ALCANI

Argomenti trattati:

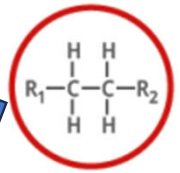
- ✓ Idrocarburi saturi: gli alcani, struttura, nomenclatura e proprietà
- ✓ Isomeri costituzionali
- ✓ Rotazione intorno a legami semplici carbonio-carbonio (conformeri, proiezioni di Newman)

Bruice: cap. 3 (paragrafi 1-2, 7-9)

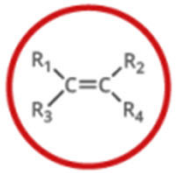
FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

FUNCTIONAL GROUPS ARE GROUPS OF ATOMS IN ORGANIC MOLECULES THAT ARE RESPONSIBLE FOR THE CHARACTERISTIC CHEMICAL REACTIONS OF THOSE MOLECULES. IN THE GENERAL FORMULAE SHOWN BELOW FOR EACH FUNCTIONAL GROUP, 'R' REPRESENTS THE REST OF THE MOLECULE, AND 'X' REPRESENTS ANY HALOGEN ATOM.

HYDROCARBONS | SIMPLE OXYGEN HETEROATOMICS | HALOGEN HETEROATOMICS | CARBONYL COMPOUNDS | NITROGEN-BASED | SULFUR-BASED | AROMATIC

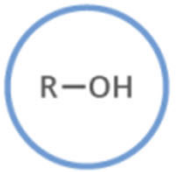


ALKANE
Naming: -ane
e.g. ethane

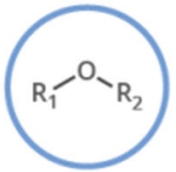


ALKENE
Naming: -ene
e.g. ethene

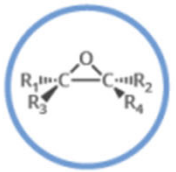
ALKYNE
Naming: -yne
e.g. ethyne



ALCOHOL
Naming: -ol
e.g. ethanol

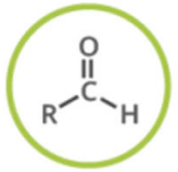


ETHER
Naming: -oxy -ane
e.g. methoxyethane

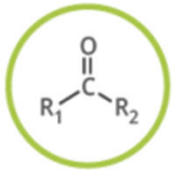


EPOXIDE
Naming: -ene oxide
e.g. ethene oxide

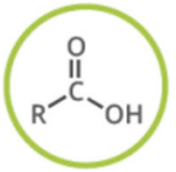
HALOALKANE
Naming: halo-
e.g. chloroethane



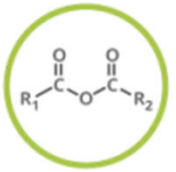
ALDEHYDE
Naming: -al
e.g. ethanal



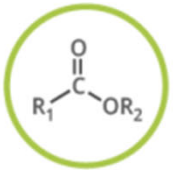
KETONE
Naming: -one
e.g. propanone



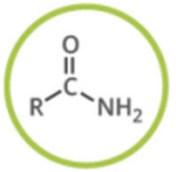
CARBOXYLIC ACID
Naming: -oic acid
e.g. ethanoic acid



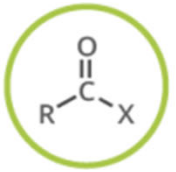
ACID ANHYDRIDE
Naming: -oic anhydride
e.g. ethanoic anhydride



ESTER
Naming: -yl -oate
e.g. ethyl ethanoate



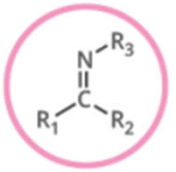
AMIDE
Naming: -amide
e.g. ethanamide



ACYL HALIDE
Naming: -oyl halide
e.g. ethanoyl chloride

AMINE
Naming: -amine
e.g. ethanamine

NITRILE
Naming: -nitrile
e.g. ethanenitrile

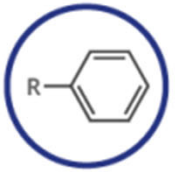


IMINE
Naming: -imine
e.g. ethanimine

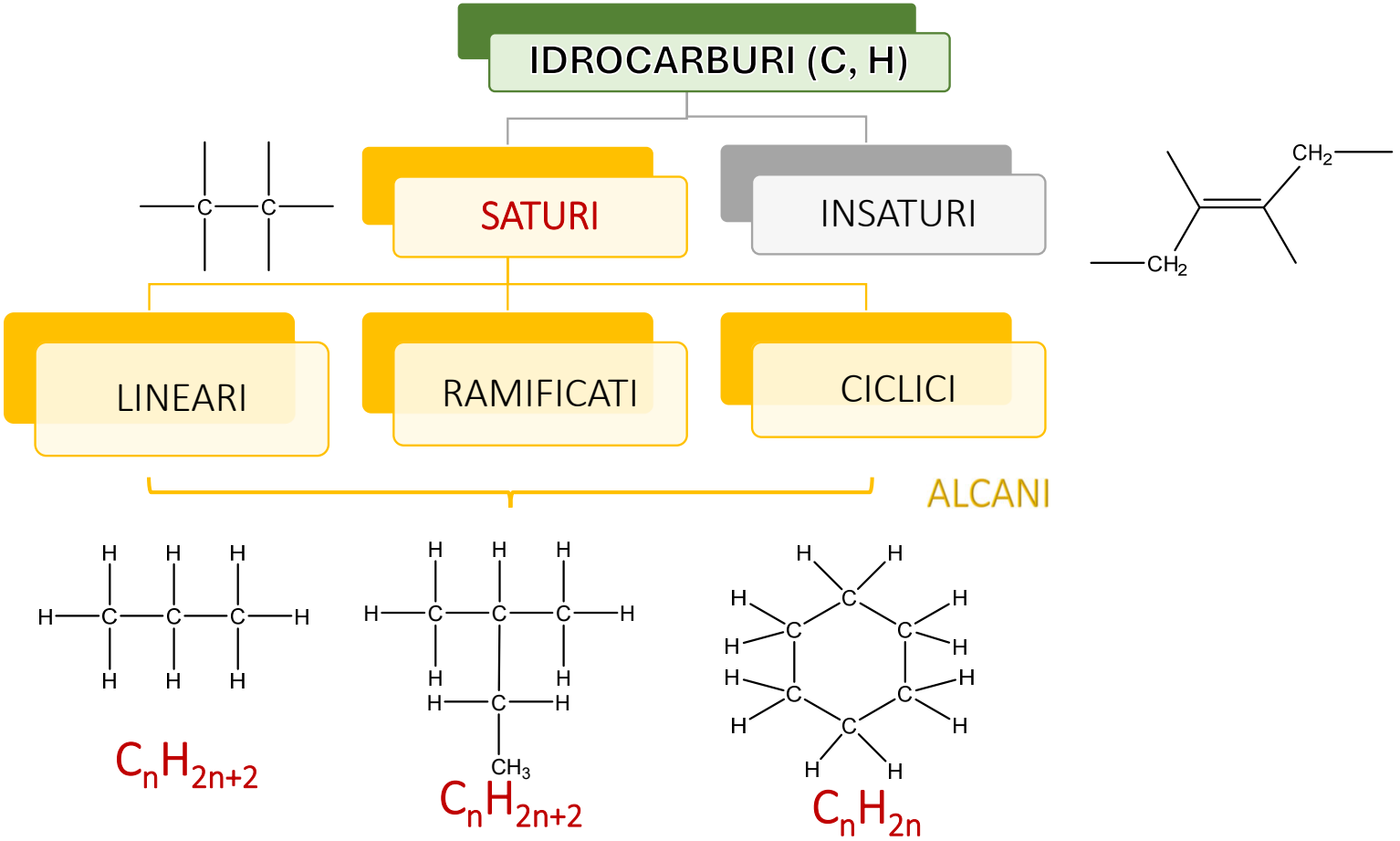
ISOCYANATE
Naming: -yl isocyanate
e.g. ethyl isocyanate

AZO COMPOUND
Naming: azo-
e.g. azoethane

THIOL
Naming: -thiol
e.g. methanethiol



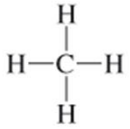
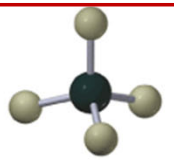
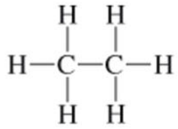
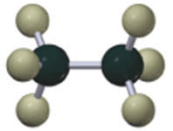
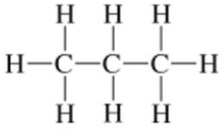
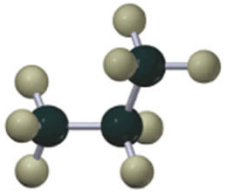
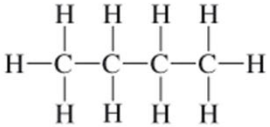
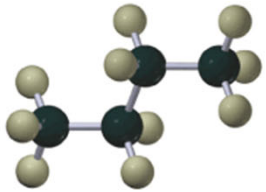
ARENE
Naming: -yl benzene
e.g. ethyl benzene


IDROCARBURI (C, H)
SATURI
INSATURI
LINEARI
RAMIFICATI
CICLICI
ALCANI
C_nH_{2n+2}
C_nH_{2n+2}
C_nH_{2n}

Formula generale: C_nH_{2n+2}

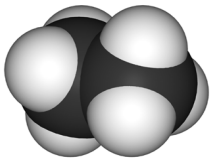
NOMENCLATURA

n=1-4

nome	struttura di Kekulé	struttura condensata	modello a sfere e bastoncini
metano		CH_4	
etano		CH_3CH_3	
propano		$CH_3CH_2CH_3$	
butano		$CH_3CH_2CH_2CH_3$	

n>5 *numero latino*-ano

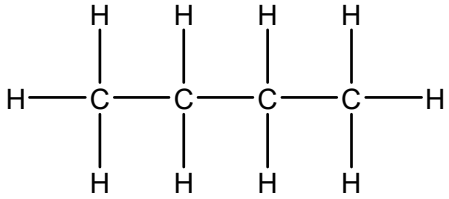
3D



mostrano NUVOLE ELETTRONICHE

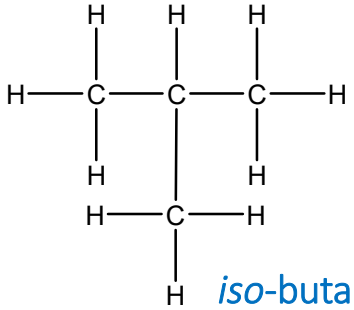
mostrano solo la posizione dei nuclei

A una STESSA formula bruta possono corrispondere DIVERSE formule di struttura



butano

C_4H_{10}



iso-butano

le 2 molecole contengono lo **STESSO NUMERO** e lo STESSO TIPO di atomi
ma
gli atomi sono **LEGATI** tra loro in **MODO DIFFERENTE**

ISOMERI COSTITUZIONALI

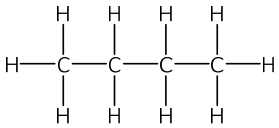
All'aumentare del numero di atomi di C aumenta esponenzialmente il numero di isomeri

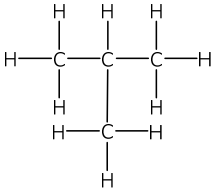
ISOMERI COSTITUZIONALI

STESSA FORMULA BRUTA, DIVERSE PROPRIETÀ

scheletro carbonioso diverso

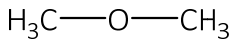
C_4H_{10}

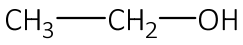




diversi gruppi funzionali

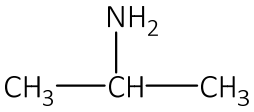
C_2H_6O

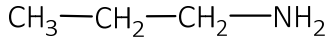




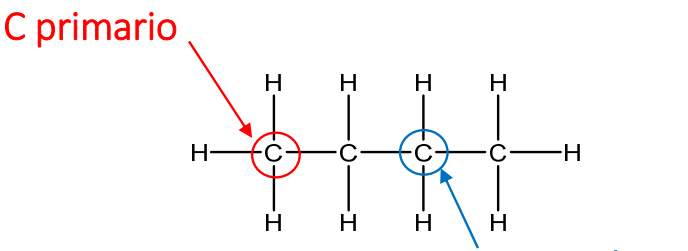
diversa posizione dei gruppi funzionali

C_3H_9N

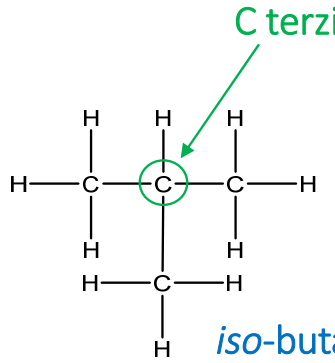




Occorre individuare REGOLE che permettano di correlare in modo univoco nome e formula di struttura



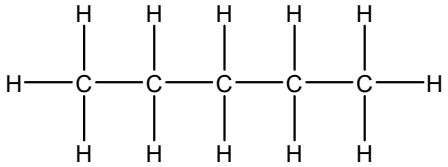
butano



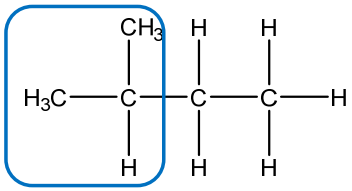
iso-butano

GLI ISOMERI COSTITUZIONALI SONO COMPOSTI DIVERSI CON PROPRIETÀ DIFFERENTI

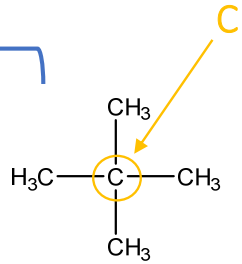
C_5H_{12}



T_{eb}=36,1°C pentano



T_{eb}=27,8°C *iso*-pentano

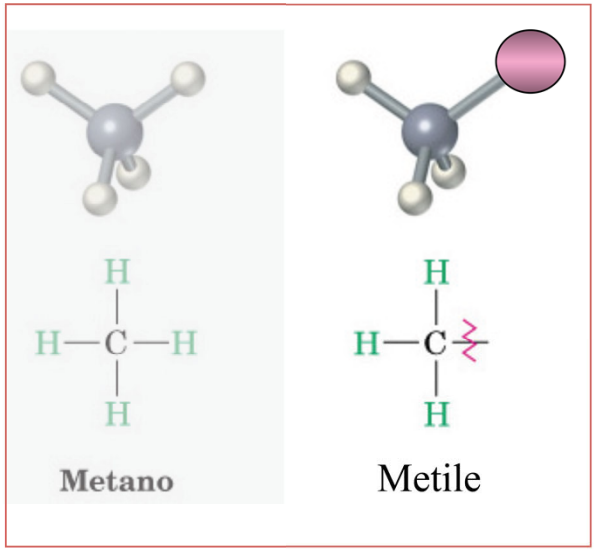


T_{eb}=9,5°C *neo*-pentano

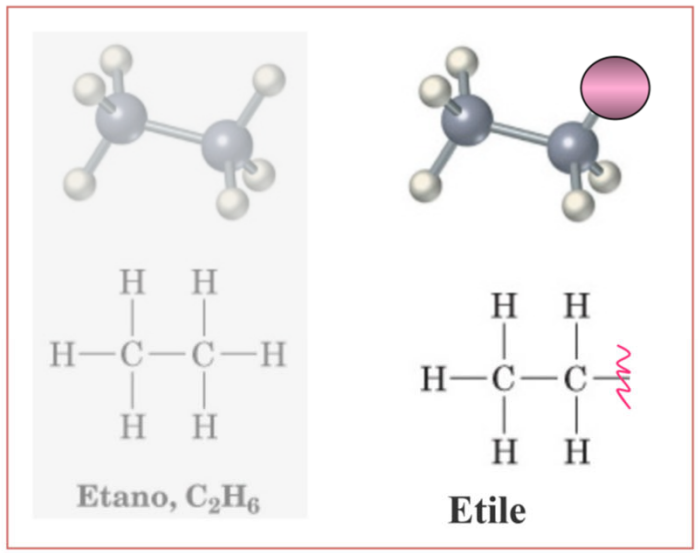
NOMENCLATURA SISTEMATICA

(IUPAC: International Union Pure and Applied Chemistry)

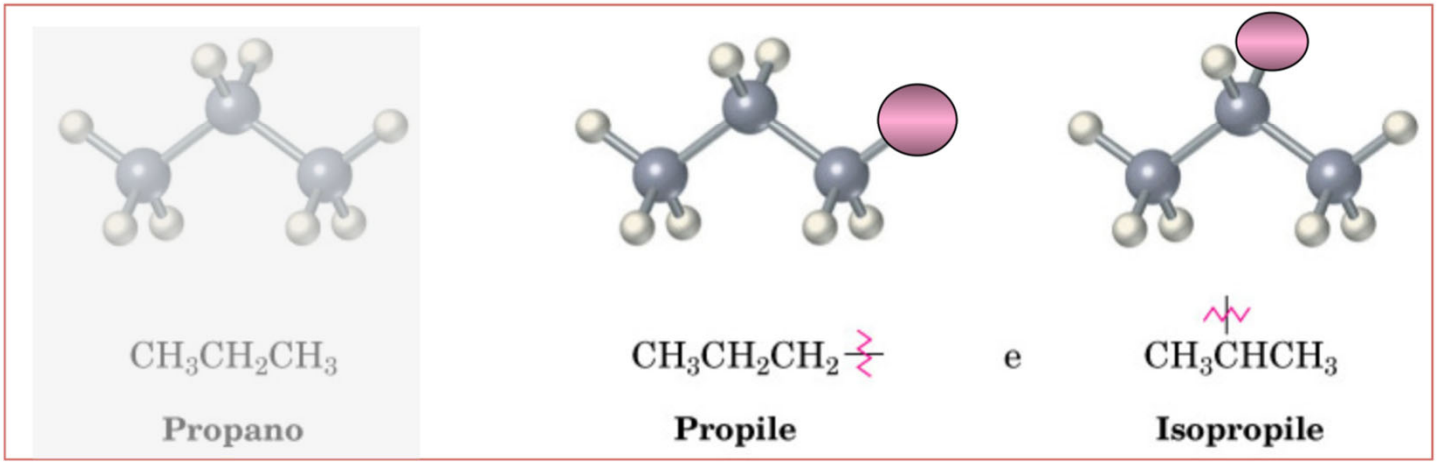
Per rimozione di un idrogeno da un alcano si ottiene un SOSTITUENTE ALCHILICO



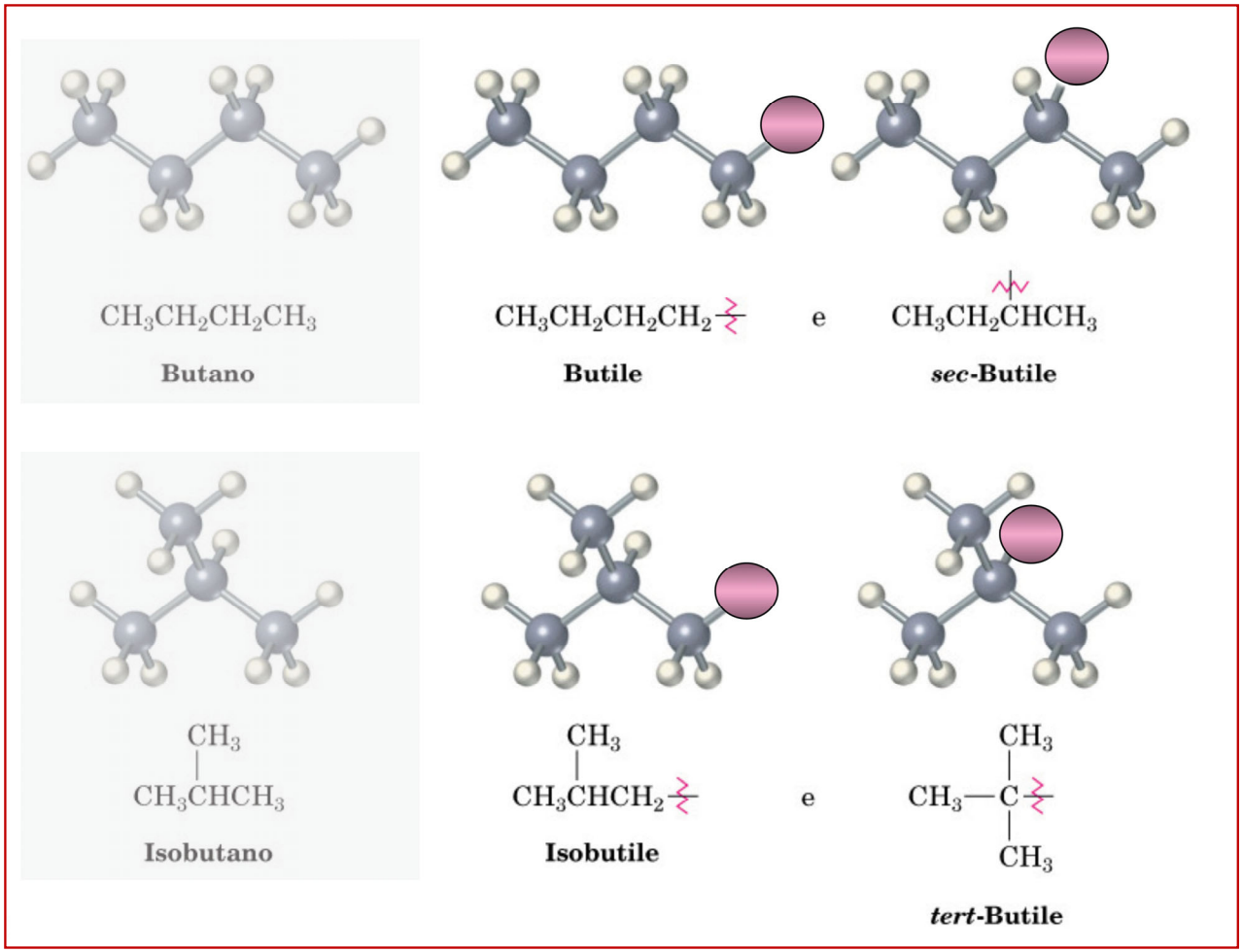
Il nome si ottiene sostituendo la desinenza –ano dell'alcano con il suffisso -ile



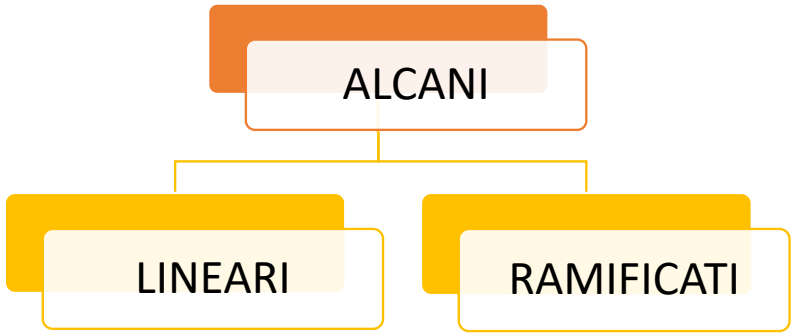
C3



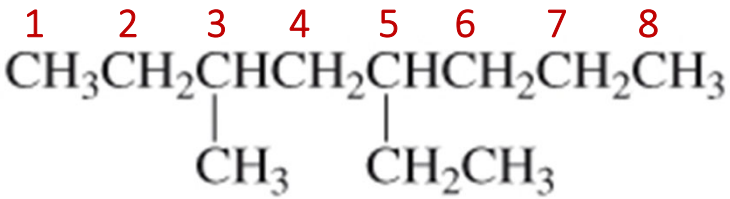
C4


$CH_3CH_2CH_2CH_3$
Butano
$CH_3CH_2CH_2CH_2$
Butile
e
$CH_3CH_2CHCH_3$
sec-Butile
CH_3
CH_3CHCH_3
Isobutano
CH_3
CH_3CHCH_2
Isobutile
e
CH_3
$CH_3—C$
CH_3
tert-Butile

NOMENCLATURA IUPAC



numero latino-ano

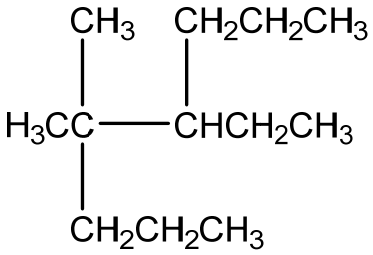


5-etil-3-metilottano
non
4-etil-6-metilottano
poiché 3 < 4

1. Individuare la catena principale (più lunga)= IDROCARBURO GENITORE
2. numerare la catena in modo che il sostituente abbia numero più basso
3. Indicare tipo e posizione del sostituente
4. I sostituenti sono elencati in ordine alfabetico (! di-, tri-…sec-, terz-…non vengono considerati)
5. Un numero e una parola sono separati da trattino; i numeri da virgola

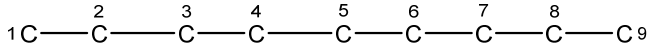
Esempi

Assegnare il nome IUPAC

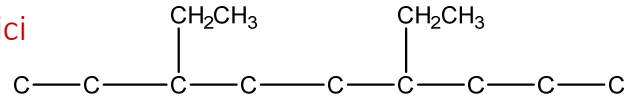


Disegnare la struttura di 3,6-dietil-3,6-dimetilnonano

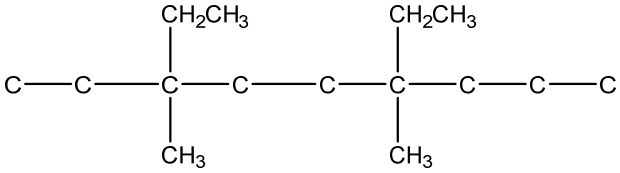
1. disegnare la catena e numerarla



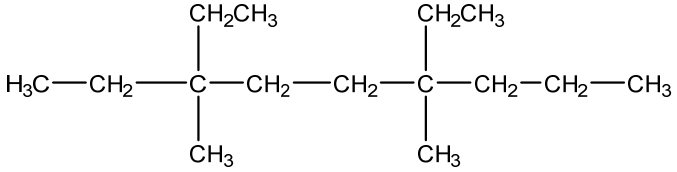
2. mettere i sostituenti etilici



3. mettere i sostituenti metilici

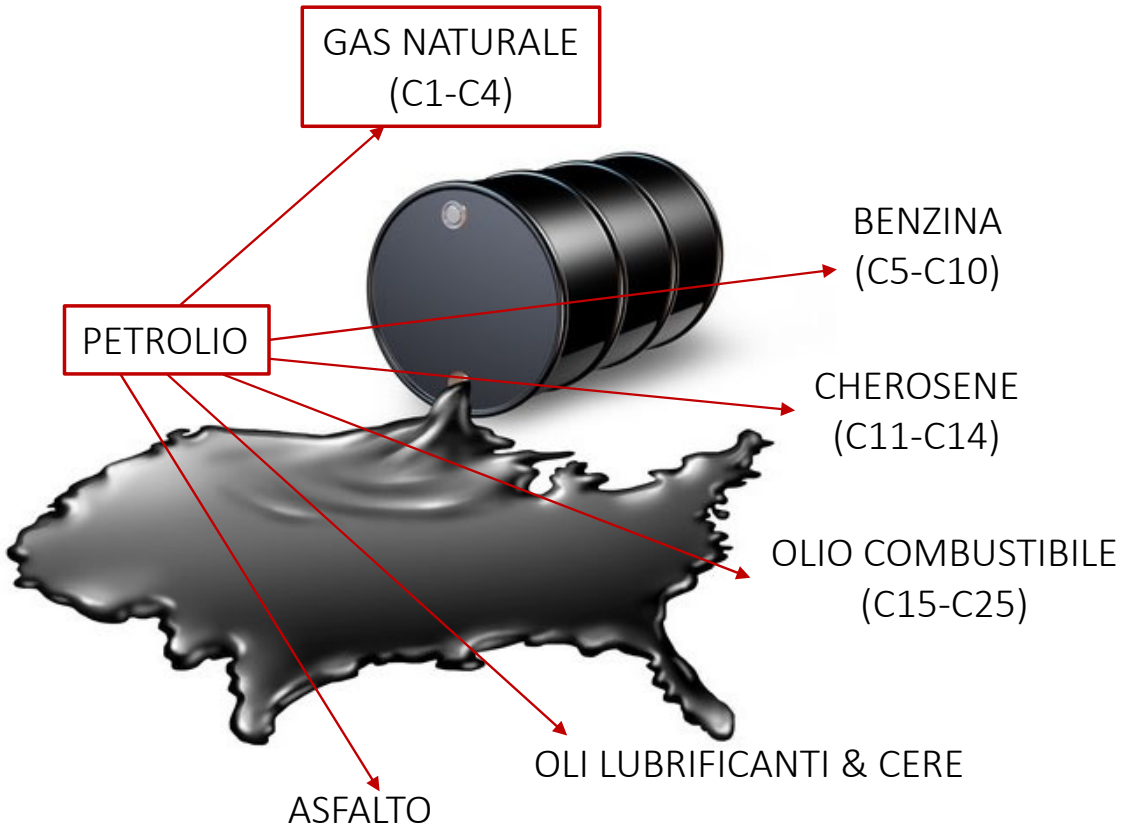


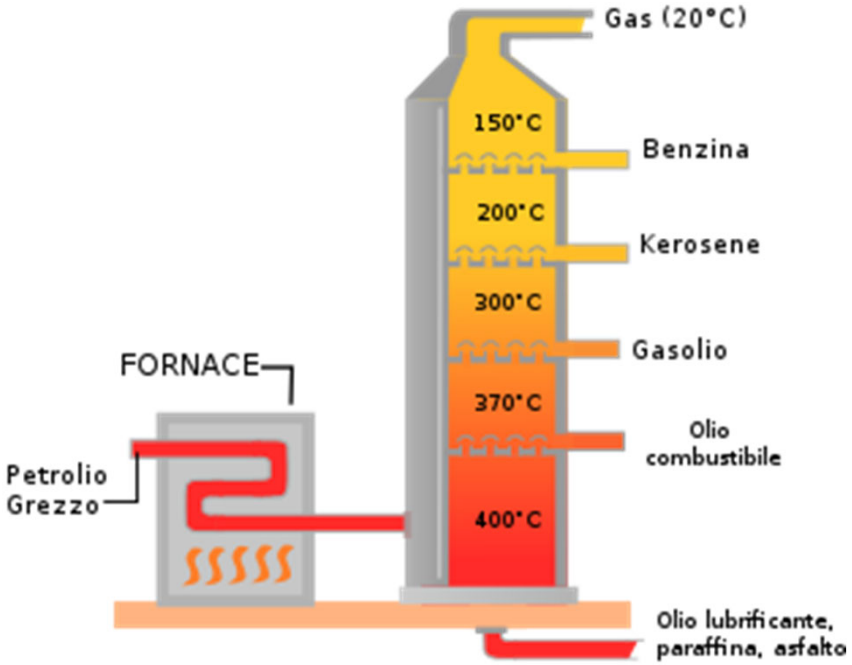
4. Aggiungere gli atomi di H necessari a completare i 4 legami per ogni C



Dove si trovano gli ALCANI?

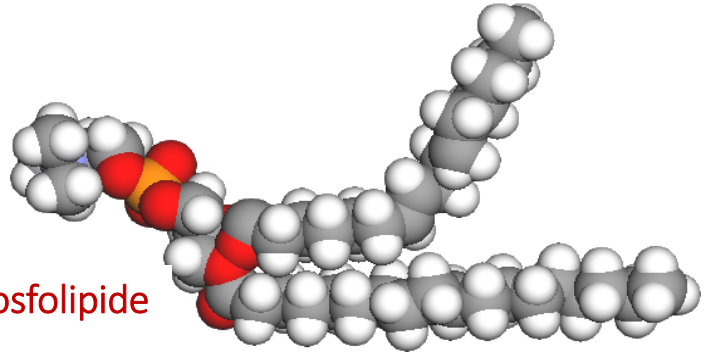
GAS NATURALE
PETROLIO
CERE VEGETALI





…. e nei sistemi biologici?

Catene alchiliche nelle molecole di LIPIDI

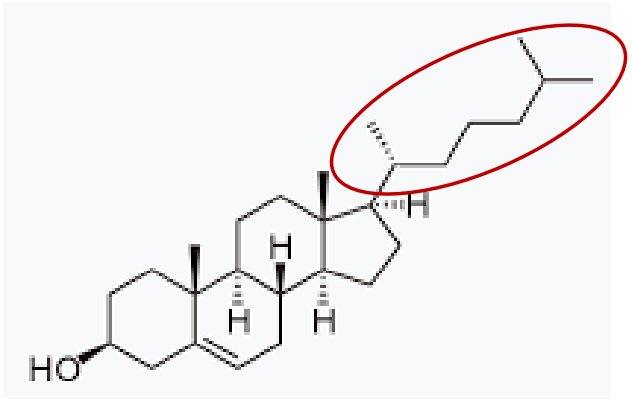


fosfolipide

Acidi grassi SATURI

palmitico

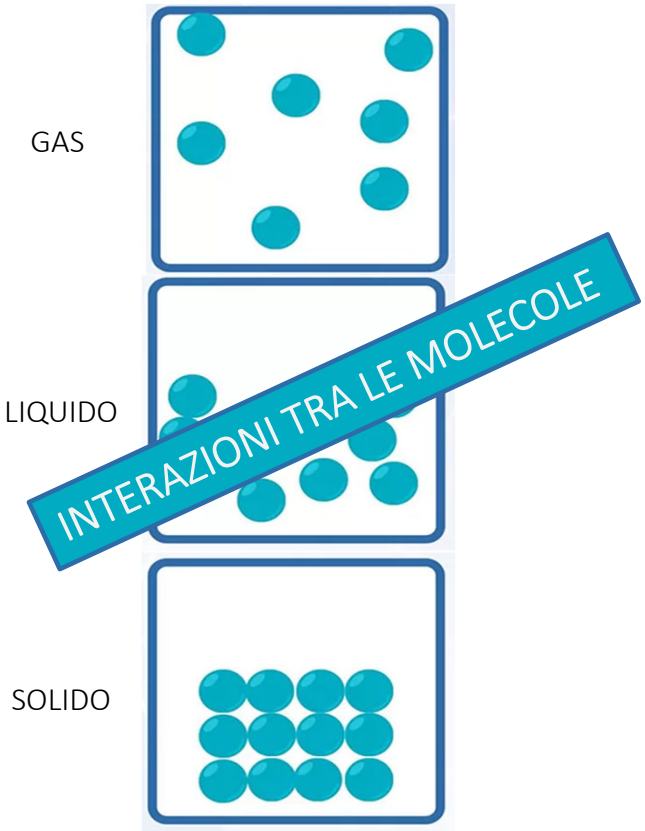
stearico



colesterolo

PROPRIETA' DEGLI IDROCARBURI

PASSAGGI DI STATO
(p. eb./p. fus.)

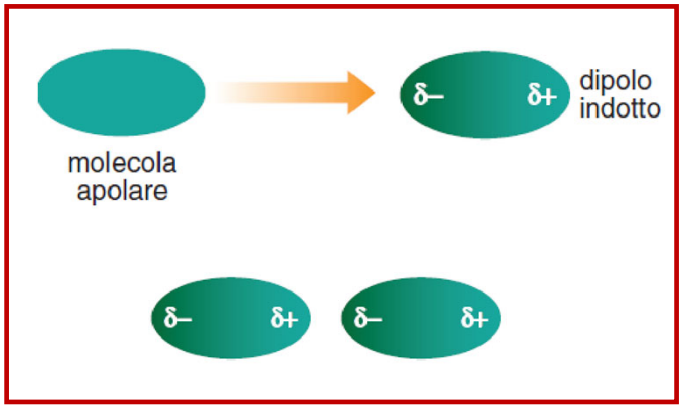


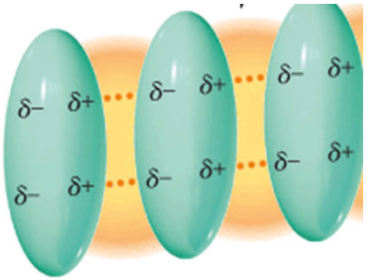
SOLUBILITA'
insolubili in acqua

FORZE INTERMOLECOLARI SONO RESPONSABILI
DELLE INTERAZIONI TRA MOLECOLE

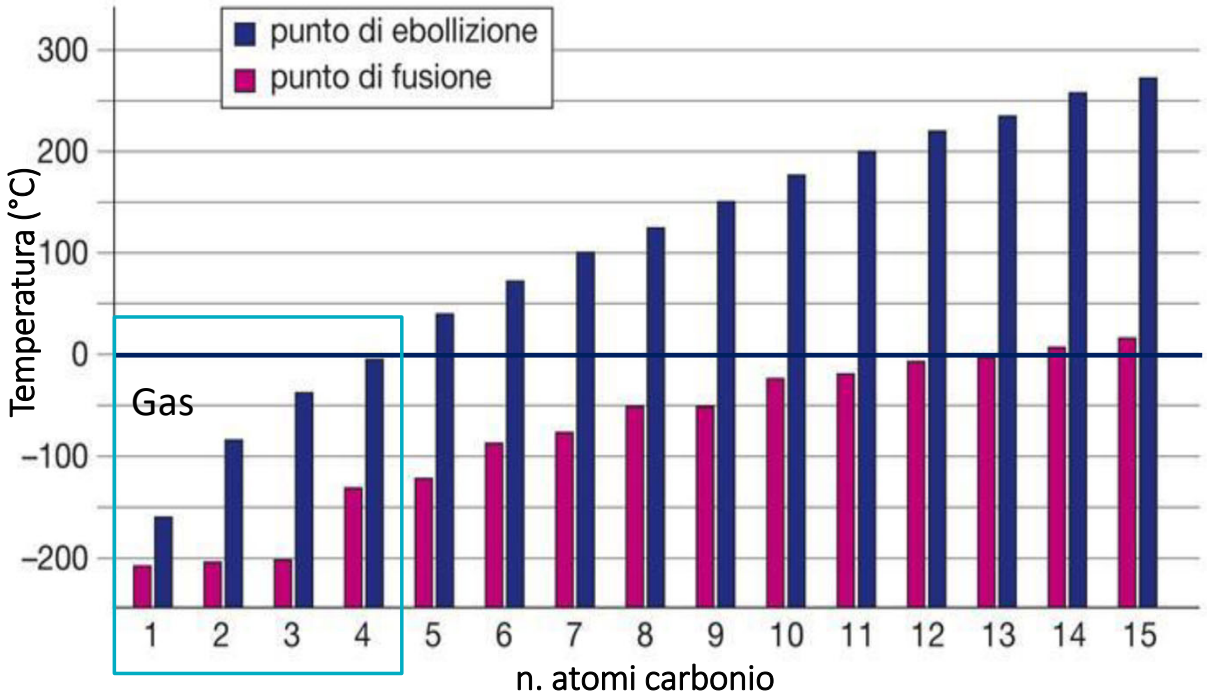
Punto di fusione e di ebollizione degli idrocarburi lineari

formazione di dipolo indotto





Interazioni tra dipoli indotti sono note come FORZE DI LONDON



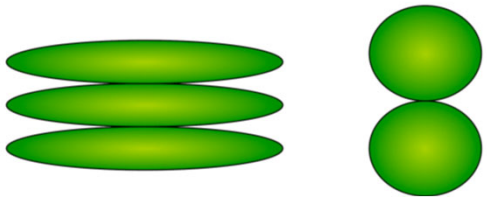
All'aumentare del numero di atomi di carbonio nella molecola aumenta il p.eb/p.f. dell'idrocarburo

Gli idrocarburi sono **molecole non-polari** e interagiscono tra loro attraverso la formazione di dipoli indotti

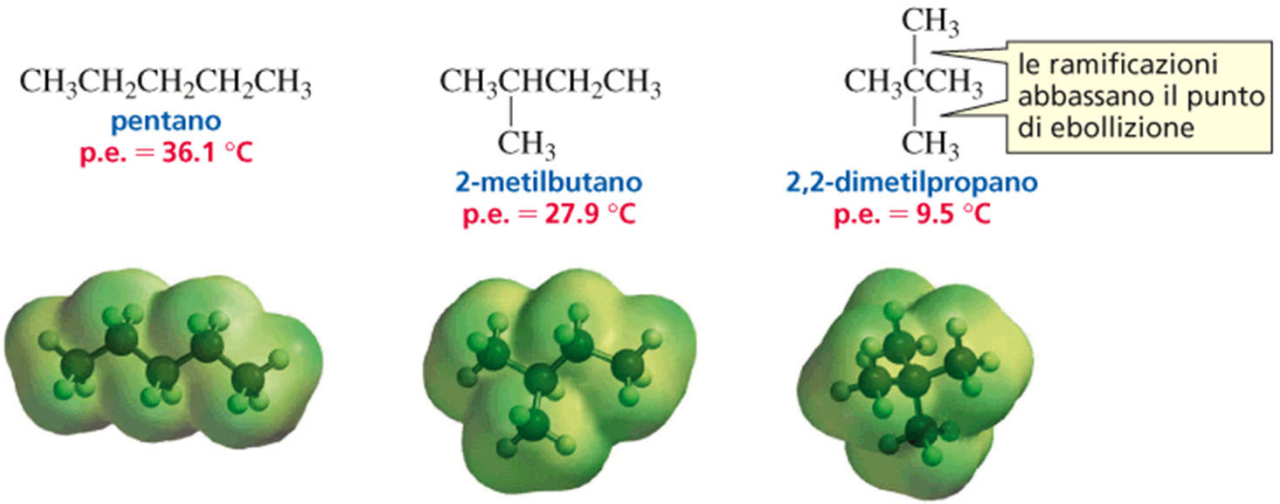
Le forze di London dipendono da:

- dal numero di elettroni nella molecola (polarizzabilità) e quindi dal suo peso molecolare (sbilanciamenti nella distribuzione elettronica più probabili)

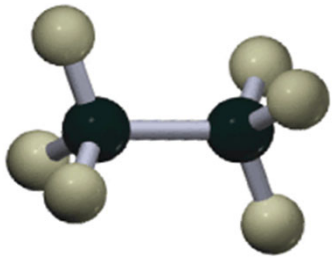
- dalla superficie di contatto tra le molecole



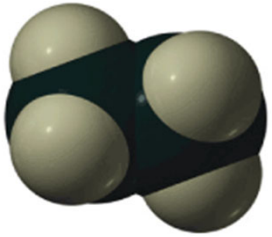
A PARITA' DI ATOMI DI CARBONIO E' IMPORTANTE
LA FORMA DELLA MOLECOLA



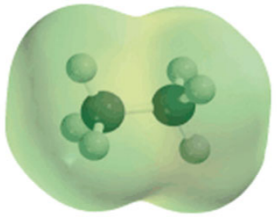
RAPPRESENTAZIONE 3D DELLE MOLECOLE NELLO SPAZIO



modello a sfere e bastoncini



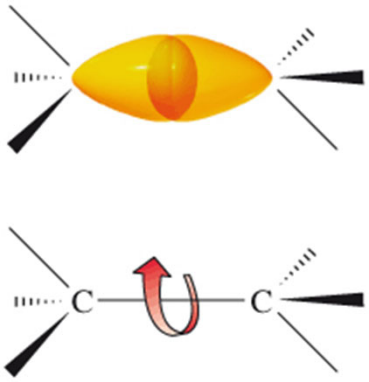
modello a spazio pieno



mappa di potenziale elettrostatico

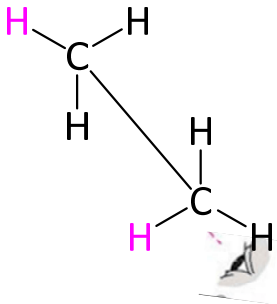
Ognuna di queste rappresentazioni fornisce una *fotografia* della molecola in *un certo istante*

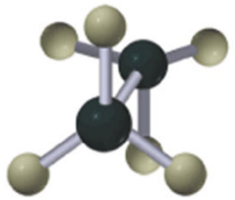
…ma le molecole sono in continuo movimento….



c'è **libera rotazione** attorno ai legami **σ** e gli atomi tendono a disporsi in modo da **rendere minime le tensioni**

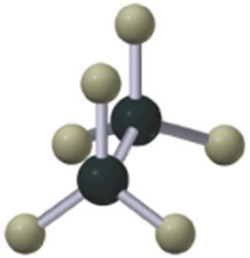
Le diverse disposizioni degli atomi nello spazio sono dette CONFORMAZIONI



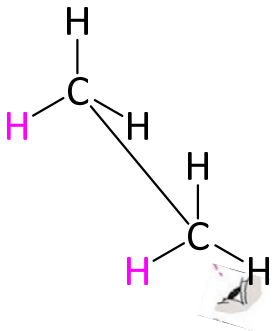


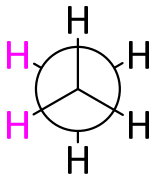
conformero sfalsato

le conformazioni hanno
DIVERSA ENERGIA



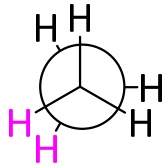
conformero eclissato





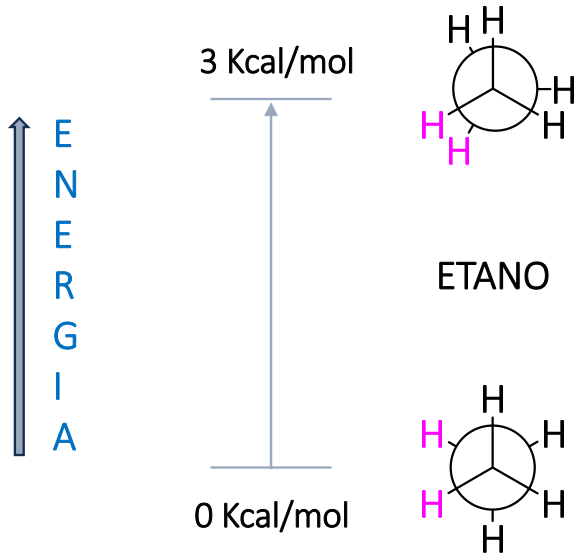
Proiezioni di Newman

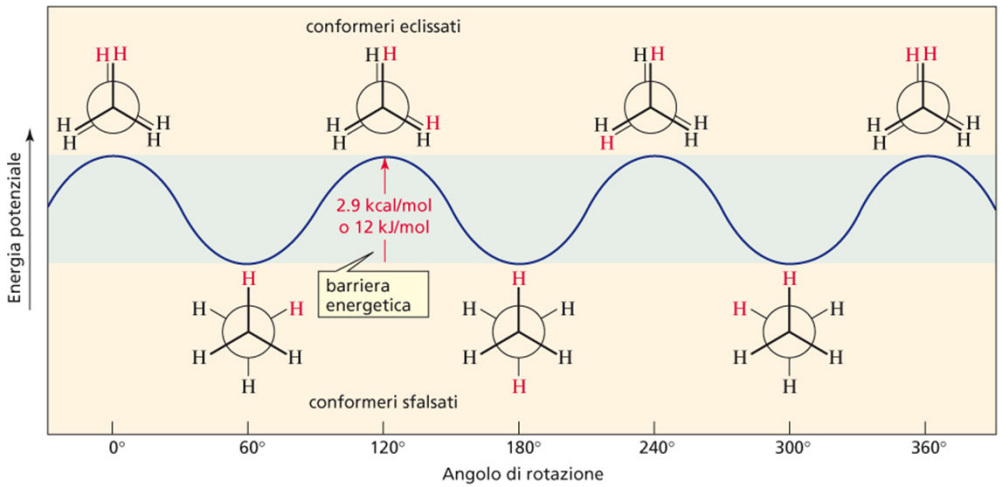
La molecola viene osservata lungo un legame C-C



CONFORMERI

La diversa energia dipende dalla **repulsione** tra le coppie di elettroni di legame, ovvero dalla TENSIONE TORSIONALE





In ogni istante il **99%** delle molecole di etano sarà in **conformazione sfalsata** (più stabile) e solo 1% in conformazione eclissata (più alta energia)

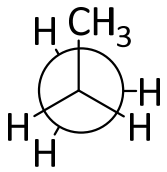
PIU' LE MOLECOLE SONO COMPLESSE PIU' AUMENTA IL NUMERO DEI CONFORMERI

$H_3C-CH_2-CH_3$

ENERGIA

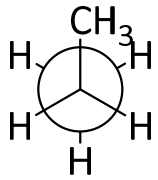
3.4 Kcal/mol
(14.2 KJ/mol)

0 Kcal/mol

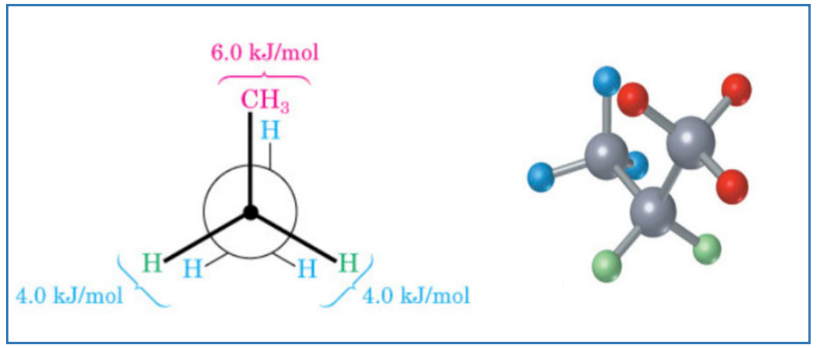


eclissata

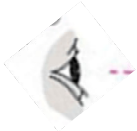
PROPANO



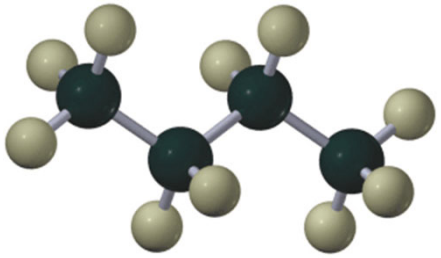
sfalsata



Nella forma eclissata oltre alle tensione torsionale (elettroni dei legami) c'è anche TENSIONE STERICA dovuta all'ingombrante gruppo metilico

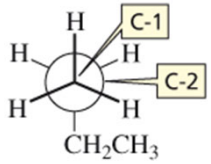


$H_3C{-}CH_2{-}CH_2{-}CH_3$

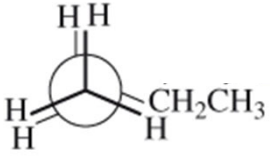


$H_3C{-}CH_2{-}CH_2{-}CH_3$

C1-C2



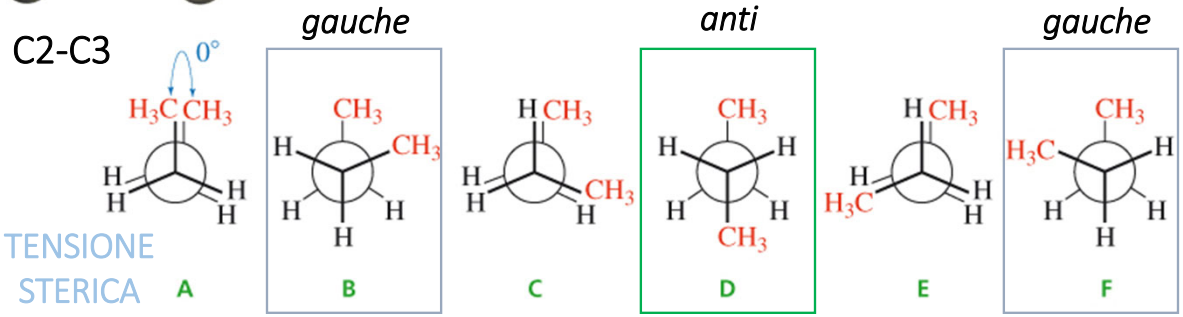
conformazione sfalsata



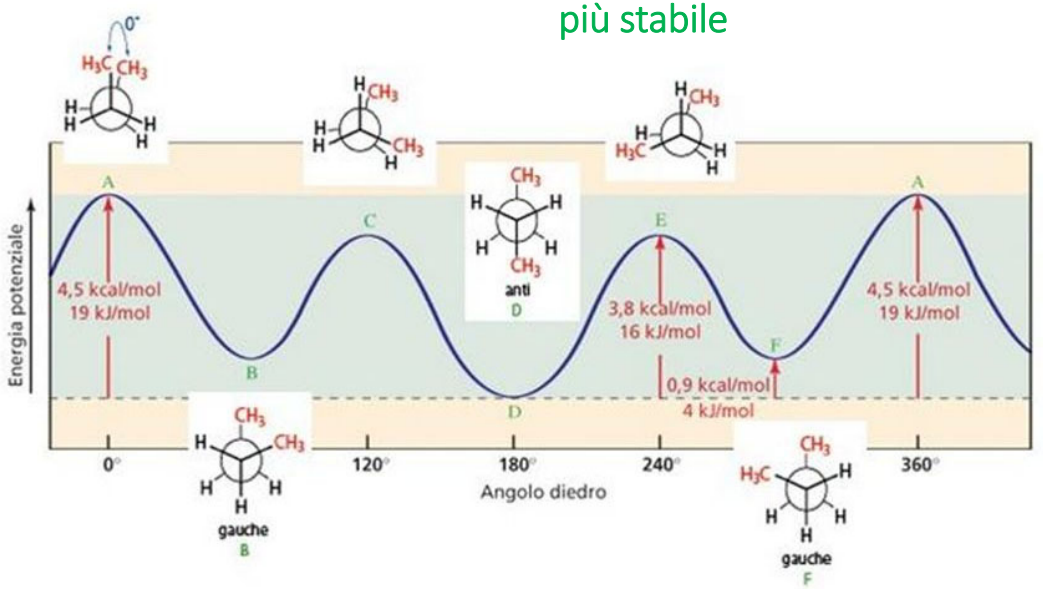
conformazione eclissata

TENSIONE TORSIONALE

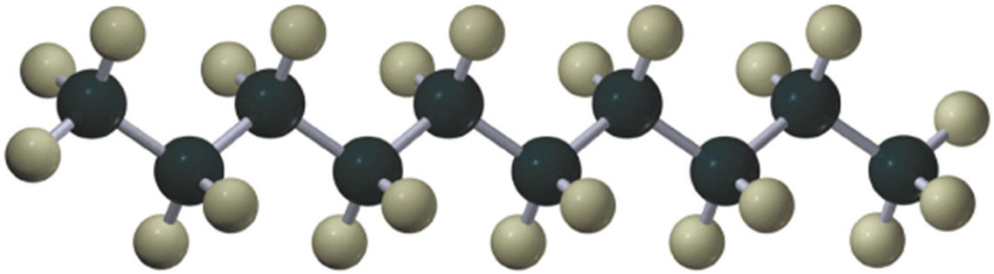
C2-C3



L'energia dei diversi conformeri (C2-C3) dipende dai diversi contributi della **tensione torsionale** e della **tensione sterica**



ALCANI A LUNGA CATENA



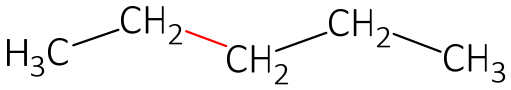
DECANO

In soluzione esistono molto conformazioni in equilibrio tra loro.
In ogni istante sarà maggiore la % di molecole nella conformazione più stabile

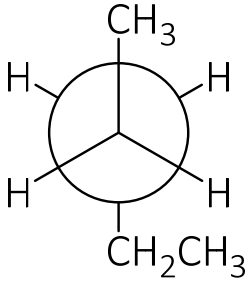
La conformazione a minore energia (quindi più stabile) è quella completamente sfalsata (*anti*)

Orientamento a zig-zag della catena di atomi di C

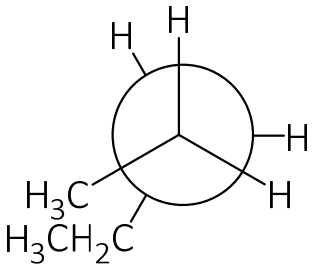
Esempi



Scrivere il conformero PIU' stabile ottenuto per rotazione attorno al legame C2-C3

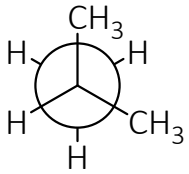


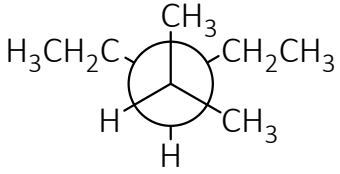
Scrivere il conformero MENO stabile ottenuto per rotazione attorno al legame C2-C3

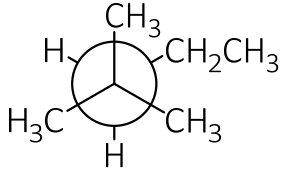


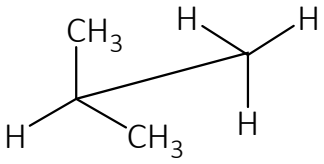
Esempi

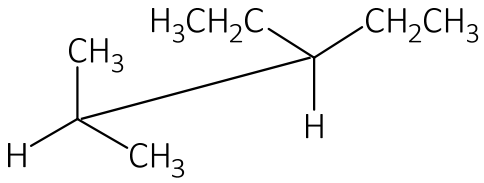
Convertire le seguenti proiezioni di Newman in strutture a segmenti:

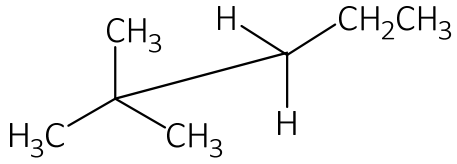










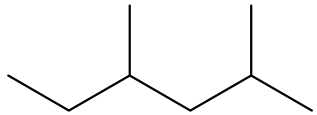


Esercizi

Il singolo legame N-H nella metilamina (CH_3NH_2) è un legame _____ formato dalla sovrapposizione di un orbitale _____ dell'azoto e di un orbitale _____ dell'idrogeno.

A. σ; sp^3; s
B. π; sp^2; s
C. σ; p; p
D. π; sp^3; s

Qual è il nome corretto da assegnare al seguente composto:



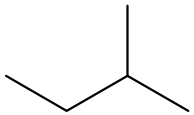
a. 2,4-dimetilesano
b. 3,5-dimetilesano
c. 2-etil-4-metilpentano

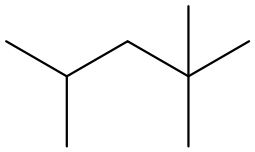
Quale dei seguenti composti ha il più basso punto di ebollizione?

a. $CH_3CH(CH_3)CH(CH_3)CH_3$
b. $CH_3CH_2CH_2CH(CH_3)_2$
c. $CH_3CH_2CH_2CH_2CH_2CH_3$
d. $CH_3CH_2CH(CH_3)CH_2CH_3$

Disegna le formule di struttura degli isomeri costituzionali con formula molecolare C_6H_{14}

Individua nei seguenti composti gli atomi di C primari, secondari, terziari e quaternari





Scrivi la formula molecolare corrispondente ai seguenti alcani: