

3 Gesättigte Kohlenwasserstoffe

3.1 Lineare und verzweigte Alkane

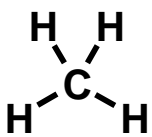
Summenformel	Konstitutionsformel	Bezeichnung
CH_4	CH_4	Methan
C_2H_6	$\text{CH}_3\text{-CH}_3$	Ethan
C_3H_8	$\text{CH}_3\text{-CH}_2\text{-CH}_3$	Propan
C_4H_{10}	$\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-CH}_3$	n-Butan
C_5H_{12}	$\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_3$	n-Pentan
C_6H_{14}	$\text{CH}_3\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_3$	n-Hexan
C_7H_{16}	$\text{CH}_3\text{-(CH}_2\text{)}_5\text{-CH}_3$	n-Heptan
C_8H_{18}	$\text{CH}_3\text{-(CH}_2\text{)}_6\text{-CH}_3$	n-Octan
C_9H_{20}	$\text{CH}_3\text{-(CH}_2\text{)}_7\text{-CH}_3$	n-Nonan
$\text{C}_{10}\text{H}_{22}$	$\text{CH}_3\text{-(CH}_2\text{)}_8\text{-CH}_3$	n-Decan
$\text{C}_{20}\text{H}_{42}$	$\text{CH}_3\text{-(CH}_2\text{)}_{18}\text{-CH}_3$	n-Eicosan
$\text{C}_{30}\text{H}_{62}$	$\text{CH}_3\text{-(CH}_2\text{)}_{28}\text{-CH}_3$	n-Triacontan
$\text{C}_n\text{H}_{2n+2}$	$\text{CH}_3\text{-(CH}_2\text{)}_{n-2}\text{-CH}_3$	n-Alkan

Homologe Reihe der geradkettigen Alkane

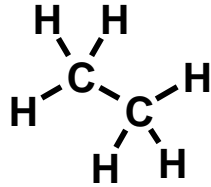
3 Gesättigte Kohlenwasserstoffe

Gesättigte, offenkettige Verbindungen: C_nH_{2n+2}

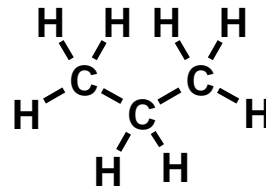
Siedepunkt steigt mit Kettenlänge um 20-30°C pro CH_2 -Gruppe an (Ethan, Propan, Butan: Gase; Pentan-Heptadecan: Flüssigkeiten; ab Octadecan: Feststoffe)



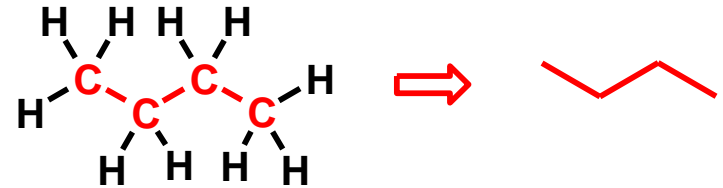
Methan
 CH_4



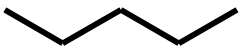
Ethan
 C_2H_6



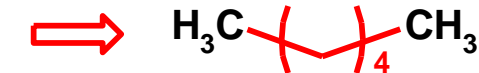
Propan
 C_3H_8



n-Butan
 C_4H_{10}



n-Pentan
 C_5H_{12}



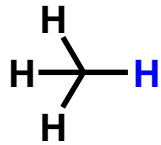
n-Hexan
 C_6H_{14}



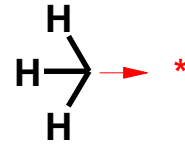
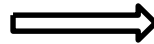
n-Dodecan
 $C_{12}H_{26}$

3 Gesättigte Kohlenwasserstoffe

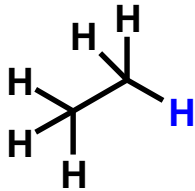
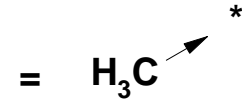
Bezeichnung von Alkylresten



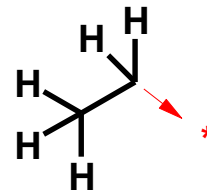
Meth **an**



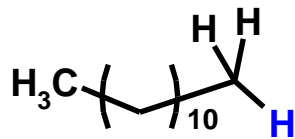
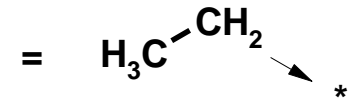
Meth **yl**



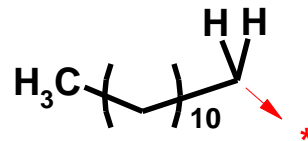
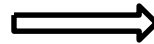
Eth **an**



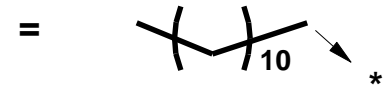
Eth **yl**



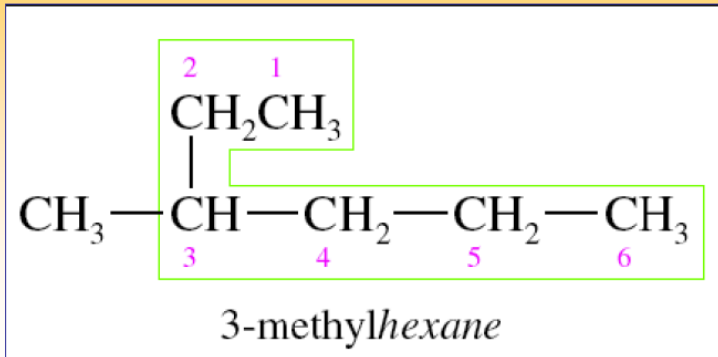
Dodec **an**



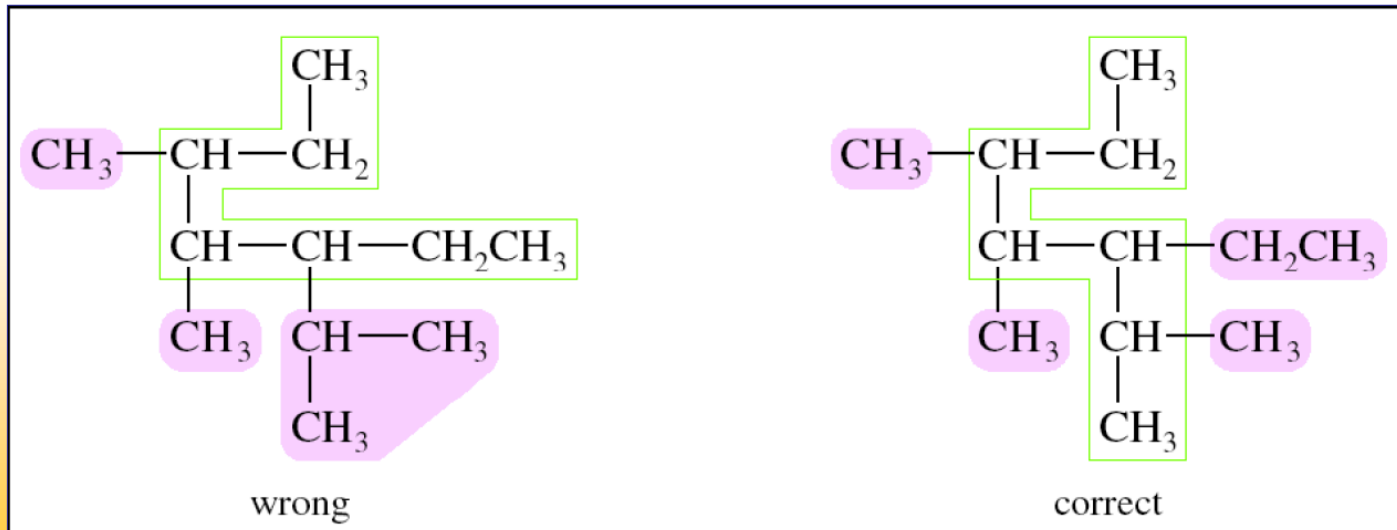
Dodec **yl**



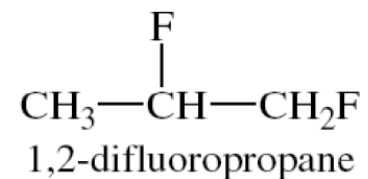
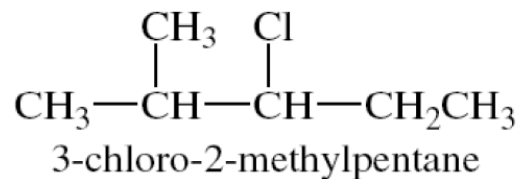
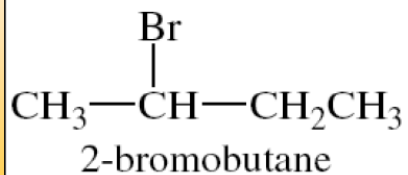
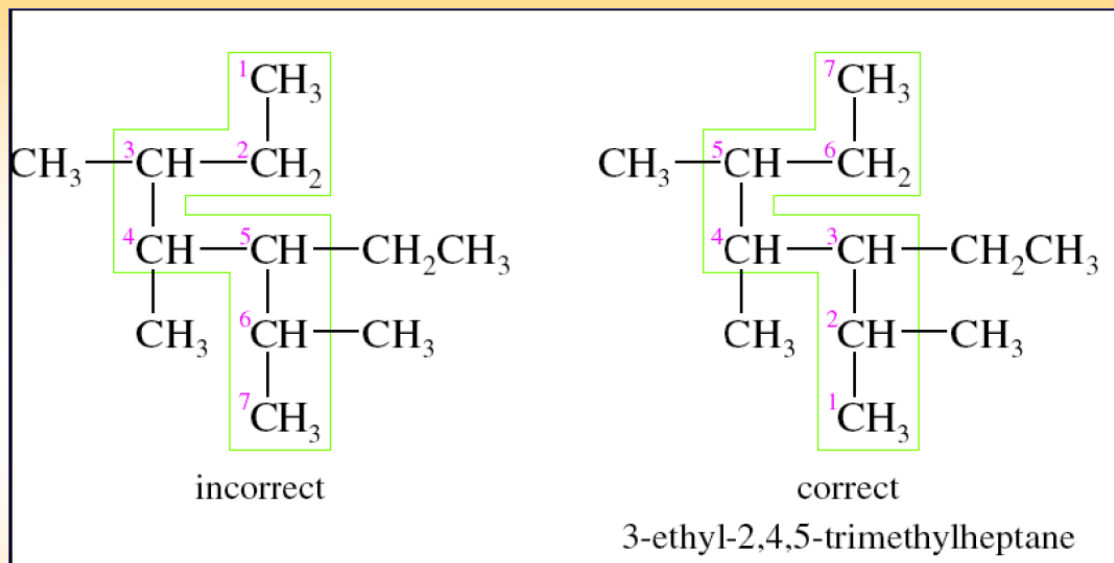
IUPAC Regeln



gleich lange Ketten:
diejenige mit den meisten
Substituenten wählen

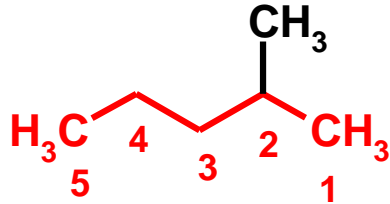


IUPAC Regeln

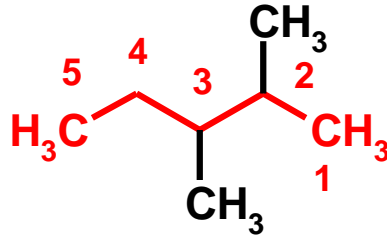


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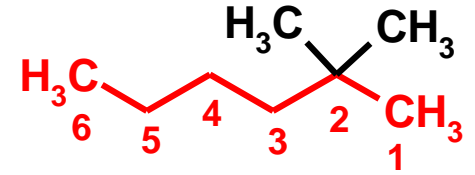
Benennung verzweigter Alkane



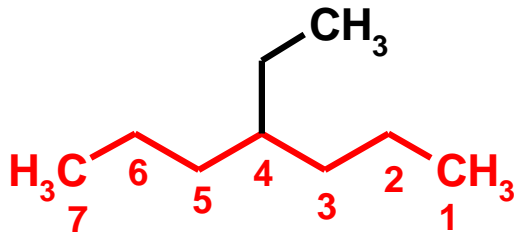
2-Methyl **pentan**



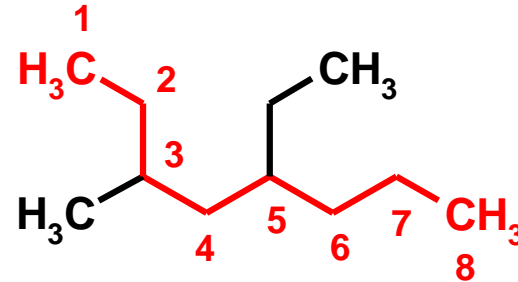
2,3-Dimethyl **pentan**



2,2-Dimethyl **hexan**



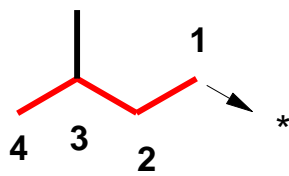
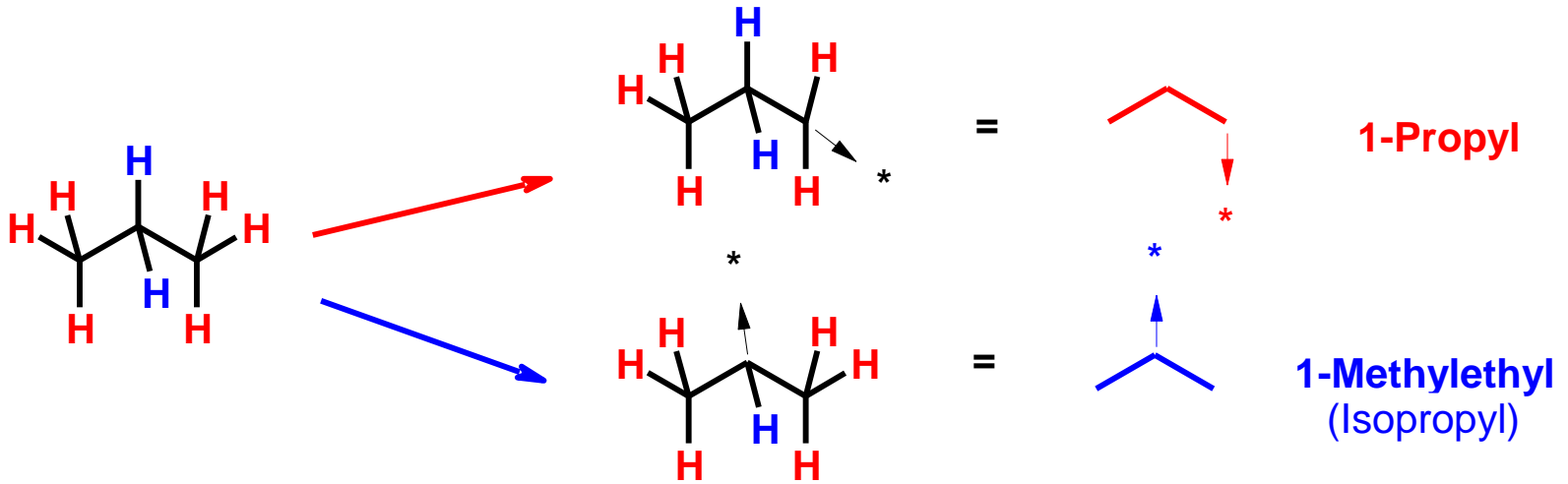
4-Ethyl **heptan**



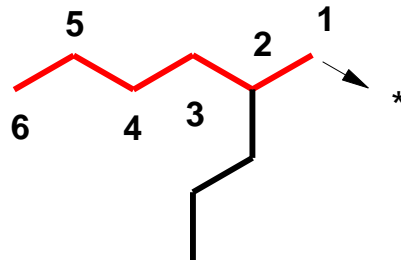
5-Ethyl-3-methyl **octan**

3 Gesättigte Kohlenwasserstoffe

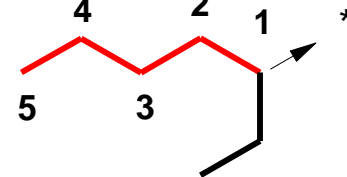
Benennung verzweigter Alkylreste



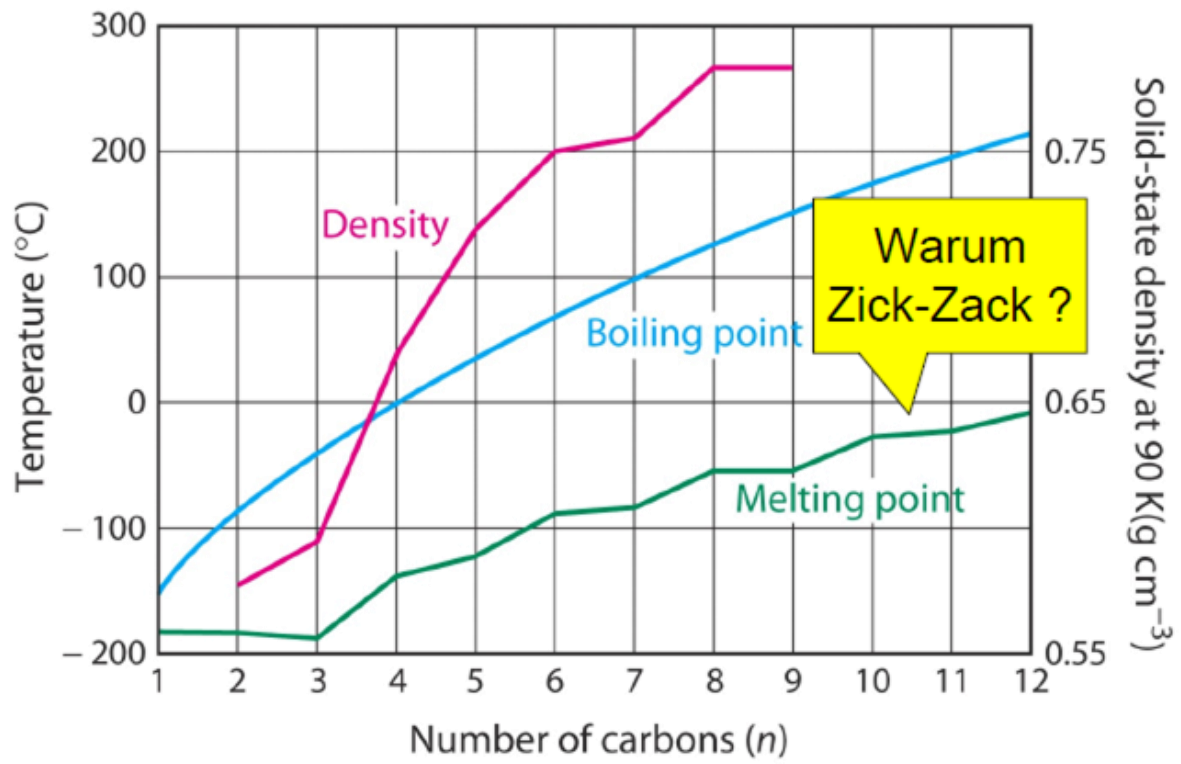
3-Methyl butyl



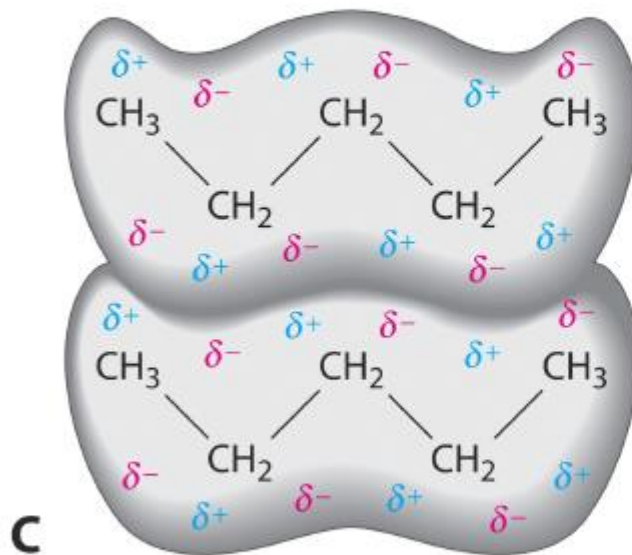
2-Propyl hexyl



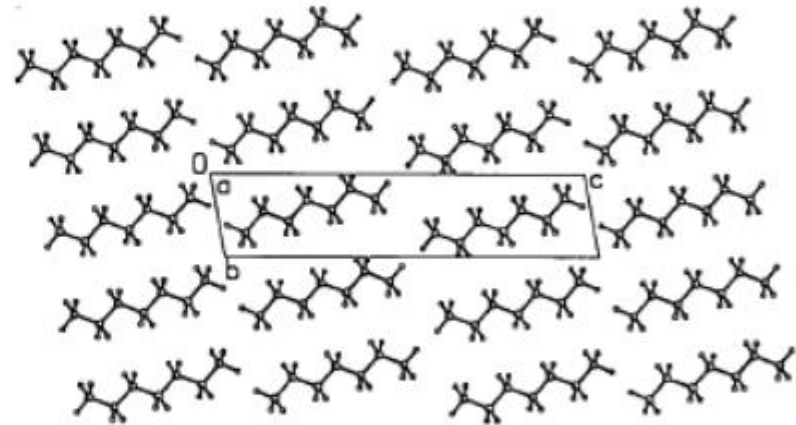
1-Ethyl pentyl



London-Kräfte



Idealisiertes
Pentan

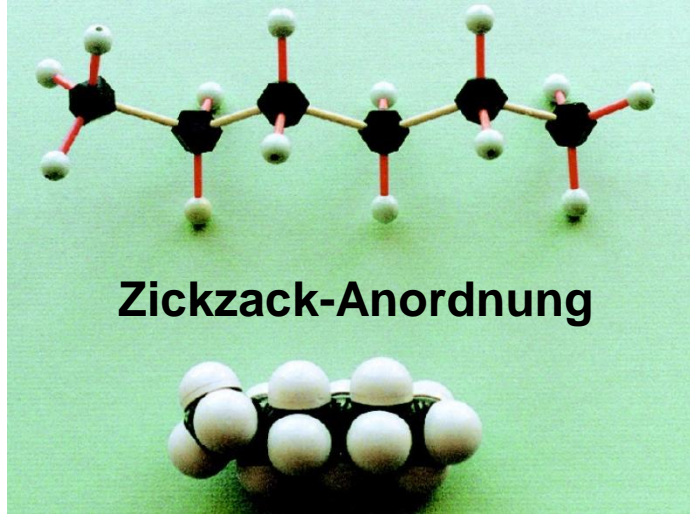


Experimentell:
Heptan

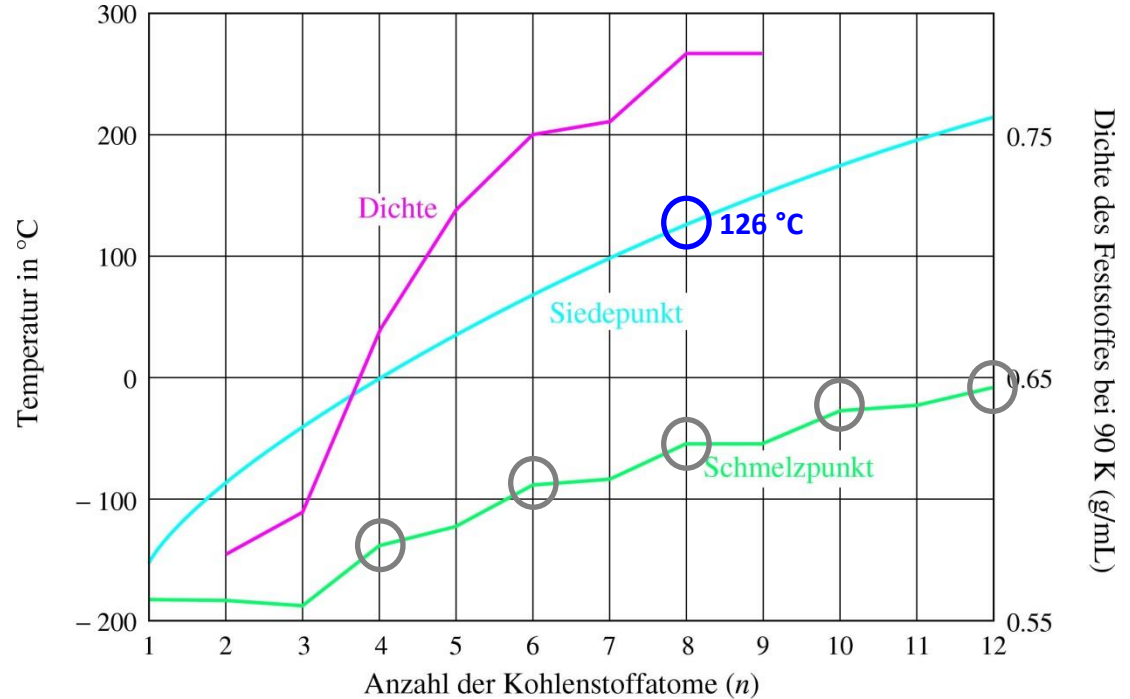
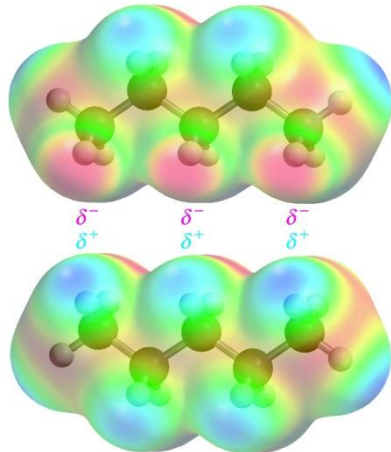
Spontane Polarisation von unpolaren Teilchen (induzierte Dipole) = Anziehung von aliphatischen Ketten!

3 Gesättigte Kohlenwasserstoffe

3.1.3 Struktur und physikalische Eigenschaften der linearen Alkane



Intermolekulare **van-der-Waals-Wechselwirkungen** (2 kJ/ mol/ CH₂-Gruppe)

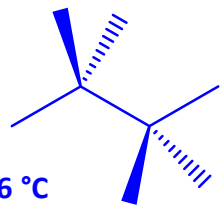


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Struktur-Eigenschafts-Beziehungen:
physikalische Eigenschaften in Abhängigkeit
von der Kettenlänge bzw. Molekulargewicht

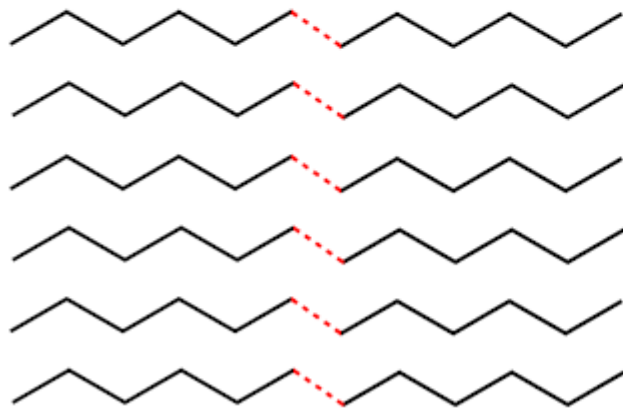
Verzweigte Alkane

Sdp. 106 °C

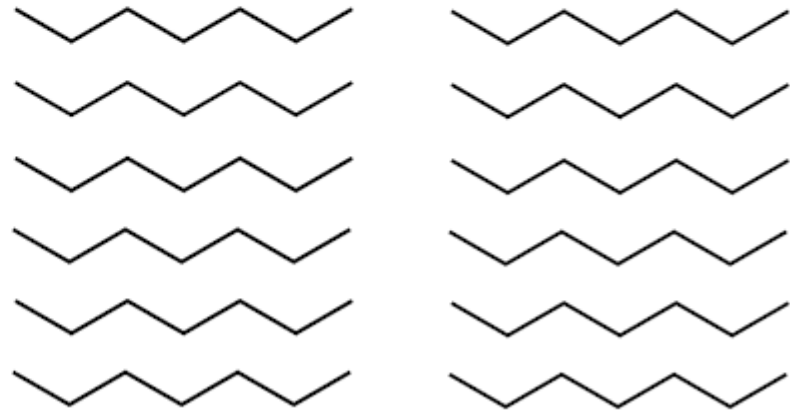


Smp gerade/ungerade Alkane

Hexan

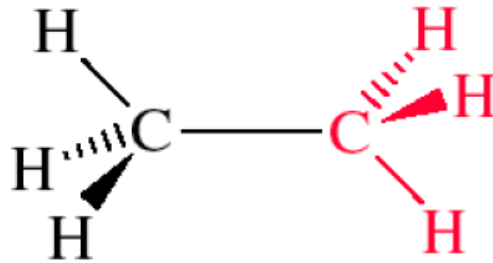


Heptan

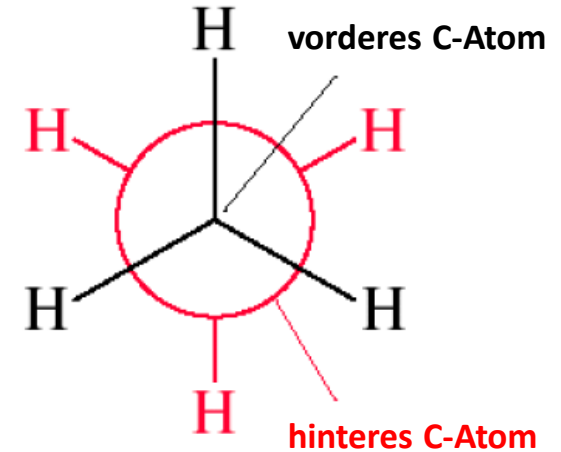


Gesättigte Kohlenstoffketten: Ethan

Newman-Projektion



=



vom Ende betrachten

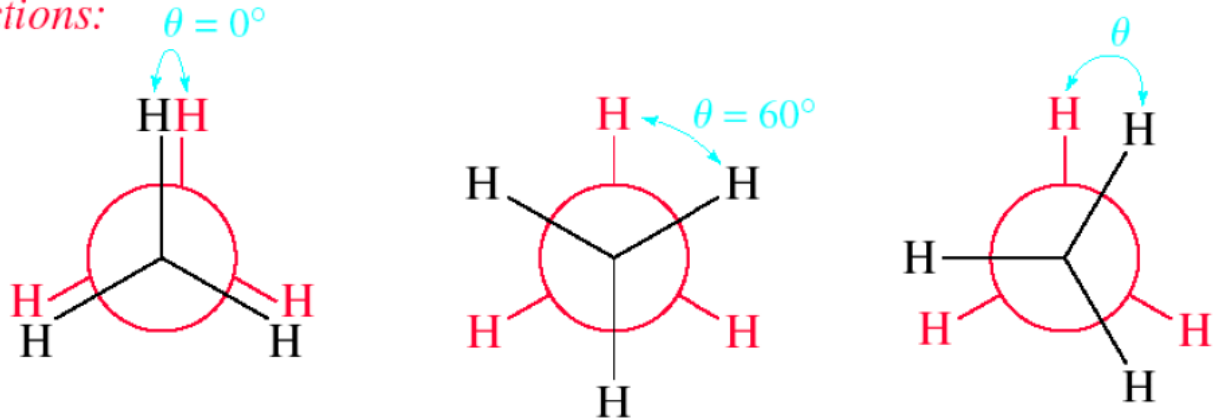
Keil/Strich-Schreibweise
zur räumlichen
Klarstellung

Newman Projektion

Gesättigte Kohlenstoffketten: Ethan

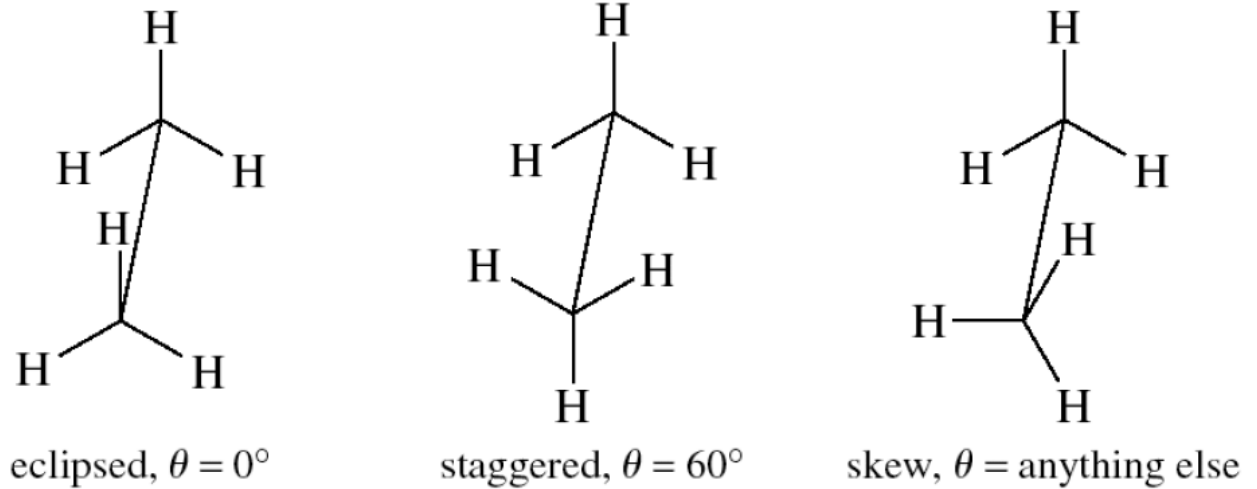
Newman projections: $\theta = 0^\circ$

Newman-Projektion



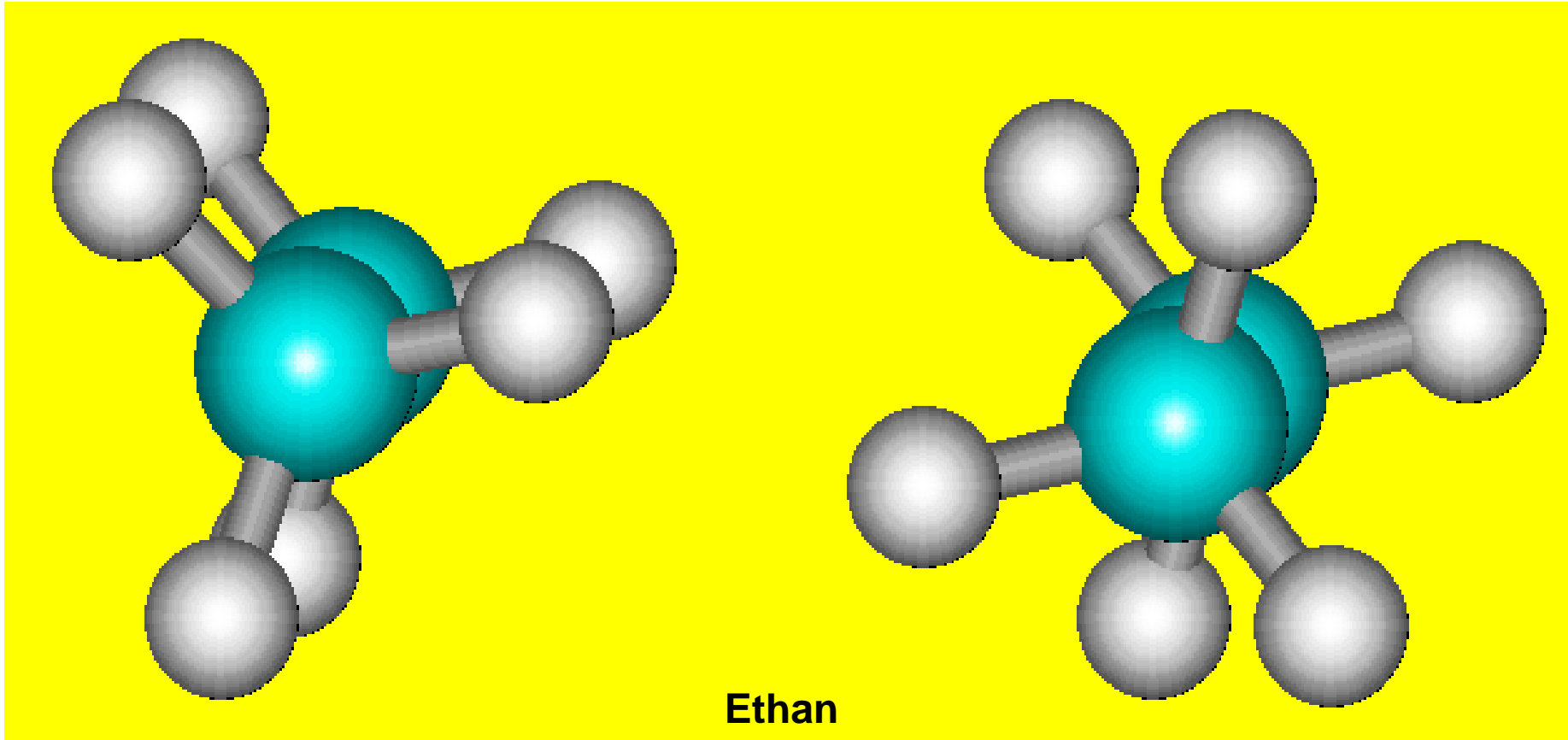
Sawhorse structures:

Sägebock-Schreibweise



3 Gesättigte Kohlenwasserstoffe

3.1.4 Dynamische Struktur der linearen Alkane: **Konformationen**



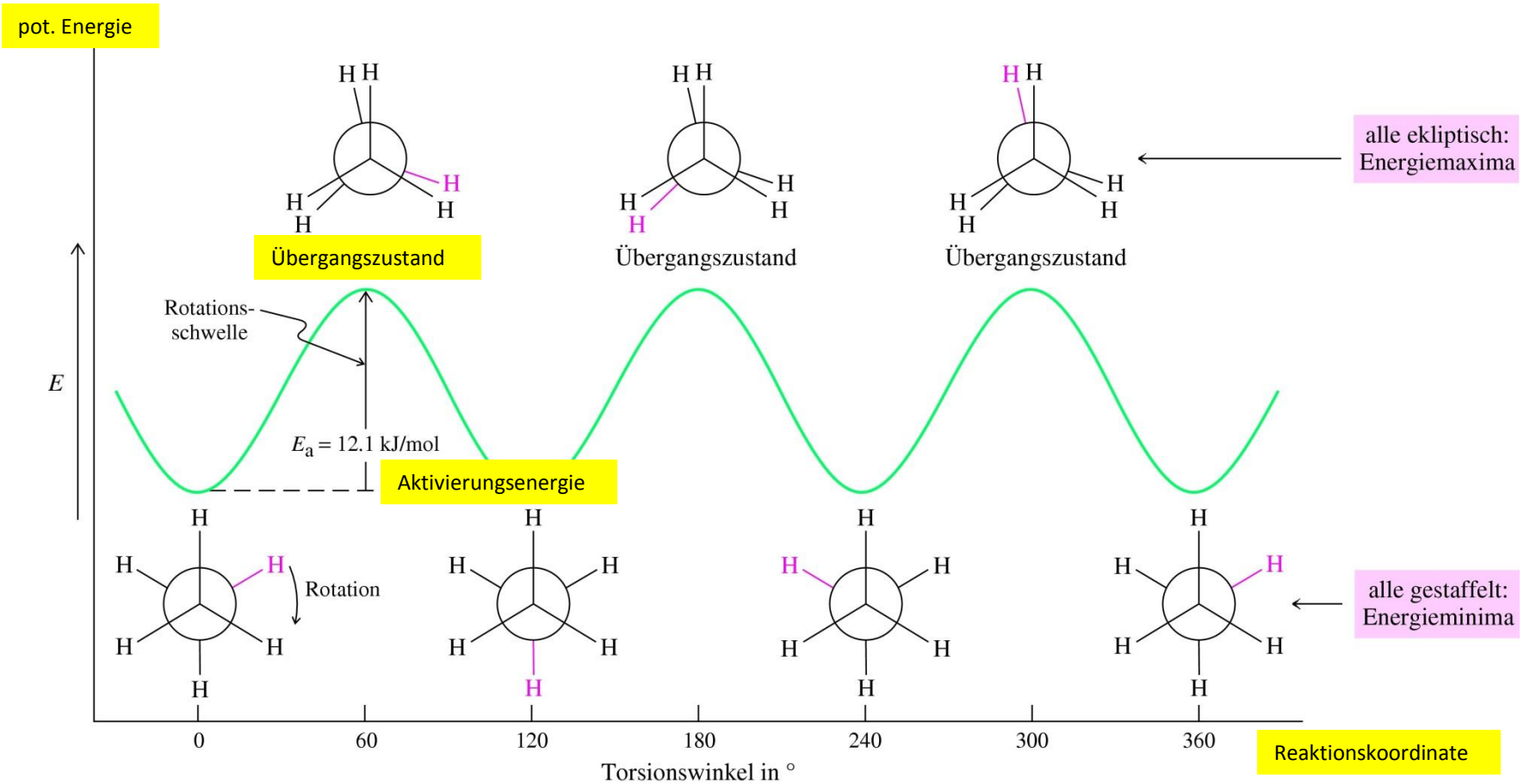
ekliptisch

Ethan

gestaffelt

3 Gesättigte Kohlenwasserstoffe

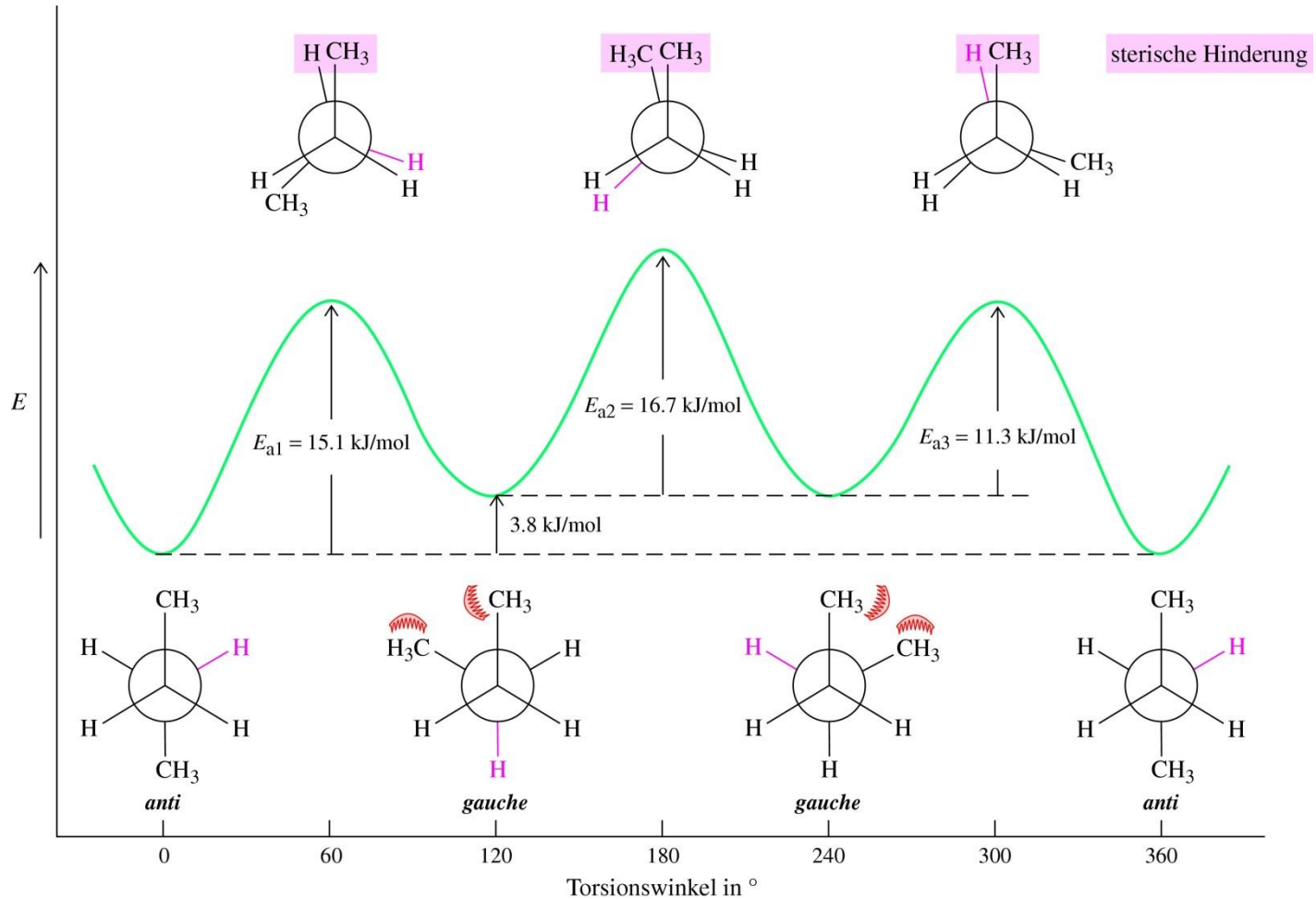
Energieprofil (potentielle Energie) der Rotamere des Ethans:
Drehung um die C-C-Einfachbindung



Die chemische Reaktivität hängt von Konformationen ab

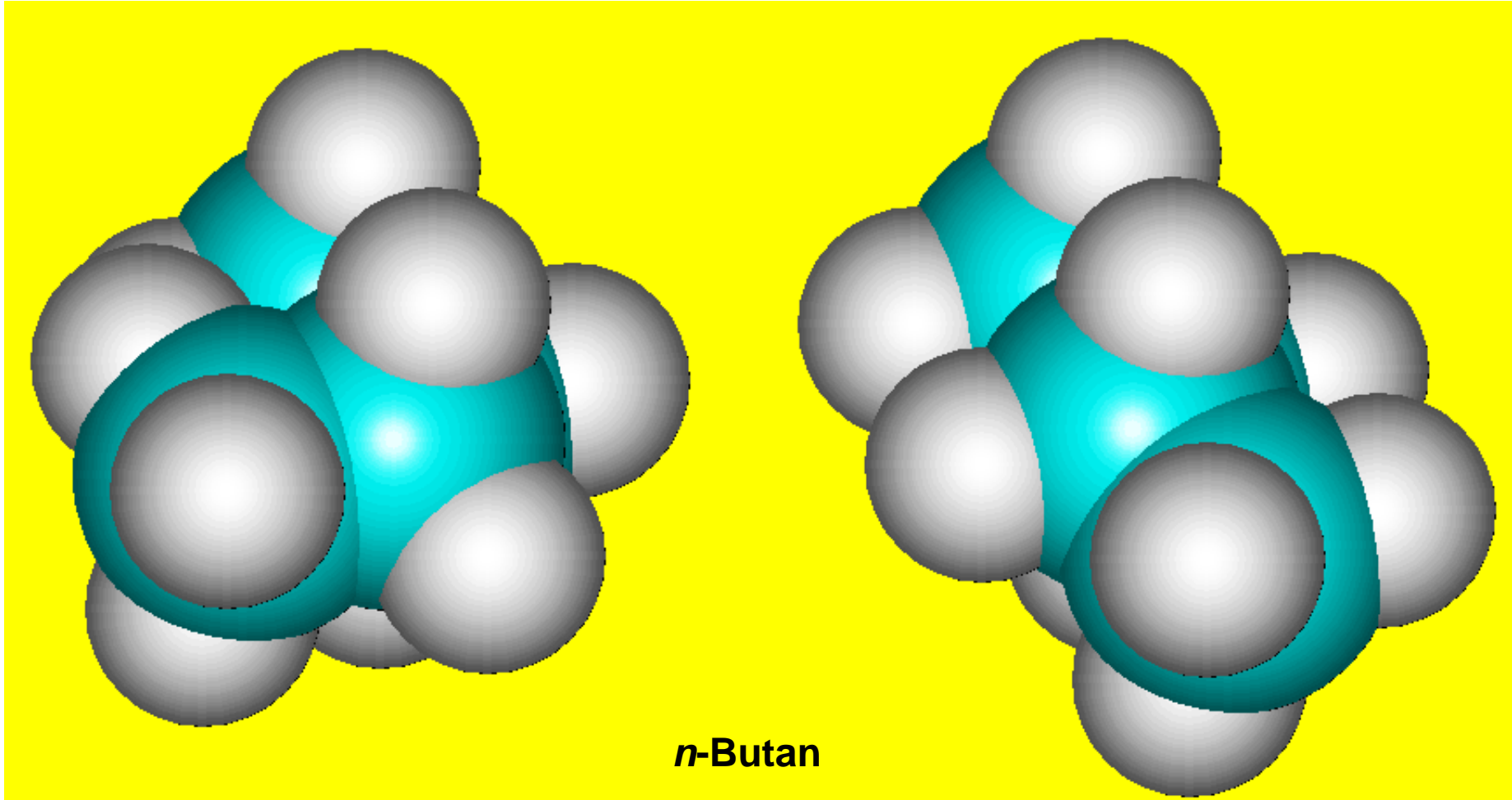
3 Gesättigte Kohlenwasserstoffe

Energieprofil der Drehung um die C₂-C₃-Bindung bei *n*-Butan



3 Gesättigte Kohlenwasserstoffe

Konformationen des n-Butans (Kalottenmodell)



synklinal = gauche

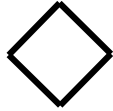
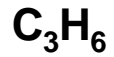
antiperiplanar = gestaffelt

3.4 Cycloalkane

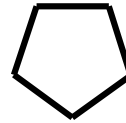
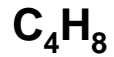
Namen und Formel von Monocyclische Alkane: C_nH_{2n}



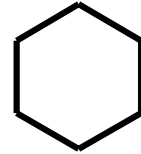
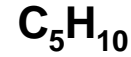
Cyclopropan



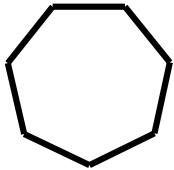
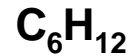
Cyclobutan



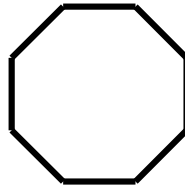
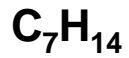
Cyclopentan



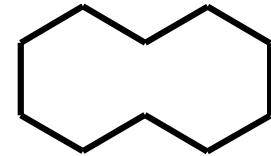
Cyclohexan



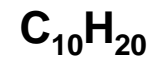
Cycloheptan



Cyclooctan

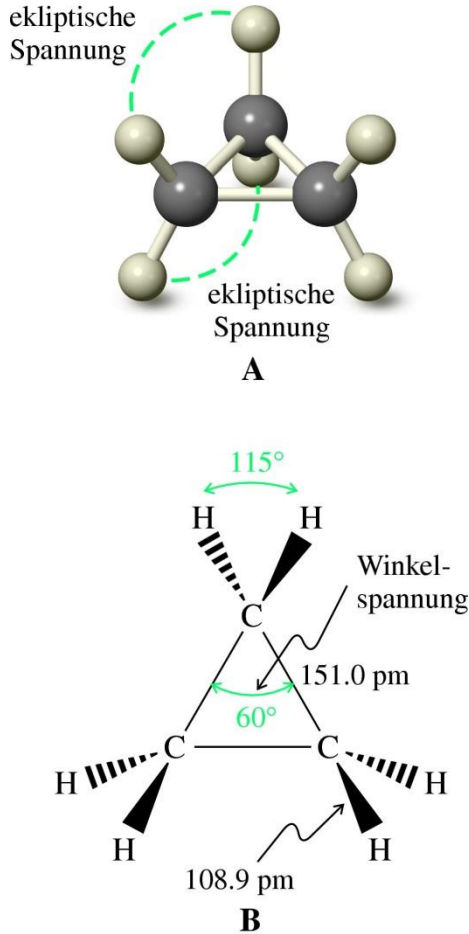


Cyclodecan

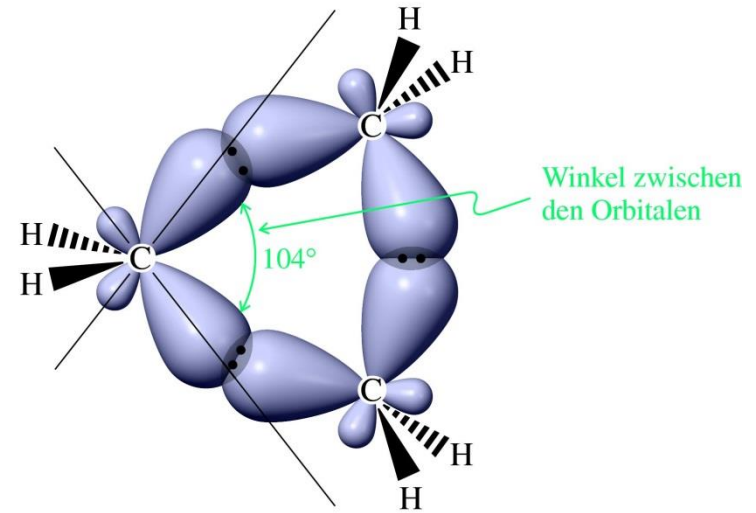
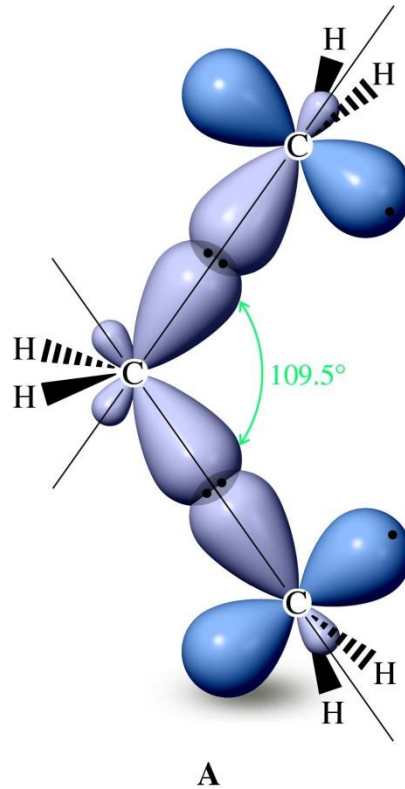


3.4 Cycloalkane

3.4.1 Ringspannung und Struktur der Cycloalkane



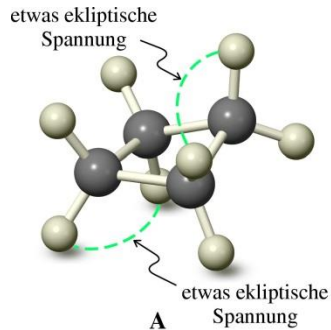
Geometrische und elektronische Struktur des Cyclopropans
Ringspannung: $\Delta H^\circ = 115 \text{ kJ/mol}$ / 38 kJ/mol pro CH_2 -Gruppe)



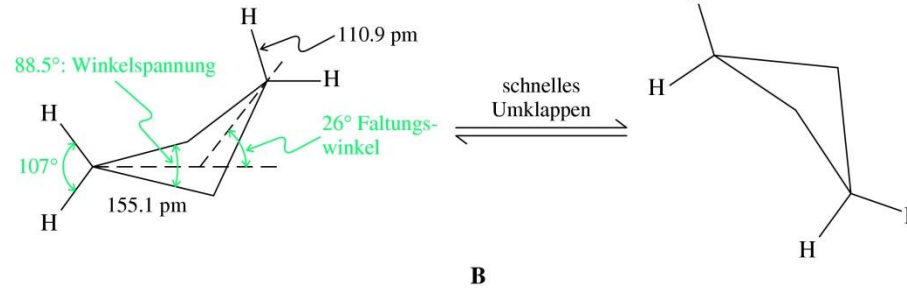
Schwächere C-C-Bindungen:
 $DH^\circ = 272 \text{ kJ/mol}$

3.4 Cycloalkane

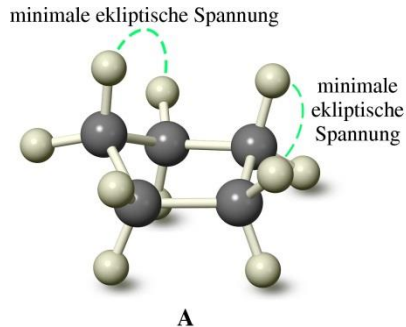
Strukturen von Cyclobutan (C₄H₈), Cyclopentan (C₅H₁₀)



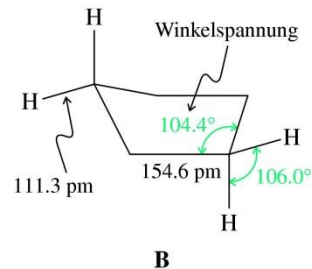
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Ringspannung: $\Delta H^\circ = 110 \text{ kJ/mol}$ / 28 kJ/mol/CH₂-Gruppe)



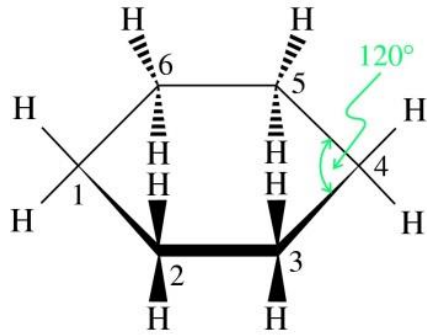
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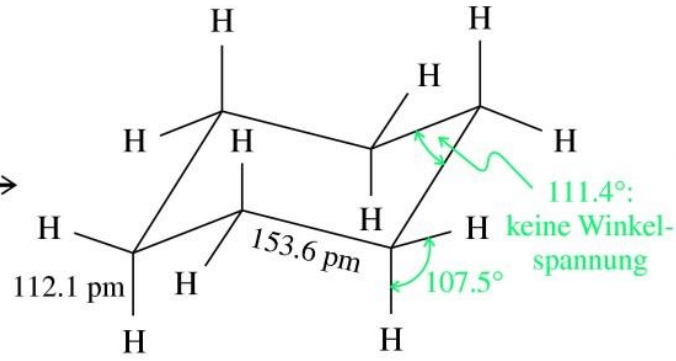
Ringspannung: $\Delta H^\circ = 27 \text{ kJ/mol}$ / 5.4 kJ/mol/CH₂-Gruppe)

3.4 Cycloalkane

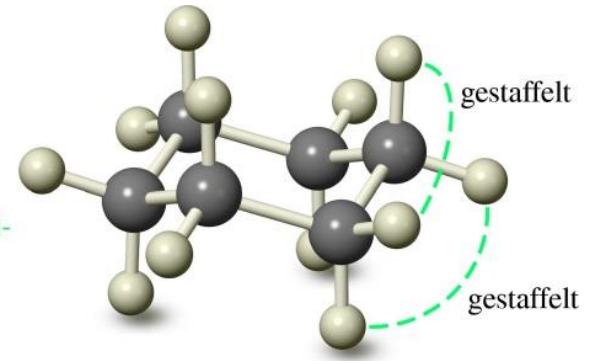
Struktur von Cyclohexan (C_6H_{12})



A
ebenes Cyclohexan
(Bindungswinkel 120° ;
12 ekliptische Wasserstoffatome)



B
Sesselkonformation des Cyclohexans
(fast tetraedrische Bindungswinkel;
keine ekliptischen Wasserstoffatome)

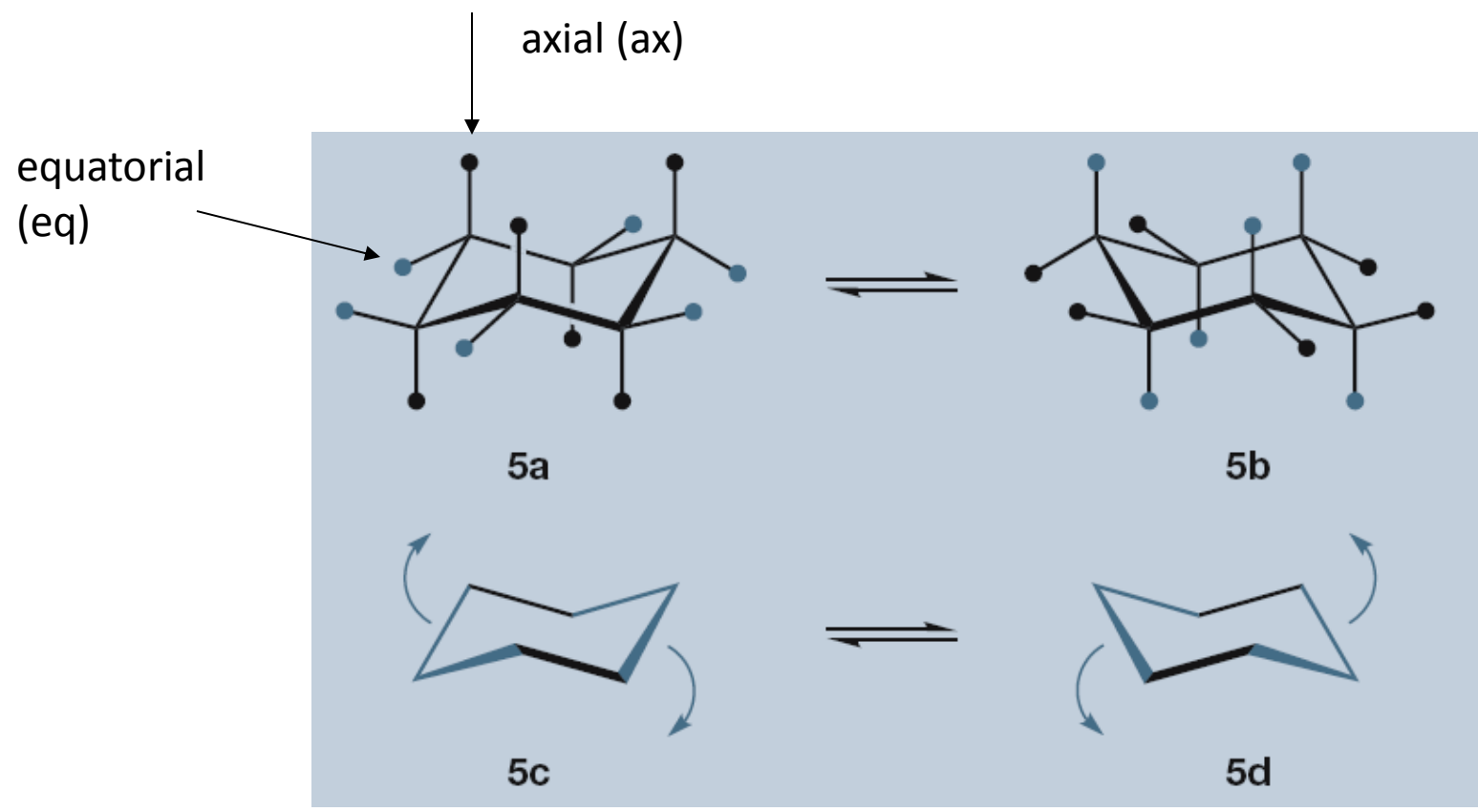


C

Ringspannung: $\Delta H^\circ = 0.4 \text{ kJ/mol}$ / 0 kJ/mol/ CH_2 -Gruppe)

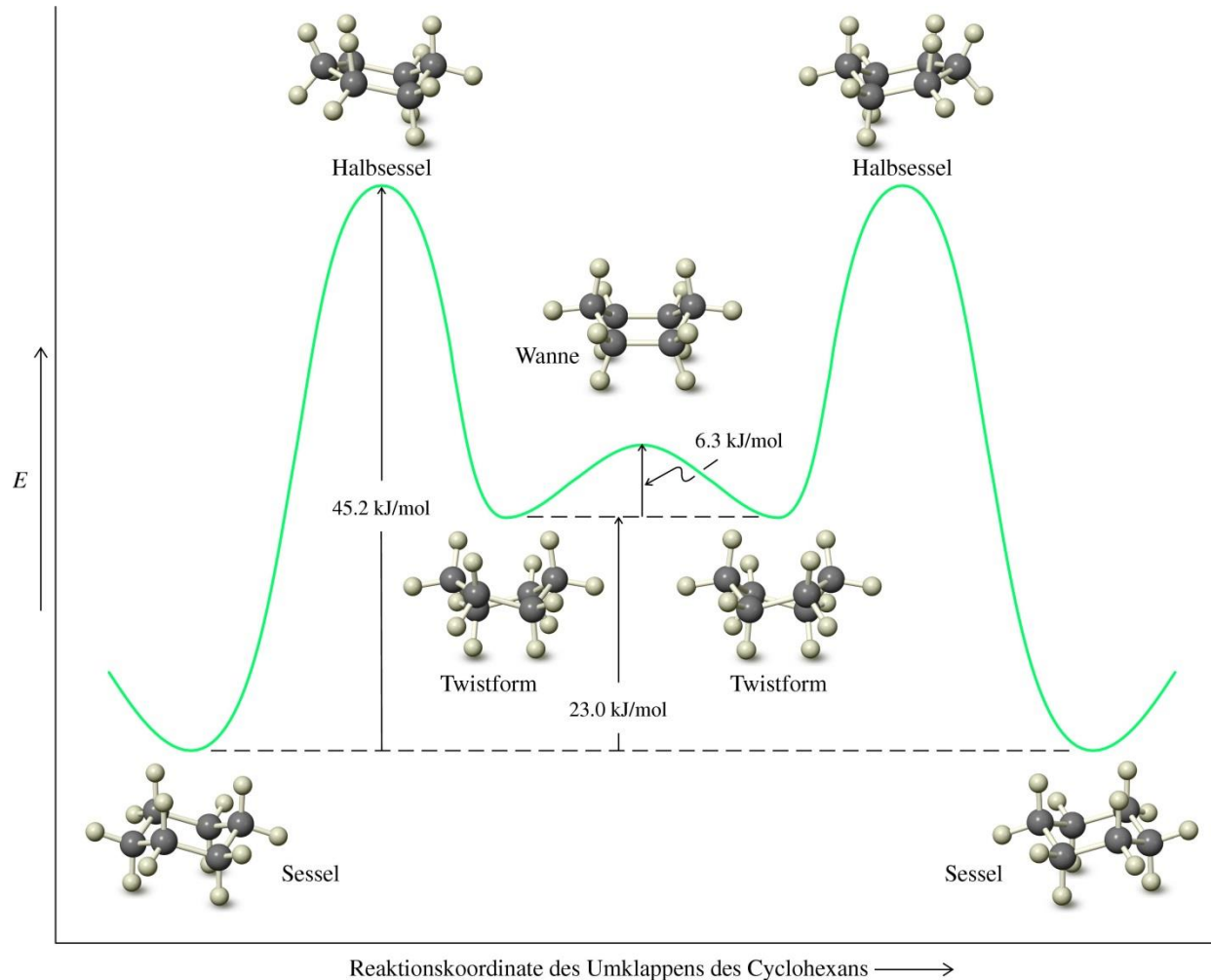
Cyclohexan ist spannungsfrei!

Bei Ringinversion werden Substituenten in equatorialer bzw. axialer Stellung ausgetauscht



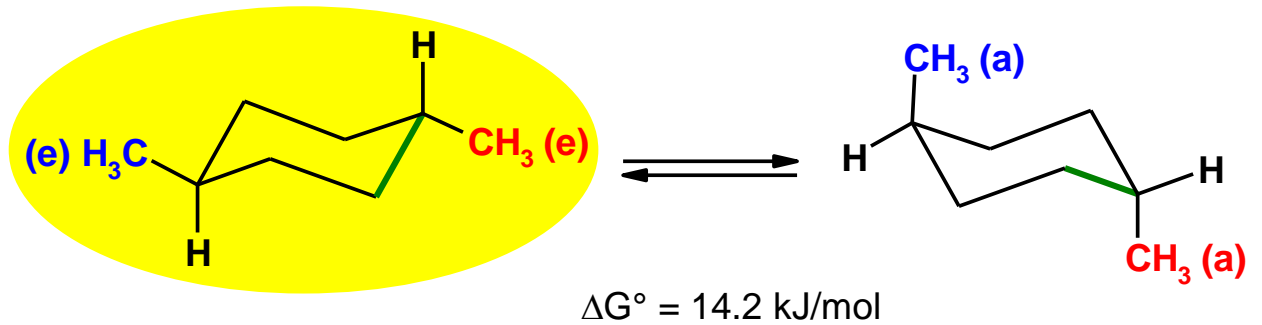
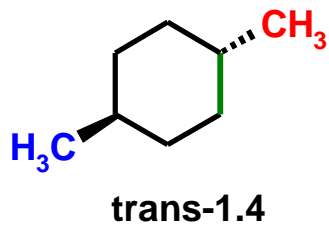
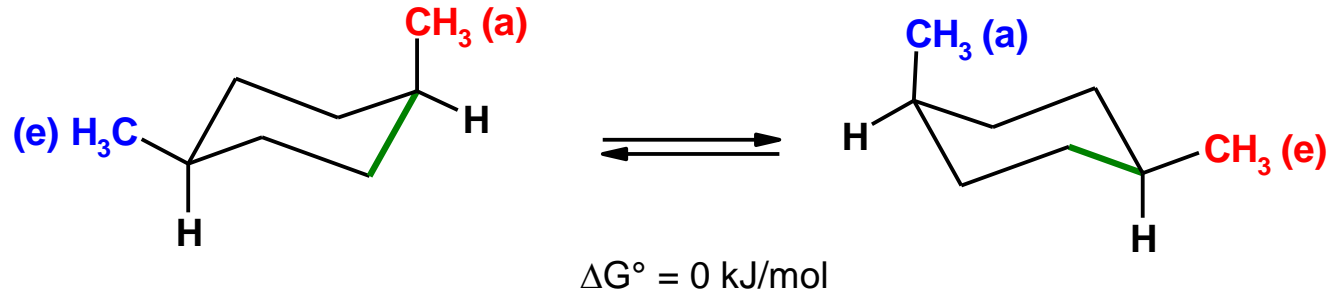
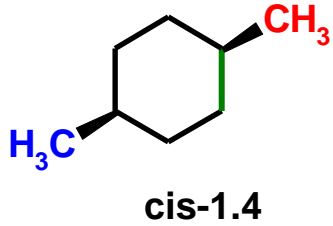
3.4 Cycloalkane

3.4.2 Cyclohexan, ein spannungsfreies Cycloalkan

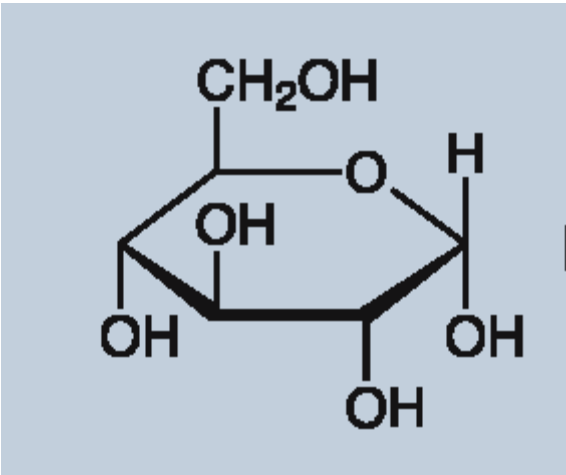


3.4 Cycloalkane

cis- und *trans*-1,4-Dimethylcyclohexan

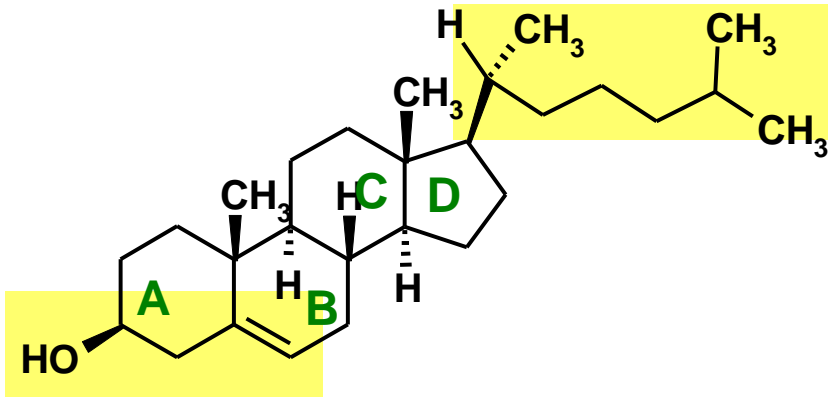


3.4 Cycloalkane

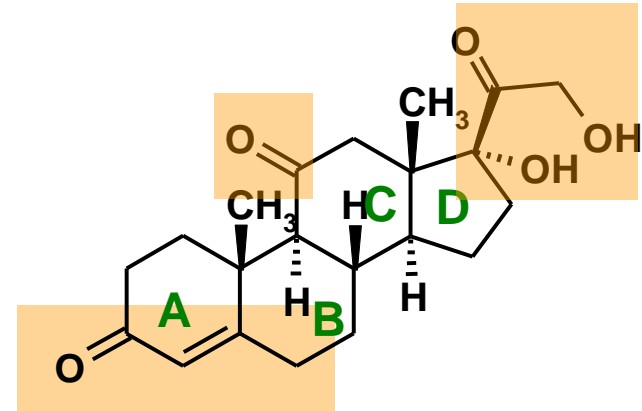


3.4 Cycloalkane

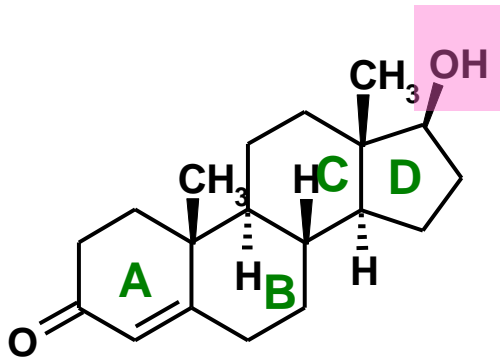
Carbocyclische Naturstoffe



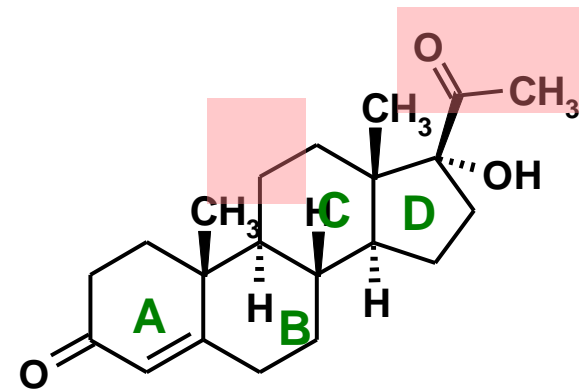
Cholesterin



Cortison



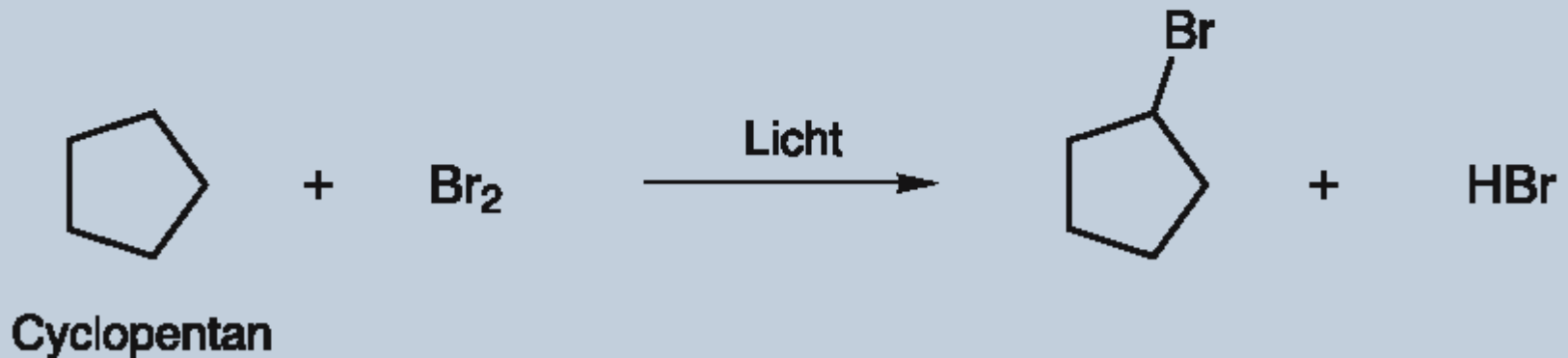
Testosteron



Progesteron

Reaktionen von Alkanen:

Reaktionen mit Sauerstoff(Verbrennung) und mit Halogenen(radikalische Chlorierung, Fluorierung usw.)



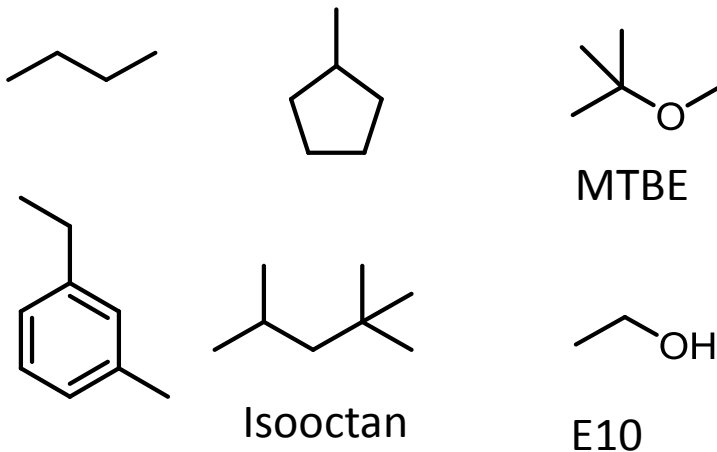
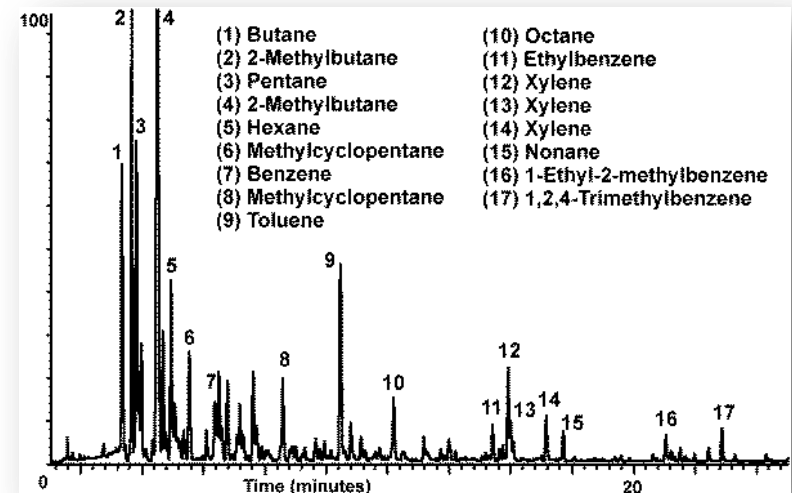
3 Gesättigte Kohlenwasserstoffe

Einschub: was ist eigentlich Benzin?



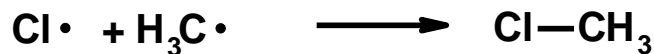
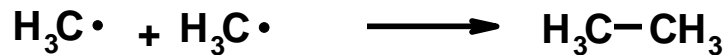
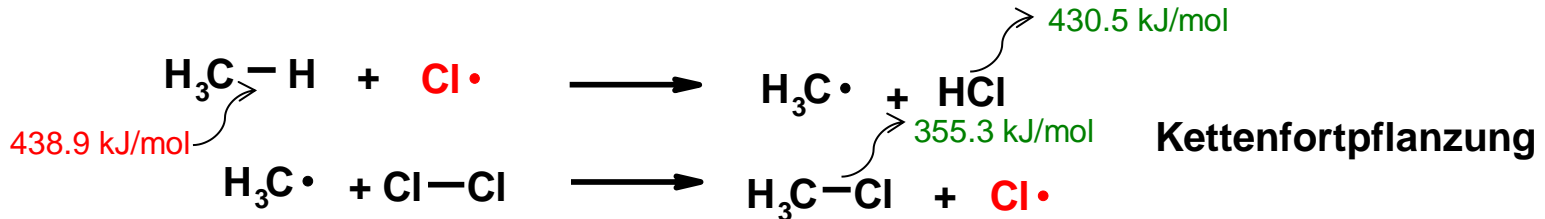
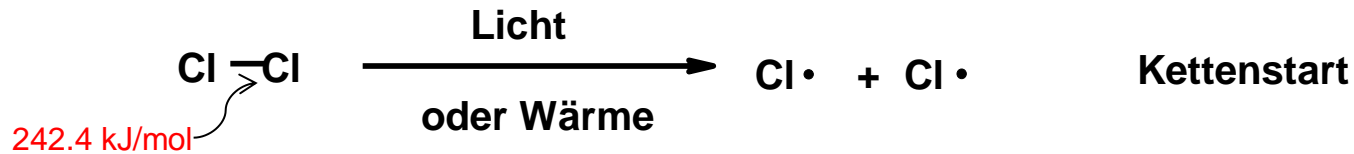
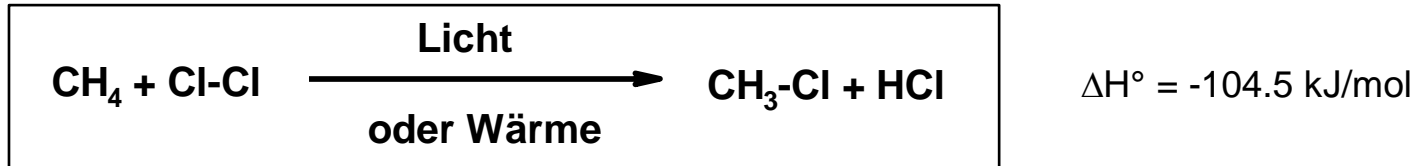
- Name hat nichts mit Carl Benz zu tun, sondern kommt über Umwege vom Benzoeharz
- Ein komplexes Gemisch aus Kohlenwasserstoffen (typ. 4-12 C Atome)
- Genaue Zusammensetzung variiert je nach Anwendung

GC-MS Analyse



3 Gesättigte Kohlenwasserstoffe

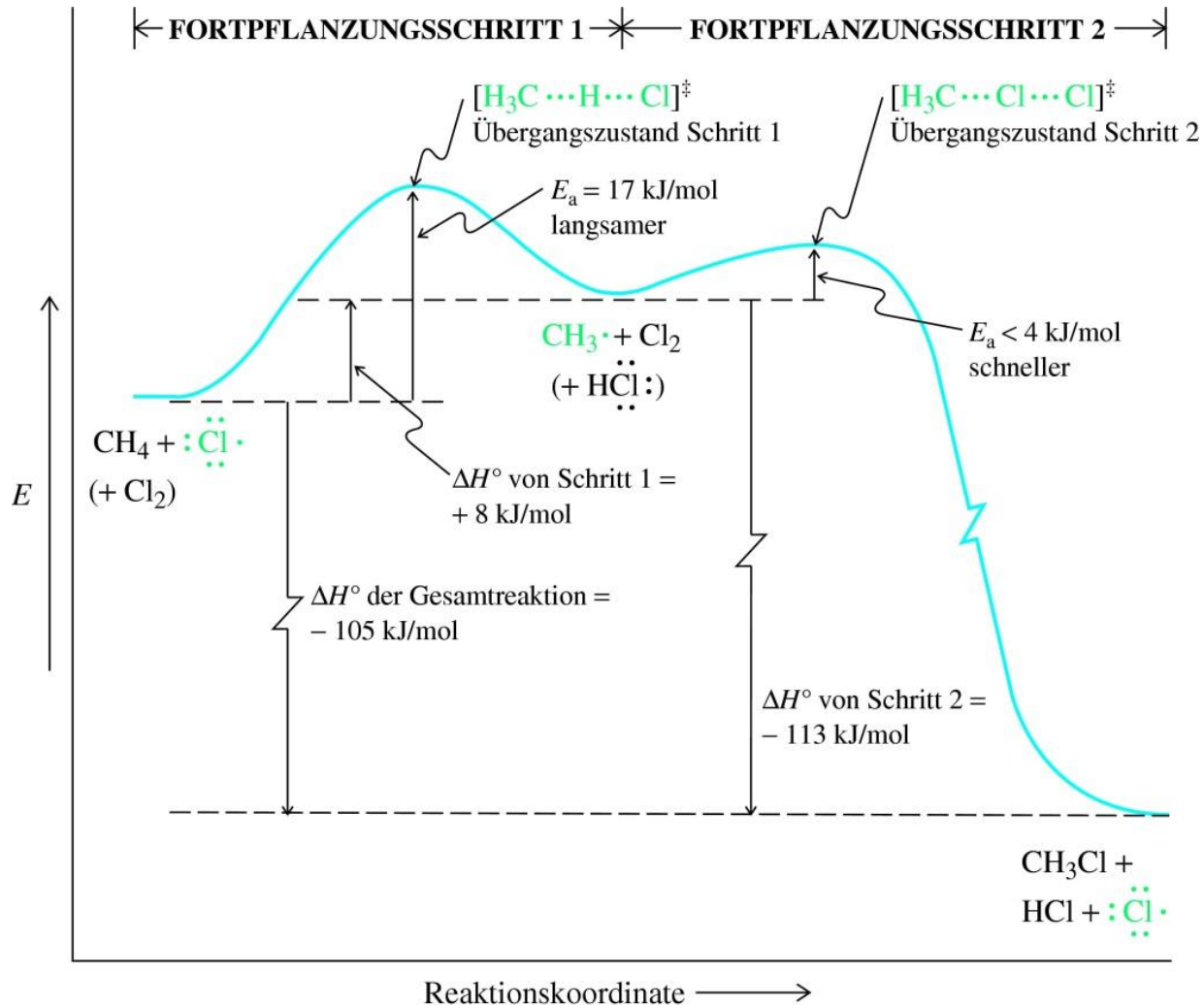
3.3.1 Chlorierung von Methan (Radikalische Substitution – Kettenmechanismus)



Kettenabbruch

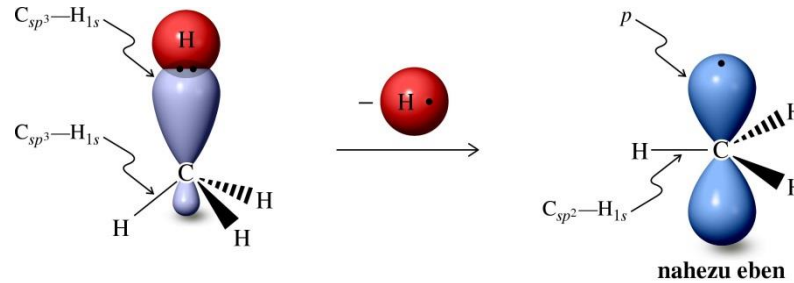
3.3 Reaktionen der Alkane

Energiediagramm des zeitlichen Verlaufs der Methanchlorierung (**Kinetik**)



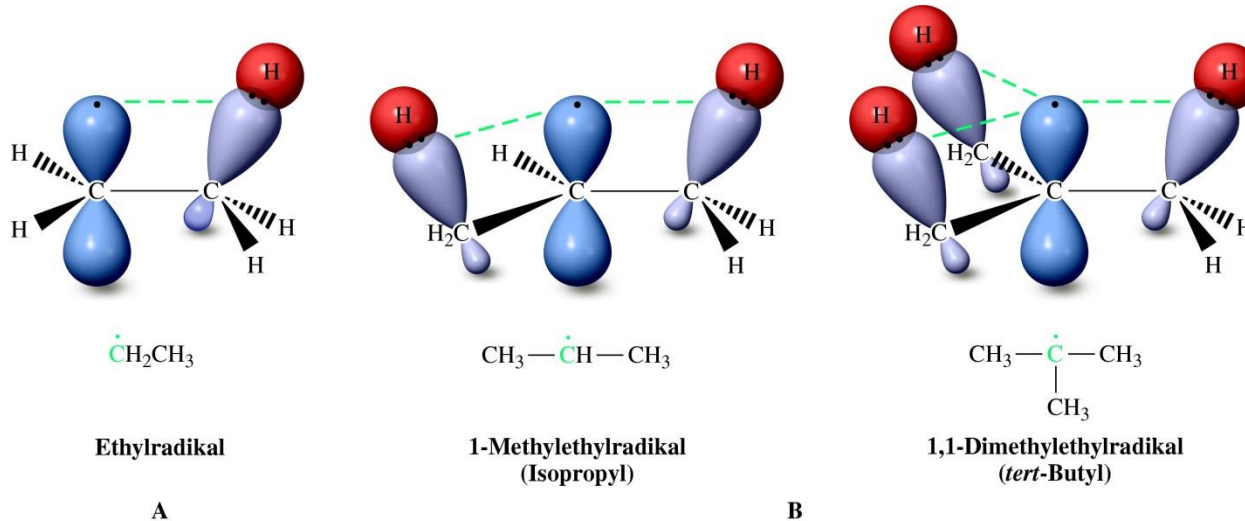
3.3 Reaktionen der Alkane

3.3.3 Struktur und Stabilisierung von Alkylradikalen: Hyperkonjugation



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Vollhardt - Organische Chemie
ISBN: 9783527327546 Abb. 03-002

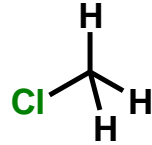
$R_3C\bullet$ -Radikale streben eine ebene Anordnung an



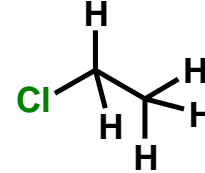
$R_3C\bullet$ -Radikale werden durch Hyperkonjugation stabilisiert (ca. 10-11 kJ/mol/ CH_3 -Gruppe)

3.3 Reaktionen der Alkane

3.3.4 Chlorierung höherer Alkane: Regioisomerie bei Chloralkanen



Chlormethan



Chlorethan

