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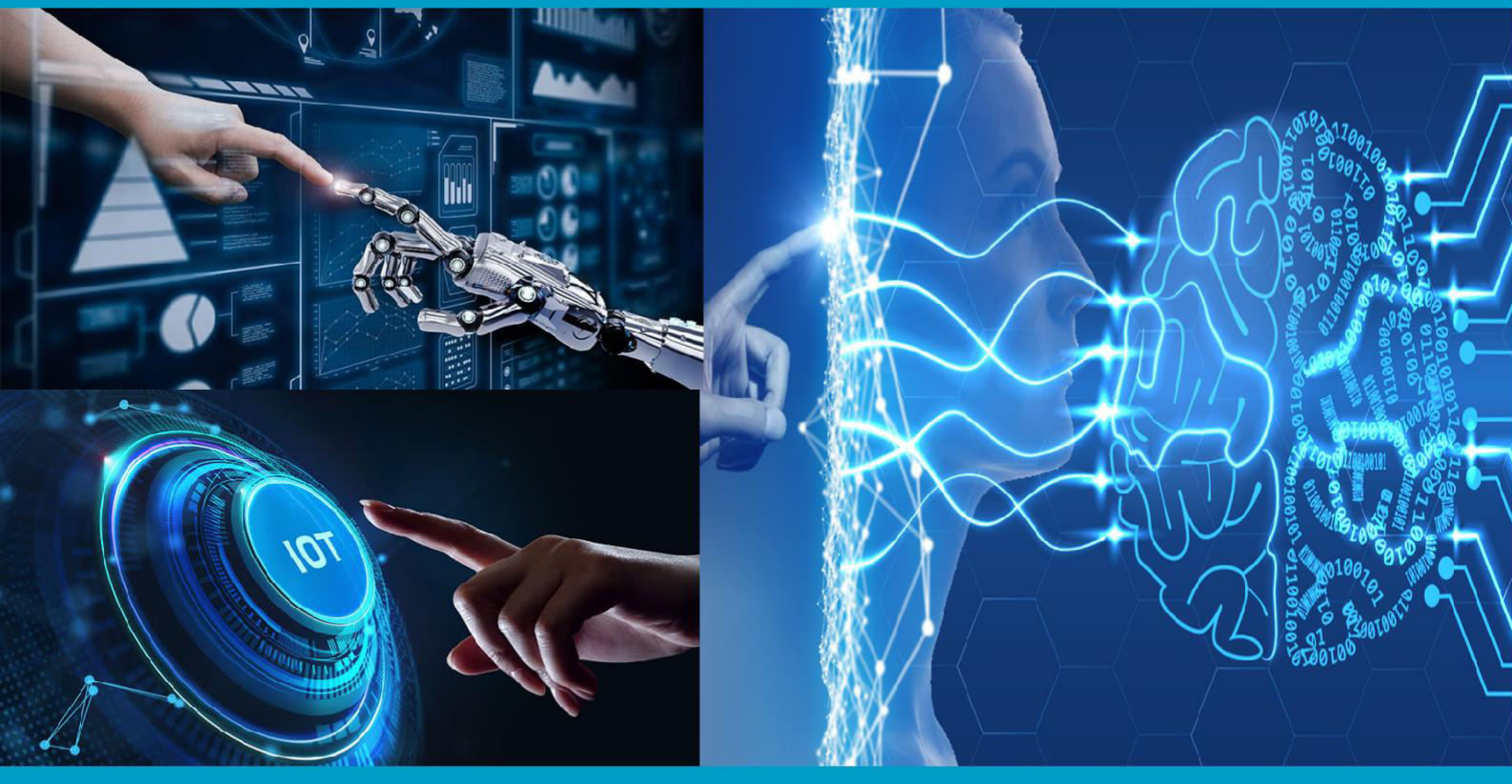

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Functional Groups are the Cause of Chemical Reactions

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ABSTRACT: In organic chemistry, a **functional group** is a substituent or moiety in a molecule that causes the molecule's characteristic chemical reactions. The same functional group will undergo the same or similar chemical reactions regardless of the rest of the molecule's composition. This enables systematic prediction of chemical reactions and behavior of chemical compounds and the design of chemical synthesis. The reactivity of a functional group can be modified by other functional groups nearby. Functional group interconversion can be used in retrosynthetic analysis to plan organic synthesis.

KEYWORDS: functional group, organic, chemical reactions, reactivity, analysis, compounds, molecule

I.INTRODUCTION

A functional group is a group of atoms in a molecule with distinctive chemical properties, regardless of the other atoms in the molecule. The atoms in a functional group are linked to each other and to the rest of the molecule by covalent bonds. For repeating units of polymers, functional groups attach to their nonpolar core of carbon atoms and thus add chemical character to carbon chains. Functional groups can also be charged, e.g. in carboxylate salts ($–COO^-$), which turns the molecule into a polyatomic ion or a complex ion. Functional groups binding to a central atom in a coordination complex are called ligands. Complexation and solvation are also caused by specific interactions of functional groups. In the common rule of thumb "like dissolves like", it is the shared or mutually well-interacting functional groups which give rise to solubility. For example, sugar dissolves in water because both share the hydroxyl functional group (–OH) and hydroxyls interact strongly with each other. Plus, when functional groups are more electronegative than atoms they attach to, the functional groups will become polar, and the otherwise nonpolar molecules containing these functional groups become polar and so become soluble in some aqueous environment.

Combining the names of functional groups with the names of the parent alkanes generates what is termed a systematic nomenclature for naming organic compounds. In traditional nomenclature, the first carbon atom after the carbon that attaches to the functional group is called the alpha carbon; the second, beta carbon, the third, gamma carbon, etc. If there is another functional group at a carbon, it may be named with the Greek letter, e.g., the gamma-amine in gamma-aminobutyric acid is on the third carbon of the carbon chain attached to the carboxylic acid group. IUPAC conventions call for numeric labeling of the position, e.g. 4-aminobutanoic acid. In traditional names various qualifiers are used to label isomers, for example, isopropanol (IUPAC name: propan-2-ol) is an isomer of n-propanol (propan-1-ol). The term moiety has some overlap with the term "functional group". However, a moiety is an entire "half" of a molecule, which can be not only a single functional group, but also a larger unit consisting of multiple functional groups. For example, an "aryl moiety" may be any group containing an aromatic ring, regardless of how many functional groups the said aryl has.

II.DISCUSSION

The following is a list of common functional groups.[3] In the formulas, the symbols R and R' usually denote an attached hydrogen, or a hydrocarbon side chain of any length, but may sometimes refer to any group of atoms.

Hydrocarbons

Hydrocarbons are a class of molecule that is defined by functional groups called hydrocarbyls that contain only carbon and hydrogen, but vary in the number and order of double bonds. Each one differs in type (and scope) of reactivity.

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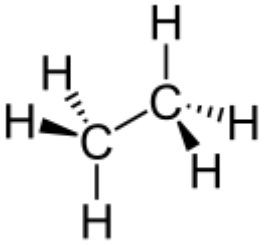
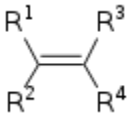
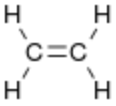
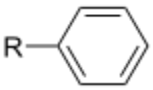
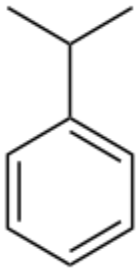
Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
Alkane	Alkyl	$R(CH_2)_nH$		alkyl-	-ane	 Ethane
Alkene	Alkenyl	$R_2C{=}CR_2$		alkenyl-	-ene	 Ethylene (Ethene)
Alkyne	Alkynyl	RC≡CR'		alkynyl-	-yne	Acetylene (Ethyne)
Benzene derivative	Phenyl	RC_6H_5 RPh		phenyl-	-benzene	 Cumene (Isopropylbenzene)

There are also a large number of branched or ring alkanes that have specific names, e.g., tert-butyl, bornyl, cyclohexyl, etc. Hydrocarbons may form charged structures: positively charged carbocations or negative carbanions. Carbocations are often named -um. Examples are tropylium and triphenylmethyl cations and the cyclopentadienyl anion.

Groups containing halogen

Haloalkanes are a class of molecule that is defined by a carbon–halogen bond. This bond can be relatively weak (in the case of an iodoalkane) or quite stable (as in the case of a fluoroalkane). In general, with the exception of fluorinated compounds, haloalkanes readily undergo nucleophilic substitution reactions or elimination reactions. The substitution on the carbon, the acidity of an adjacent proton, the solvent conditions, etc. all can influence the outcome of the reactivity.

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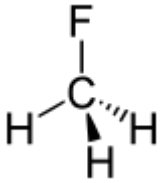
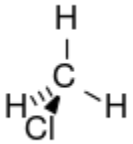
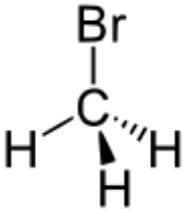
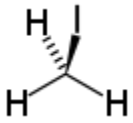
haloalkane	halo	RX		halo-	alkyl **halide**	 Chloroethane (Ethyl chloride)
fluoroalkane	fluoro	RF		fluoro-	alkyl **fluoride**	 Fluoromethane (Methyl fluoride)
chloroalkane	chloro	RCl		chloro-	alkyl **chloride**	 Chloromethane (Methyl chloride)
bromoalkane	bromo	RBr		bromo-	alkyl **bromide**	 Bromomethane (Methyl bromide)
iodoalkane	iodo	RI		iodo-	alkyl **iodide**	 Iodomethane (Methyl iodide)

Groups containing oxygen

Compounds that contain C-O bonds each possess differing reactivity based upon the location and hybridization of the C-O bond, owing to the electron-withdrawing effect of sp-hybridized oxygen (carbonyl groups) and the donating effects of sp^2-hybridized oxygen (alcohol groups).

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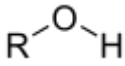
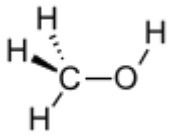
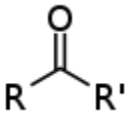
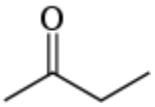
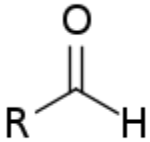
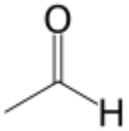
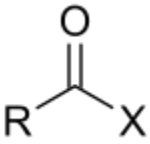
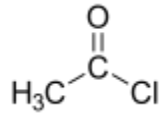
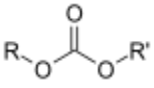
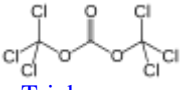
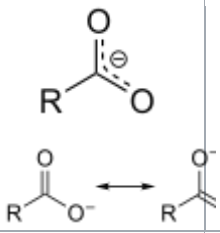
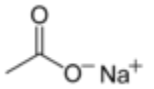
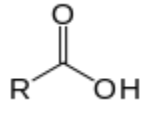
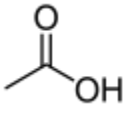
Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
Alcohol	Hydroxyl	ROH		hydroxy-	**-ol**	 Methanol
Carbonyl function	Carbonyl	CO				
Ketone	Ketone	RCOR'		-oyl- (-COR') or oxo- (=O)	**-one**	 Butanone (Methyl ethyl ketone)
Aldehyde	Aldehyde	RCHO		formyl- (-COH) or oxo- (=O)	**-al**	 Acetaldehyde (Ethanal)
Acyl halide	Haloformyl	RCOX		carbonofluoridoyl- carbonochloridoyl- carbonobromidoyl- carbonoiodidoyl-	-oyl **fluoride** -oyl **chloride** -oyl **bromide** -oyl **iodide**	 Acetyl chloride (Ethanoyl chloride)
Carbonate	Carbonate ester	ROCOOR'		(alkoxycarbonyl)oxy-	alkyl **carbonate**	 Triphosgene (bis(trichloromethyl) carbonate)
Carboxylate	Carboxylate	$RCOO^-$		carboxy-	-oate	 Sodium acetate (Sodium ethanoate)
Carboxylic acid	Carboxyl	RCOOH		carboxy-	-oic **acid**	

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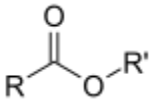
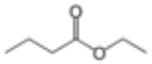
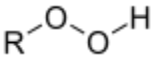
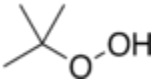
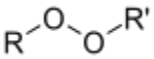
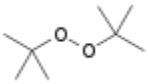
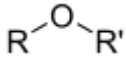
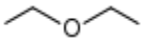
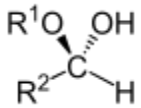
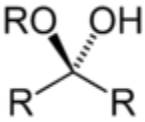
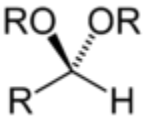
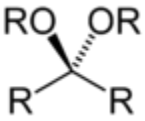
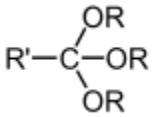
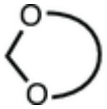
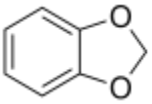
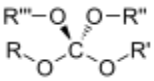
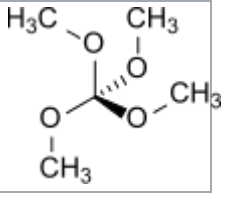
						Acetic acid (Ethanoic acid)
Ester	Carboalkoxy	RCOOR'		alkanoyloxy- or alkoxycarbonyl	alkyl alkan**oate**	 Ethyl butyrate (Ethyl butanoate)
Hydroperoxide	Hydroperoxy	ROOH		hydroperoxy-	alkyl **hydroperoxide**	 tert-Butyl hydroperoxide
Peroxide	Peroxy	ROOR'		peroxy-	alkyl **peroxide**	 Di-tert-butyl peroxide
Ether	Ether	ROR'		alkoxy-	alkyl **ether**	 Diethyl ether (Ethoxyethane)
Hemiacetal	Hemiacetal	$R_2CH(OR_1)(OH)$		alkoxy -ol	-al alkyl **hemiacetal**	
Hemiketal	Hemiketal	RC(OR″)(OH)R'		alkoxy -ol	-one alkyl **hemiketal**	
Acetal	Acetal	RCH(OR')(OR")		dialkoxy-	-al dialkyl **acetal**	
Ketal (or Acetal)	Ketal (or Acetal)	RC(OR")(OR‴)R'		dialkoxy-	-one dialkyl **ketal**	
Orthoester	Orthoester	RC(OR')(OR")(OR‴)		trialkoxy-		
Heterocycle (if cyclic)	Methylenedioxy	(–OCH_2O–)		methylenedioxy-	-dioxole	 1,2-Methylenedioxybenzene (1,3-Benzodioxole)
Orthocarbonate ester	Orthocarbonate ester	C(OR)(OR')(OR")(OR‴)		tetralkoxy-	tetraalkyl **orthocarbonate**	

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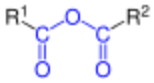
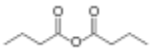
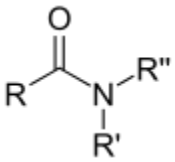
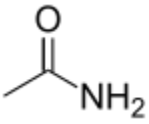
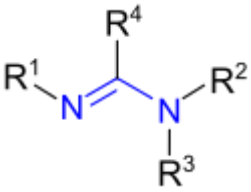
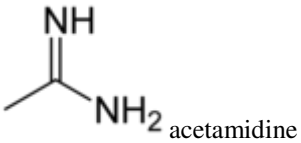
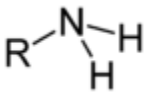
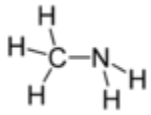
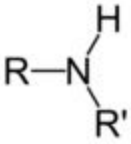
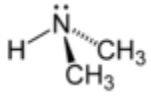
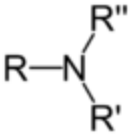
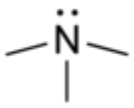
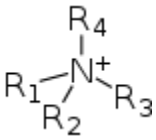
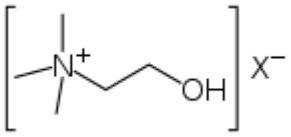
						Tetramethoxymethane
Organic acid anhydride	Carboxylic anhydride	$R_1(CO)O(CO)R_2$			anhydride	 Butyric anhydride

III.RESULTS

Groups containing nitrogen

Compounds that contain nitrogen in this category may contain C-O bonds, such as in the case of amides.

Chemical class	Group	Formula	Structural Formula	Prefix	Example
Amide	Carboxamide	RCONR'R"		carboxamido- or carbamoyl-	 Acetamide (Ethanamide)
Amidine	Amidine	$RC(NR)NR_2$		amidino-	 acetamidine (acetimidamide)
Amines	Primary amine	RNH_2		amino-	 Methylamine (Methanamine)
	Secondary amine	R'R"NH		amino-	 Dimethylamine
	Tertiary amine	R_3N		amino-	 Trimethylamine
	4° ammonium ion	R_4N^+		ammonio-	 Choline

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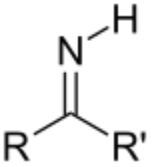
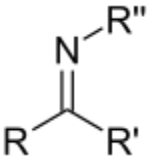
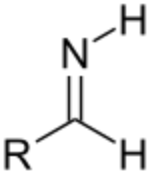
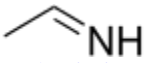
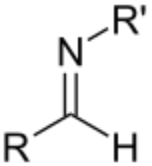
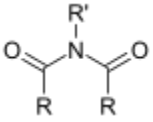
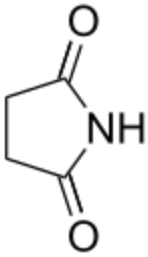
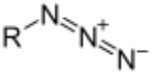
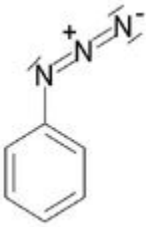
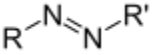
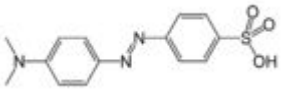
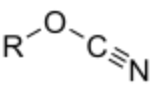
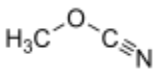
Imine	Primary ketimine	RC(=NH)R'		imino-	
	Secondary ketimine			imino-	
	Primary aldimine	RC(=NH)H		imino-	 Ethanimine
	Secondary aldimine	RC(=NR')H		imino-	
Imide	Imide	$(RCO)_2NR'$		imido-	 Succinimide (Pyrrolidine-2,5-dione)
Azide	Azide	RN_3		azido-	 Phenyl azide (Azidobenzene)
Azo compound	Azo (Diimide)	RN_2R'		azo-	 Methyl orange (p-dimethylamino-azobenzenesulfonic acid)
Cyanates	Cyanate	ROCN		cyanato-	 Methyl cyanate

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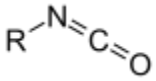
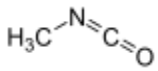
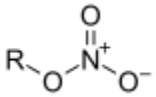
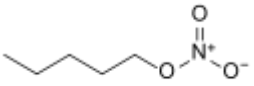
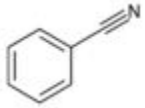
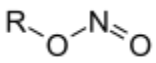
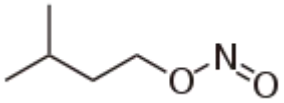
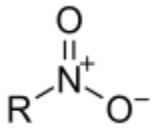
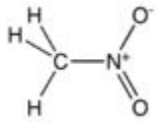
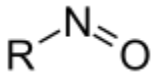
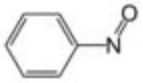
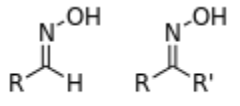
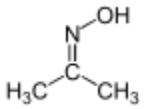
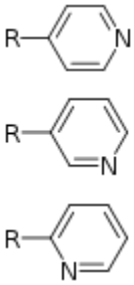
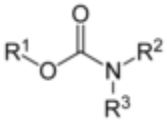
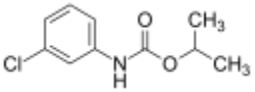
	Isocyanate	RNCO		isocyanato-	 Methyl isocyanate
Nitrate	Nitrate	$RONO_2$		nitrooxy-, nitroxy-	 Amyl nitrate (1-nitrooxypentane)
Nitrile	Nitrile	RCN		cyano-	 Benzonitrile (Phenyl cyanide)
	Isonitrile	RNC		isocyano-	Methyl isocyanide
Nitrite	Nitrosooxy	RONO		nitrosooxy-	 Isoamyl nitrite (3-methyl-1-nitrosooxybutane)
Nitro compound	Nitro	RNO_2		nitro-	 Nitromethane
Nitroso compound	Nitroso	RNO		nitroso- (Nitrosyl-)	 Nitrosobenzene
Oxime	Oxime	RCH=NOH	 aldoxime ketoxime		 Acetone oxime (2-Propanone oxime)
Pyridine derivative	Pyridyl	RC_5H_4N		4-pyridyl (pyridin-4-yl) 3-pyridyl (pyridin-3-yl) 2-pyridyl (pyridin-2-yl)	 Nicotine
Carbamate ester	Carbamate	$RO(C{=}O)NR_2$		(-carbamoyl)oxy-	 Chlorpropham (Isopropyl (3-

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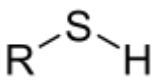
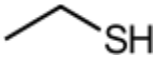
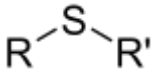
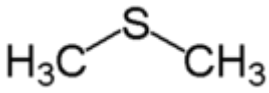
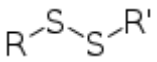
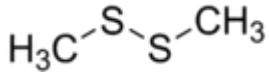
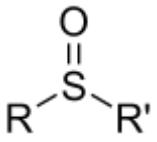
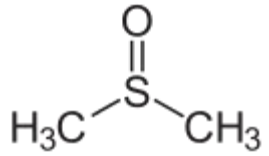
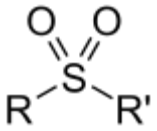
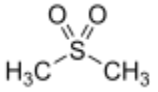
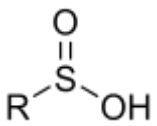
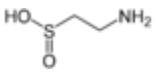
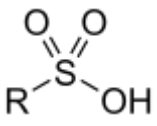
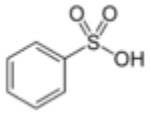
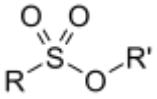
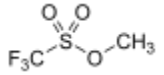
					chlorophenyl)carbamate)

Groups containing sulfur

Compounds that contain sulfur exhibit unique chemistry due to sulfur's ability to form more bonds than oxygen, its lighter analogue on the periodic table. Substitutive nomenclature (marked as prefix in table) is preferred over functional class nomenclature (marked as suffix in table) for sulfides, disulfides, sulfoxides and sulfones.

Chemical class	Group	Formula	Structural Formula	Example
Thiol	Sulfhydryl	RSH		 Ethanethiol
Sulfide (Thioether)	Sulfide	RSR'		 (Methylsulfanyl)methane (prefix) or Dimethyl sulfide (suffix)
Disulfide	Disulfide	RSSR'		 (Methyldisulfanyl)methane (prefix) or Dimethyl disulfide (suffix)
Sulfoxide	Sulfinyl	RSOR'		 (Methanesulfinyl)methane (prefix) or Dimethyl sulfoxide (suffix)
Sulfone	Sulfonyl	RSO_2R'		 (Methanesulfonyl)methane (prefix) or Dimethyl sulfone (suffix)
Sulfinic acid	Sulfino	RSO_2H		 2-Aminoethanesulfinic acid
Sulfonic acid	Sulfo	RSO_3H		 Benzenesulfonic acid
Sulfonate ester	Sulfo	RSO_3R'		 Methyl trifluoromethanesulfonate or Methoxysulfonyl trifluoromethane (prefix)

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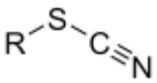
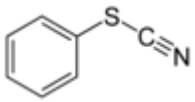
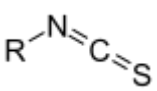
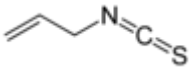
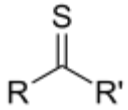
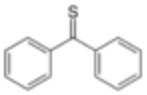
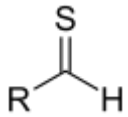
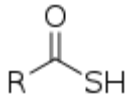
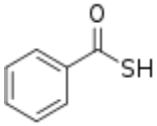
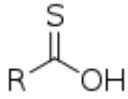
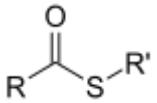
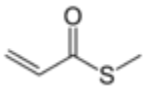
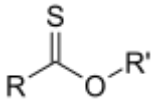
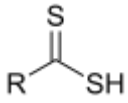
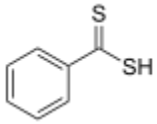
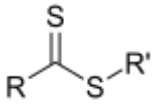
Thiocyanate	Thiocyanate	RSCN		 Phenyl thiocyanate
	Isothiocyanate	RNCS		 Allyl isothiocyanate
Thioketone	Carbonothioyl	RCSR'		 Diphenylmethanethione (Thiobenzophenone)
Thial	Carbonothioyl	RCSH		
Thiocarboxylic acid	Carbothioic S-acid	RC=OSH		 Thiobenzoic acid (benzothioic S-acid)
	Carbothioic O-acid	RC=SOH		
Thioester	Thiolester	RC=OSR'		 S-methyl thioacrylate (S-methyl prop-2-enethioate)
	Thionoester	RC=SOR'		
Dithiocarboxylic acid	Carbodithioic acid	RCS_2H		 Dithiobenzoic acid (Benzenecarbodithioic acid)
Dithiocarboxylic acid ester	Carbodithio	RC=SSR'		

Groups containing phosphorus

Compounds that contain phosphorus exhibit unique chemistry due to the ability of phosphorus to form more bonds than nitrogen, its lighter analogue on the periodic table.

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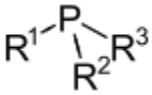
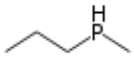
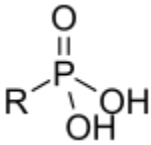
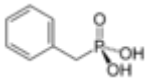
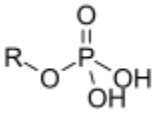
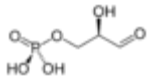
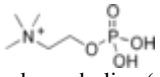
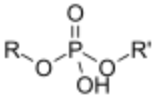
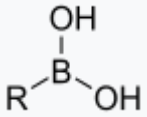
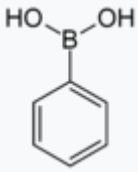
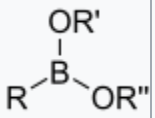
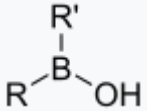
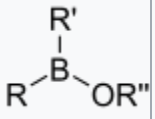
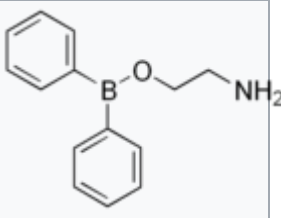
Chemical class	Group	Formula	Structural Formula	Example
Phosphine (Phosphane)	Phosphino	R_3P		 Methylpropylphosphane
Phosphonic acid	Phosphono			 Benzylphosphonic acid
Phosphate	Phosphate			 Glyceraldehyde 3-phosphate (suffix)
				 O-Phosphonocholine (prefix) (Phosphocholine)
Phosphodiester	Phosphate	$HOPO(OR)_2$		DNA
				O-[(2-Guanidinoethoxy)hydroxyphosphoryl]-L-serine (prefix) (Lombricine)

Groups containing boron

Compounds containing boron exhibit unique chemistry due to their having partially filled octets and therefore acting as Lewis acids.

Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
Boronic acid	Borono	$RB(OH)_2$		Borono-	substituent **boronic acid**	 Phenylboronic acid
Boronic ester	Boronate	$RB(OR)_2$		O-[bis(alkoxy)alkylboronyl]-	substituent **boronic acid** di(substituent) **ester**	
Borinic acid	Borino	R_2BOH		Hydroxyborino-	di(substituent) **borinic acid**	
Borinic ester	Borinate	R_2BOR		O-[alkoxydialkylboronyl]-	di(substituent) **borinic acid** substituent **ester**	 Diphenylborinic acid 2-aminoethyl ester (2-Aminoethoxydiphenyl borate)

Groups containing metals

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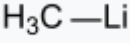
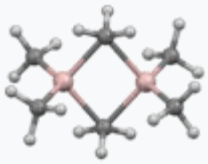
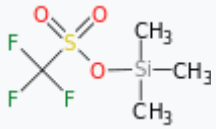
Chemical Class	Structural Formula	Prefix	Suffix	Example
Alkyllithium	RLi	(tri/di)alkyl-	-lithium	 methyllithium
Alkylmagnesium halide	RMgX (X=Cl, Br, I)[note 1]		-magnesium halide	 methylmagnesium chloride
Alkylaluminium	Al_2R_6		-aluminium	 trimethylaluminium
Silyl ether	R_3SiOR		-silyl ether	 trimethylsilyl triflate

Fluorine is too electronegative to be bonded to magnesium; it becomes an ionic salt instead.

Names of radicals or moieties

These names are used to refer to the moieties themselves or to radical species, and also to form the names of halides and substituents in larger molecules.
When the parent hydrocarbon is unsaturated, the suffix ("-yl", "-ylidene", or "-ylidyne") replaces "-ane" (e.g. "ethane" becomes "ethyl"); otherwise, the suffix replaces only the final "-e" (e.g. "ethyne" becomes "ethynyl").[4]
When used to refer to moieties, multiple single bonds differ from a single multiple bond. For example, a methylene bridge (methanediyl) has two single bonds, whereas a methylene group (methylidene) has one double bond. Suffixes can be combined, as in methylidyne (triple bond) vs. methylylidene (single bond and double bond) vs. methanetriyl (three double bonds).

There are some retained names, such as methylene for methanediyl, 1,x-phenylene for phenyl-1,x-diyl (where x is 2, 3, or 4),[5] carbyne for methylidyne, and trityl for triphenylmethyl.

Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
Single bond		R•		Ylo-[6]	-yl	Methyl group Methyl radical
Double bond		R:		?	-ylidene	Methylidene
Triple bond		R:		?	-ylidyne	Methylidyne
Carboxylic acyl radical	Acyl	R−C(=O)•		?	-oyl	Acetyl

CONCLUSIONS

A **group-contribution method** in chemistry is a technique to estimate and predict thermodynamic and other properties from molecular structures. In today's chemical processes hundreds of thousands of components are used. The Chemical Abstracts Service registry lists 56 million substances,[1] but many of these are only of scientific interest.
Process designers need to know some basic chemical properties of the components and their mixtures. Experimental measurement is often too expensive.
Predictive methods can replace measurements if they provide sufficiently good estimations. The estimated properties cannot be as precise as well-made measurements, but for many purposes the quality of estimated properties is sufficient. Predictive methods can also be used to check the results of experimental work.[3]

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A group-contribution method uses the principle that some simple aspects of the structures of chemical components are always the same in many different molecules. The smallest common constituents are the atoms and the bonds. The vast majority of organic components, for example, are built of carbon, hydrogen, oxygen, nitrogen, halogens, and maybe sulfur or phosphorus. Together with a single, a double, and a triple bond there are only ten atom types (not including astatine) and three bond types to build thousands of components. The next slightly more complex building blocks of components are functional groups, which are themselves built from few atoms and bonds.[4]

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1. Compendium of Chemical Terminology (IUPAC "Gold Book") functional group
2. ^ March, Jerry (1985), Advanced Organic Chemistry: Reactions, Mechanisms, and Structure (3rd ed.), New York: Wiley, ISBN 0-471-85472-7
3. ^ Brown, Theodore (2002). Chemistry: the central science. Upper Saddle River, NJ: Prentice Hall. p. 1001. ISBN 0130669970.
4. ^ Moss, G. P.; W.H. Powell. "RC-81.1.1. Monovalent radical centers in saturated acyclic and monocyclic hydrocarbons, and the mononuclear EH4 parent hydrides of the carbon family". IUPAC Recommendations 1993. Department of Chemistry, Queen Mary University of London. Archived from the original on 9 February 2015. Retrieved 25 February 2015.
5. ^ "R-2. 5 Substituent Prefix Names Derived from Parent Hydrides". IUPAC. 1993. section P-56.2.1
6. ^ "Revised Nomenclature for Radicals, Ions, Radical Ions and Related Species (IUPAC Recommendations 1993: RC-81.3. Multiple radical centers)". Archived from the original on 2017-06-11. Retrieved 2014-12-02.

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