WILEY-VCH

Catalysis from A to Z

A Concise Encyclopedia

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Library of Congress Card No. applied for

A catalogue record for this book is available from the British Library

Die Deutsche Bibliothek – CIP Cataloguing-in-Publication-Data
A catalogue record for this publication is available from Die Deutsche Bibliothek

ISBN 3-527-29855-X

Printed on acid-free and chlorine-free paper

Composition: Kühn & Weyh Software GmbH, D-79111 Freiburg
Printing: betz-druck GmbH, D-64291 Darmstadt
Bookbinding: Wilh. Osswald + Co., D-67433 Neustadt
Printed in the Federal Republic of Germany

Preface

"Wir bekommen begründeten Anlaß zu vermuten, daß in lebenden Pflanzen und Tieren Tausende von katalytischen Prozessen zwischen den Geweben und Flüssigkeiten vor sich gehen."

*J.J. Berzelius (1836)**

Catalysis occurs always and everywhere. Catalysis is not a separate scientific discipline of limited scope, but rather a cross-linking science that embraces all chemistry and biology. There is hardly any scientist in these and related areas who does not encounter catalytic phenomena in his work. Beyond that, many catalytic processes are known to the educated member of the public, to the politician as well as to any other informed person. Anyone who knows about Mozart, Ravel, and Gershwin should know about catalysis as well. There is no life without the miracles of catalytic reactions in plants, animals, and human beings.

Because of this broad importance of catalysis both in science and in daily life, four scientists covering the main fields of catalysis have edited the present encyclopedia, which is the first comprehensive "Catalysis from A to Z". Approximately 3000 keywords have been explained by 165 authors and coauthors, who are all active in their respective areas. It was our aim to edit a concise handbook which is quickly at hand if one wants to know the meaning of certain catalytic or catalysis-related terminology. We hope that the present book proves a useful compendium for everyone whose occasional or permanent interest is catalysis – scholars, high-school teachers, professors, chemists, bioscientists, and physicists, both within and beyond the academic world.

We have been fortunate to have conferred on a multiplicity of topics with experts. Nevertheless we might have overlooked keywords and entries which are important for catalysis. Please keep the editors informed of any such cases.

We thank the team of Wiley-VCH, Dr. F. Sagi from Lyon (France) for supporting the French translations, and especially our freelance copyeditor, Mrs. Diana P.E. Boatman, M.A., M.R.S.C, C. Chem, from Redhill, Surrey (UK), for their endless patience and help during the difficult process of completion.

Frankfurt, München, Berlin, La Jolla
January 2000

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* "We have good reasons to assume that thousands of catalytic processes take place in living organisms between the tissues and the body fluids" (*Ann. Chim. et Phys.* **1836**, 146–151).

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How to Use this Encyclopedia

Abbreviations Used

abbr.	abbreviation
acc.	according to, accordingly
calcn(s).	calculation(s)
calc(d)(ng).	calculat(ed)(ing)
cat(s).	catalyst(s), catalytical(ly), catalysis, catalyzing, catalyze(s)
comb(s).	combination(s)
comp(s).	component(s)
conc(s).	concentration(s)
cond(s).	condition(s)
conv(s).	conversion(s)
cpd(s).	compound(s)
3D	three dimensional
DE	German patent
ee	enantiomeric excess
EP	European patent
equ(s).	equation(s)
equil(s).	equilibrium, equilibria
equiv.	equivalent
FR	French patent
GB	British Patent
H	hydrogen
hc(s).	hydrocarbon(s)
het.	heterogen, heterogeneous(ly)
hom.	homogen, homogeneous(ly)
manuf(d)(ng).	manufacture(d)(ing)
m/m	molar ratio
N	nitrogen
O	oxygen
prep(d)(n).	prepared, preparation
press.	pressure
proc(s).	process(es)
prod(s).	production, product(s)
®	trade mark
rac.	racemic
rt	room temperature
S	sulfur
sc.	supercritical
spec(s).	specification(s)
synth.	synthesis, synthethic, synthesize, synthetically
temp(s).	temperature(s)
UHV	ultra high vacuum

US	US patent
UV	ultra violet light
w/o	with or without
wt.%	weight%
w/w	by weight (e.g., %)
→	cross reference, cf.
⇢	reaction

Plurals of noun abbreviations are formed by adding "s" to the singular abbr. (such as abbrs.).

References

The references at the end of most of the entries illustrate developments or important aspects of the keyword, being mainly from recent publications. References which are mentioned often are given with only the name of the author and are compiled under "General references cited" (cf. below). Other information is cited mainly from recent publications in journals; in this case we dispensed with the names of the authors. Of course, no attempt has been made to provide a complete literature review of the topics covered by each keyword.

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Cross References

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Translations

Each keyword is translated into French (**F**) and German (**G**); identical translations are indicated by **E=F=G**.

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A

AA 1: → acetic acid; 2: → acrylic acid; 3: → adipic acid; 4: → acrylamide; 5: atomic absorption, → atomic absorption spectroscopy (AAS)

AAA → acetic acid anhydride

AAS → atomic absorption spectroscopy

ABB process → Lummus procs.

ab-initio calculations Nonrelativistic quantum mechanical ab-initio calcns. (aics.) aim at approximate solutions of the *Schrödinger equ. without making use of experimental values. The first step in an aic. is the solution of the one-electron *Hartree–Fock (HF) equs., which approximate the many-electron wave function as a prod. of one-electron functions. The prod. of the one-electron functions has the form of a determinant, called the Slater determinant, because a simple prod. would violate the Pauli principle. The integro-differential HF equs. are usually approximated by the *LCAO, which expands the one-electron functions as a set of basis functions called the basis set. The LCAO approximation leads to linear equs. which can be solved iteratively in the *SCF procedure. Most aics. also make use of the Born–Oppenheimer approximation, i.e., the electrons move in the field of fixed nuclei. The quality of an HF-LCAO aic. is determined by the size of the basis set. Since the HF-LCAO equs. are variational, the calcd. energy is always higher than the true energy. The difference between the correct (nonrelativistic) energy and the HF energy with an infinite basis set is called the *correlation energy. There are several methods for calcng. correlation energy in aics. The most popular ones are Møller–Plesset perturbation theory, configuration interaction (CI), multi-configuration SCF (MCSCF), and coupled-cluster theory. Aics. can thus be carried out at many levels of theory, the quality of which depends on the size of the basis set and the accuracy of the correlation treatment. High-level aics. may challenge the accuracy of experimental values, but they can become very expensive. Relativistic aics. try to solve the Dirac equs., which give relativistic total energies. Solving the Dirac equs. is substantially more complicated than solving the Schrödinger equ., because the former equs. involve a four-comp. Hamiltonian. Most aics. circumvent this problem by using *pseudopotentials. Aics. can also predict physical properties of atoms and molecules such as ionization potentials, electron affinities, equil. geometries, bond dissociation energies, activation and reaction enthalpies, rotational and vibrational spectra, NMR chemical shifts, coupling constants, etc. In this respect they are interesting for cat. as well. The theoretical properties are obtained from calcn. of first or second derivatives of the energy with respect to coordinates or electromagnetic fields. **F** calculs d'ab-initio; **G** Ab-initio-Rechnungen. G. FRENKING

Ref.: Thomas/Thomas, p. 400.

ABS 1: alkylbenzene sulfonate, manuf. by *alkylation of benzene and subsequent *sulfonation; 2: a co- or graft-*copolymer of acrylonitrile, butadiene, and styrene, where the disperse phase formed by a butadiene elastomer is distributed in a continuous phase consisting of a styrene–acrylonitrile copolymer. B. CORNILS

abzymes → catalytic antibodies

ac, Ac acetyl (MeCO–) or acyl (MeCO–O–) groups in *complex cpds. or as *ligands. Acc. to

the IUPAC rules for nomenclature abbrs. for *ligands should be written with small letters.

B. CORNILS

Ac_2O → acetic (acid) anhydride, AAA

accelerator → activator, *promoter, *co-catalyst

acceptor ligands are *ligands which usually form stable *complexes with *transition metals in low positive, zero, or negative oxidation states. These ligands bear low-energy, empty orbitals (acceptor orbitals) and are able to accept electrons (ligand acidity) from a metal center. This occurs upon interaction with filled metal-centered orbitals of the same symmetry (metal–ligand *back-bonding) and reduces the electron density at the metal center brought about by the ligand-to-metal σ- or π-donation of electrons. Depending on the symmetry of the *overlapping orbitals with respect to the metal–ligand axis, als. can be classified into π-acceptors (π-acids, e.g. CO, N_2, *phosphines, alkenes, *carbenes) and δ-acceptors (e.g. *arenes, *cp). Another classification differentiates between single-faced and double-faced als. π-Als. exert a strong ligand field leading usually to complexes with a low-spin *configuration. **E=F=G.**

A.C. FILIPPOU

Ref.: DeKock, Gray, *Chemical Structure and Bonding*, University Science Books, Sausalito 1989.

accessibility of het. cats. means the facility of diffusion of heat and mass into and out of their *surfaces. The physicochemical background is a considerable topic in cat. reaction engineering. Important factors to be taken into account are, inter alia, gradients of temps. and concs., and *diffusion coefficients, reaction charateristics, *porosity, oscillations (steady/unsteady states), spatial distribution of the *active sites (*distribution of metals), etc. In many cases, *selectivity, *stability, and a. must be considered together; retroactive consequences to the choice of reactors and their design are not excluded. **F** accessibilité; **G** Zugänglichkeit.

B. CORNILS

Ref.: Anderson/Boudart, Vol. 8, Chapter 3.

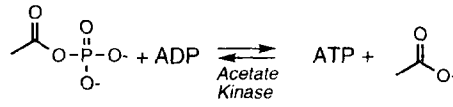
acac, ACAC acetylacetone anions in *complex cpds. or as *ligands

acetamidocinnamate amidohydrolase This *enzyme cat. the *hydrolysis of acetamidocinnamic acid to phenylpyruvic acid and acetamide. This transformation has been used synth. in the prod. of L-phenylalanine from acetamidocinnamic acid by *coupling this reaction with enzymatic *transamination. **E=F=G.**

P.S. SEARS

Ref.: *J. Biotechnol.* **1986**, *4*, 293.

acetate kinase (EC 2.7.2.1) cat. the synth. of adenosine 5-triphosphate (*ATP) from acetyl phosphate (AcP) and adenosine 5′-diphosphate (*ADP).



The reaction is in favor of *ATP formation, and the *enzyme also accepts other *NDPs. The reaction has been used in the *regeneration of ATP for enzymatic synth. **E=F=G.**

C.-H. WONG

acetic acid (AA, AcOH) is an important intermediate, manuf. preferably by cat. procs. such as *oxidation of hydrocarbons (procs. of *Celanese LPO, *Bayer, *BP, *Hüls), acetaldehyde *oxidation (*Hoechst AA, *Daicel, *Rhône-Poulenc), or *carbonylation of methanol (procs. of *BASF, *Monsanto). **F** acide acétique; **G** Essigsäure.

B. CORNILS

Ref.: Kirk/Othmer-1, Vol. 1, p. 121; Ullmann, Vol. A1, p. 45; Cornils/Herrmann-1, p. 104; McKetta-1, Vol. 1, p. 216; *Chem. Tech.* **1971**, 600.

acetic acid anhydride (AAA, Ac_2O, acetic anhydride) important intermediate, manufd. by oxidative *dehydration of acetaldehyde (*Hoechst AAA proc.) or by *carbonylation of *methyl acetate or dimethyl ether