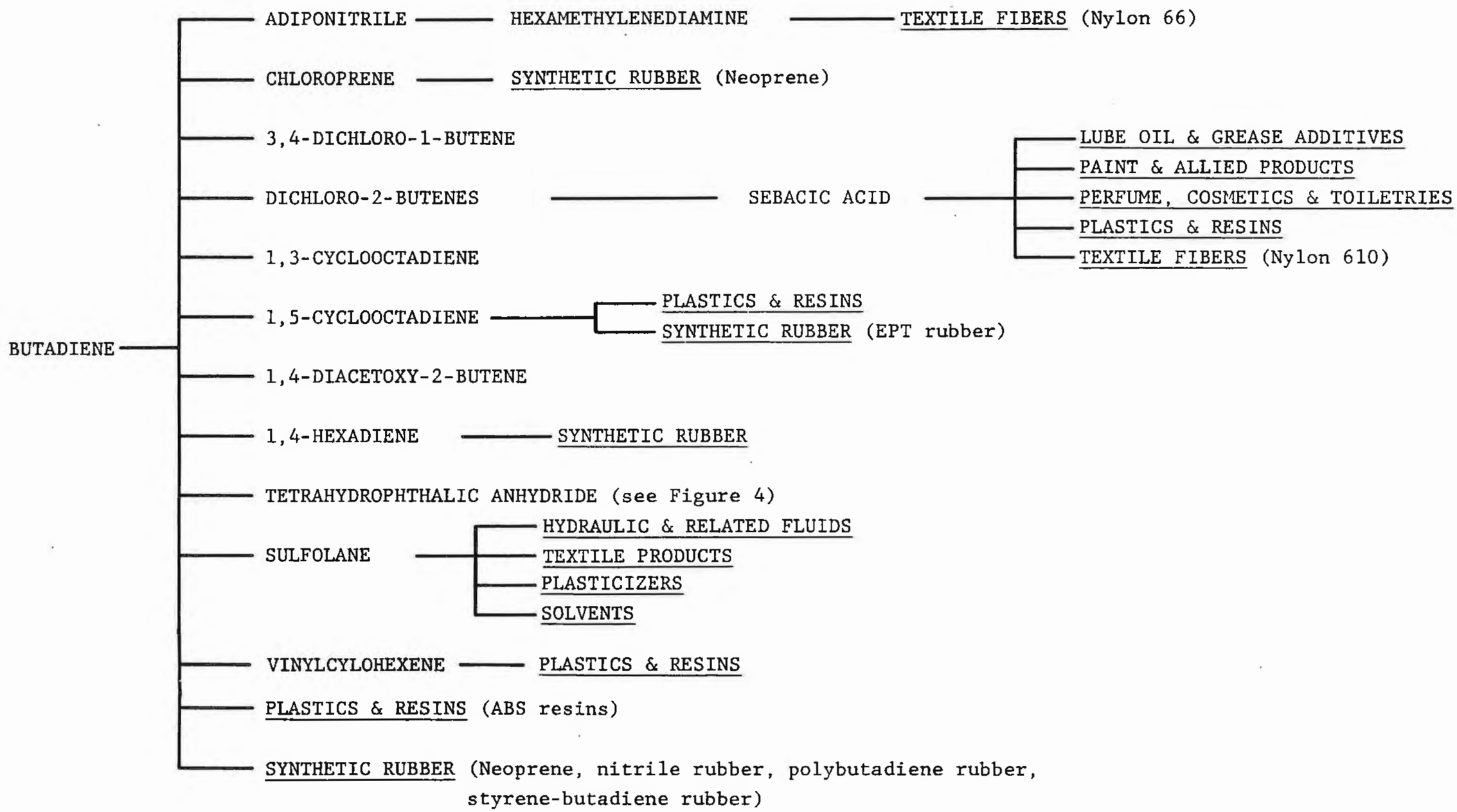


Figure 6. ISOBUTYLENE

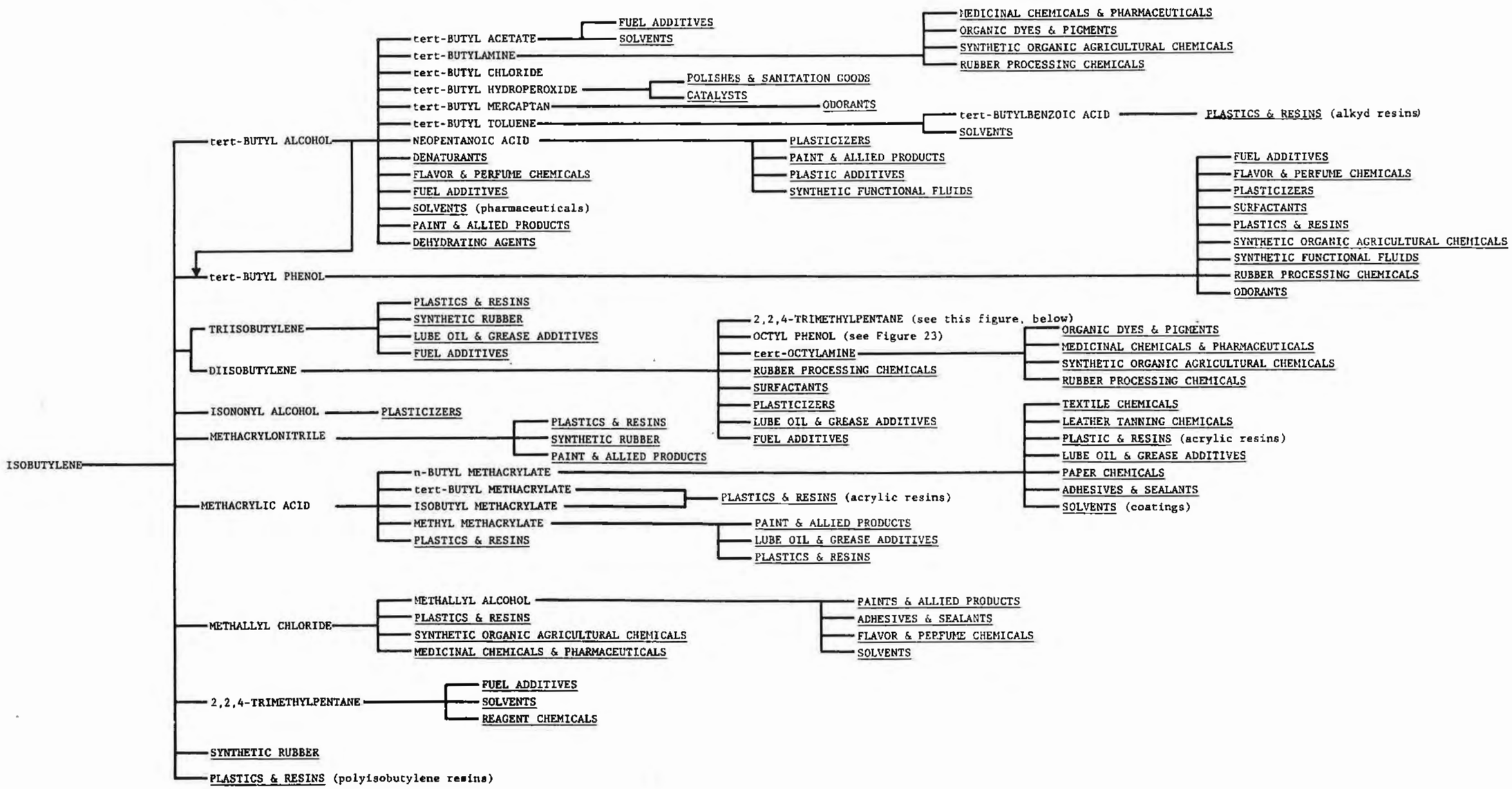


Figure 7. ETHYLENE

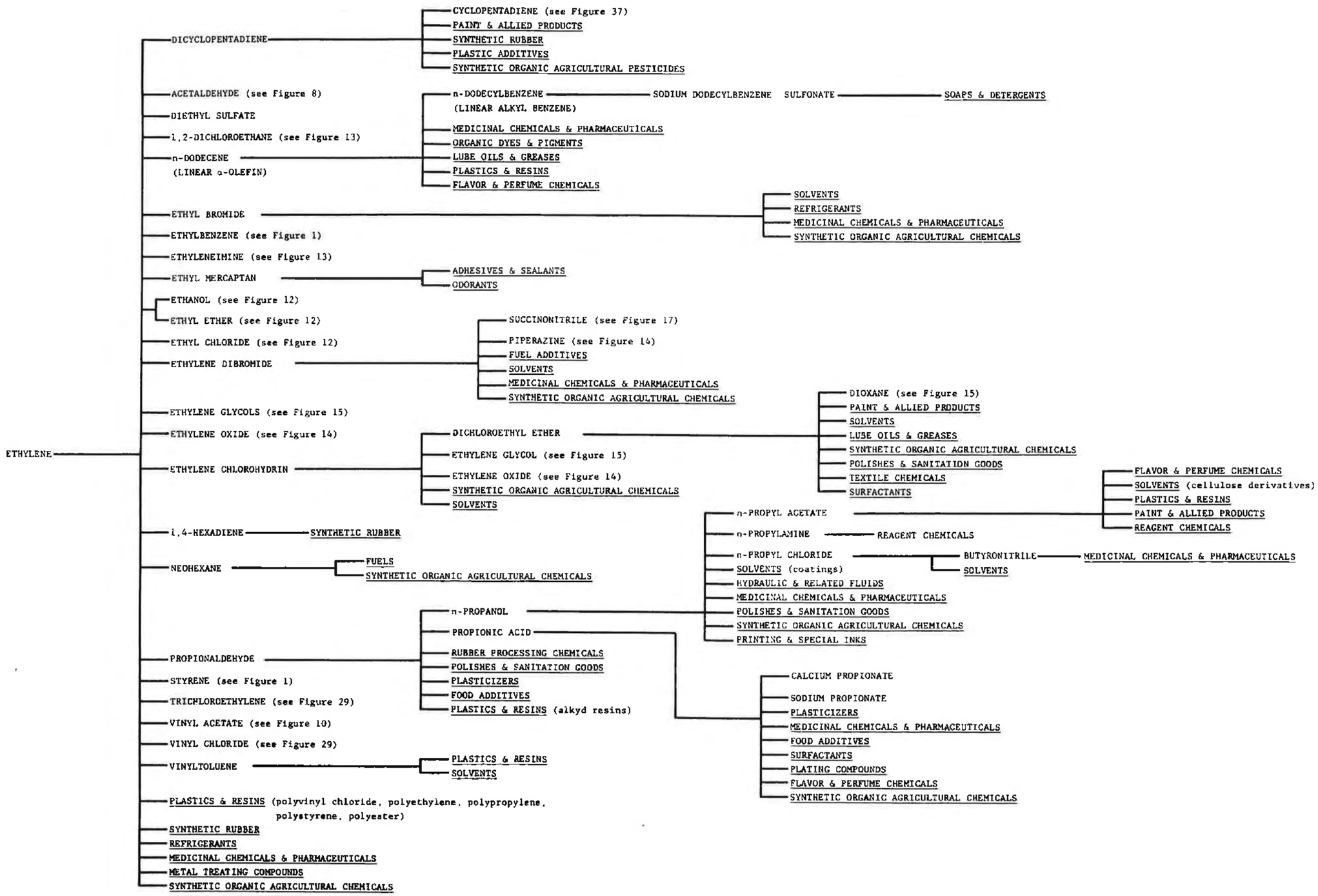
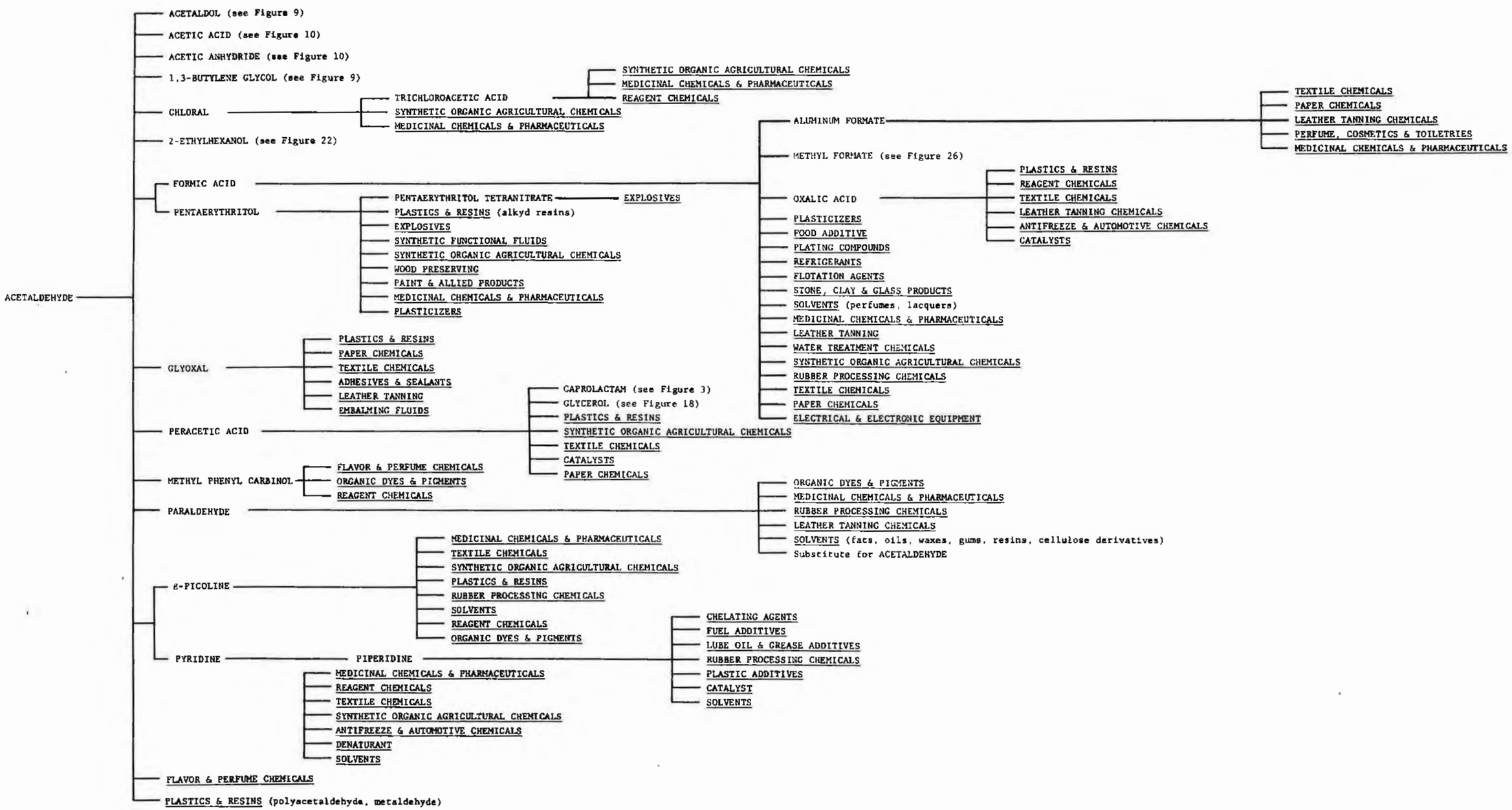


Figure 8. ACETALDEHYDE



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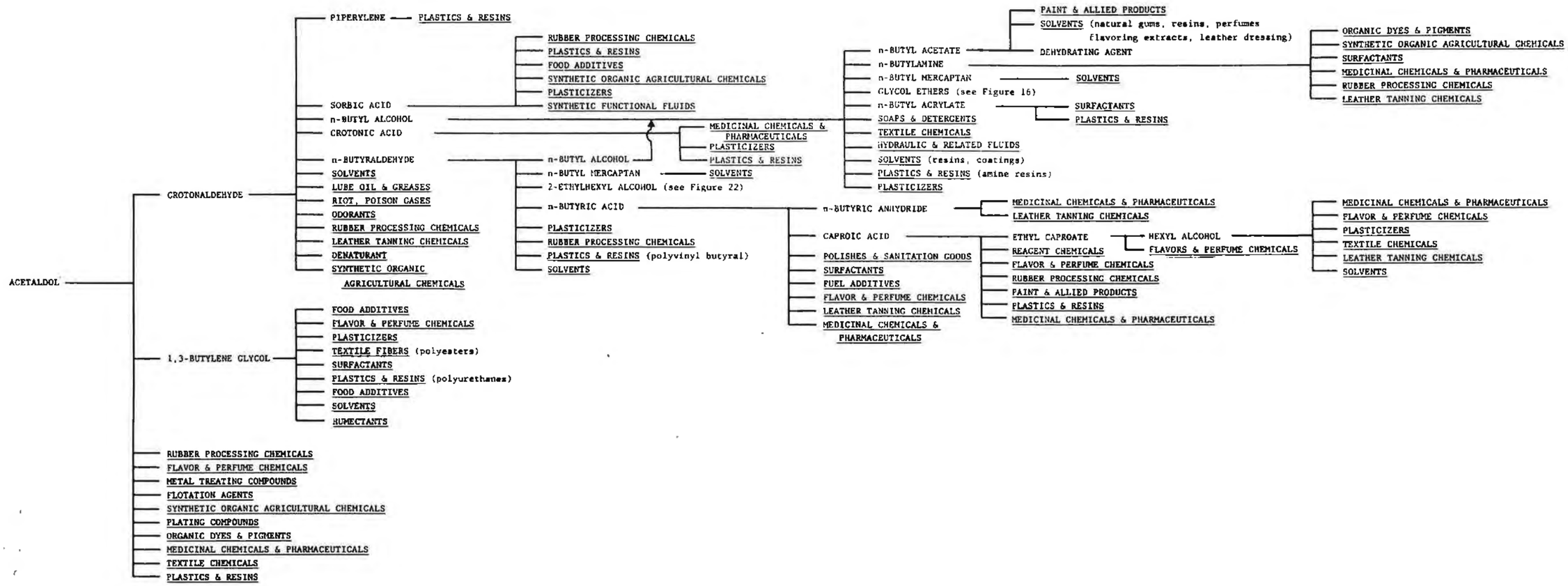


Figure 10. ACETIC ACID

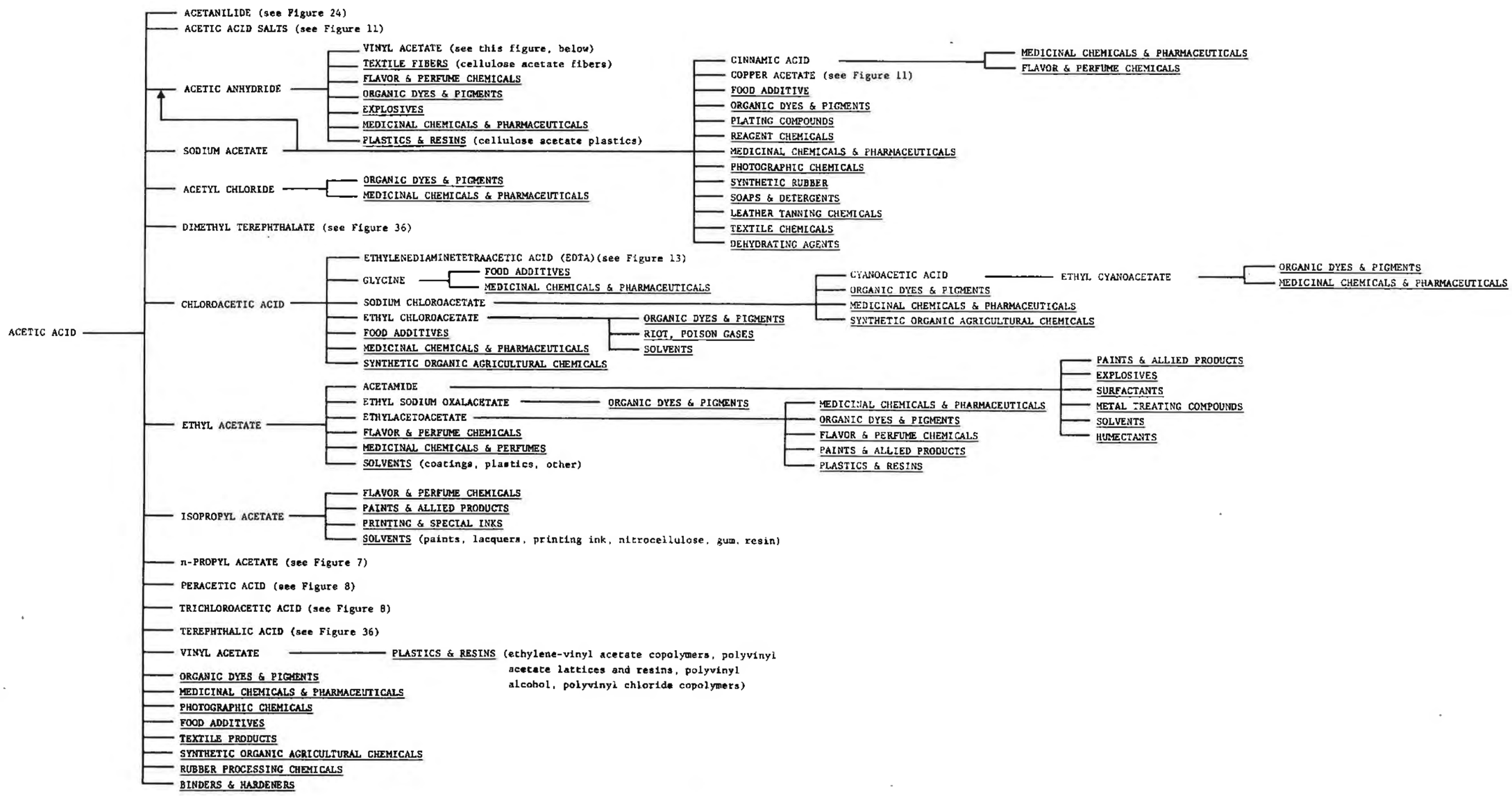


Figure 11. ACETIC ACID SALTS

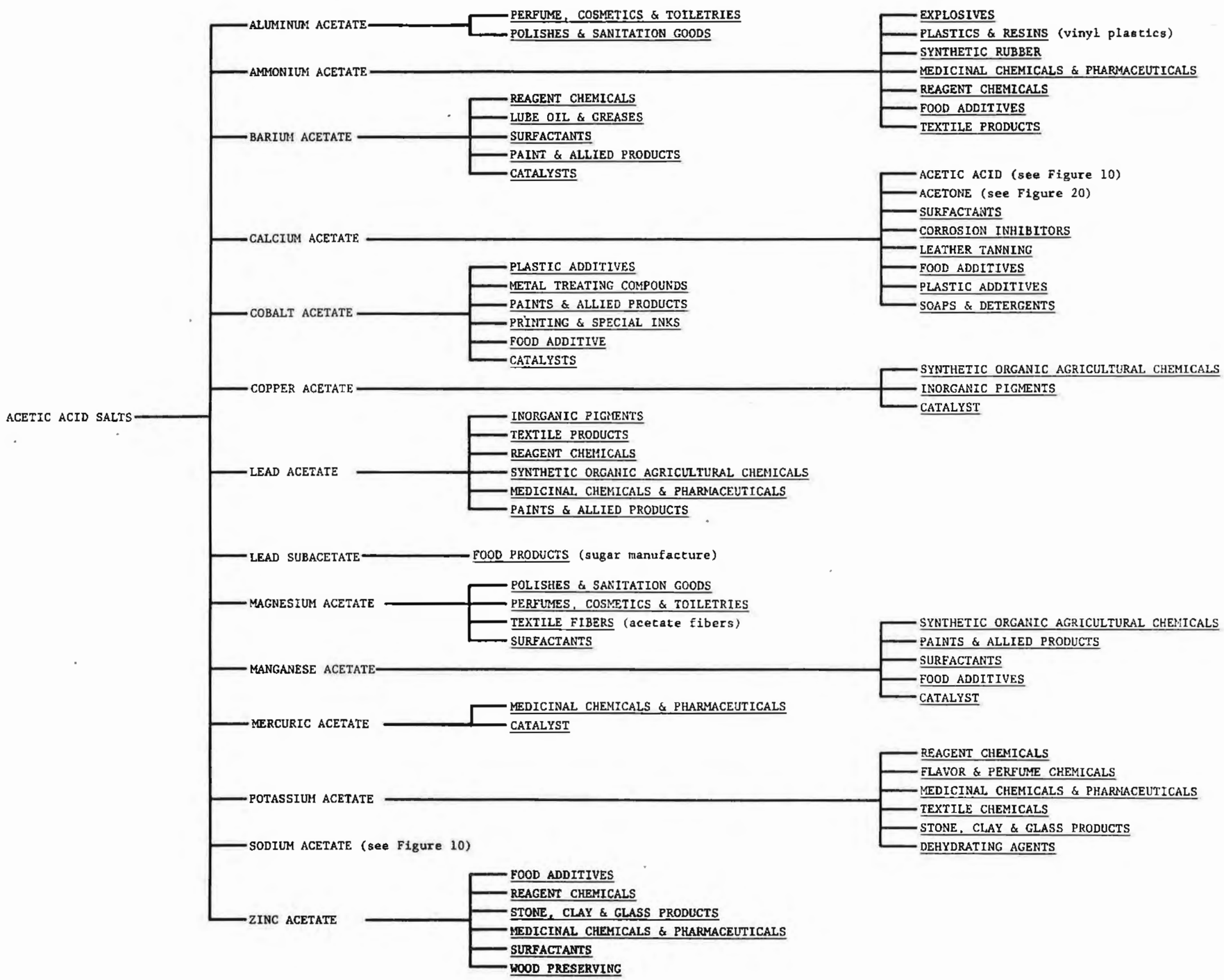


Figure 12. ETHANOL

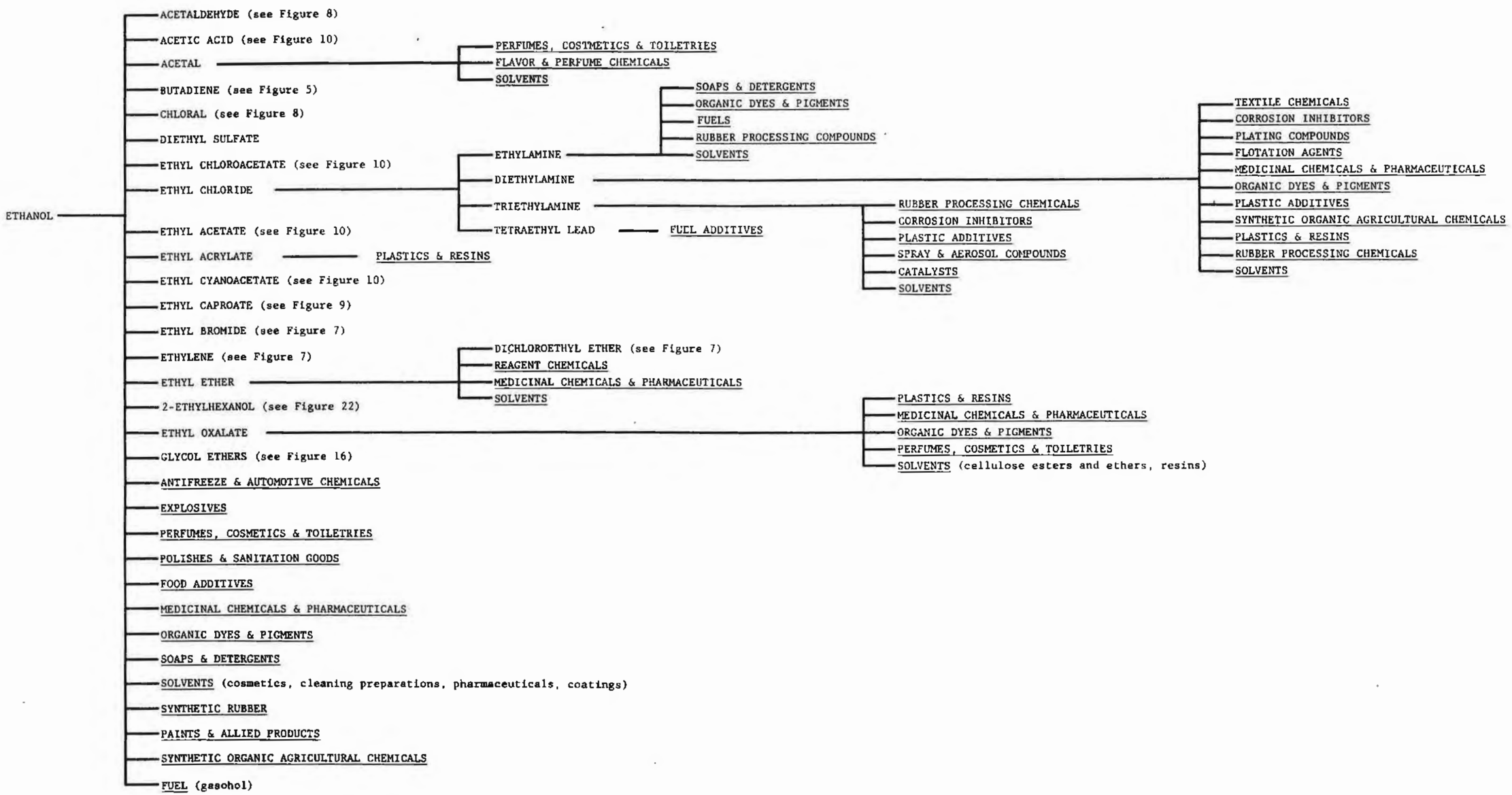


Figure 13. 1,2-DICHLOROETHANE (ETHYLENE DICHLORIDE)

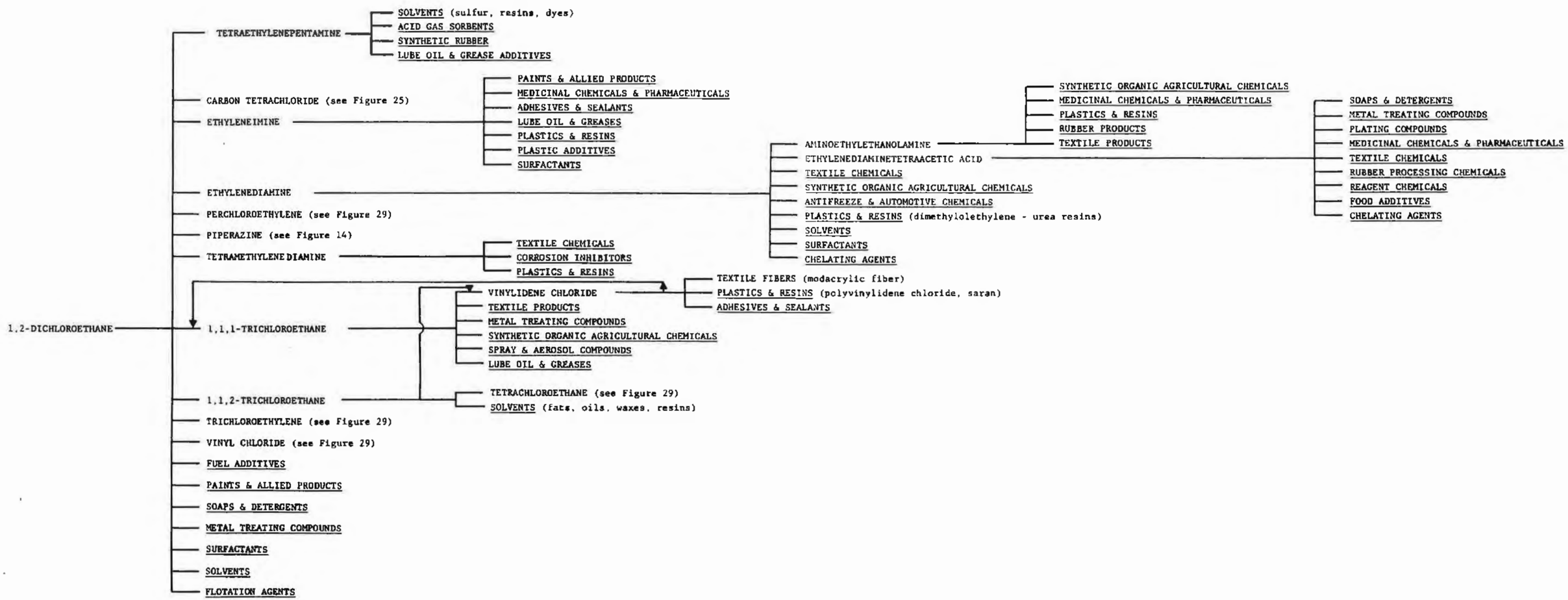


Figure 14. ETHYLENE OXIDE

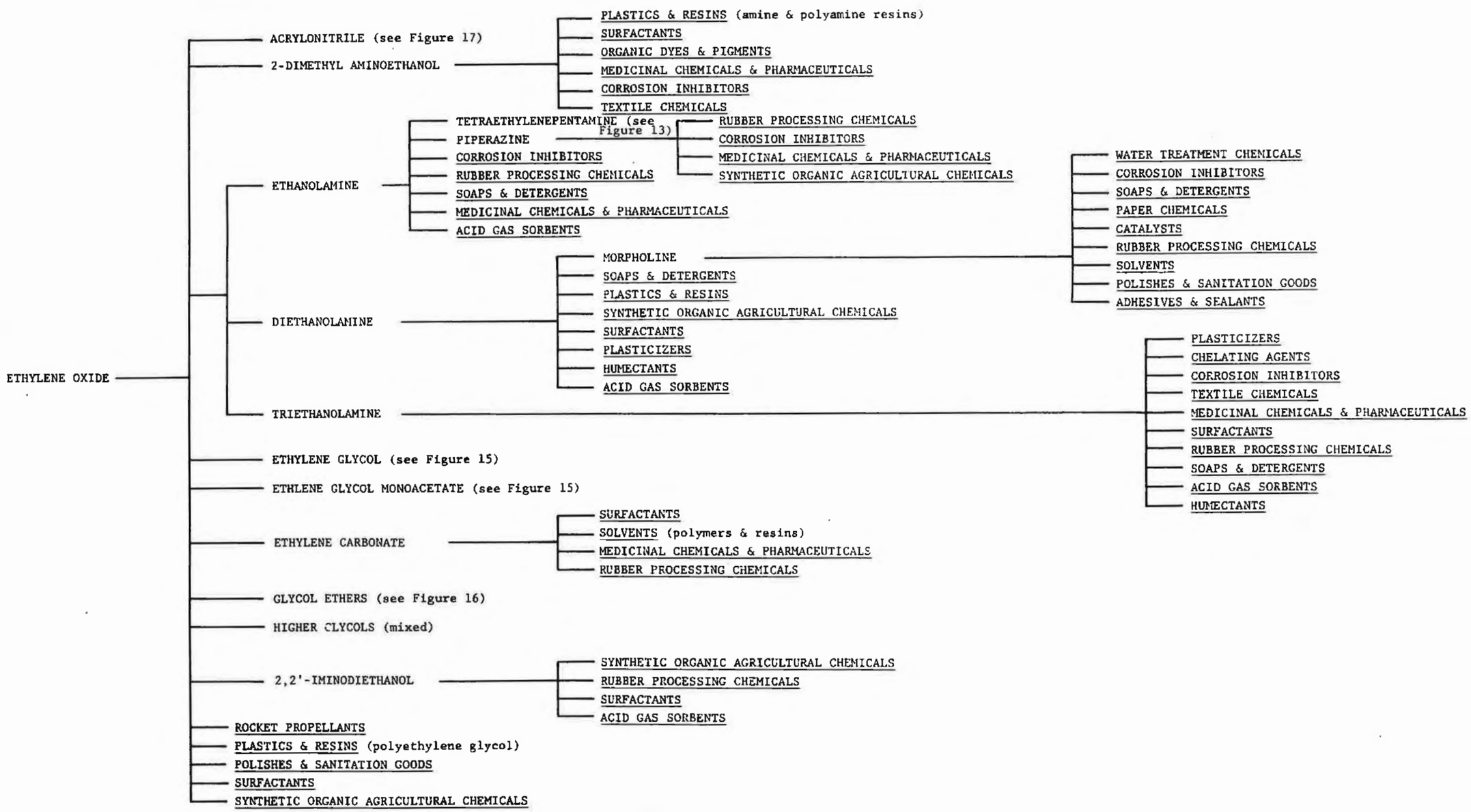


Figure 15. ETHYLENE GLYCOL

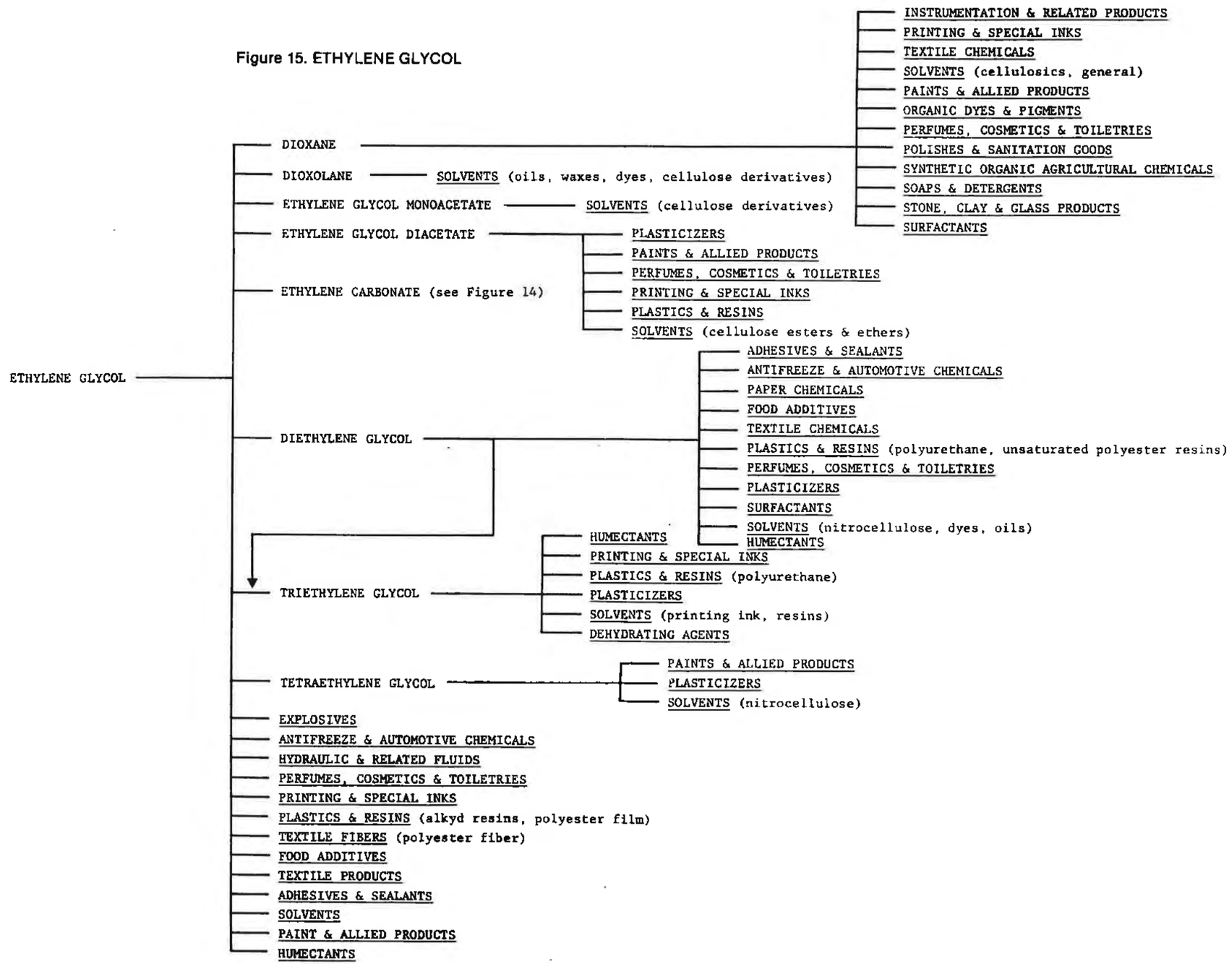


Figure 16. GLYCOL ETHERS

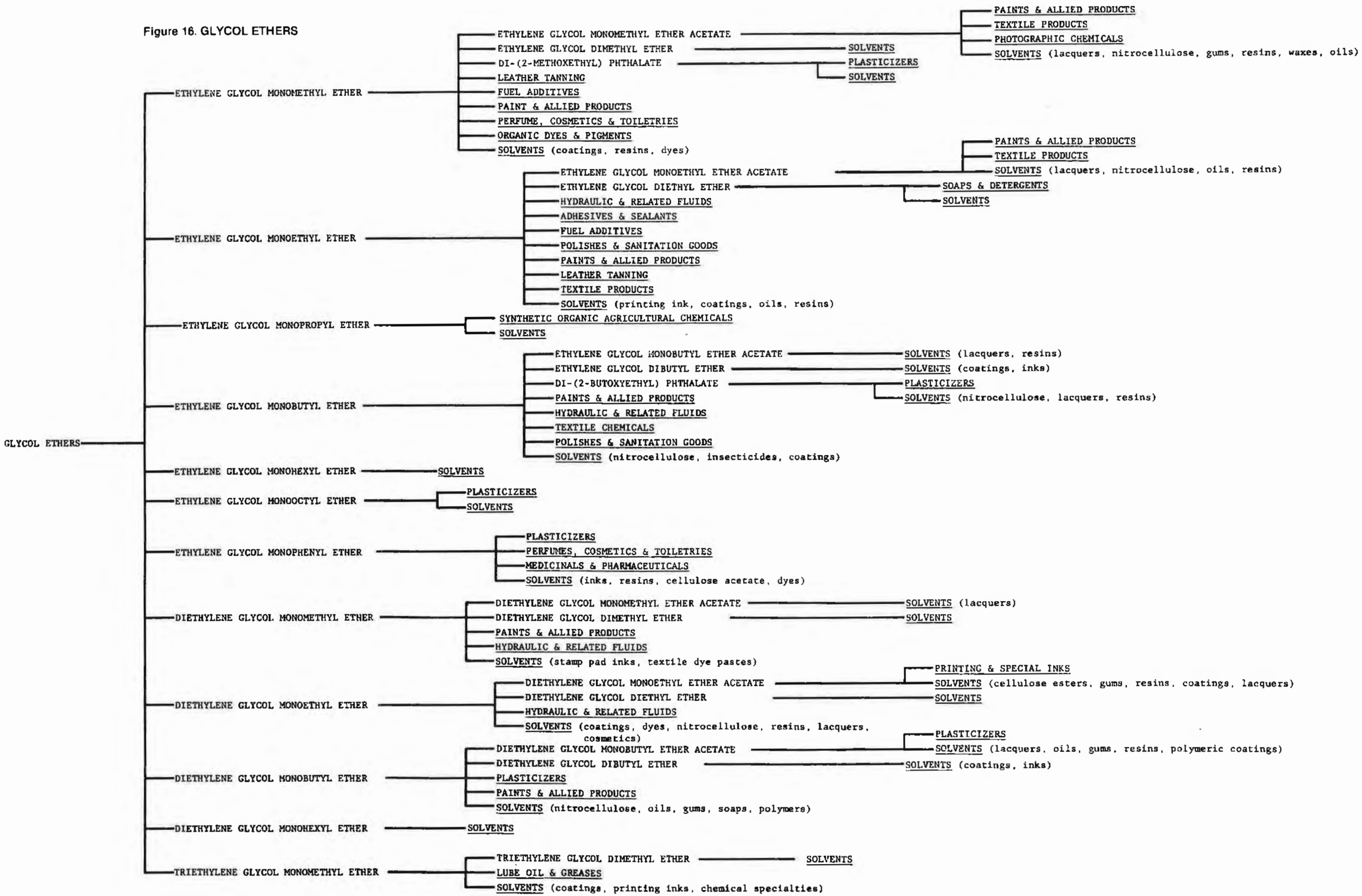
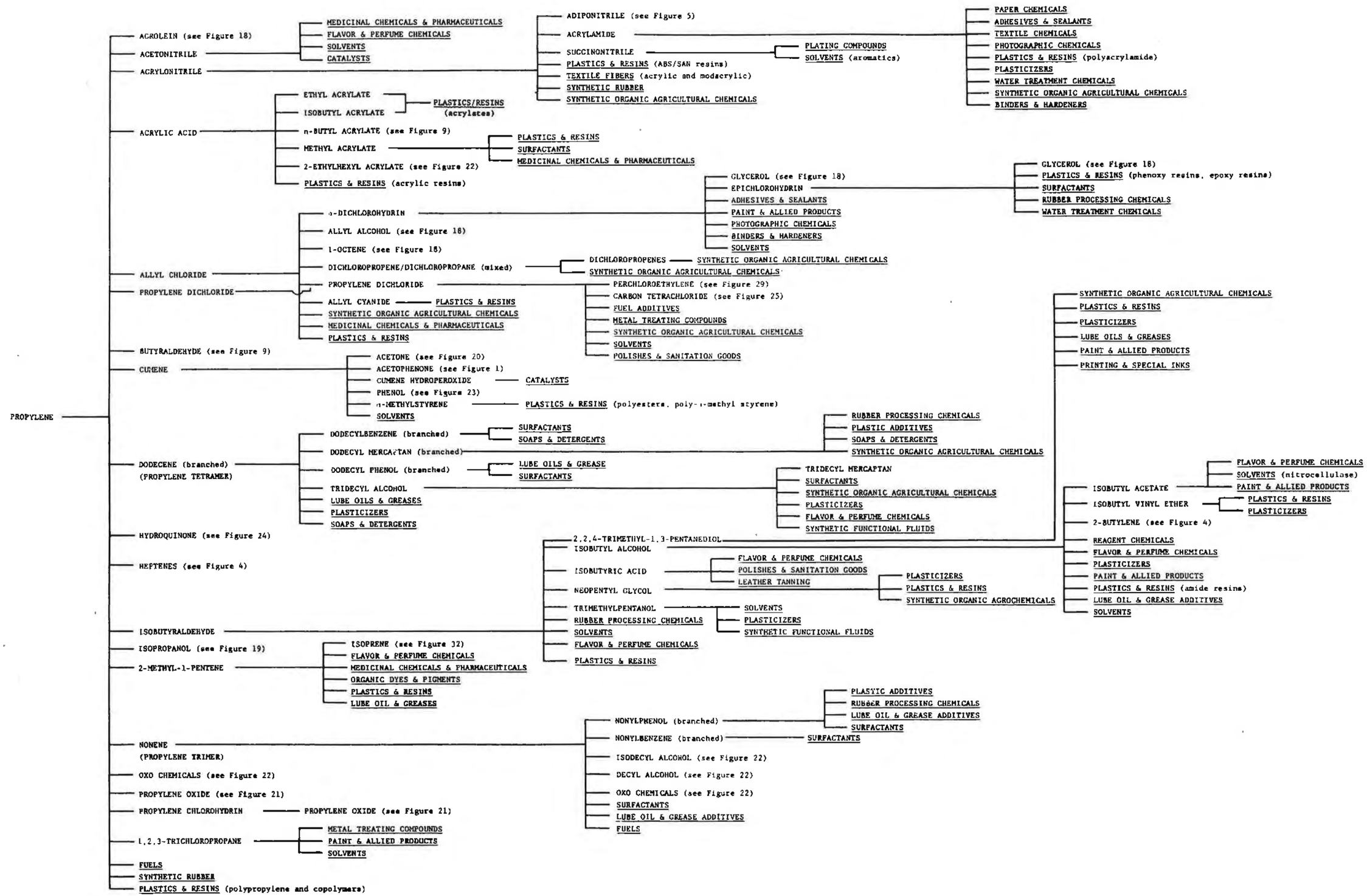


Figure 17. PROPYLENE



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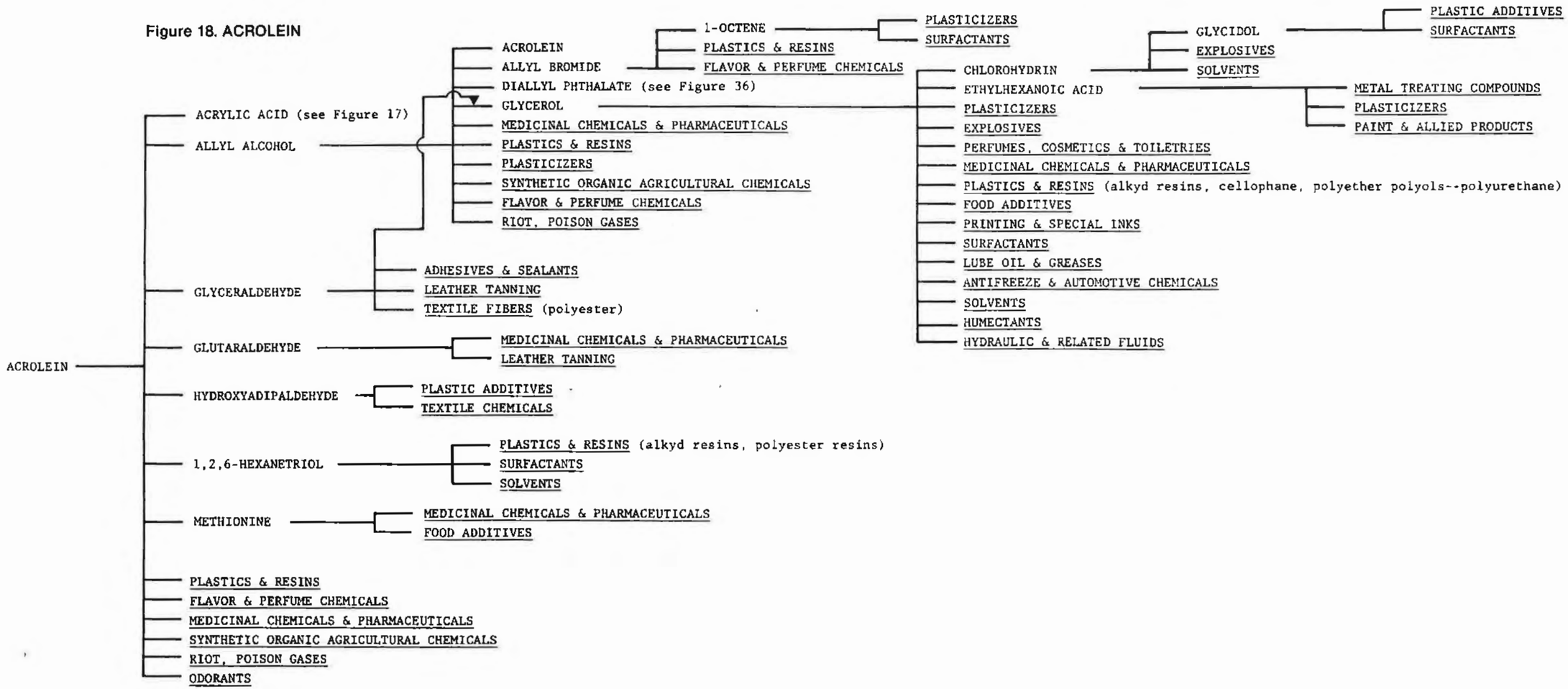

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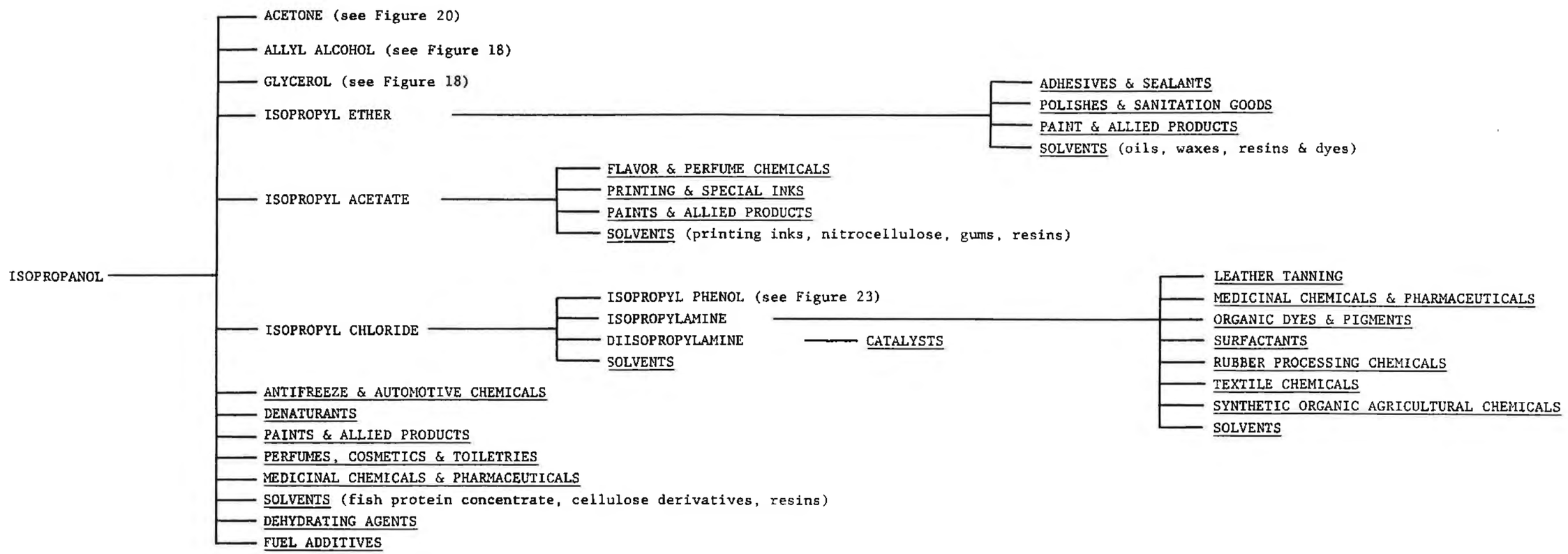

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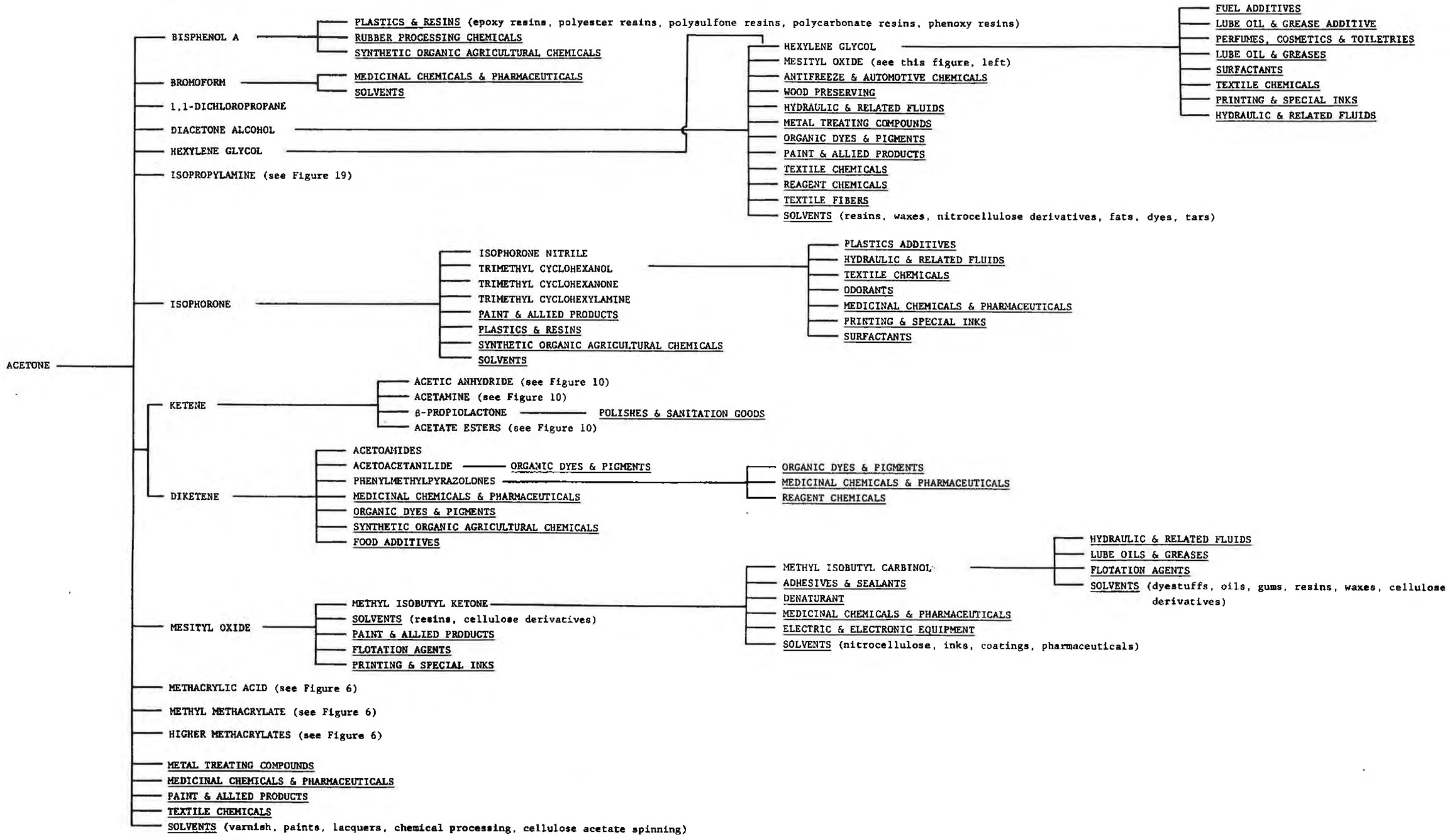

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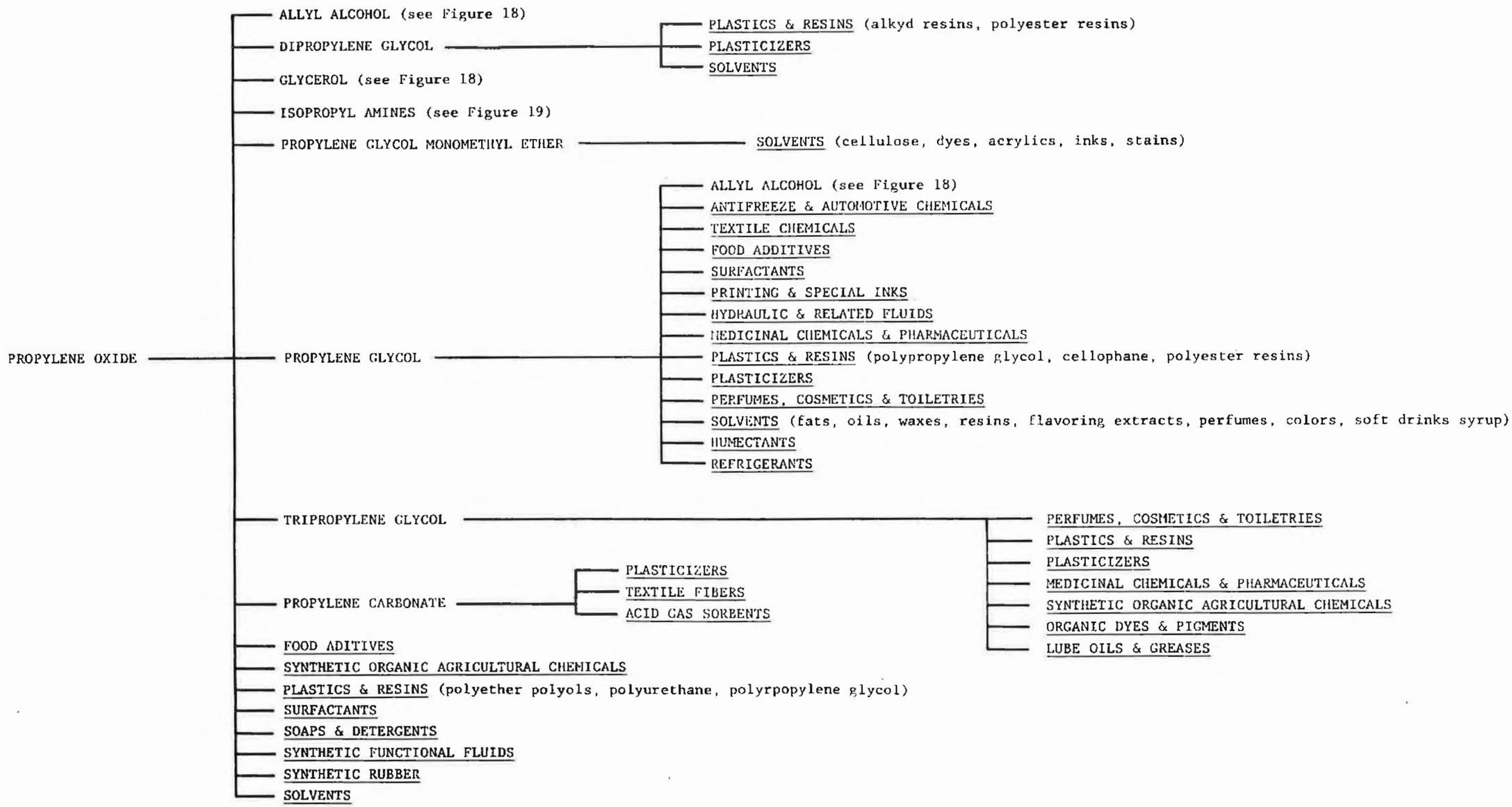
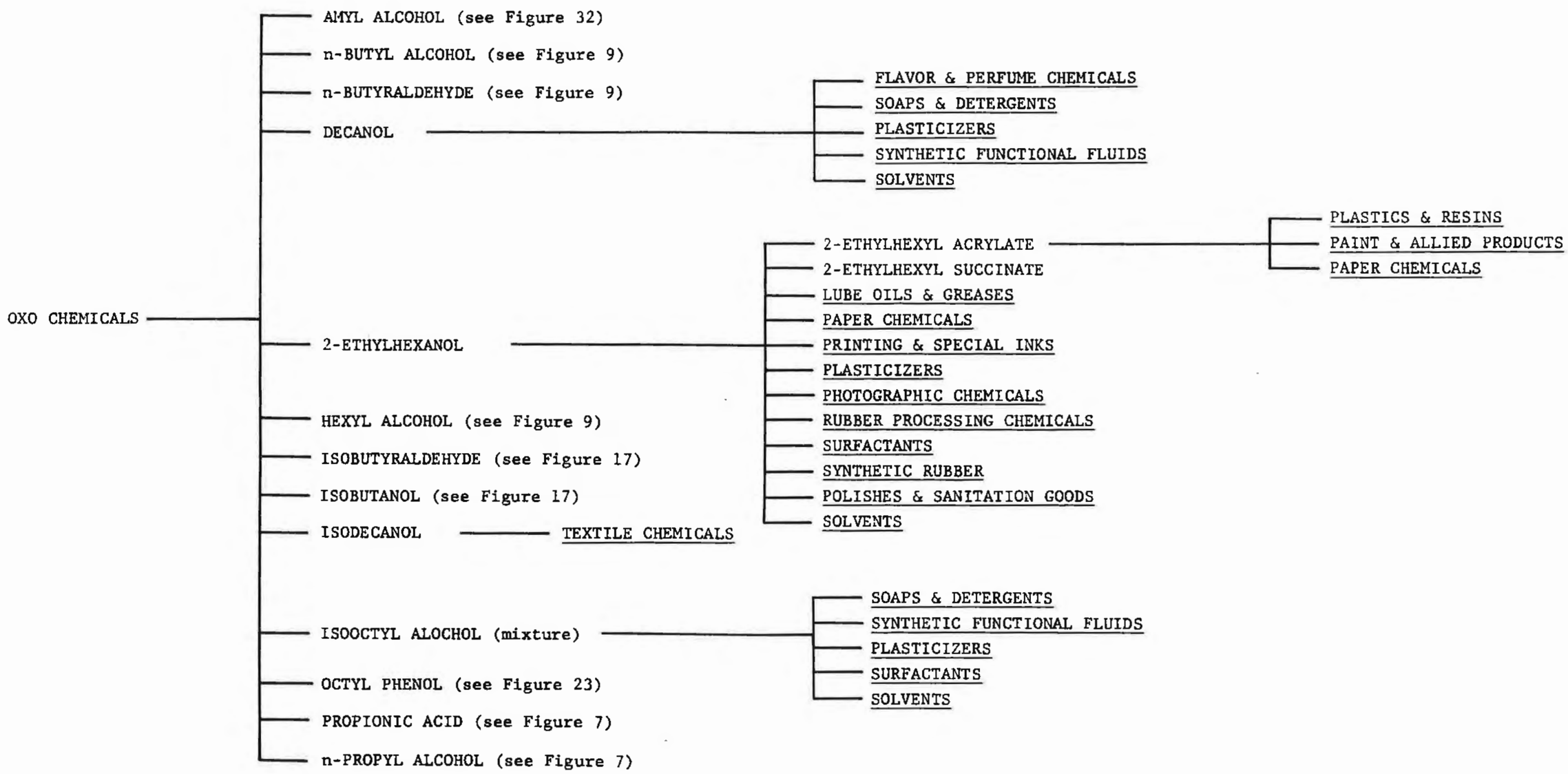


Figure 22. OXO CHEMICALS



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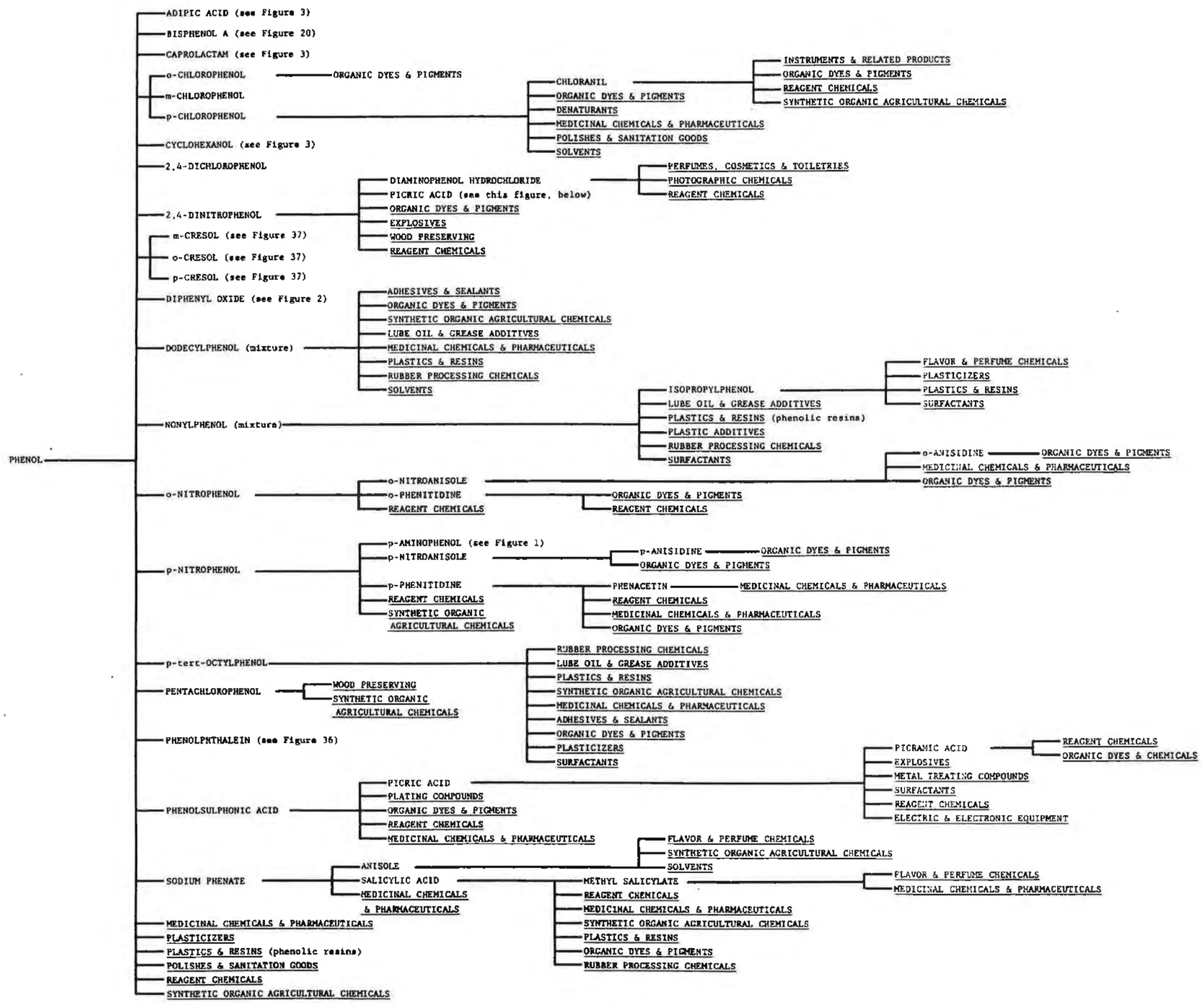

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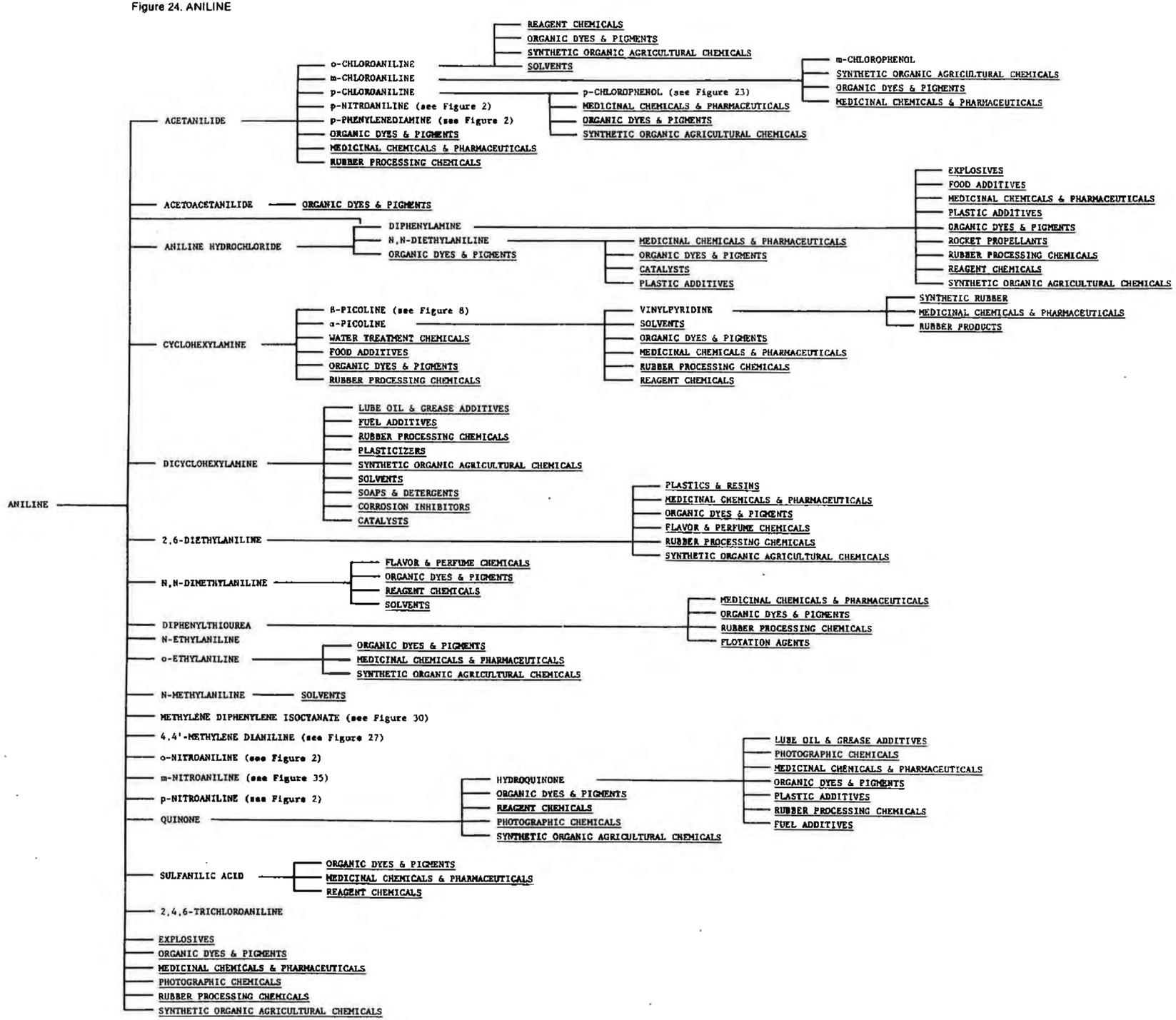


Figure 25. METHANE

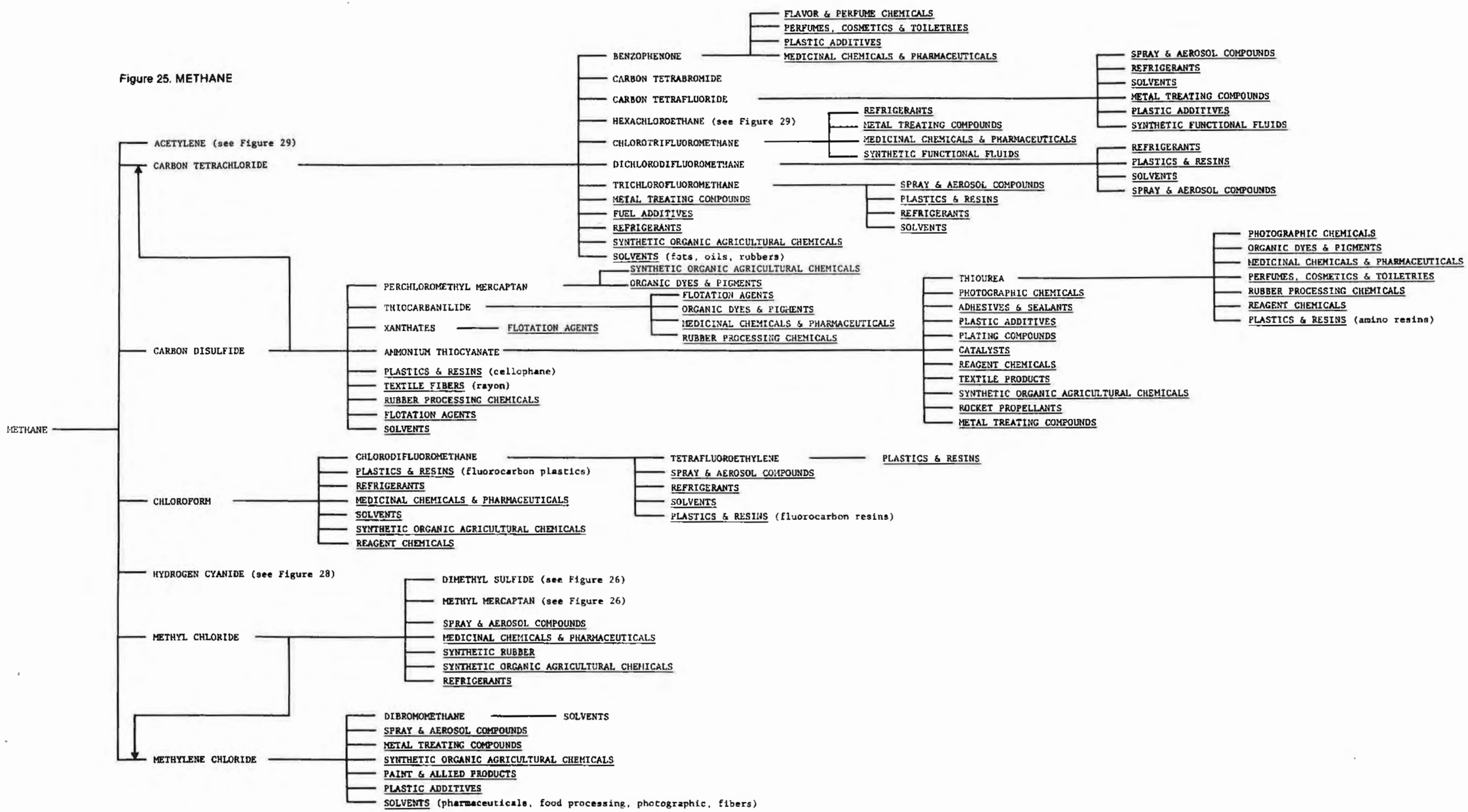
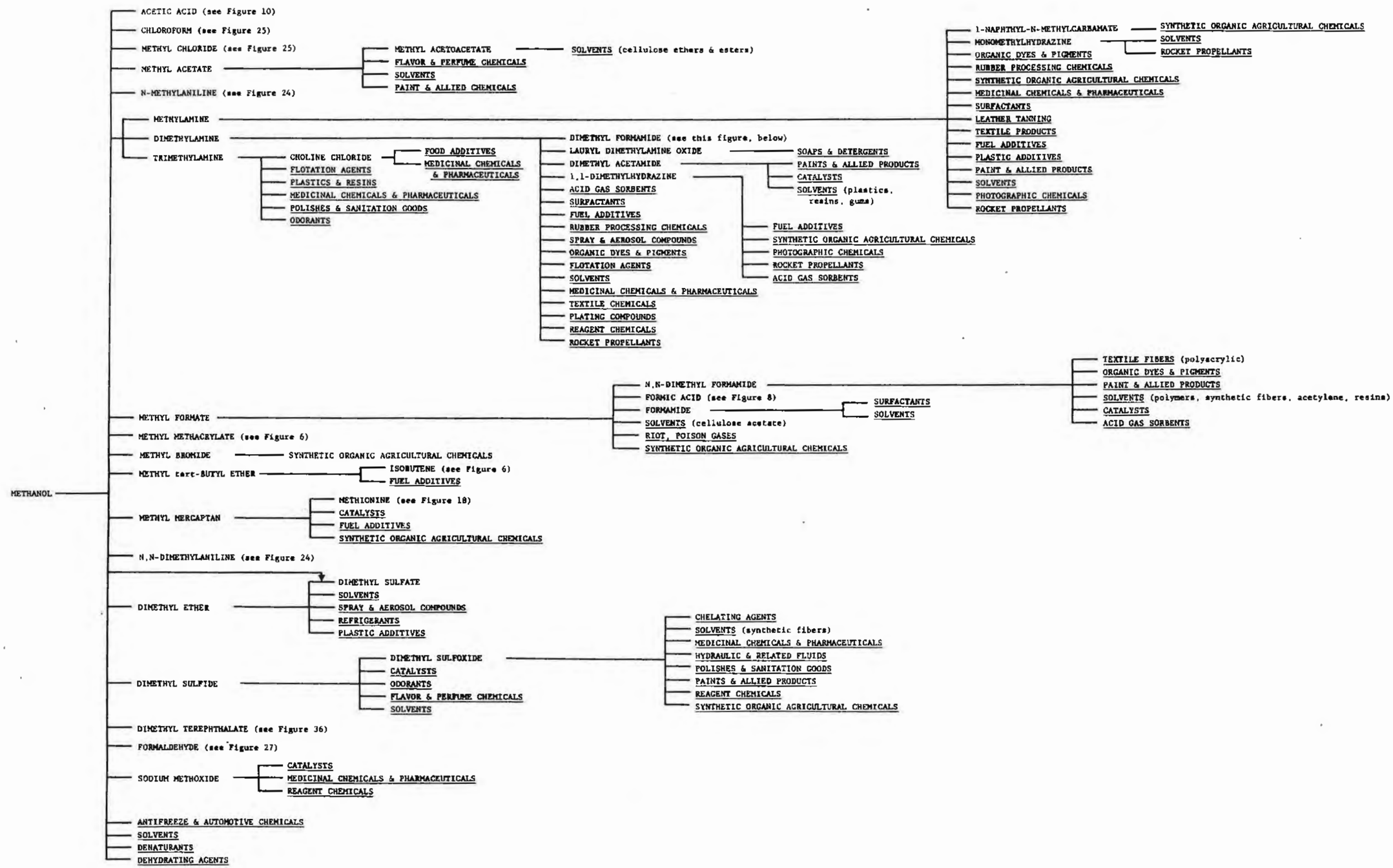


Figure 26. METHANOL



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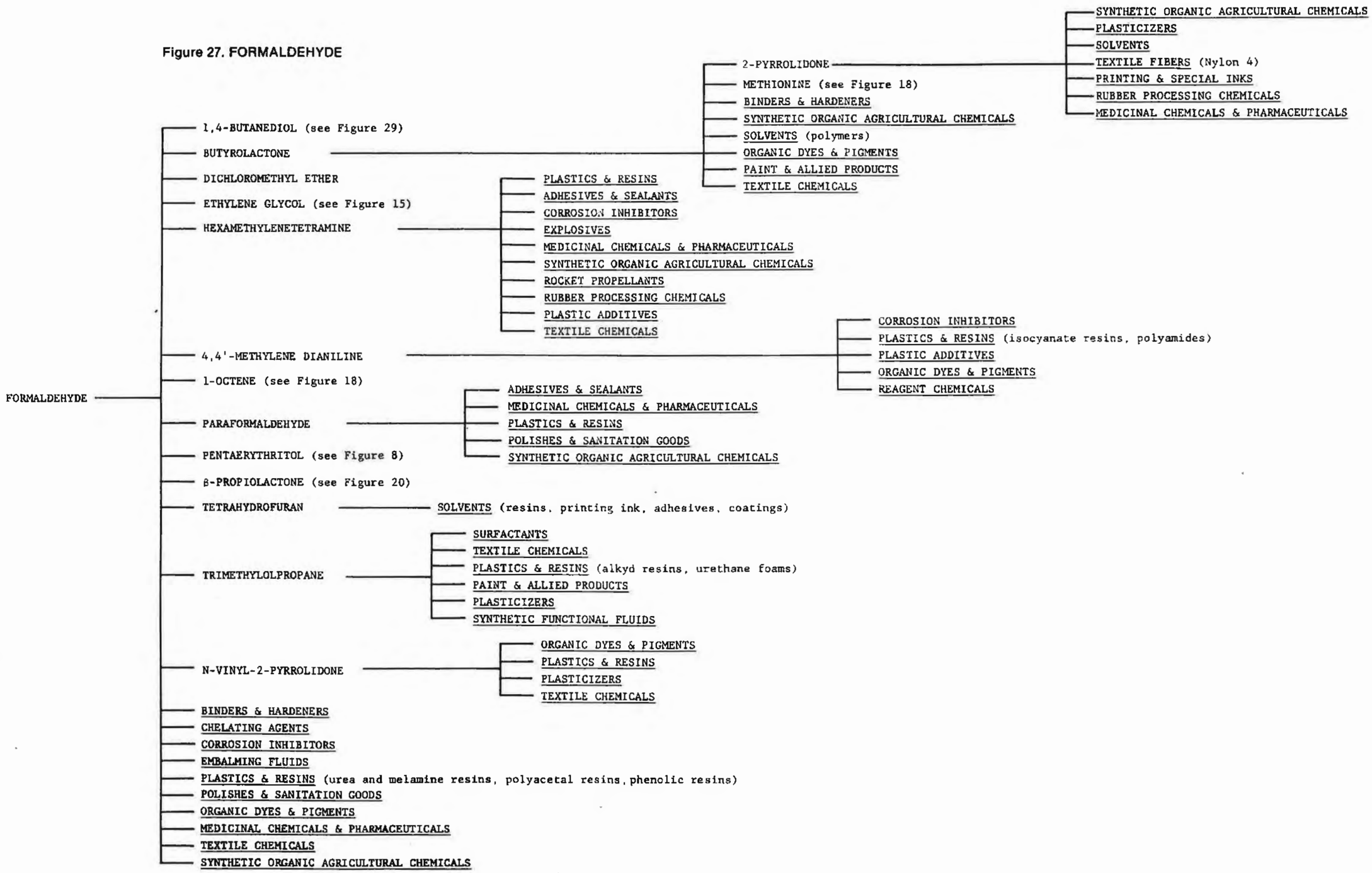

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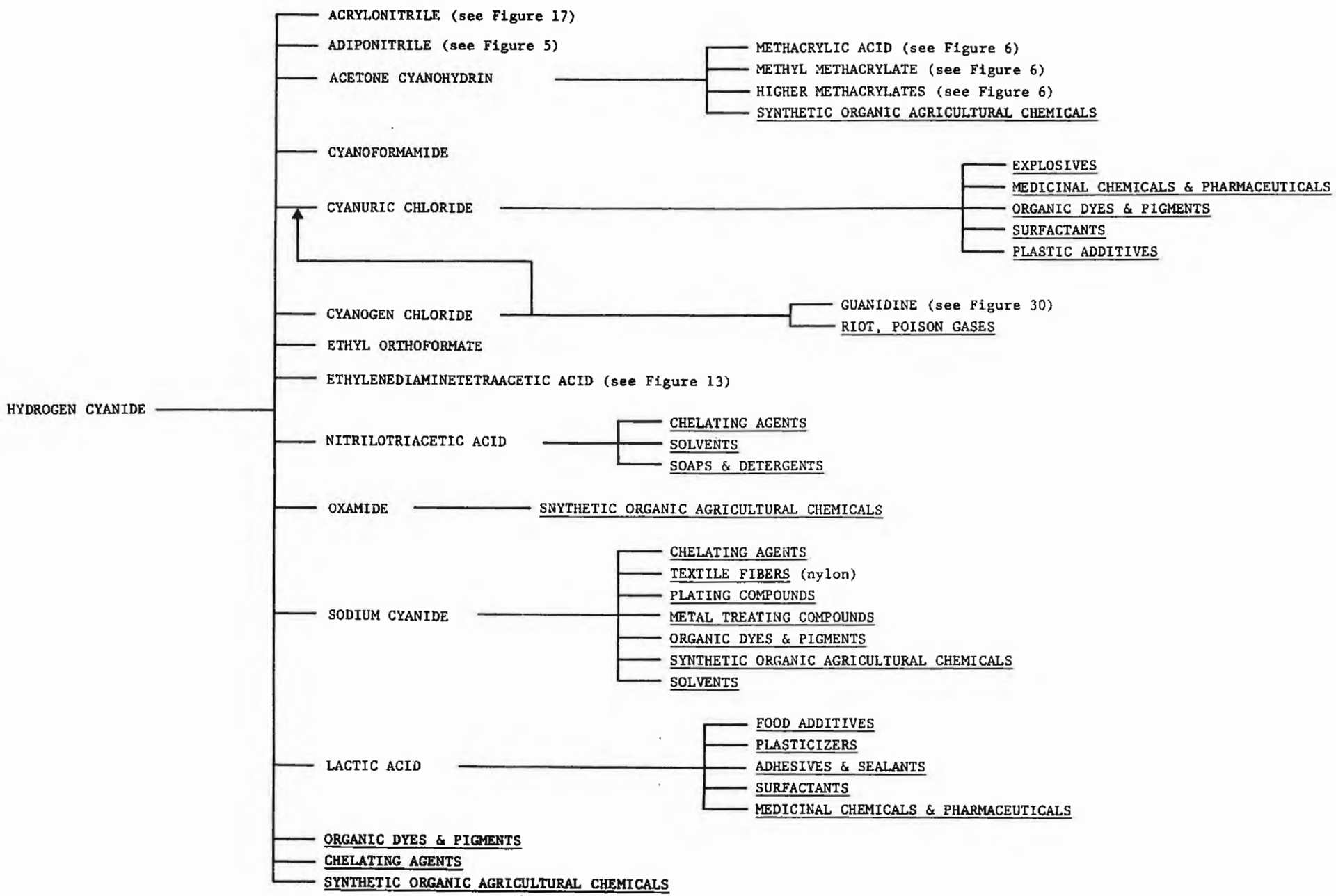

Figure 29. ACETYLENE

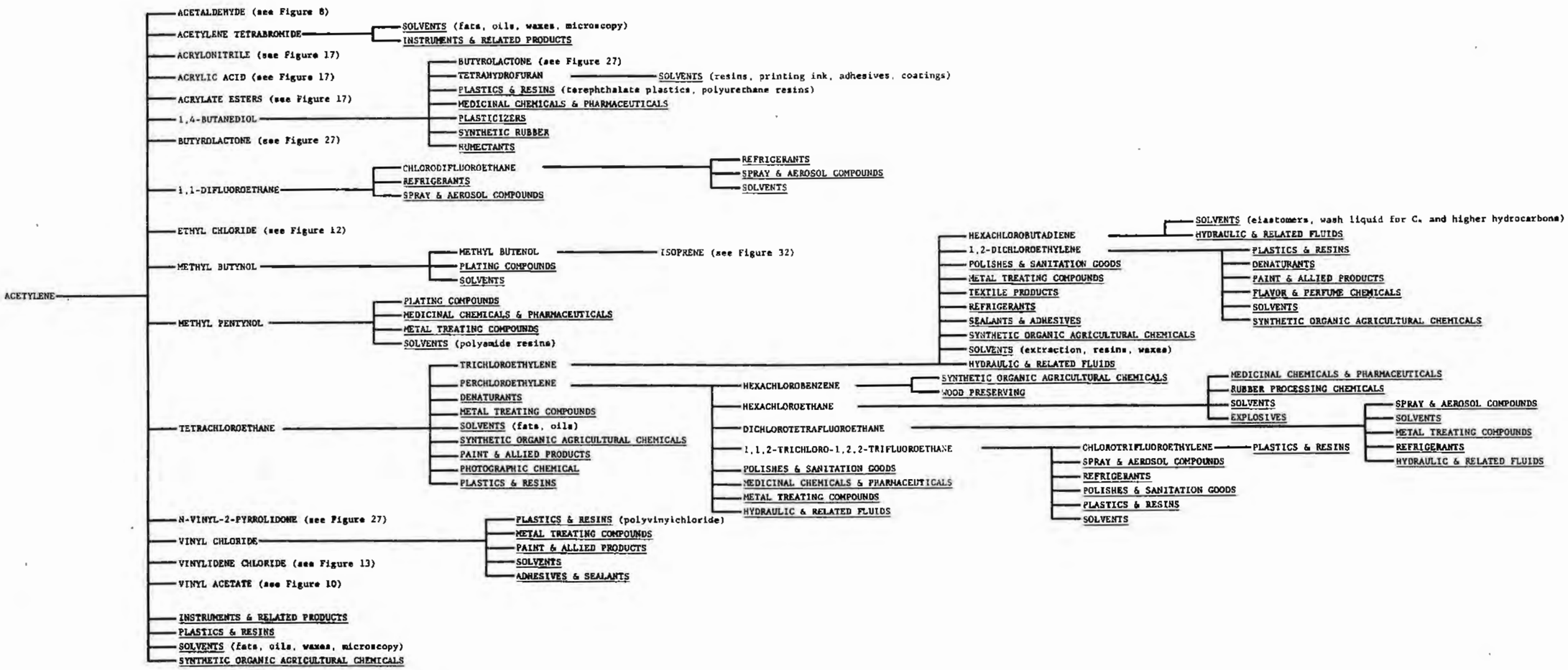

Figure 30. SYNTHESIS GAS

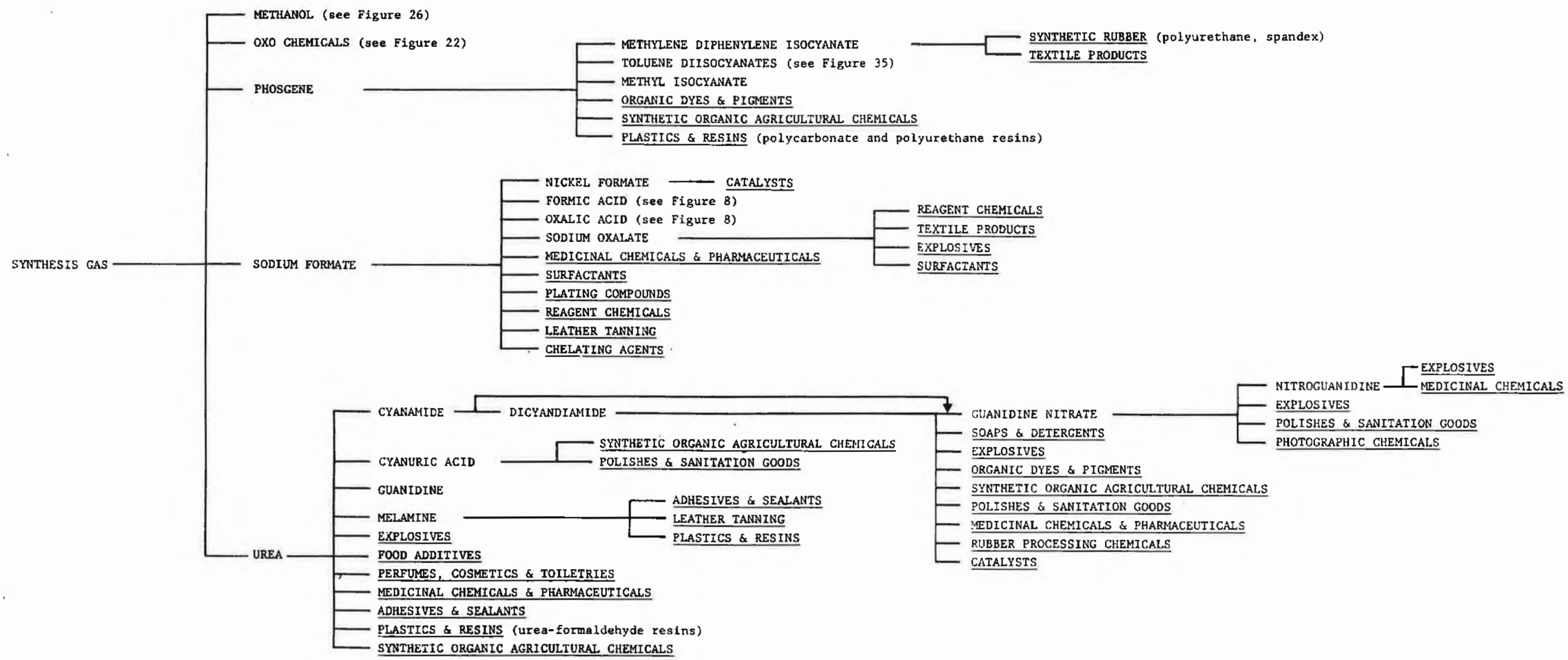

Figure 31. ETHANE, PROPANE, BUTANE

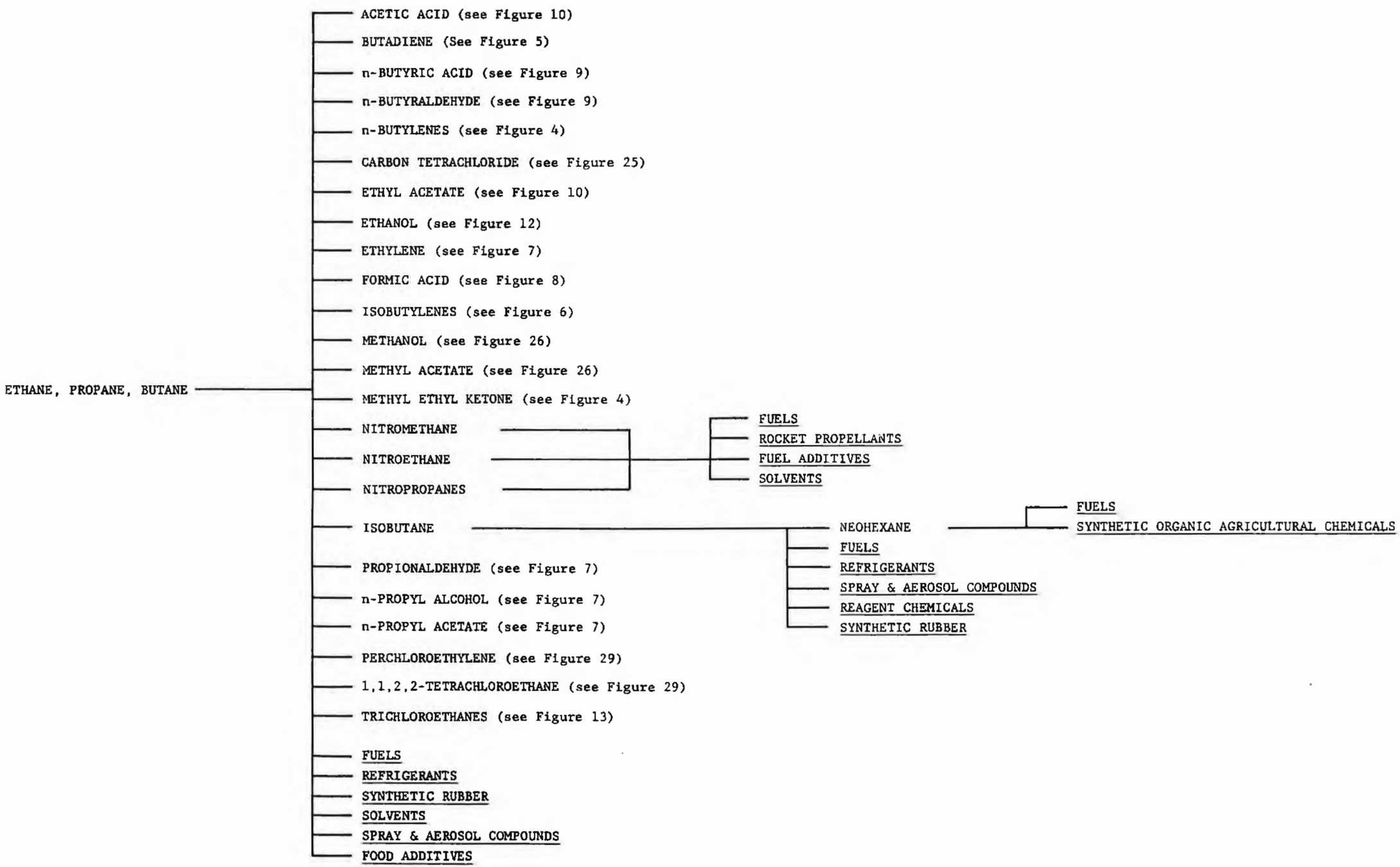

Figure 32. PENTANE, ISOPENTANE

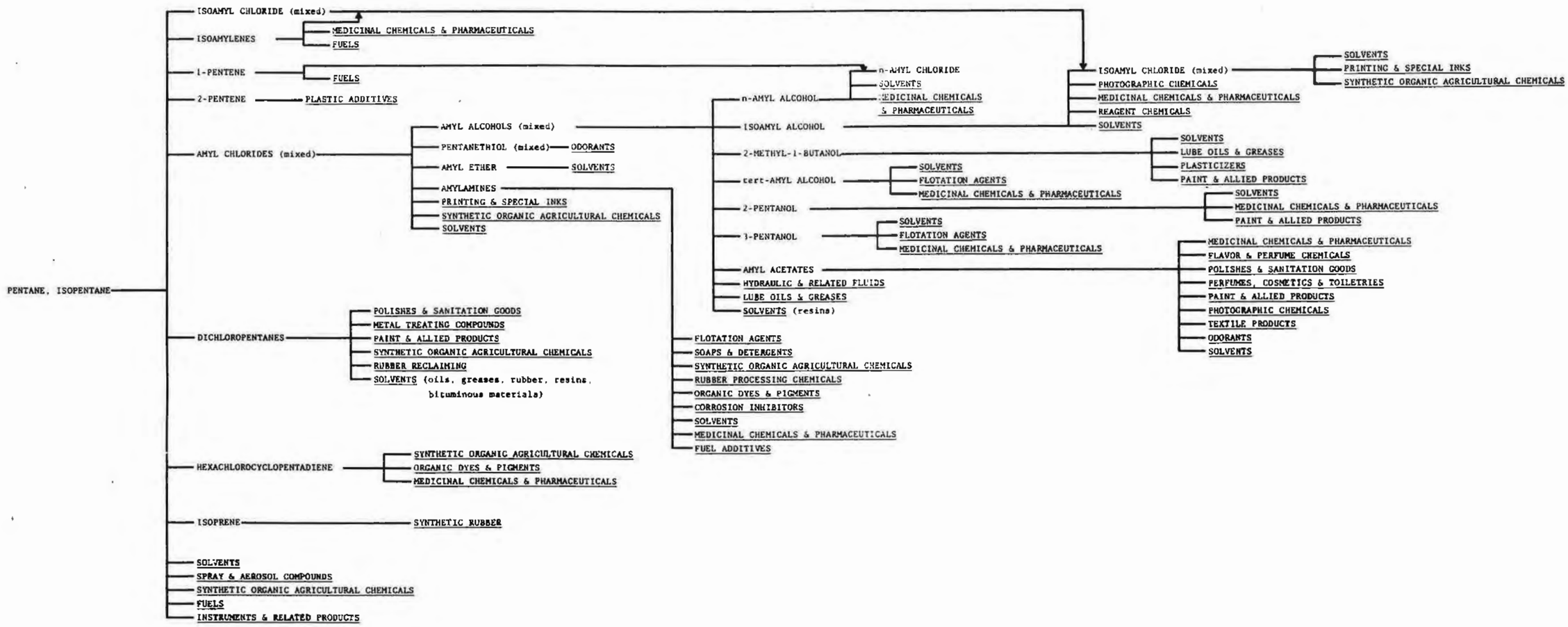

Figure 33. TOLUENE

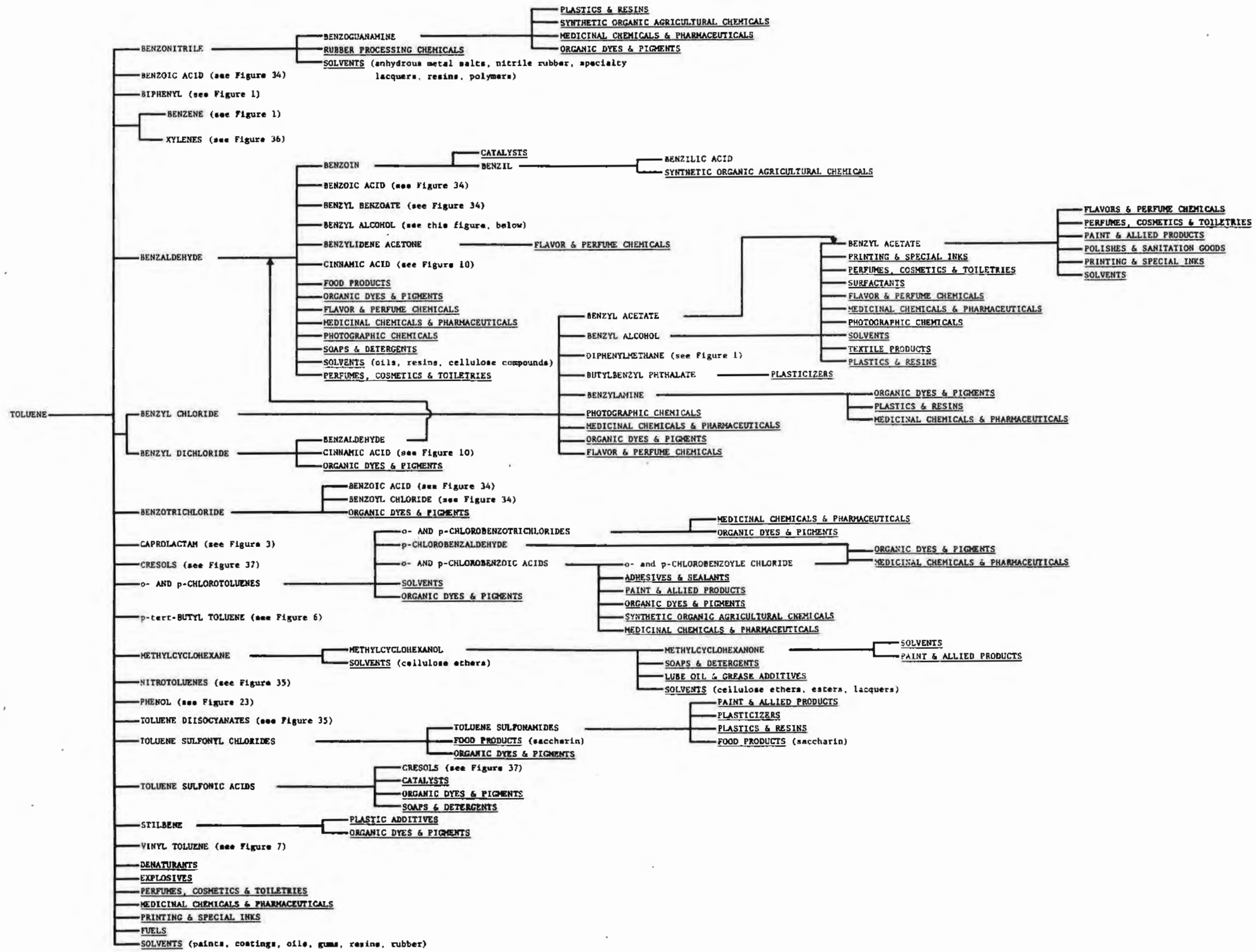

Figure 34. BENZOIC ACID

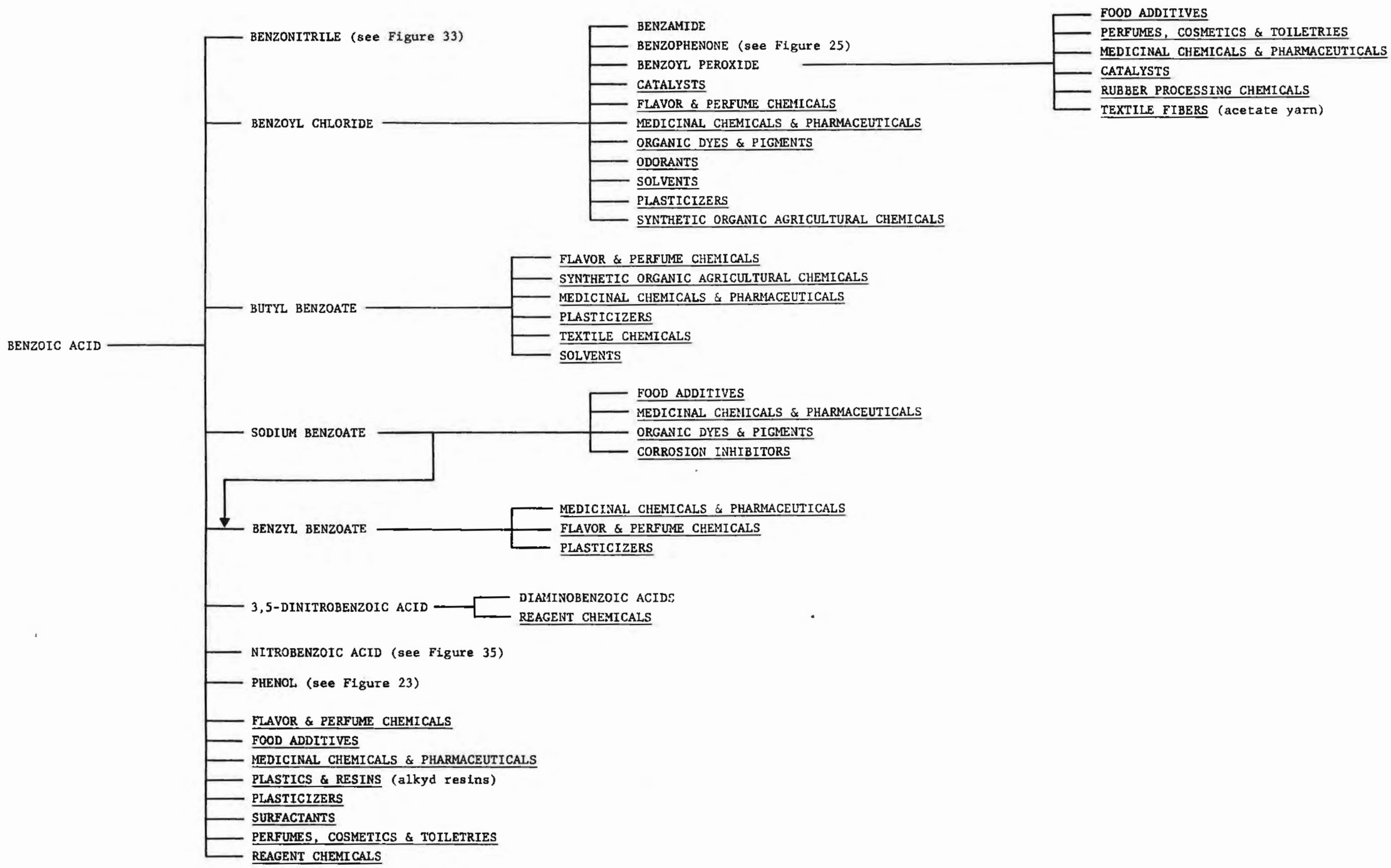

Figure 35. NITROTOLUENES

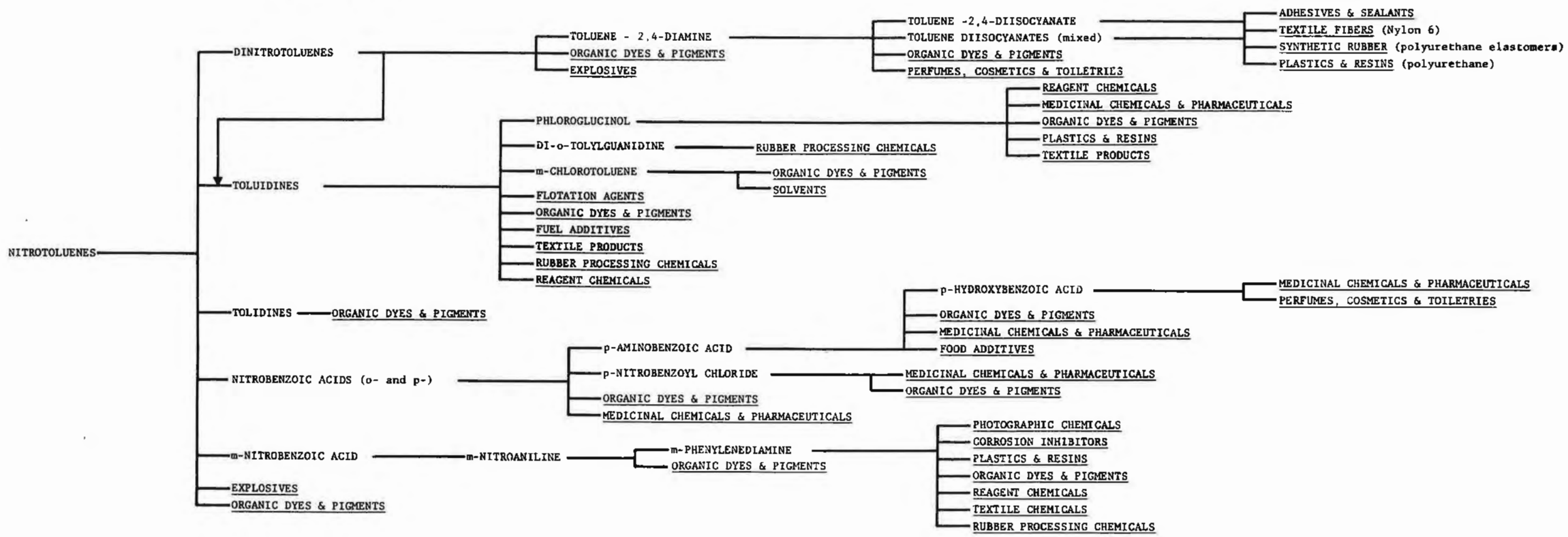

Figure 36. XYLENES

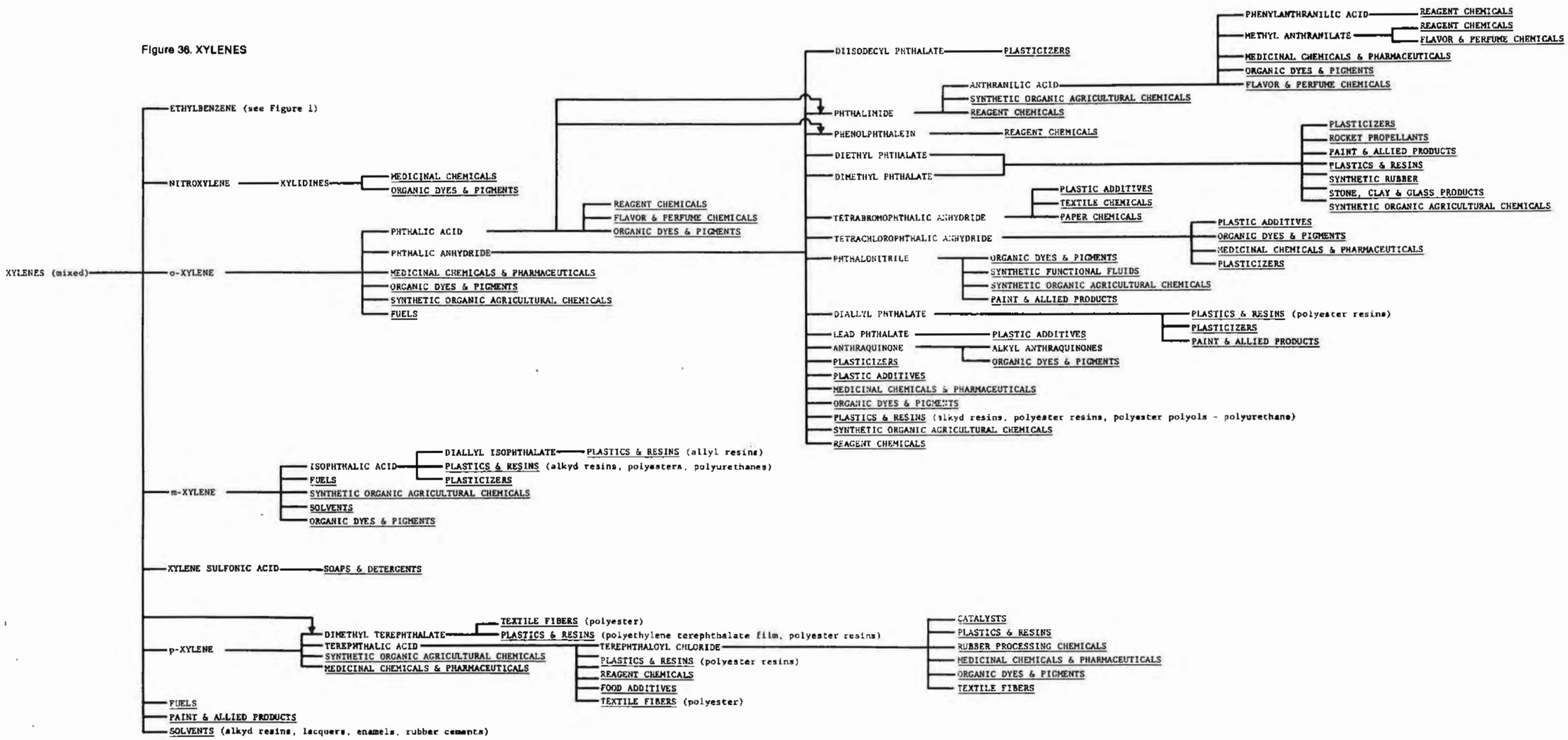
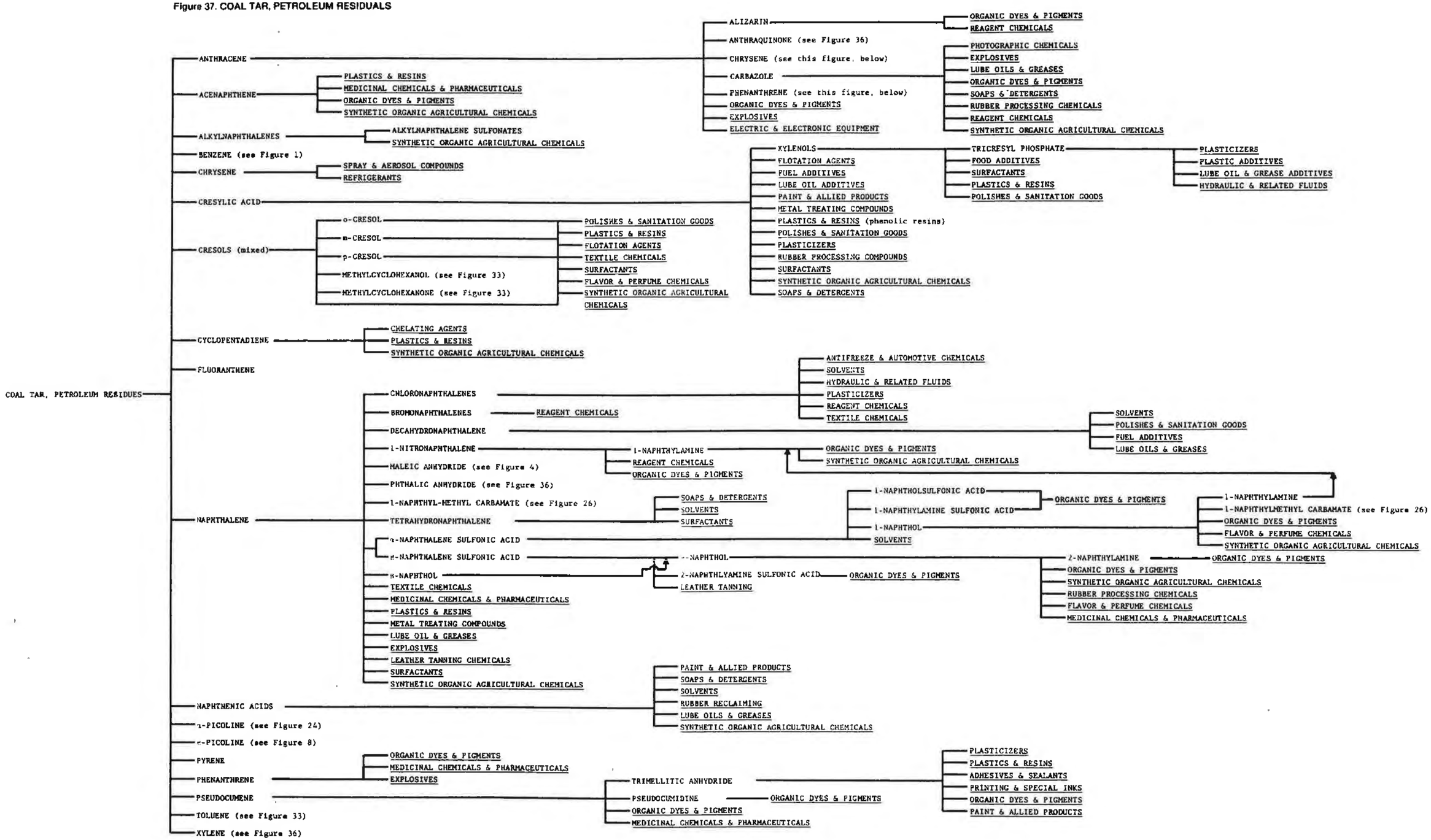
Figure 37. COAL TAR, PETROLEUM RESIDUALS