Which Carbocation Is Most Stable

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. 52d24af2a6 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... 52d24af2a6

Tertiary carbon Tertiary carbons form the most stable carbocations due to a combination of factors. The three alkyl groups on the A tertiary carbon atom is a carbon atom bound to three other carbon atoms. They are called saturated hydrocarbons because they only contain carbon-carbon single bonds. example of this is shown in the figure. For this reason, tertiary carbon atoms are found only in hydrocarbons containing at least four carbon atoms. Tertiary carbon atoms can occur, for example, in branched alkanes, but not in linear alkanes. Tertiary carbons have a hybridization of sp3 52d24af2a6

Decay technique In chemistry, the decay technique is a method to generate chemical species such as radicals, carbocations, and other potentially unstable covalent structures 52d24af2a6

Magic acid Gillespie also used the acid system to generate electron-deficient Magic acid (FSO3H·SbF5) is a superacid consisting of a mixture, most commonly in a 1:1 molar ratio, of fluorosulfuric acid (HSO3F) and antimony pentafluoride (SbF5). 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. 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. developed in the 1960s by Gillespie, and was to be used to study stable carbocations 52d24af2a6

Pyramidal carbocation A pyramidal carbocation is a type of carbocation with a specific configuration. The four-sided pyramidal ion will carry a charge of 1+, and the five-sided pyramid will carry 2+. 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. In the images (at upper right), the black spot on the vertical line represents the hovering carbon atom. 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 ions 52d24af2a6

== Explanation == 52d24af2a6 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... 52d24af2a6 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. 52d24af2a6 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. 52d24af2a6

Markovnikov's rule The rule was formulated by Russian chemist Vladimir Markovnikov in 1870. The chemical basis for Markovnikov's Rule is the formation of the most stable carbocation during the addition process. Adding the hydrogen ion In organic chemistry, Markovnikov's rule or Markownikoff's rule describes the outcome of some addition reactions. carbon–hydrogen bonds 52d24af2a6

E1cB-elimination reaction Usually a moderate to strong base is present. of the α-carbon. E1cB is a two-step process, the first step of which may or may not be reversible. First, a base abstracts the relatively acidic proton to generate a stabilized anion. The carbocation is then deprotonated resulting in the formation of a new 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. Unimolecular refers to the fact that the rate-determining step of this reaction only involves one molecular entity. Elimination refers to the fact that the mechanism is an elimination reaction and will lose two substituents. 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. This results in the formation of a carbocation intermediate. The name of the mechanism - E1cB - stands for Elimination Unimolecular conjugate Base. Finally, conjugate base refers to the formation of the carbanion intermediate, which is the conjugate base of the starting material 52d24af2a6

== History == 52d24af2a6 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... 52d24af2a6 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... 52d24af2a6

Hammond's postulate carbocation is relatively stable and therefore close in energy to the R-X reactant, then the tertiary transition state will have a structure that is fairly 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: 52d24af2a6

Carbenium ion They are isoelectronic with monoboranes such as B(CH3)3. In carbenium ions, the charge is localized. of carbocations, which is a general term for diamagnetic carbon-based cations. Carbenium ions are a major subset of carbocations, which is a general term for diamagnetic carbon-based cations. In parallel with carbenium ions is another subset of carbocations, the 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. In parallel with carbenium ions is another subset of carbocations, the carbonium ions with the formula R5+ 52d24af2a6

George S. Hammond carbocation is relatively stable and therefore close in energy to the R-X reactant, then the tertiary transition state will have a structure that is fairly 52d24af2a6

== History == 52d24af2a6 == Nomenclature == 52d24af2a6

2-Norbornyl cation lies on methylene carbon 6. This is surprising as primary carbocations are much less stable than secondary carbocations. However, the 2-norbornyl cation 52d24af2a6

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. 52d24af2a6 == Nomenclature == 52d24af2a6