A Dictionary of Chemistry

SIXTH EDITION

Edited by JOHN DAINTITH

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computational chemistry The use of computers in chemical research. With the increase in processing power of computers, calculations on individual molecules and on chemical systems have become important tools for research and industrial development. With simple molecules, predictions can be made about electronic structure and properties using *ab-initio calculations. For more complex molecules *semiempirical calculations are used. The field has been particularly expanded by the *density-functional method of treating large molecules and by the availability of software for analysing molecular behaviour and structure. See also MOLECULAR MODEL-LING.

concentrated Describing a solution that has a relatively high concentration of solute.

concentration The quantity of dissolved substance per unit quantity of a solution. Concentration is measured in various ways. The amount of substance dissolved per unit volume of the solution (symbol c) has units of mol dm⁻³ or mol l⁻¹. It is now called amount concentration (formerly molarity). The mass concentration (symbol ρ) is the mass of solute per unit volume of solution. It has units of kg dm⁻³, g cm⁻³, etc. The **molality** is the amount of substance per unit mass of solvent, commonly given in units of mol kg⁻¹. See also MOLE FRAC-TION.

concentration cell See CELL.

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concentration gradient (diffusion gradient) The difference in concentration between a region of a solution or gas that has a high density of particles and a region that has a relatively lower density of particles. By random motion, particles will move from the area of high concentration towards the area of low concentration, by the process of *diffusion, until the particles are evenly distributed in the solution or gas.

concerted reaction A type of reaction in which there is only one stage rather than a series of steps. The $S_N 2$ mechanism in *nucleophilic substitutions is an example. See also PERICYCLIC REACTIONS.

condensation The change of a vapour or gas into a liquid. The change of phase is accompanied by the evolution of heat (*see* LATENT HEAT).

condensation polymerization *See* POLYMER.

condensation pump See DIFFU-SION PUMP.

condensation reaction A chemical reaction in which two molecules combine to form a larger molecule with elimination of a small molecule (e.g. H_2O). See ALDEHYDES; KETONES.

condenser A device used to cool a vapour to cause it to condense to a liquid. *See* LIEBIG CONDENSER.

conducting polymer An organic polymer that conducts electricity. Conducting polymers have a crystalline structure in which chains of conjugated unsaturated carbon– carbon bonds are aligned. Examples are polyacetylene and polypyrrole. There has been considerable interest in the development of such materials because they would be cheaper and lighter than metallic conductors. They do, however, tend to be chemically unstable and, so far, no commercial conducting polymers have been developed. **conduct** of titratic conducti is contin reactant point is t undergoe method j

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normal i: **conduci** BANDS.

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Condy's cium and (mangana

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configu sional sp: $(q_1, q_2, \dots, c$



eclipsed con

@=methyl;

Conformatio



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Conformation

conformation

conductiometric titration A type of titration in which the electrical conductivity of the reaction mixture is continuously monitored as one reactant is added. The equivalence point is the point at which this undergoes a sudden change. The method is used for titrating coloured solutions, which cannot be used with normal indicators.

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conduction band See Energy BANDS.

conductivity water See DISTILLED WATER.

Condy's fluid A mixture of calcium and potassium permanganates (manganate(VII)) used as an antiseptic.

configuration 1. The arrangement of atoms or groups in a molecule.2. The arrangement of electrons about the nucleus of an *atom.

configuration space The *n*-dimensional space with coordinates $(q_1, q_2, ..., q_n)$ associated with a system



eclipsed conformation

🍘 = methyl group

Conformations of butane (sawhorse projection)



bisecting conformation

eclipsed conformation

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anti conformation

Conformations of R_CHO (Newman projection)

that has *n* degrees of freedom, where the values *q* describe the degrees of freedom. For example, in a gas of *N* atoms each atom has three positional coordinates, so the configuration space is 3*N*-dimensional. If the particles also have internal degrees of freedom, such as those caused by vibration and rotation in a molecule. then these must be included in the configuration space, which is consequently of a higher dimension. *See also* STATISTICAL MECHANICS.

conformation One of the very large number of possible spatial arrangements of atoms that can be interconverted by rotation about a single bond in a molecule. In the case of ethane, H_3C - CH_3 , one methyl group can rotate relative to the other. There are two extreme cases. In one, the C-H bonds on one group align with the C-H bonds on the other (as viewed along the C-C bond). This is an **eclipsed** conformation) and corresponds to a maximum in a



gauche conformation

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