

C07D

HETEROCYCLIC COMPOUNDS

Definition statement

This place covers:

Organic compounds containing at least one heterocyclic ring, and with no ring comprising a steroid, saccharide or peptide moiety. Said compounds should generally comprise the following elements or periodic groups only, C, H, halogen, N, O, S, Se, Te.

The only exception to this requirement is that the compounds may contain metal atoms, but only as the cations of heterocyclic organic acid salts, alcoholates, phenolates or mercaptides, or as chelating atoms, e.g. in porphyrins.

Preparation of such compounds, including purification, separation, stabilisation or use of additives, unless a separate place is provided elsewhere in the classification scheme.

Rings are considered as "heterocycles" only if they contain at least one atom selected from halogen, N, O, S, Se or Te as a ring member. Heterocyclic rings may be present as distinct entities or condensed, either with carbocycles or among themselves.

[C07D 201/00- C07D 259/00](#)

Heterocyclic compounds having only nitrogen as ring hetero atom

[C07D 261/00- C07D 273/00](#)

Heterocyclic compounds having nitrogen and oxygen as the only ring hetero atoms

[C07D 275/00- C07D 285/00](#)

Heterocyclic compounds having nitrogen and sulfur as the only ring hetero atoms

[C07D 291/00](#)

Heterocyclic compounds having nitrogen and oxygen and sulfur as the only ring hetero atoms

[C07D 293/00](#)

Heterocyclic compounds containing rings having nitrogen and selenium or nitrogen and tellurium, with or without oxygen or sulfur atoms, as the ring hetero atoms

[C07D 295/00](#)

Heterocyclic compounds containing polymethylene-imine rings with at least five ring members, 3-azabicyclo [3.2.2] nonane, piperazine, morpholine or thiomorpholine rings, having only hydrogen atoms directly attached to the ring carbon atoms

[C07D 301/00- C07D 329/00](#)

Heterocyclic compounds having oxygen atoms, with or without sulfur, selenium or tellurium atoms, as ring hetero atoms

[C07D 331/00- C07D 345/00](#)

Heterocyclic compounds having sulfur, selenium or tellurium atoms as the only ring hetero atoms

[C07D 347/00](#)

Heterocyclic compounds containing halogen as ring hetero atoms

[C07D 401/00- C07D 421/00](#)

Heterocyclic compounds containing two or more hetero rings (*)

[C07D 451/00- C07D 519/00](#)

Heterocyclic compounds containing condensed hetero ring systems (**)

[C07D 521/00](#) Heterocyclic compounds containing unspecified hetero rings

(*) Groups [C07D 401/00-C07D 421/00](#)

Cover compounds containing two or more relevant hetero rings at least two of which are covered by different main groups of groups [C07D 203/00- C07D 347/00](#), neither condensed among themselves nor condensed with a common carbocyclic ring or ring system

(**) Groups [C07D 451/00- C07D 517/00](#)

Cover compounds containing one system of two or more relevant hetero rings condensed among themselves or condensed with a common carbocyclic ring system, with or without other non-condensed hetero rings.

Relationships with other classification places

In class [C07](#), the last place priority rule is used, i.e. in the absence of an indication to the contrary, a compound is classified in the last appropriate subclass. Hence, while individual heterocycle-containing amino acids are classified in this subclass [C07D](#), peptides are generally classified in subclass [C07K](#). Similarly, compounds containing saccharide radicals are classified in subclass [C07H](#), and heterocyclic steroids are classified in subclass [C07J](#). (Detailed instructions which compounds are considered as [C07H](#), [C07J](#) or [C07K](#) can be found in the corresponding CPC Definitions.) Heterocycles incorporating elements other than C, H, halogen, N, O, S, Se or Te are classified in subclass [C07F](#), but only if the metal-containing compound has a metal carbon bond or if the metal is attached to at least two different ligands. Salts, chelates, alcoholates (except Ti/Zr), phenates involving a single ligand are classified as the parent compound (metal containing porphyrin [C07D 487/22](#)).

This subclass is a structure-oriented entry for the compounds themselves and does not cover the application or use of the compounds under the subclass definition.

For classifying such information other entries exist, for example:

- Heterocyclic compounds for producing dyes are classified in subclass [C09B](#).
- Compounds or compositions for preservation of bodies of humans, animals, plants, or parts thereof, as biocides, e.g. disinfectants, pesticides, herbicides, as pest repellants or attractants, and as plant growth regulators are classified in subclass [A01N](#).
- Preparations for medical, dental, or toilet purposes or methods of using compounds for the same purposes are classified in subclass [A61K](#). (N.B.: when the compound per se is novel, the medicinal preparation and/or methods of use are not classified in [A61K 31/00](#) in CPC).

Multiple classification:

Biocidal, pest attractant, or plant growth regulatory activity of chemical compounds or preparations is further classified in subclass [A01P](#) (this subclass does only exist in IPC). Therapeutic activity of chemical compounds is further classified in subclass [A61P](#). Uses of cosmetics or similar toilet preparations are further classified in subclass [A61Q](#).

Oligomers are classified as low molecular compounds in [C07D](#) and as macromolecular compounds in [C08](#).

References

Limiting references

This place does not cover:

Heterocyclic organic compounds containing elements other than carbon, hydrogen, halogen, oxygen, nitrogen, sulfur, selenium or tellurium	C07F
Sugars	C07H
Steroids	C07J
Peptides	C07K
Macromolecular compounds	C08
Dyes and pigments	C09B
Liquid crystalline compounds	C09K 19/00
Preparation of heterocyclic organic compounds using enzymes or fermentation processes	C12P
Electrolytic production of organic compounds	C25B 3/00
Processes for producing compounds in which simultaneously electricity is generated	C25B 5/00
Electrophoretic production of compounds	C25B 7/00

Informative references

Attention is drawn to the following places, which may be of interest for search:

Pesticides	A01N
Biocidal activity	A01P (IPC)
Food or functional food (nutraceuticals)	A23L
Cosmetics	A61K 8/00 , A61Q
Medicinal preparations containing organic ingredients	A61K 31/00
Therapeutic activity	A61P
Physical or Chemical Processes or Apparatus in General	B01
Catalysts	B01J
Generic methods and apparatus therefor used in organic chemistry, such as oxidation, reduction, addition, substitution, purification, separation, stabilisation	C07B
Adhesives	C09J
Luminescent, e.g. electroluminescent, chemiluminescent materials	C09K 11/00
Combinatorial libraries containing organic compounds	C40B 40/00

Special rules of classification

In this subclass, in the absence of an indication to the contrary, a compound is classified in the last appropriate place.

Chemical compounds and their preparation are classified in the groups for the type of compound prepared. The processes of preparation are also classified in the groups for the types of reaction employed, if of interest. The compounds prepared are also classified in the groups for the types of compounds prepared, if of interest.

Salts of a compound, unless specifically provided for, are classified as that compound. Salts, adducts or complexes formed between two or more organic compounds are classified according to all compounds forming the salts, adducts or complexes.

Where a molecule may exist in tautomeric forms, classification is made for the form which appears latest in the scheme. Therefore, double bonds between ring members and non-ring members and double bonds between ring members themselves are considered equivalent in determining the degree of hydrogenation of the ring.

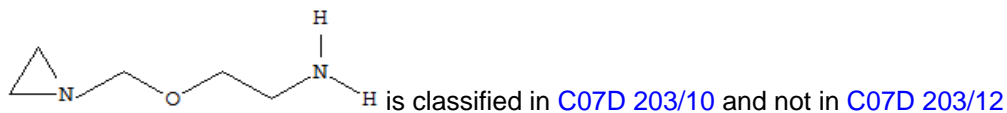
Compounds containing a single heterocycle are classified in the range [C07D 203/00-C07D 347/00](#) (cf. Table 1). Compounds containing two or more heterocycles, none of which are condensed among themselves nor condensed with a carbocyclic ring, and all of which are covered by the same main group, are also classified in this range.

Compounds containing two or more hetero rings individually covered by different main groups, and not part of the same condensed ring system are classified in the range [C07D 401/00-C07D 421/00](#) (cf. Table 2).

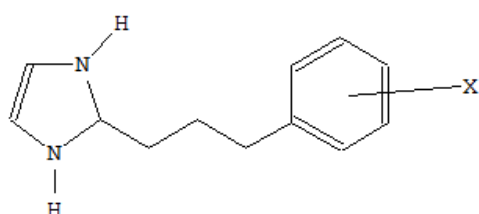
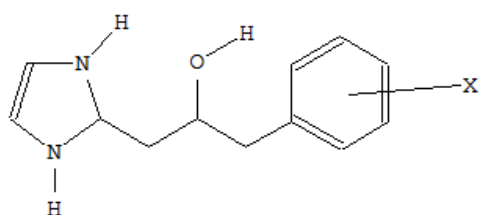
Compounds containing two or more hetero rings, being part of the same condensed ring system, are classified in the range [C07D 451/00-C07D 519/00](#) (cf. Table 3 and 4).

Heterocyclic compounds which contain rings of five or more members, wherein only nitrogen is present as a ring heteroatom, and wherein the ring carbon atoms are fully saturated and only bound to hydrogen atoms, are classified in main group [C07D 295/00](#). Morpholines and thiomorpholines unsubstituted on the ring carbon atoms are also classified here.

An acyclic side-chain linked to the hetero ring is considered to be terminated by every bond to:
1) an element other than carbon 2) a carbon atom having three bonds to hetero atoms, with at the most one bond to halogen, e.g. ester or nitrile radicals. For example, the compound:



Where a heterocycle is linked to a carbocycle by an acyclic chain, and both the chain and the carbocycle are further substituted by either hetero atoms or carbon atoms with three bonds to hetero atoms, not more than one hetero atom being a halogen, the molecule is classified according to the substituents on the acyclic chain. See the following example:

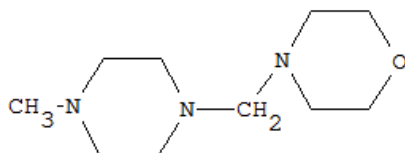


X = - NH₂, - NHCOCH₃, or - COOCH₃.

[C07D 451/00-C07D 517/00](#) cover compounds containing one system of two or more relevant hetero rings condensed among themselves or condensed with a common carbocyclic ring system, with or without other non-condensed hetero rings. For the purpose of classification in groups [C07D 451/00-C07D 519/00](#), the degree of hydrogenation of the ring system is not taken into consideration. For the purpose of classification in groups [C07D 451/00](#) [C07D 463/00](#),

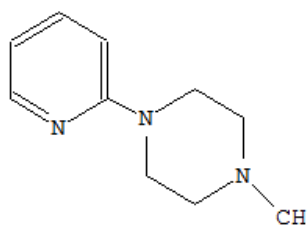
[C07D 473/00-C07D 477/00](#), [C07D 489/00](#), [C07D 499/00-C07D 507/00](#), the wording of the groups has to be understood, in the absence of an indication to the contrary, as including ring systems further condensed with carbocyclic rings or ring systems, but excluding ring systems further condensed with other hetero rings, either directly or through a common carbocyclic ring system, e.g. sparteine is classified in group [C07D 471/22](#), not in group [C07D 455/02](#). In groups [C07D 471/00](#), [C07D 487/00](#), [C07D 491/00-C07D 498/00](#) or [C07D 513/00-C07D 517/00](#), the subdivision is based on the number of relevant hetero rings.

Where a compound contains at least one ring covered by group [C07D 295/00](#) and at least one other hetero ring, the hetero ring covered by group [C07D 295/00](#) is treated as an acyclic chain containing nitrogen atoms for the purposes of classification and is not considered to be a hetero ring in this



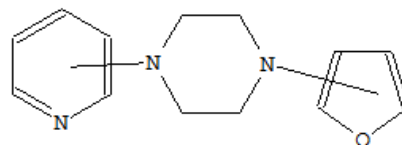
context. Thus, e.g.

[C07D 295/02](#), and NOT [C07D 413/06](#) and



[C07D 213/74](#), and NOT [C07D 401/04](#)

[C07D 405/12](#), and NOT [C07D 405/14](#)



What is classified as a compound?

Classified are real examples of claimed compounds, i.e. those which are prepared or for which physical data are given, and which are individually named or drawn in the claims. The same applies for compounds disclosed as reaction intermediates.

Not classified are generic formulae (Markush formulae, even if they have only one variable group), lists of "prophetic compounds" which fall within the scope of the claims but which were not actually prepared and compounds disclosed in the description but which are not claimed as compounds per se.

What is classified as a process for the preparation of a compound?

Classified are only preparation examples of claimed processes. A process is classified in a process group if a dedicated process group exists (e.g. [C07D 201/00](#) or [C07D 301/00](#)). Where there is no process group for making a particular compound the process is classified according to the product obtained in the claimed process.

Further classification information:

Tables 1-4 provide an overview of the main groups in [C07D](#).

Structural chemical formulae for various subgroups (in particular for specific ring systems as shown in table 3 below) are available in the classification scheme on the WIPO web-site.

Table 1: Overview of main groups [C07D 201/00](#) - [C07D 347/00](#):

	Number of heteroatoms / Number of carbon atoms / Ring characteristics
Only N:	
C07D 201/00	Preparation of unsubstituted lactams
C07D 203/00	1N / 2C / _

C07D 205/00	1N / 3C / _
C07D 207/00	1N / 4C / _
C07D 209/00	_ / _ / condensed pyrroles
C07D 211/00	1N / 5C / hydrogenated
C07D 213/00	1N / 5C / aromatic
C07D 215/00	_ / _ / quinolines
C07D 217/00	_ / _ / isoquinolines
C07D 219/00	_ / _ / acridines
C07D 221/00	_ / _ / other condensed pyridines
C07D 223/00	1N / 6C / _
C07D 225/00	1N / > 6C / _
C07D 227/00	Heterocyclic compounds according to more than one of groups C07D 203/00 - C07D 225/00
C07D 229/00	2N / 1C,2C / _
C07D 231/00	2N / 3C / (1,2)
C07D 233/00	2N / 3C / (1,3)
C07D 235/00	_ / _ / condensed imidazoles
C07D 237/00	2N / 4C / (1,2)
C07D 239/00	2N / 4C / (1,3)
C07D 241/00	2N / 4C / (1,4)
C07D 243/00	2N / 5C / _
C07D 245/00	2N / > 5C / _
C07D 247/00	Heterocyclic compounds according to more than one of groups C07D 229/00 - C07D 245/00
C07D 249/00	3N / 2C / (1,2,3)
C07D 251/00	3N / 3C / (1,3,5)
C07D 253/00	3N / 3C / (1,2,4), (1,2,3)
C07D 255/00	3N / _ / C07D 251/00 - C07D 253/00
C07D 257/00	4N / _ / _
C07D 259/00	> 4N / _ / _
Only N+O:	
C07D 261/00	1N+1O / 3C / (1,2)
C07D 263/00	1N+1O / 3C / (1,3)
C07D 265/00	1N+1O / 4C / _
C07D 267/00	1N+1O / >4C / _
C07D 269/00	Heterocyclic compounds according to more than one of groups C07D 261/00 - C07D 267/00
C07D 271/00	2N+1O / 2C / _
C07D 273/00	N+O / _ / C07D 261/00 - C07D 271/00
Only N+S:	

C07D 275/00	1N+1S / 3C / (1,2)
C07D 277/00	1N+1S / 3C / (1,3)
C07D 279/00	1N+1S / 4C / _
C07D 281/00	1N+1S / >4C / _
C07D 283/00	Heterocyclic compounds according to more than one of groups C07D 275/00 - C07D 281/00
C07D 285/00	N+S/ _ / ≠ 275-283
Only N+O+S:N+Se/ Te(+O) (+S)	
C07D 291/00	N+O+S / _ / _
C07D 293/00	N+Se/Te(+O) (+S) / _ / _
C07D 295/00	compounds containing polymethylene-imine rings with at least five ring members, 3-azabicyclo [3.2.2] nonane, piperazine, morpholine or thiomorpholine rings, having only hydrogen atoms directly attached to the ring carbon atoms
Only O; O+S; O+Se/Te (+S):	
C07D 301/00	Preparation of oxiranes
C07D 303/00	1O / 2C / _
C07D 305/00	1O / 3C / _
C07D 307/00	1O / 4C / _
C07D 309/00	1O / 5C / _
C07D 311/00	/ _ / _ / condensed pyrans
C07D 313/00	1O / > 5C / _
C07D 315/00	Heterocyclic compounds according to more than one of groups C07D 303/00 - C07D 313/00
C07D 317/00	2O / 3C / _
C07D 319/00	2O / 4C / _
C07D 321/00	2O / >4C / _
C07D 323/00	> 2O / _ / _
C07D 325/00	Heterocyclic compounds according to more than one of groups C07D 317/00 - C07D 323/00
C07D 327/00	O+S / _ / _
C07D 329/00	O+Se/Te(+S) / _ / _
Only S; S+Se/Te:	
C07D 331/00	1S / 2C,3C / _
C07D 333/00	1S / 4C / _
C07D 335/00	1S / 5C / _
C07D 337/00	1S / > 5C / _
C07D 339/00	2S / _ / _
C07D 341/00	> 2S / _ / _
C07D 343/00	S+Se/Te / _ / _

Only Se/Te:	
C07D 345/00	Se, Te; Se+Te / _ / _
Containing halogen:	
C07D 347/00	_ / _ / containing halogen

NOTES to Table 1:

condensed derivatives are together with the parent hetero ring, unless a specific main group is provided

hydrogenated derivatives are together with the parent hetero ring, with the exception of [C07D 211/00](#), [C07D 213/00](#)

the relative position of the hetero atoms in the hetero ring is given between brackets

Table 2: Overview of main groups [C07D 401/00](#) - [C07D 421/00](#):

	At least one of the rings contains as heteroatoms ...
C07D 401/00	only N, at least one of them being a C5N ring
C07D 403/00	only N, not provided for by C07D 401/00
C07D 405/00	only O, and at least one ring with only N
C07D 407/00	only O, not provided for by C07D 405/00
C07D 409/00	only S
C07D 411/00	only O+S
C07D 413/00	only N+O
C07D 415/00	containing the THIAMINE skeleton
C07D 417/00	only N+S
C07D 419/00	only N+O+S
C07D 421/00	Se/Te; halogen; (+O) (+S) (+N)

Tables 3 and 4: Overview of main groups [C07D 451/00](#) - [C07D 521/00](#):

Table 3: Overview of specific condensed systems:

C07D 451/00	8-Azabicyclo[3.2.1]octane (tropane) 6,7-Epoxy-8-azabicyclo[3.2.1]octane (scopolamine) and cyclic acetals; 9-Azabicyclo[3.3.1]nonane (granatane)
C07D 453/00	Quinuclidine or isoquinuclidine containing ring systems (e.g. quinine derivatives)
C07D 455/00	Quinolizine containing ring systems (e.g. berberine or emetine)
C07D 457/00	Indolo[4,3-f,g]quinoline, (e.g. Ergot alkaloids)
C07D 459/00	Benz[g]indolo[2,3-a]quinolizine (yohimbine) and lactones (reserpine acid lactone)
C07D 461/00	Indolo [3,2,1-d,e]pyrido [3,2,1-i,]] [1,5]-naphthyridine ring systems, e.g. vincamine (dimeric indolo alkaloids C07D 519/04)
C07D 463/00	Carbacephalosporins
C07D 473/00	Purine

C07D 475/00	Pteridine
C07D 477/00	Thienamycins (Carbapenicillins)
C07D 489/00	4aH-8,9c-Iminoethanophenanthro[4,5-b,c,d]furan ring systems, (e.g. morphine) and 6,14-carbon bridged derivatives (oripavines)
C07D 499/00	Penicillins
C07D 501/00	Cephalosporins
C07D 503/00	Oxapenicillins
C07D 505/00	Oxacephalosporins
C07D 507/00	Condensed beta-lactam ring systems, not provided for by groups C07D 463/00 , C07D 477/00 or C07D 499/00- C07D 505/00
C07D 519/02 and C07D 519/04	Ergot and Vinca alkaloids containing two or more condensed systems in the molecule

Table 4: Overview of other condensed systems:

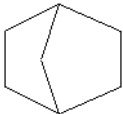
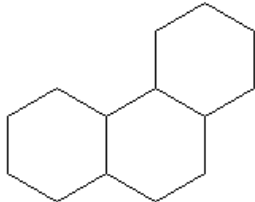
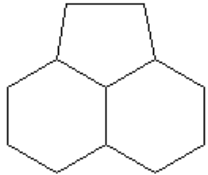
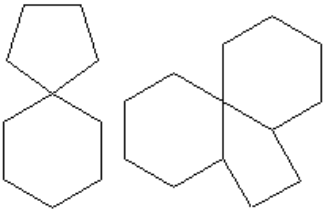
(compounds of Table 3 take precedence)

	The ring system contains as heteroatoms ...
C07D 471/00	only nitrogen atoms, with at least one (hydro) pyridine, not provided for by Table 3
C07D 487/00	only nitrogen atoms, not provided for by Table 3 and by C07D 471/00
C07D 491/00	at least one ring containing only oxygen atoms and at least one ring containing only nitrogen atoms, not provided for by C07D 451/00 , C07D 459/00 , C07D 463/00 , C07D 477/00 or C07D 489/00
C07D 493/00	only oxygen atoms
C07D 495/00	at least one ring containing only sulfur atoms
C07D 497/00	at least one ring containing only oxygen and sulfur atoms
C07D 498/00	at least one ring containing only nitrogen and oxygen atoms
C07D 513/00	at least one ring containing only nitrogen and sulfur atoms (penicillin C07D 499/00 ; cephalosporin C07D 501/00)
C07D 515/00	at least one ring containing only nitrogen, oxygen and sulfur atoms
C07D 517/00	at least one ring containing selenium, tellurium or halogen atoms, with or without other hetero atoms
C07D 519/00	two or more condensed systems in the molecule not provided for by C07D 453/00 or C07D 455/00
C07D 521/00	unspecified hetero rings

Glossary of terms

In this place, the following terms or expressions are used with the meaning indicated:

Acyclic	The absence of a ring structure. Acyclic chains may be linear or branched.
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Bridged	<p>Where two condensed rings share at least three adjacent ring members:</p> 
Carbocyclic	Where all ring members in a ring are carbon atoms.
Condensed	Where at least two rings share at least one ring member.
Condensed ring system	<p>A ring system in which all rings are condensed among themselves, i.e. a ring system wherein the scission of a single connection between two ring atoms cannot result in the division of the ring system into separate entities. Two or more hetero rings are considered part of the same condensed ring system if they are condensed among themselves or to a common carbocycle or carbocyclic system.</p>
Heterocyclic	<p>Wherein at least one ring member in a molecule containing a ring of atoms is not a carbon atom. For the purposes of classification in this subclass, a narrower definition applies wherein heteroatoms may only be chosen from nitrogen, oxygen, sulfur, selenium, tellurium or halogen.</p>
Ortho-condensed	<p>Where two condensed rings share two adjacent ring atoms in common. A ring system is deemed ortho-condensed if each ring shares only one face with any other ring, and no ring has two adjacent shared faces:</p> 
Peri-condensed	<p>Where three rings in a condensed ring system share a single ring atom in common:</p> 
Spiro-condensed	<p>Where two condensed rings share only one atom in common:</p>  <p>"free" "frozen"</p>
Number of relevant rings	<p>In a condensed ring system, this equals the minimum number of scissions necessary to convert the ring system into an acyclic chain, a scission being the disconnection of two bonded atoms, without regard for the bond order.</p>

Relevant rings	These are the rings which account for all the bonds in a condensed system. In order to prevent ambiguity in classifying a condensed ring system, the rings which identify the ring system are determined according to the following hierarchy of criteria: the rings with the lowest number of members; the rings with the highest number of hetero atoms as ring members; the rings with the lowest number of members shared between rings; the rings with the latest place in the classification scheme.
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C07D 521/00

Heterocyclic compounds containing unspecified hetero rings

Special rules of classification

This group is only used for the classification of compounds the chemical structure of which is not specified, i.e. only in those cases where the compounds cannot be classified in any of groups:

[C07D 201/00](#) - [C07D 519/00](#).