Which Carbocation Is The Most Stable

The apparent coordination number of five, or even six, associated with the carbon atom at the top of the pyramid is a rarity as compared to the usual maximum of four. 01b42efdd2 == Theory == 01b42efdd2

Carbenium ion of carbocations, which is a general term for diamagnetic carbon-based cations. They are isoelectronic with monoboranes such as B(CH3)3. In parallel with carbenium ions is another subset of carbocations, the carbonium A carbenium ion is a positive ion with the structure RR′R″C+, that is a chemical species with carbon atom having only three covalent bonds, thus bearing a +1 formal charge. Carbenium ions are a major subset of carbocations, which is a general term for diamagnetic carbon-based cations. In carbenium ions, the charge is localized. In parallel with carbenium ions is another subset of carbocations, the carbonium ions with the formula R5+ 01b42efdd2

Tertiary carbon Tertiary carbon atoms can occur, for example, in branched alkanes, but not in linear alkanes. The three alkyl groups on the tertiary carbon contribute to A tertiary carbon atom is a carbon atom bound to three other carbon atoms. For this reason, tertiary carbon atoms are found only in hydrocarbons containing at least four carbon atoms. They are called saturated hydrocarbons because they only contain carbon-carbon single bonds. Tertiary carbons have a hybridization of sp3. Tertiary carbons form the most stable carbocations due to a combination of factors. figure 01b42efdd2

2-Norbornyl cation 2. methylene carbon 6. However, the 2-norbornyl cation can be In organic chemistry, the term 2-norbornyl cation (or 2-bicyclo[2. This is surprising as primary carbocations are much less stable than secondary carbocations. 1]heptyl cation) describes a carbonium ionic derivative of norbornane. A salt of the 2-norbornyl cation was crystallized and characterized by X-ray crystallography to confirm the non-classical structure 01b42efdd2

E1cB-elimination reaction Elimination refers to the fact that the mechanism is an elimination reaction and will lose two substituents. E1cB is a two-step process, the first step of which may or may not be reversible. of a carbocation intermediate. The name of the mechanism - E1cB - stands for Elimination Unimolecular conjugate Base. The lone pair of electrons on the anion then moves to the neighboring atom, thus expelling the leaving group and forming a double or triple bond. Usually a moderate to strong base is present. The carbocation is then deprotonated resulting in the formation of a new pi bond. Unimolecular refers to the fact that the rate-determining step of this reaction only involves one molecular entity. First, a base abstracts the relatively acidic proton to generate a stabilized anion. The molecule involved must also have The E1cB elimination reaction is a type of elimination reaction which occurs under basic conditions, where the hydrogen to be removed is relatively acidic, while the leaving group (such as -OH or -OR) is a relatively poor one. Finally, conjugate base

refers to the formation of the carbanion intermediate, which is the conjugate base of the starting material 01b42efdd2

If two states, as, for example, a transition state and an unstable intermediate, occur consecutively during a reaction process and have nearly the same energy content, their interconversion will involve only a small reorganization of the molecular structures. 01b42efdd2 The rule states that with the addition of a protic acid HX or other polar reagent to an asymmetric alkene, the acid hydrogen (H) or electropositive part gets attached to the carbon with more hydrogen substituents, and the halide (X) group or electronegative part gets attached to the carbon with more alkyl substituents. This is in contrast to Markovnikov's original definition, in which the rule states that the X component is added to the carbon with the fewest hydrogen atoms while the hydrogen atom is added to the carbon with the greatest number of hydrogen atoms. 01b42efdd2 Whitmore earned both his bachelor's degree (1911) and Ph.D. (1914) from Harvard University, where his Ph.D. advisor was Charles Loring Jackson. Several prominent contemporaries of Whitmore at Harvard were E.K. Bolton, Farrington Daniels, Roger Adams, James B. Sumner and James Bryant Conant. After graduating from Harvard he became a professor and taught at the University of Minnesota, Northwestern University, and The Pennsylvania State University. 01b42efdd2 == Explanation == 01b42efdd2 At Penn State, Whitmore served as the Dean of the School of Chemistry and Physics from 1929–1947, succeeding his former Harvard colleague Gerald Wendt in the position. He hired several prominent scientists as faculty members, including Russell Marker and Merrell Fenske. 01b42efdd2 A native of Maine, he was born and raised in Auburn; he attended nearby Bates College in Lewiston, Maine, where he graduated magna cum laude with a B.S. in chemistry in 1943. He completed his... 01b42efdd2

Frank C. Whitmore Nevertheless, Whitmore published these findings which today are accepted as the most logical Frank Clifford Whitmore (October 1, 1887 – June 24, 1947), nicknamed "Rocky", was a prominent chemist who submitted significant evidence for the existence of carbocation mechanisms in organic chemistry. like a carbocation would never be stable enough to exist 01b42efdd2

The R is the functional group attached to a tertiary carbon. If the functional group was an OH group, this compound would be commonly called tert-butanol or t-butanol. When a functional group is attached to a tertiary carbon, the prefix -tert (-t) is used in the common name for the compound. An example of this is shown in the figure. 01b42efdd2 The term "superacid" was first used in 1927 when James Bryant Conant found that perchloric acid could protonate ketones and aldehydes to form salts in nonaqueous solution. The term itself was coined by Gillespie, after Conant combined sulfuric acid with fluorosulfuric acid, and found the solution to be several million times more acidic than sulfuric acid alone. The magic acid system was developed in the 1960s by Gillespie, and was to be used to study stable carbocations. Gillespie also used the acid system to generate electron-deficient inorganic cations. The name... 01b42efdd2 E1cB should be thought of as being on one end of a continuous spectrum, which includes the E1 mechanism at the opposite end and the E2 mechanism in the middle. The E1... 01b42efdd2 He was a chemist at the California Institute of

Technology, and subsequently headed both the Departments of Chemistry and Chemical Engineering at the university. He conducted research at the University of Oxford and University of Basel as a Guggenheim Fellow and National Science Foundation Fellow, respectively. He served as the foreign secretary of the National Academy of Sciences from 1974 to 1978. 01b42efdd2 == Nomenclature == 01b42efdd2

Hammond's postulate Therefore, since the tertiary carbocation is relatively stable and therefore close in energy to the R-X reactant, then the tertiary transition state Hammond's postulate (or alternatively the Hammond–Leffler postulate), is a hypothesis in physical organic chemistry which describes the geometric structure of the transition state in an organic chemical reaction. First proposed by George Hammond in 1955, the postulate states that:. methyl 01b42efdd2

== Academic career == 01b42efdd2 He was born in 1887 in the town of North Attleborough, Massachusetts. 01b42efdd2

Markovnikov's rule of the most stable carbocation during the addition process. Adding the hydrogen ion to one carbon atom in the alkene creates a positive charge on the other In organic chemistry, Markovnikov's rule or Markownikoff's rule describes the outcome of some addition reactions. The rule was formulated by Russian chemist Vladimir Markovnikov in 1870 01b42efdd2

== History == 01b42efdd2 Therefore, the geometric structure of a state can be predicted by comparing its energy to the species neighboring it along the reaction coordinate. For example, in an exothermic reaction the transition state is closer in energy to the reactants than to the products. Therefore, the transition state will be more geometrically similar to the reactants than to the products. In contrast, however, in an endothermic reaction the transition state is closer in energy to the products than to the reactants. So, according to Hammond's postulate the structure of the transition state would resemble the products more than the reactants. This type of comparison... 01b42efdd2

George S. Hammond His research garnered him the Norris Award in 1968, the Priestley Medal in 1976, the National Medal of Science in 1994, and the Othmer Gold Medal in 2003. He served as the executive chairman of the Allied Chemical Corporation from 1979 to 1989. This is a two-step mechanism. Hammond's research is also known for its influence on the philosophy of science. The more stable the carbocation intermediate is, the faster the reaction George Simms Hammond (May 22, 1921 – October 5, 2005) was an American scientist and theoretical chemist who developed "Hammond's postulate", and fathered organic photochemistry,–the general theory of the geometric structure of the transition state in an organic chemical reaction. depends on the removal of a single molecular species 01b42efdd2

== History == 01b42efdd2

Pyramidal carbocation The four-sided pyramidal ion will carry a charge of 1+, and the five-sided pyramid will carry 2+. In the images (at upper right), the black spot on the

vertical line represents the hovering carbon atom. This ion exists as a third class, besides the classical and non-classical ions. In these ions, a single carbon atom hovers over a four- or five-sided polygon, in effect forming a pyramid. This ion exists as a third class, besides the classical and non-classical A pyramidal carbocation is a type of carbocation with a specific configuration. A pyramidal carbocation is a type of carbocation with a specific configuration 01b42efdd2

Whitmore was a member of several academic societies, namely the American Academy of Arts and Sciences (1939), the American Philosophical Society (1943), and the United States National... 01b42efdd2 Studying these cations was sparked, at the time, by amazing results in computational chemistry. While calculating the optimal geometry of the mono-cation which arises from the extraction of chloride from 3-chlorotricyclo[2.1.0.02,5]pentane, the three bridges were expected to orient in space with angles of roughly 120°. The calculations however showed the four-sided pyramid to be the most stable configuration. At the top of this pyramid, there resides a carbon atom, still connected to a hydrogen. The original expected structure turned out to... 01b42efdd2

Magic acid The magic acid system was developed in the 1960s by Gillespie, and was to be used to study stable carbocations. This conjugate Brønsted–Lewis superacid system was developed in the 1960s by Ronald Gillespie and his team at McMaster University, and has been used by George Olah to stabilise carbocations and hypercoordinated carbonium ions in liquid media. alone. Magic acid and other superacids are also used to catalyze isomerization of saturated hydrocarbons, and have been shown to protonate even weak bases, including methane, xenon, halogens, and molecular hydrogen. Gillespie also used the acid system Magic acid ($FSO_3H{\cdot}SbF_5$) is a superacid consisting of a mixture, most commonly in a 1:1 molar ratio, of fluorosulfuric acid (HSO_3F) and antimony pentafluoride (SbF_5) 01b42efdd2

== Nomenclature == 01b42efdd2