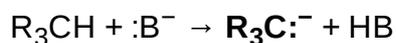


Carbanion

A **carbanion** is an anion in which carbon is trivalent (forms three bonds) and bears a formal negative charge (in at least one significant resonance form).^[1]

Formally, a carbanion is the conjugate base of a **carbon acid**:



where B stands for the base. The carbanions formed from deprotonation of alkanes (at an sp³ carbon), alkenes (at an sp² carbon), arenes (at an sp² carbon), and alkynes (at an sp carbon) are known as **alkyl**, **alkenyl** (**vinyl**), **aryl**, and **alkynyl** (**acetylide**) **anions**, respectively.

Carbanions have a concentration of electron density at the negatively charged carbon, which, in most cases, reacts efficiently with a variety of electrophiles of varying strengths, including carbonyl groups, imines/iminium salts, halogenating reagents (e.g., *N*-bromosuccinimide and diiodine), and proton donors. A carbanion is one of several reactive intermediates in organic chemistry. In organic synthesis, organolithium reagents and Grignard reagents are commonly treated and referred to as "carbanions." This is a convenient approximation, although these species are generally clusters or complexes containing highly polar, but still covalent bonds metal–carbon bonds (M^{δ+}–C^{δ−}) rather than true carbanions.

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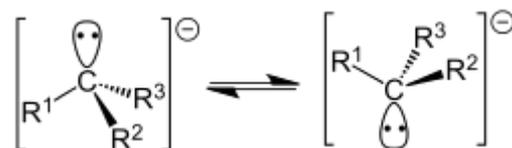
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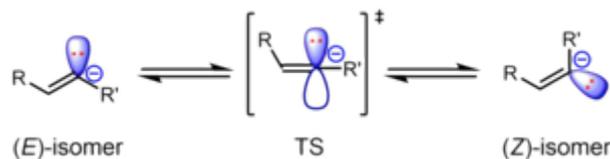
Geometry

Absent π delocalization, the negative charge of a carbanion is localized in an sp^x hybridized orbital on carbon as a lone pair. As a consequence, *localized* alkyl, alkenyl/aryl, and alkynyl carbanions assume trigonal pyramidal, bent, and linear geometries, respectively. By Bent's rule, placement of the carbanionic lone pair electrons in an orbital with significant s character is favorable, accounting for the pyramidalized and bent geometries of alkyl and alkenyl carbanions, respectively. Valence shell electron pair repulsion (VSEPR) theory makes similar predictions. This contrasts with carbocations, which have a preference for unoccupied nonbonding orbitals of pure atomic p character, leading to planar and linear geometries, respectively, for alkyl and alkenyl carbocations.

However, *delocalized* carbanions may deviate from these geometries. Instead of residing in a hybrid orbital, the carbanionic lone pair may instead occupy a p orbital (or an orbital of high p character). A p orbital has a more suitable shape and orientation to overlap with the neighboring π system, resulting in more effective charge delocalization. As a consequence, alkyl carbanions with neighboring conjugating groups (e.g., allylic anions, enolates, nitronates, etc.) are generally planar rather than pyramidized. Likewise, delocalized alkenyl carbanions sometimes favor a linear instead of bent geometry. More often, a bent geometry is still preferred for substituted alkenyl anions, though the linear geometry is only *slightly* less stable, resulting in facile equilibration between the (*E*) and (*Z*) isomers of the (bent) anion through a linear transition state.^[2] For instance, calculations indicate that the parent vinyl anion, $\text{H}_2\text{C}=\text{CH}^\ominus$, has an inversion barrier of 27 kcal/mol, while allenyl anion, $\text{H}_2\text{C}=\text{C}=\text{CH}^\ominus$ ($\leftrightarrow \text{H}_2\text{C}^\ominus-\text{C}\equiv\text{CH}$), whose negative charge is stabilized by delocalization, has an inversion barrier of only 4 kcal/mol, reflecting stabilization of the linear transition state by better π delocalization.^[3]



An alkyl carbanion is trigonal pyramidal.



Vinyl anions are bent. 1,2-Disubstituted vinyl anions have *E* and *Z* isomers that undergo inversion through a linear transition state.

Trends and occurrence

Carbanions are typically nucleophilic and basic. The basicity and nucleophilicity of carbanions are determined by the substituents on carbon. These include

1. The inductive effect. Electronegative atoms adjacent to the charge will stabilize the charge;
2. The extent of conjugation of the anion. Resonance effects can stabilize the anion. This is especially true when the anion is stabilized as a result of aromaticity.

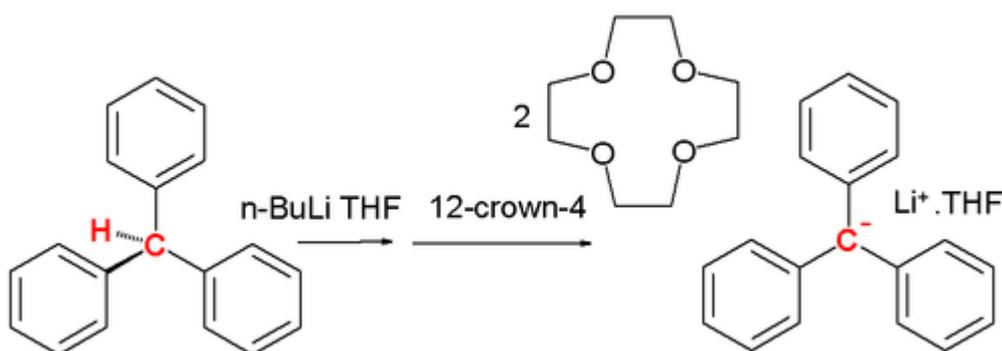
Geometry also affects the orbital hybridization of the charge-bearing carbanion. The greater the s-character of the charge-bearing atom, the more stable the anion.

Organometallic reagents like butyllithium (hexameric cluster, $[\text{BuLi}]_6$) or methylmagnesium bromide (ether complex, $\text{MeMgBr}(\text{OEt})_2$) are often referred to as "carbanions," at least in a retrosynthetic sense. However, they are really clusters or complexes containing a polar covalent bond, though with electron density heavily polarized toward the carbon atom. In fact, true carbanions without stabilizing substituents are not available in the condensed phase, and these species must be studied in the gas phase.

For some time, it was not known whether simple alkyl anions could exist as free species; many theoretical studies predicted that even methanide anion CH_3^- should be an unbound species (i.e., the electron affinity of CH_3^\bullet was predicted to be negative). Such a species would decompose immediately by spontaneous ejection of an electron and would therefore be too fleeting to observe directly by mass spectrometry.^[4] However, in 1978, methyl anion was unambiguously synthesized by subjecting ketene to electric discharge, and the electron affinity (EA) of CH_3^\bullet was determined by photoelectron spectroscopy to be $+1.8 \text{ kcal mol}^{-1}$, making it a bound species, but just barely so. The structure of CH_3^- was found to be pyramidal (C_{3v}) with $\angle\text{H}-\text{C}-\text{H} = 108^\circ$ and inversion barrier of $1.3 \text{ kcal mol}^{-1}$, while CH_3^\bullet was determined to be planar (D_{3h} point group).^[5]

Simple primary, secondary and tertiary sp^3 carbanions (e.g., CH_3CH_2^- , $(\text{CH}_3)_2\text{CH}^-$, and $(\text{CH}_3)_3\text{C}^-$) were subsequently determined to be unbound species (EA of $\text{CH}_3\text{CH}_2^\bullet$, $(\text{CH}_3)_2\text{CH}^\bullet$, $(\text{CH}_3)_3\text{C}^\bullet = -6, -7.4, -3.6$ kcal mol^{-1} , respectively) indicating that α substitution is destabilizing. However, relatively modest stabilizing effects can render them bound. For example, cyclopropyl and cubyl anions are bound due to increased s character of the lone pair orbital, while neopentyl and phenethyl anion are also bound, as a result of negative hyperconjugation of the lone pair with the β -substituent ($n_{\text{C}} \rightarrow \sigma^*_{\text{C-C}}$). The same holds true for anions with benzylic and allylic stabilization. Gas-phase carbanions that are sp^2 and sp hybridized are much more strongly stabilized and are often prepared directly by gas-phase deprotonation.^[6]

In the condensed phase only carbanions that are sufficiently stabilized by delocalization have been isolated as truly ionic species. In 1984, Olmstead and Power presented the lithium crown ether salt of the triphenylmethanide carbanion from triphenylmethane, *n*-butyllithium and 12-crown-4 (which forms a stable complex with lithium cations) at low temperatures:^[7]



Adding *n*-butyllithium to triphenylmethane (pK_a in DMSO of $\text{CHPh}_3 = 30.6$) in THF at low temperatures followed by 12-crown-4 results in a red solution and the salt complex $[\text{Li}(12\text{-crown-4})]^+[\text{CPh}_3]^-$ precipitates at -20°C . The central C–C bond lengths are 145 pm with the phenyl ring propellered at an average angle of 31.2° . This propeller shape is less pronounced with a tetramethylammonium counterion. A crystal structure for the analogous diphenylmethanide anion ($[\text{Li}(12\text{-crown-4})]^+[\text{CHPh}_2]^-$), prepared from diphenylmethane (pK_a in DMSO of $\text{CH}_2\text{Ph}_2 = 32.3$), was also obtained. However, the attempted isolation of a complex of the benzyl anion $[\text{CH}_2\text{Ph}]^-$ from toluene (pK_a in DMSO of $\text{CH}_3\text{Ph} \approx 43$) was unsuccessful, due to rapid reaction of the formed anion with the THF solvent.^[8] The free benzyl anion has also been generated in the solution phase by pulse radiolysis of dibenzylmercury.^[9]

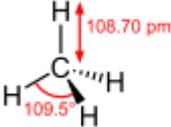
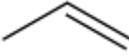
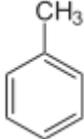
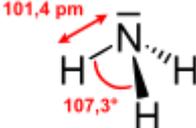
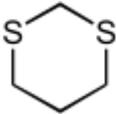
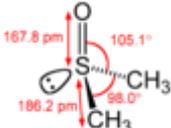
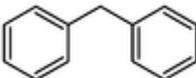
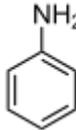
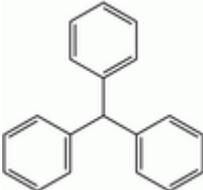
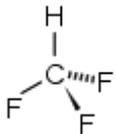
Early in 1904^[10] and 1917,^[11] Schlenk prepared two red-colored salts, formulated as $[\text{NMe}_4]^+[\text{CPh}_3]^-$ and $[\text{NMe}_4]^+[\text{CH}_2\text{Ph}]^-$, respectively, by metathesis of the corresponding organosodium reagent with tetramethylammonium chloride. Since tetramethylammonium cations cannot form a chemical bond to the carbanionic center, these species are believed to contain free carbanions. While the structure of the former was verified by X-ray crystallography almost a century later,^[12] the instability of the latter has so far precluded structural verification. The reaction of the putative " $[\text{NMe}_4]^+[\text{CH}_2\text{Ph}]^-$ " with water was reported to liberate toluene and tetramethylammonium hydroxide and provides indirect evidence for the claimed formulation.

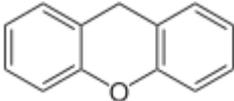
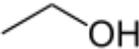
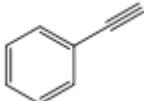
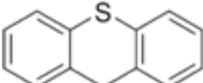
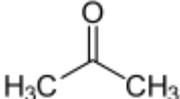
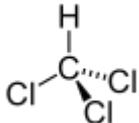
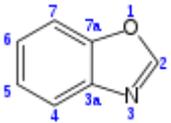
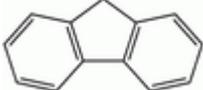
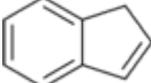
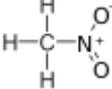
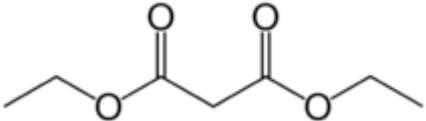
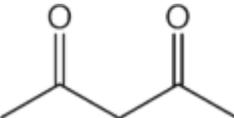
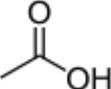
One tool for the detection of carbanions in solution is proton NMR.^[13] A spectrum of cyclopentadiene in DMSO shows four vinylic protons at 6.5 ppm and two methylene bridge protons at 3 ppm whereas the cyclopentadienyl anion has a single resonance at 5.50 ppm. The use of ^6Li and ^7Li NMR has provided structural and reactivity data for a variety of organolithium species.

Carbon acids

Any compound containing hydrogen can, in principle, undergo deprotonation to form its conjugate base. A compound is a **carbon acid** if deprotonation results in loss of a proton from a carbon atom. Compared to compounds typically considered to be acids (e.g., mineral acids like nitric acid, or carboxylic acids like acetic acid), carbon acids are typically many orders of magnitude weaker, although exceptions exist (see below). For example, benzene is not an acid in the classical Arrhenius sense, since its aqueous solutions are neutral. Nevertheless, it is very weak Brønsted acid with an estimated pK_a of 49 which may undergo deprotonation in the presence of a superbases like the Lochmann–Schlosser base ($n\text{-BuLi}:\text{KO}t\text{-Bu}$). As conjugate acid-base pairs, the factors that determine the relative stability of carbanions also determine the ordering of the pK_a values of the corresponding carbon acids. Furthermore, pK_a values allow the prediction of whether a proton transfer process will be thermodynamically favorable: In order for the deprotonation of an acidic species HA with base B^- to be thermodynamically favorable ($K > 1$), the relationship $pK_a(\text{BH}) > pK_a(\text{AH})$ must hold.

These values below are pK_a values determined in DMSO, which has a broader useful range (~ 0 to ~ 35) than values determined in water (~ 0 to ~ 14) and better reflect the basicity of the carbanions in typical organic solvents. Values below less than 0 or greater than 35 are indirectly estimated; hence, the numerical accuracy of these values is limited. Aqueous pK_a values are also commonly encountered in the literature, particularly in the context of biochemistry and enzymology. Moreover, aqueous values are often given in introductory organic chemistry textbooks for pedagogical reasons, although the issue of solvent dependence is often glossed over. In general, pK_a values in water and organic solvent diverge significantly when the anion is capable of hydrogen bonding. For instance, in the case of water, the values differ dramatically: pK_a in water of water = 14.0,^[14] while pK_a in DMSO of water = 31.4,^[15] reflecting the differing ability of water and DMSO to stabilize hydroxide anion. On the other hand, for cyclopentadiene, the numerical values are comparable: $pK_a^{\text{aq}}(\text{Cp-H}) = 15$, while $pK_a^{\text{DMSO}}(\text{Cp-H}) = 18$.^[15]

name	formula	structural formula	pK _a ^{DMSO}
<u>Cyclohexane</u>	C ₆ H ₁₂		~ 60
<u>Methane</u>	CH ₄		~ 56
<u>Benzene</u>	C ₆ H ₆		~ 49 ^[16]
<u>Propene</u>	C ₃ H ₆		~ 44
<u>Toluene</u>	C ₆ H ₅ CH ₃		~ 43
<u>Ammonia (N-H)</u>	NH ₃		~ 41
<u>Dithiane</u>	C ₄ H ₈ S ₂		~ 39
<u>Dimethyl sulfoxide</u>	(CH ₃) ₂ SO		35.1
<u>Diphenylmethane</u>	C ₁₃ H ₁₂		32.3
<u>Acetonitrile</u>	CH ₃ CN	CH₃-C≡N	31.3
<u>Aniline (N-H)</u>	C ₆ H ₅ NH ₂		30.6
<u>Triphenylmethane</u>	C ₁₉ H ₁₆		30.6
<u>Fluoroform</u>	CHF ₃		30.5 ^[17]

<u>Xanthene</u>	$C_{13}H_{10}O$		30.0
<u>Ethanol (O-H)</u>	C_2H_5OH		29.8
<u>Phenylacetylene</u>	C_8H_6		28.8
<u>Thioxanthene</u>	$C_{13}H_{10}S$		28.6
<u>Acetone</u>	C_3H_6O		26.5
<u>Chloroform</u>	$CHCl_3$		24.4 ^[17]
<u>Benzoxazole</u>	C_7H_5NO		24.4
<u>Fluorene</u>	$C_{13}H_{10}$		22.6
<u>Indene</u>	C_9H_8		20.1
<u>Cyclopentadiene</u>	C_5H_6		18.0
<u>Nitromethane</u>	CH_3NO_2		17.2
<u>Diethyl malonate</u>	$C_7H_{12}O_4$		16.4
<u>Acetylacetone</u>	$(H_3CC(O))_2CH_2$		13.3
<u>Hydrogen cyanide</u>	HCN	$H-C\equiv N$	12.9
<u>Acetic acid (O-H)</u>	CH_3COOH		12.6
<u>Malononitrile</u>	$C_3H_2N_2$		11.1

<u>Dimedone</u>	C ₈ H ₁₂ O ₂		10.3
<u>Meldrum's acid</u>	C ₆ H ₈ O ₄		7.3
<u>Hexafluoroacetylacetone</u>	(F ₃ CC(O)) ₂ CH ₂		2.3
<u>Hydrogen chloride</u> (Cl-H)	HCl	HCl (g)	-2.0 ^[18]
<u>Triflic acid</u>	HC(SO ₂ CF ₃) ₃		~ -16 ^[19]

Table 1. Carbon acid acidities by pK_a in DMSO.^[20] These values may differ significantly from aqueous pK_a values.

Note that acetic acid, ammonia, aniline, ethanol, and hydrogen chloride are not carbon acids, but are common acids shown for comparison.

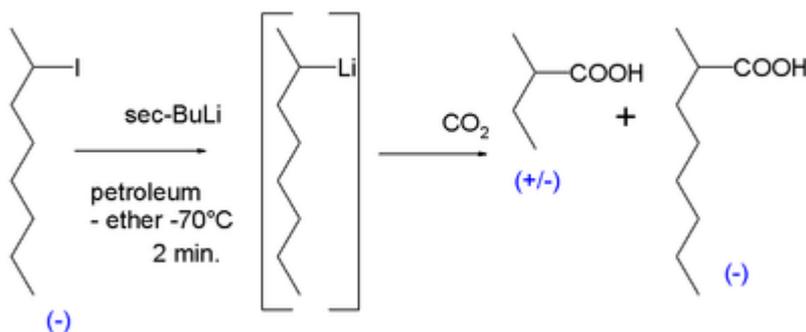
As indicated by the examples above, acidity increases (pK_a decreases) when the negative charge is delocalized. This effect occurs when the substituents on the carbanion are unsaturated and/or electronegative. Although carbon acids are generally thought of as acids that are much weaker than "classical" Brønsted acids like acetic acid or phenol, the cumulative (additive) effect of several electron accepting substituents can lead to acids that are as strong or stronger than the inorganic mineral acids. For example, trinitromethane (HC(NO₂)₃), tricyanomethane (HC(CN)₃), pentacyanocyclopentadiene (HC₅(CN)₅), and fulminic acid (HCNO) are all strong acids with aqueous pK_a values that indicate complete or nearly complete proton transfer to water. Triflic acid, with three strongly electron withdrawing triflyl groups, has an estimated pK_a well below -10. On the other end of the scale, hydrocarbons bearing only alkyl groups are thought to have pK_a values in the range of 55 to 65. The range of acid dissociation constants for carbon acids thus spans over 70 orders of magnitude.

The acidity of the α -hydrogen in carbonyl compounds enables these compounds to participate in synthetically important C–C bond-forming reactions including the aldol reaction and Michael addition.

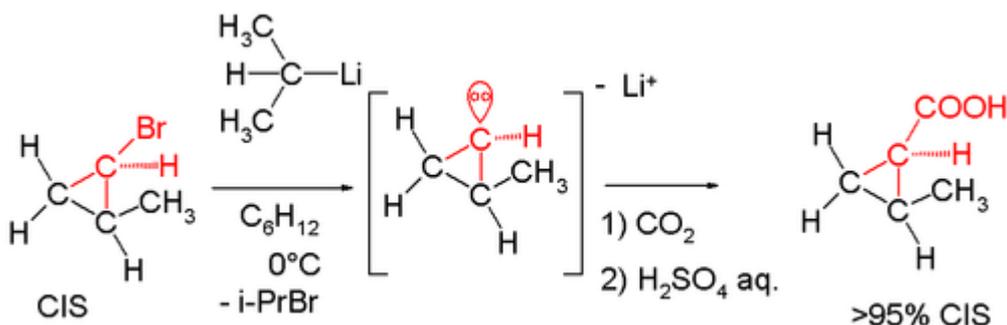
Chiral carbanions

With the molecular geometry for a carbanion described as a trigonal pyramid the question is whether or not carbanions can display chirality, because if the activation barrier for inversion of this geometry is too low any attempt at introducing chirality will end in racemization, similar to the nitrogen inversion. However, solid evidence exists that carbanions can indeed be chiral for example in research carried out with certain organolithium compounds.

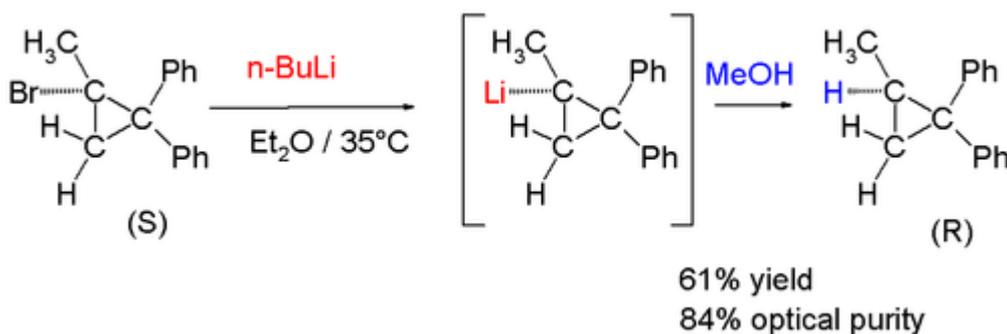
The first ever evidence for the existence of chiral organolithium compounds was obtained in 1950. Reaction of chiral 2-iodooctane with *sec*-butyllithium in petroleum ether at $-70\text{ }^{\circ}\text{C}$ followed by reaction with dry ice yielded mostly racemic 2-methylbutyric acid but also an amount of optically active 2-methyloctanoic acid which could only have formed from likewise optical active 2-methylheptyllithium with the carbon atom linked to lithium the carbanion.^[21]



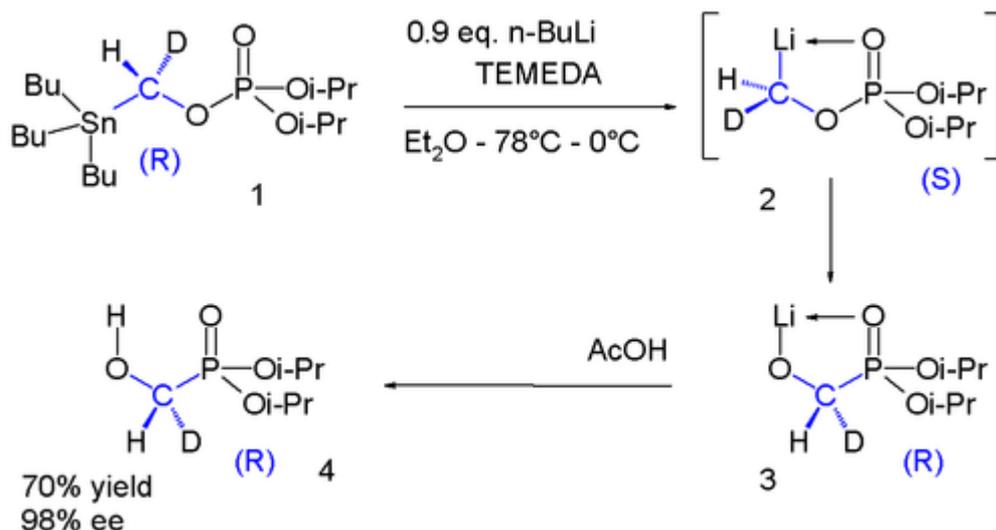
On heating the reaction to $0\text{ }^{\circ}\text{C}$ the optical activity is lost. More evidence followed in the 1960s. A reaction of the *cis* isomer of 2-methylcyclopropyl bromide with *sec*-butyllithium again followed by carboxylation with dry ice yielded *cis*-2-methylcyclopropylcarboxylic acid. The formation of the *trans* isomer would have indicated that the intermediate carbanion was unstable.^[22]



In the same manner the reaction of (+)-(*S*)-1-bromo-1-methyl-2,2-diphenylcyclopropane with *n*-butyllithium followed by quench with methanol resulted in product with retention of configuration.^[23]



Of recent date are chiral methyl lithium compounds:^[24]



The phosphate **1** contains a chiral group with a hydrogen and a deuterium substituent. The stannyl group is replaced by lithium to intermediate **2** which undergoes a phosphate-phosphorane rearrangement to phosphorane **3** which on reaction with acetic acid gives alcohol **4**. Once again in the range of -78 °C to 0 °C the chirality is preserved in this reaction sequence.^[25]

History

A carbanionic structure first made an appearance in the reaction mechanism for the benzoin condensation as correctly proposed by Clarke and Arthur Lapworth in 1907.^[26] In 1904 Wilhelm Schlenk prepared $\text{Ph}_3\text{C}^-\text{NMe}_4^+$ in a quest for pentavalent nitrogen (from tetramethylammonium chloride and Ph_3CNa)^[10] and in 1914 he demonstrated how triarylmethyl radicals could be reduced to carbanions by alkali metals ^[27] The phrase carbanion was introduced by Wallis and Adams in 1933 as the negatively charged counterpart of the carbonium ion^{[28][29]}

See also

- Carbocation
- Enolates
- Nitrile anion

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External links

- Large database of Bordwell pKa values at www.chem.wisc.edu Link (<https://web.archive.org/web/20081009060809/http://www.chem.wisc.edu/areas/reich/pkatable/>)
 - Large database of Bordwell pKa values at daecr1.harvard.edu Link (https://web.archive.org/web/20061212181531/http://daecr1.harvard.edu/pdf/evans_pKa_table.pdf)
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