

## Chapter 1 : The Synthetic Organic Chemist's Companion by Michael C. Pirrung

*The Organic Chemists' Companion provides a practical, hands-on resource for students and practitioners of organic synthesis. It presents the fundamentals and guides the reader through the entire process of organic synthesis. It includes basic instructions on everything from on handling reagents.*

Visit our Beautiful Books page and find lovely books for kids, photography lovers and more. Organic Chemistry Flap copy How to Use the Solvent selection chart Solvents known to swell polystyrene are shown in blue. Protic solvents are shown in red. Aprotic solvents are shown in black. N-methylformamide and N-methylacetamide are shown slightly lower than their  $t_1$  coordinates, 5. This chart is based on: Strategies for solvent selection. B , 39, This work used principal components analysis of solvent properties [mp, bp, dielectric constant  $\epsilon$  , dipole moment  $m$  , refractive index  $n$  , ET spectroscopically determined effect on a solvatochromatic dye , and  $\log P$ ]. The eigenvectors were projected into two dimensions,  $t_1$  and  $t_2$ , representing a conflation of properties that most differentiate these solvents, accounting for? Polarity correlates with  $t_1$ , while polarizability correlates with  $t_2$ . Solvents in the vicinity of one another in this chart should have similar properties. Solvents are positioned approximately to improve clarity. For reactions with a known solvent dependence, select solvents in the vicinity of the known best solvent  $s$ . For reactions with an unknown solvent dependence: Select solvents that give uniform coverage of the solvent space  $i$ . Both aprotic and protic solvents might be selected when compatible with reaction conditions. Select solvents as dissimilar as possible. A D-optimal design selects solvents at the extreme periphery of the solvent space. A quadratic D-optimal design also includes a solvent near the origin. Packed with tips, data, and real-life examples, this handbook: Reactions on a Small Scale - mmol. Other equipment and considerations. Conducting the Reaction Itself. Reagents supplied as dispersions. Syringe and inert atmosphere techniques. General procedure for transfer of materials by syringe. Reactions above atmospheric pressure. Thin layer chromatography TLC. Cutting glass TLC plates. High pressure liquid chromatography HPLC. Reactions producing triphenylphosphine oxide. Reactions involving boron compounds. Reactions involving copper salts. Reactions involving aluminum reagents. Reactions involving tin reagents. Oxalic acid-coated silica gel. Silver nitrate-impregnated silica gel. Methods for Structure Elucidation. Nuclear magnetic resonance spectroscopy. Cleaning Up After the Reaction. Strategies for Reaction Organization. NMR spectral data of common contaminants of organic reaction products. Synthetic solvent selection chart. Recipes for TLC stains. Acidities of organic functional groups. Acidities of organic functional groups in DMSO. Web resources for synthetic chemistry. The book is written in a concise, easy to read style, and it includes numerous illustrations. The book is written in a concise, easy-to-read style, and it includes numerous illustrations.

**Chapter 2 : CHEMISTRY LOVERS: Synthetic Organic Chemists Companion**

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According to the concept of vitalism vital force theory, organic matter was endowed with a "vital force". Around 1828, Michel Chevreul started a study of soaps made from various fats and alkalis. He separated the different acids that, in combination with the alkali, produced the soap. Since these were all individual compounds, he demonstrated that it was possible to make a chemical change in various fats which traditionally come from organic sources, producing new compounds, without "vital force". The event is now generally accepted as indeed disproving the doctrine of vitalism. His discovery, made widely known through its financial success, greatly increased interest in organic chemistry. Ehrlich popularized the concepts of "magic bullet" drugs and of systematically improving drug therapies. A phosphorus-ligand bond, tricyclohexyl phosphine, PCy<sub>3</sub>, is below center; another PCy<sub>3</sub> ligand appears at the top of the image where its rings are obscuring one another. The ring group projecting to the right, an alkylidene, contains a metal-carbon double bond to ruthenium. Early examples of organic reactions and applications were often found because of a combination of luck and preparation for unexpected observations. The latter half of the 19th century however witnessed systematic studies of organic compounds. The development of synthetic indigo is illustrative. The production of indigo from plant sources dropped from 19, tons in to 1, tons by thanks to the synthetic methods developed by Adolf von Baeyer. In 1884, 17, tons of synthetic indigo were produced from petrochemicals. The multiple-step synthesis of complex organic compounds is called total synthesis. Total synthesis of complex natural compounds increased in complexity to glucose and terpineol. For example, cholesterol-related compounds have opened ways to synthesize complex human hormones and their modified derivatives. Since the start of the 20th century, complexity of total syntheses has been increased to include molecules of high complexity such as lysergic acid and vitamin B<sub>12</sub>. The discovery of petroleum and the development of the petrochemical industry spurred the development of organic chemistry. Converting individual petroleum compounds into different types of compounds by various chemical processes led to organic reactions enabling a broad range of industrial and commercial products including, among many others: The majority of chemical compounds occurring in biological organisms are in fact carbon compounds, so the association between organic chemistry and biochemistry is so close that biochemistry might be regarded as in essence a branch of organic chemistry. Although the history of biochemistry might be taken to span some four centuries, fundamental understanding of the field only began to develop in the late 19th century and the actual term biochemistry was coined around the start of 20th century. Research in the field increased throughout the twentieth century, without any indication of slackening in the rate of increase, as may be verified by inspection of abstraction and indexing services such as BIOSIS Previews and Biological Abstracts, which began in the 1950s as a single annual volume, but has grown so drastically that by the end of the 20th century it was only available to the everyday user as an online electronic database. Traditional methods of separation include distillation, crystallization, and solvent extraction. Organic compounds were traditionally characterized by a variety of chemical tests, called "wet methods", but such tests have been largely displaced by spectroscopic or other computer-intensive methods of analysis. Nuclear magnetic resonance NMR spectroscopy is the most commonly used technique, often permitting complete assignment of atom connectivity and even stereochemistry using correlation spectroscopy. The principal constituent atoms of organic chemistry are hydrogen and carbon, which exist naturally with NMR-responsive isotopes, respectively <sup>1</sup>H and <sup>13</sup>C. A destructive method used to determine the elemental composition of a molecule. See also mass spectrometry, below. Mass spectrometry indicates the molecular weight of a compound and, from the fragmentation patterns, its structure. High resolution mass spectrometry can usually identify the exact formula of a compound and is used in lieu of elemental analysis. In former times, mass spectrometry was restricted to neutral molecules exhibiting some volatility, but advanced ionization techniques allow one to obtain the "mass spec" of virtually any organic compound. Crystallography can be useful for determining molecular geometry when a single

crystal of the material is available. Highly efficient hardware and software allows a structure to be determined within hours of obtaining a suitable crystal. Traditionally refractive index and density were also important for substance identification. Properties Physical properties of organic compounds typically of interest include both quantitative and qualitative features. Quantitative information includes melting point, boiling point, and index of refraction. Qualitative properties include odor, consistency, solubility, and color. Melting and boiling properties Organic compounds typically melt and many boil. In contrast, while inorganic materials generally can be melted, many do not boil, tending instead to degrade. In earlier times, the melting point  $m$ . The melting and boiling points correlate with the polarity of the molecules and their molecular weight. Some organic compounds, especially symmetrical ones, sublime, that is they evaporate without melting. A well-known example of a sublimable organic compound is para-dichlorobenzene, the odiferous constituent of modern mothballs. Solubility Neutral organic compounds tend to be hydrophobic; that is, they are less soluble in water than in organic solvents. Exceptions include organic compounds that contain ionizable which can be converted in ions groups as well as low molecular weight alcohols, amines, and carboxylic acids where hydrogen bonding occurs. Organic compounds tend to dissolve in organic solvents. Solvents can be either pure substances like ether or ethyl alcohol, or mixtures, such as the paraffinic solvents such as the various petroleum ethers and white spirits, or the range of pure or mixed aromatic solvents obtained from petroleum or tar fractions by physical separation or by chemical conversion. Solubility in the different solvents depends upon the solvent type and on the functional groups if present in the solution. Solid state properties Various specialized properties of molecular crystals and organic polymers with conjugated systems are of interest depending on applications, e. For historical reasons, such properties are mainly the subjects of the areas of polymer science and materials science. The names of organic compounds are either systematic, following logically from a set of rules, or nonsystematic, following various traditions. Systematic nomenclature starts with the name for a parent structure within the molecule of interest. This parent name is then modified by prefixes, suffixes, and numbers to unambiguously convey the structure. Given that millions of organic compounds are known, rigorous use of systematic names can be cumbersome. Thus, IUPAC recommendations are more closely followed for simple compounds, but not complex molecules. To use the systematic naming, one must know the structures and names of the parent structures. Parent structures include unsubstituted hydrocarbons, heterocycles, and monofunctionalized derivatives thereof. Nonsystematic nomenclature is simpler and unambiguous, at least to organic chemists. Nonsystematic names do not indicate the structure of the compound. They are common for complex molecules, which includes most natural products. Thus, the informally named lysergic acid diethylamide is systematically named 6aR,9R-N,N-diethylmethyl-4,6,6a,7,8,9-hexahydroindolo-[4,3-fg] quinolinecarboxamide. With the increased use of computing, other naming methods have evolved that are intended to be interpreted by machines. Structural drawings Organic molecules are described more commonly by drawings or structural formulas, combinations of drawings and chemical symbols. The line-angle formula is simple and unambiguous. In this system, the endpoints and intersections of each line represent one carbon, and hydrogen atoms can either be notated explicitly or assumed to be present as implied by tetravalent carbon. History By an explosion in the number of chemical compounds being discovered occurred assisted by new synthetic and analytical techniques. Grignard described the situation as "chaos le plus complet" as due to the lack of convention it was possible to have multiple names for the same compound. This led to the creation of the Geneva rules in Acetic acid, shown here, is an example. The concept of functional groups is central in organic chemistry, both as a means to classify structures and for predicting properties. A functional group is a molecular module, and the reactivity of that functional group is assumed, within limits, to be the same in a variety of molecules. Functional groups can have decisive influence on the chemical and physical properties of organic compounds. Molecules are classified on the basis of their functional groups. Alcohols, for example, all have the subunit C-O-H. All alcohols tend to be somewhat hydrophilic, usually form esters, and usually can be converted to the corresponding halides. Most functional groups feature heteroatoms atoms other than C and H. Organic compounds are classified according to functional groups, alcohols, carboxylic acids, amines, etc. Aliphatic compound The aliphatic hydrocarbons are subdivided into three groups of homologous series according to

their state of saturation: The rest of the group is classed according to the functional groups present. Such compounds can be "straight-chain", branched-chain or cyclic. The degree of branching affects characteristics, such as the octane number or cetane number in petroleum chemistry. Both saturated alicyclic compounds and unsaturated compounds exist as cyclic derivatives. The most stable rings contain five or six carbon atoms, but large rings macrocycles and smaller rings are common. The smallest cycloalkane family is the three-membered cyclopropane  $\text{CH}_2$  3. Saturated cyclic compounds contain single bonds only, whereas aromatic rings have an alternating or conjugated double bond. Cycloalkanes do not contain multiple bonds, whereas the cycloalkenes and the cycloalkynes do. Aromatic compounds Benzene is one of the best-known aromatic compounds as it is one of the simplest and most stable aromatics. Aromatic hydrocarbons contain conjugated double bonds. This means that every carbon atom in the ring is  $\text{sp}^2$  hybridized, allowing for added stability. Particular instability antiaromaticity is conferred by the presence of  $4n$  conjugated  $\pi$  electrons. Heterocyclic compounds Main article: Heterocyclic compound The characteristics of the cyclic hydrocarbons are again altered if heteroatoms are present, which can exist as either substituents attached externally to the ring exocyclic or as a member of the ring itself endocyclic. In the case of the latter, the ring is termed a heterocycle. Pyridine and furan are examples of aromatic heterocycles while piperidine and tetrahydrofuran are the corresponding alicyclic heterocycles. The heteroatom of heterocyclic molecules is generally oxygen, sulfur, or nitrogen, with the latter being particularly common in biochemical systems. Heterocycles are commonly found in a wide range of products including aniline dyes and medicines. Additionally, they are prevalent in a wide range of biochemical compounds such as alkaloids, vitamins, steroids, and nucleic acids e. Rings can fuse with other rings on an edge to give polycyclic compounds.

## Chapter 3 : The Synthetic Organic Chemist's Companion : Michael C. Pirrung :

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Reactions on a Small Scale 1 25 mmol. Other equipment and considerations. Conducting the Reaction Itself. Reagents supplied as dispersions. Syringe and inert atmosphere techniques. General procedure for transfer of materials by syringe. Reactions above atmospheric pressure. Thin layer chromatography TLC. Cutting glass TLC plates. High pressure liquid chromatography HPLC. Reactions producing triphenylphosphine oxide. Reactions involving boron compounds. Reactions involving copper salts. Reactions involving aluminum reagents. Reactions involving tin reagents. Triethylamine treated silica gel. Oxalic acid coated silica gel. Silver nitrate impregnated silica gel. Methods for Structure Elucidation. Nuclear magnetic resonance spectroscopy. Cleaning Up After the Reaction. Strategies for Reaction Organization. NMR spectral data of common contaminants of organic reaction products. Synthetic solvent selection chart. Recipes for TLC stains. Acidities of organic functional groups. Acidities of organic functional groups in DMSO. Web resources for synthetic chemistry. Rezensionen "There is a wealth of practical advice on both everyday lab practices and also special problems. The book is written in a concise, easy to read style, and it includes numerous illustrations.

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*Michael C. Pirrung, PhD, is a Professor of Chemistry and UC Presidential Chair at the University of [calendrierdelascience.com](http://calendrierdelascience.com) received his PhD in organic chemistry at UC-Berkeley in under the direction of Clayton Heathcock and did postdoctoral work with Gilbert Stork at Columbia as an NSF postdoctoral fellow.*

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