SATURATED HYDROCARBONES – alkanes and cycloalkanes

RADICAL REACTION

Sulfochloration $R-H + Cl_2 + SO_2 \longrightarrow R-SO_2Cl$

$Cl_2 \longrightarrow 2\ Cl^{\bullet}$ **iniciation**

$CH_4 + Cl^{\bullet} \longrightarrow CH_3^{\bullet} + HCl$

$CH_3^{\bullet} + SO_2 \longrightarrow CH_3-SO_2^{\bullet}$

$CH_3-SO_2^{\bullet} + Cl_2 \longrightarrow CH_3-SO_2Cl + Cl^{\bullet}$ **propagation**

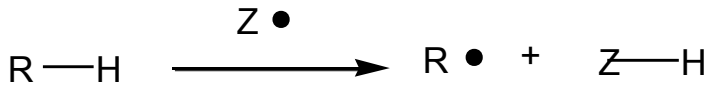
Pay attention for inhibitors of radical reactions! They are able to stop reaction of propagation.

$CH_3^{\bullet} + O_2 \longrightarrow CH_3-O-O^{\bullet}$

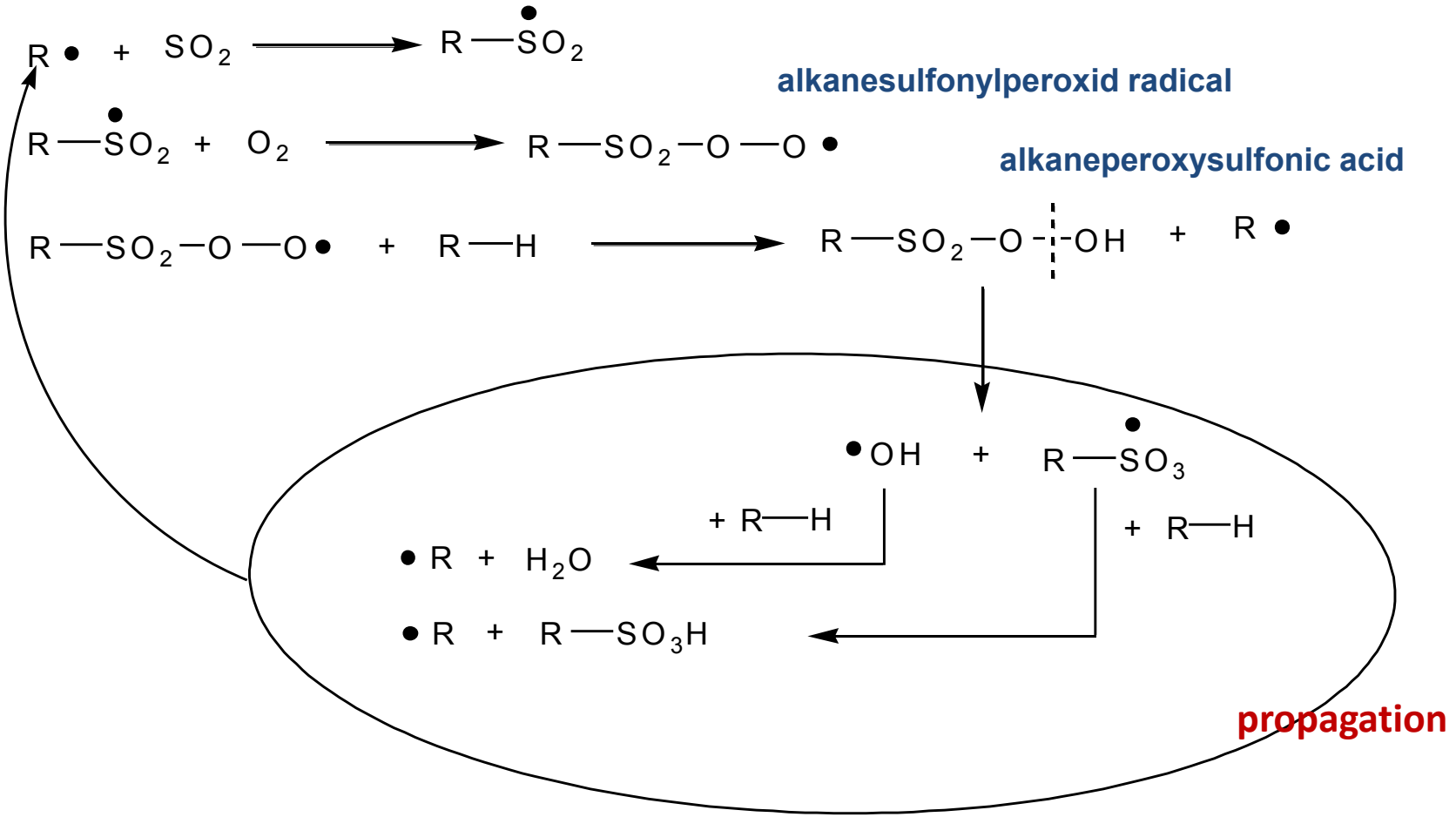
Oxygen, for instance, is forming with radicals peroxyalkyl radical (which is less reactive)

SATURATED HYDROCARBONES – alkanes and cycloalkanes

Sulfoxidation $R-H + SO_2 + O_2 \longrightarrow R-SO_3H$



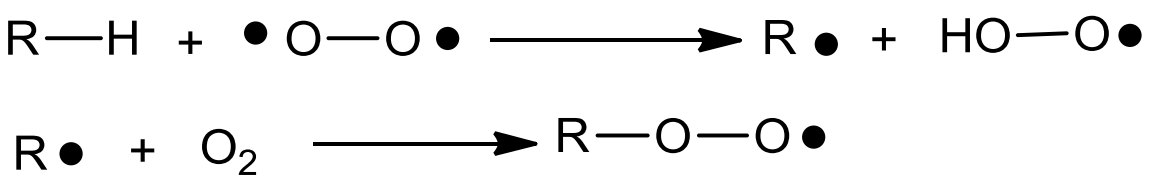
iniciation



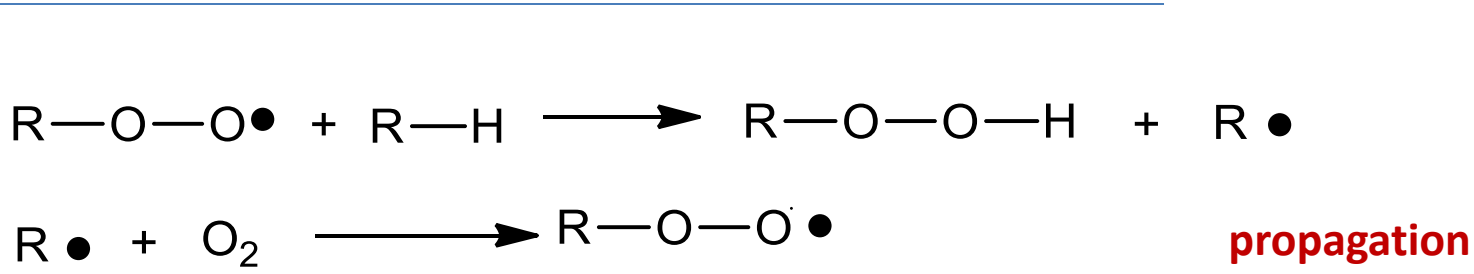
propagation

SATURATED HYDROCARBONES – alkanes and cycloalkanes

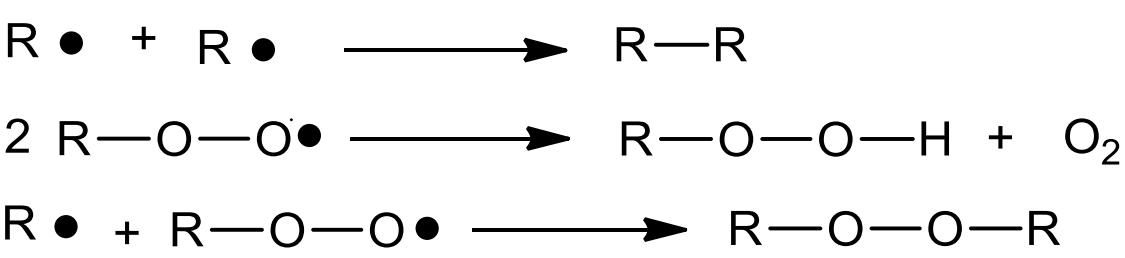
Autoxidation $R-CH_2-R + O_2 \longrightarrow R-CO-R + (2\ R-CHO)$



iniciation



propagation

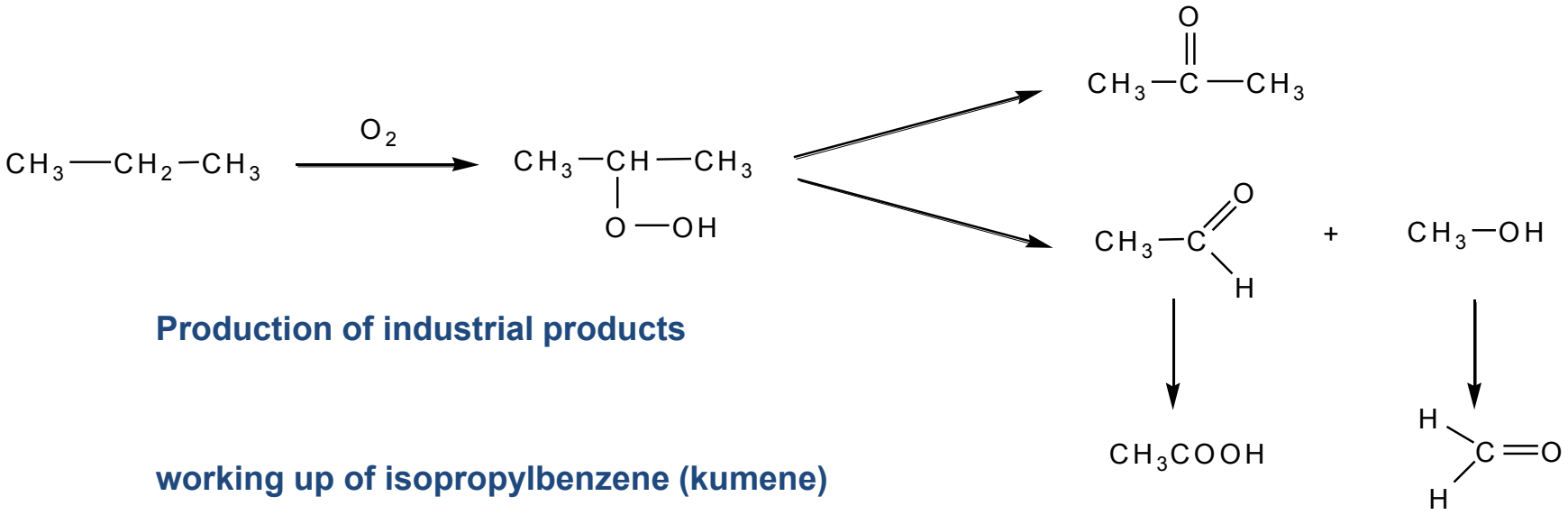


termination

SATURATED HYDROCARBONES – alkanes and cycloalkanes

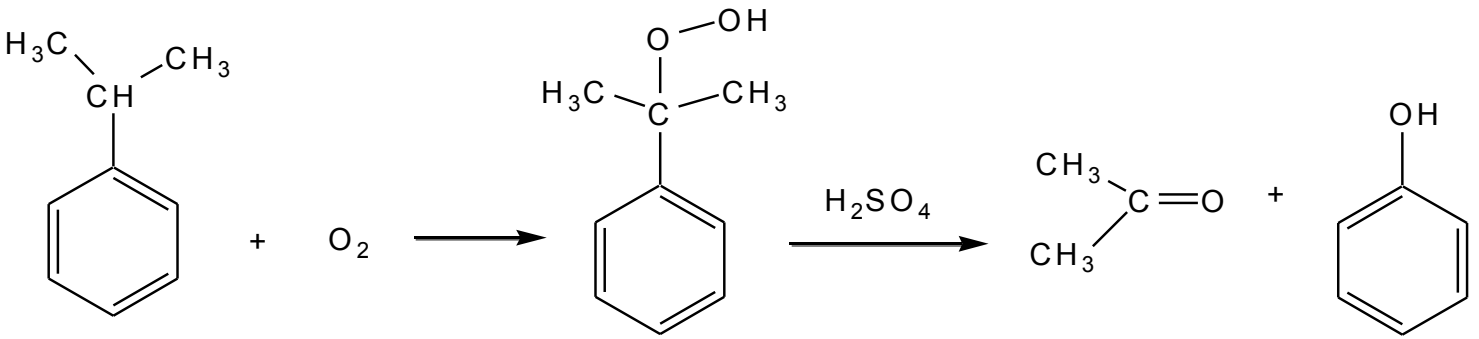
Autoxidation $R-CH_2-R + O_2 \longrightarrow R-CO-R + (2\,R-CHO)$

Practical presentations



Production of industrial products

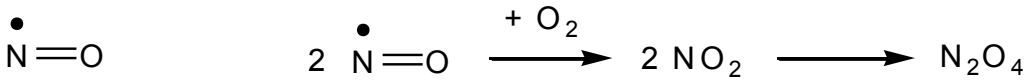
working up of isopropylbenzene (kumene)



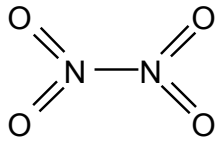
SATURATED HYDROCARBONES – alkanes and cycloalkanes

Nitration - nitrogen oxides , diluted nitric acid (400° C) ⟶ R – NO_2

Reaction is accompanied by bonds C-C splitting

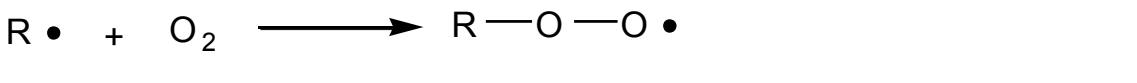


The source of reagents for nitration is a mixture of nitrogen oxides

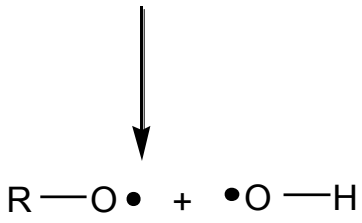


Burning

iniciation



propagation

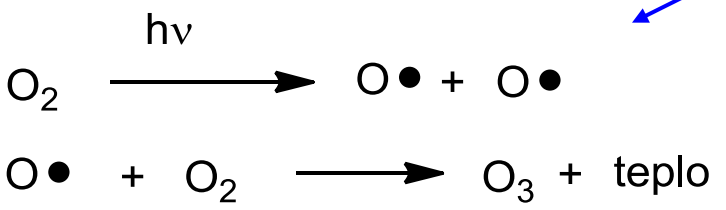


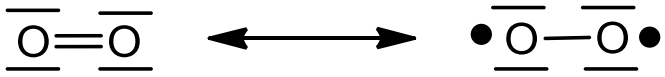
source for further chain reactions

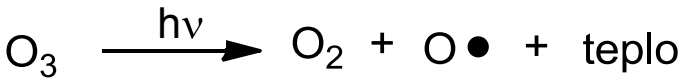
SATURATED HYDROCARBONES – alkanes and cycloalkanes

Radical reactions in atmosphere

ozonosphere – 25 km over surface of earth



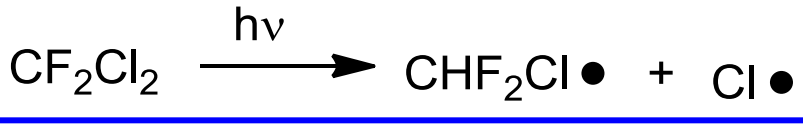




ozone when decomposes is protecting the earth against UV-light – radiation is transferred to heat

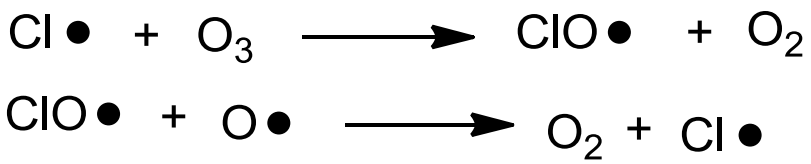
Freones – hydrocarbones with bond chlorine and fluorine
(application in cooling systems, inert solvents, spray medium)

Decomposition of freone



iniciation

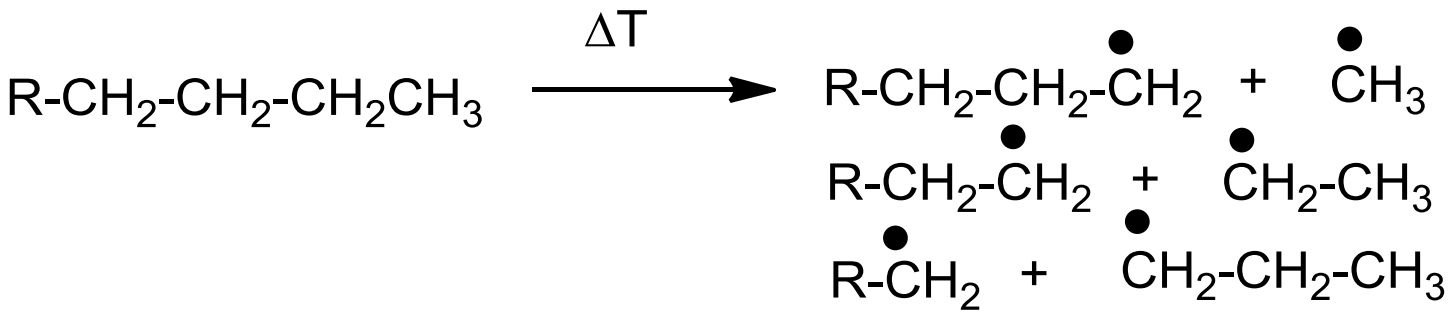
Crutzen, Molina, Rowland (1995 NP)



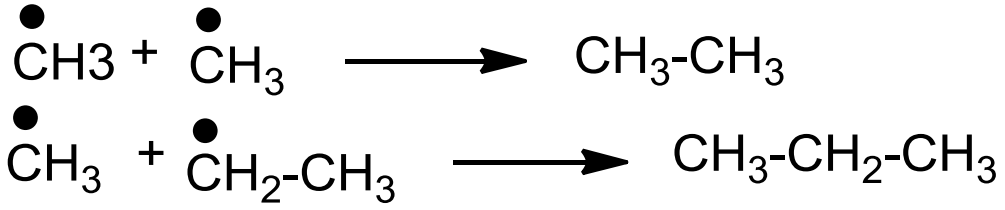
propagation

SATURATED HYDROCARBONES – alkanes and cycloalkanes

CRACKING - C-C bonds splitting $\Delta H_{C\text{-}C}$ = 346 kJ/mol 700 – 900° C

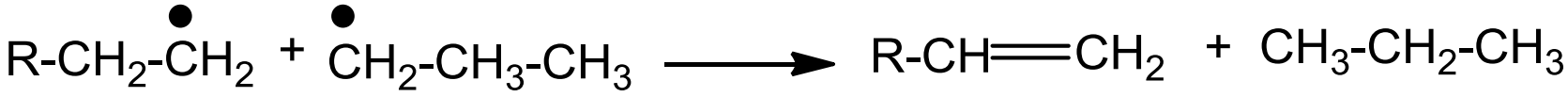


TERMINATION



recombination – formation of smaller molecules than before cracking

disproportionation



HYDROCRACK (250 – 450° C + catalyst + H_2 + pressure)

SATURATED HYDROCARBONES – alkanes and cycloalkanes

The source of saturated and nonsatureted hydrocarbons, aromates and compounds containing sulfur and nitrogen compounds are **earth gas and oil**

Boiling point ° C	Number of carbon atoms	Application
under 30	2 - 4	Gassous components - heating
30 - 180	4 - 9	Gasoline - engines
160 - 230	8 - 16	Kerosene – heating, engines
200 - 320	10 - 18	Fuel oil – diesel engines
300 – 450	16 – 30	Heavy oil- heating
higher		Vax, asphalt , koke

Oktano number: heptane 0
isooktan (2,2,4-trimethylpentan) 100

Ecologie of hydrocarbones

STRUCTURE AND STEREOCHEMIE OF COMPOUDS WITH $C_{sp}3$

Carbon atom in sp^3 hybrid state (picture)

chiral_3.wrl

Two carbon atoms in sp^3 state, Fischer projection, perspektive projection, mutual transformation

chiral21.wrl

Configuration – Cahn, Ingold, Prelog rules for priority of substituents

STRUCTURE AND STEREOCHEMIE OF COMPOUDS WITH $C_{sp}3$

	Cahn, Ingold, Prelog – rules for priority assesment of substituents (groups)
1	The higher proton number, the higher priority
2	When two atoms have the same proton numbers (isotopes), higher priority owns the atom with higher mass
3	When we are not able decide about priority applying the two rules above, we must compare proton numbers at neighbouring more distant atoms (at the second atoms from the stereogenic centrum) , and when we are not successful we must continue to the third and further atoms.
4	Atoms bound with multiple bonds are evaluated as the atom would be multiply bound by a single bond