

Notes under Subclass C07D:

1. This subclass does not cover compounds containing saccharide radicals (as defined in the Note on scope following the title of subclass C07H), which are covered by subclass C07H.
2. In this subclass, in compounds containing a hetero ring covered by group C07D295/00 and at least one other hetero ring, the hetero ring covered by group C07D295/00 is considered as an acyclic chain containing nitrogen atoms.
3. In this subclass, the following terms or expressions are used with the meanings indicated:
 - a. "hetero ring" is a ring having at least one halogen, nitrogen, oxygen, sulfur, selenium, or tellurium atom as a ring member;
 - b. "bridged" means the presence of at least one fusion other than ortho, peri or spiro;
 - c. two rings are "condensed" if they share at least one ring member, i.e. "spiro" and "bridged" are considered as condensed;
 - d. "condensed ring system" is a ring system in which all rings are condensed among themselves;
 - e. "number of relevant rings" in a condensed ring system equals the number of scissions necessary to convert the ring system into one acyclic chain;
 - f. "relevant rings" in a condensed ring system, i.e. the rings which taken together describe all the links between every atom of the ring system, are chosen according to the following criteria consecutively:
 - 1) lowest number of ring members
 - 2) highest number of hetero atoms as ring members
 - 3) lowest number of members shared with other rings
 - 4) last place in the classification scheme.
4. In this subclass, in the absence of an indication to the contrary:
 - a. compounds having only one hetero ring are classified in the last appropriate place in one of the groups C07D203/00 to C07D347/00. The same applies for compounds having more hetero rings covered by the same main group, neither condensed among themselves nor condensed with a common carbocyclic ring system;
 - b. compounds having two or more hetero rings covered by different main groups neither condensed among themselves nor condensed with a common carbocyclic ring system are classified in the last appropriate

place in one of the groups C07D401/00 to C07D421/00;

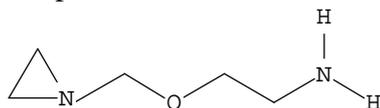
- c. compounds having two or more relevant hetero rings, covered by the same or by different main groups, which are condensed among themselves or condensed with a common carbocyclic ring system, are classified in the last appropriate place in one of the groups C07D451/00 to C07D519/00.

5. In this subclass:

- a. where a compound may exist in tautomeric forms, it is classified as though existing in the form which is classified last in the system. 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. Formulae are considered to be written in Kekulé form;

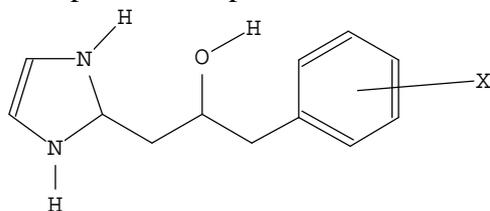
- b. [N: an acyclic side-chain linked to the hetero ring is considered to be terminated by every bond to:

- 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:

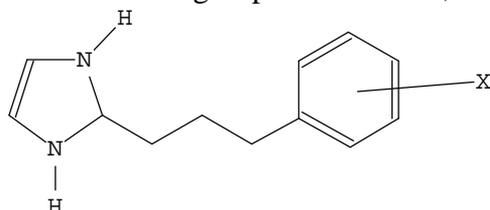


is classified in C07D203/10 and not in C07D203/12]

- c. hydrocarbon radicals containing a carbocyclic ring and an acyclic chain by which it is linked to the hetero ring and being substituted on both the carbocyclic ring and the acyclic chain by hetero atoms or by carbon atoms having three bonds to hetero atoms with at the most one bond to halogen, are classified according to the substituents on the acyclic chain. For example, the compound



is classified in group C07D233/22, and the compound



is classified in groups C07D233/24 and C07D233/26, where X

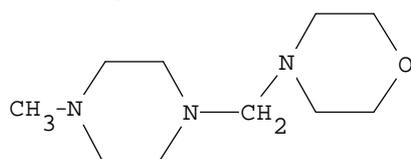
= -NH₂, -NHCOCH₃, or -COOCH₃.

6. [N: In groups C07D401/00 to C07D421/14, i.e. for compounds having two or more hetero rings (not classified in C07D451/ to C07D519/), which are covered per se by different main groups of C07D203/00 to C07D347/00, following supplementary definitions and rules apply:

a. Heterocyclic compounds containing two or more hetero rings and belonging to C07D401/00 to C07D421/14 are only classified on the level of the main group according to Table A, plus the standard subdivision according to Table B (e.g. C07D409/12), and use is no longer made of the individual notations of the component heterorings according to Table C, as from July 1st, 2005.

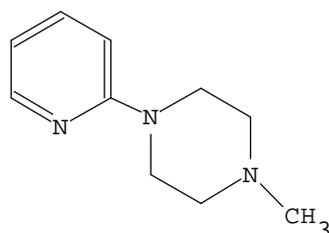
b. According to note on scope (2) of C07D, hetero rings belonging to C07D295/00, (e.g. cyclamines), are not considered to be hetero rings in this context.

Thus, e.g.



C07D295/02D, and NOT C07D413/06

and



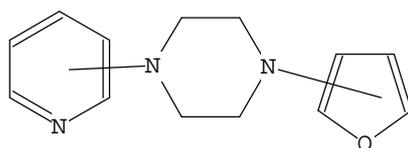
C07D213/74, and NOT C07D401/04

c. Complementary Notation for linked hetero rings used before 01.07.2005

(No longer used)

- 1) Until 01.07.2005 the classification for linked hetero rings was based on a complementary notation system, the complementary notations relating to EACH of the hetero rings present in the molecule - with the exception of those belonging to C07D295/00.

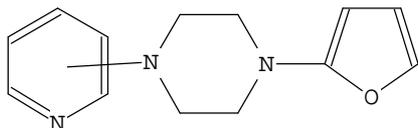
Thus, e.g.



C07D405/12, and NOT C07D405/14

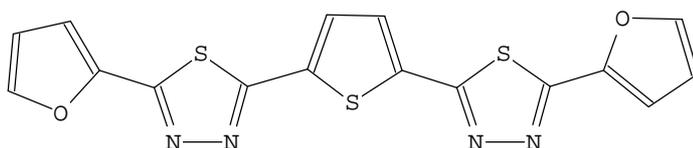
- 2) To facilitate the determination of the main group, Table A gives in a succinct way the content of these groups; the standard subdivision of these main groups is listed in Table B. (Note: main group C07D415/00 is NOT subdivided!)
 In Table C are listed the notations used for the component hetero rings. In all these tables, the last-place rule is mandatory, as no hierarchical levels are involved!

The notations were NOT written in the official IPC manner, e.g.



NOT: C07D405/12 (C07D405/12, C07D307/00, C07D213/00),
 BUT: C07D405/12+307B+213

- 3) Compounds containing four or more relevant hetero rings, at least two of which are covered by the same main group C07D203/00 to C07D347/00 were classified in a relevant C07D4../14R group; this classification symbol is followed by the complementary notations for the hetero rings, each individual notation being only given one time, e.g.

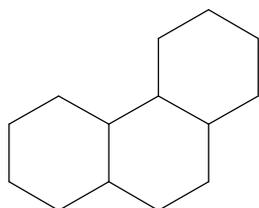


C07D417/14R + 333B + 307B + 285B

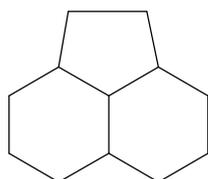
7. [N: For groups C07D451/00 to C07D521/00, i.e. for compounds having two or more relevant hetero rings, covered by the same or by different main groups, **condensed** among themselves or **condensed** with a common carbocyclic ring or ring system, following supplementary definitions and rules apply:

a. Definitions:

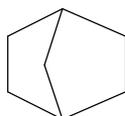
Ortho-condensed: polycyclic compounds in which two rings have two, and only two, atoms in common, e.g.



Peri-condensed: polycyclic compounds in which one ring contains two, and only two, atoms in common with each of two or more rings of a contiguous, (i.e. condensed among themselves) series of rings, e.g.



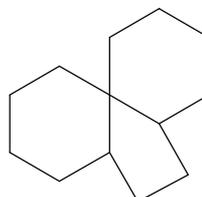
Bridged: two rings having three or more atoms in common, i.e. the bridge contains at least one atom in addition to the bridge-heads, e.g.



Spiro-condensed: a spiro union is one formed by a single atom which is the only common member of two rings: free spiro and frozen spiro union, e.g.

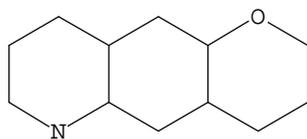


”free”

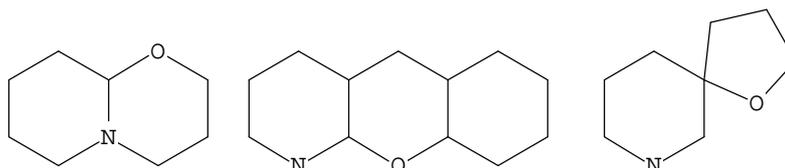


“frozen”

Not directly condensed hetero rings: are hetero rings having no atoms in common, e.g.

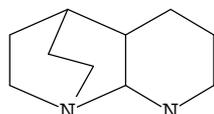


Directly condensed hetero rings: are hetero rings having at least one common atom, e.g.



b. Rules:

- 1) When no "specific" group is provided ("specific" groups: Table F; "no specific" groups: Table G), all relevant rings having hetero atoms as ring members are shown as complementary information; their classification marks are indicated in and by the symbols of Table H. However, if the number of necessary marks exceeds 7, the complementary information is not used
- 2) For compounds having two or more condensed ring systems, each having two or more relevant hetero rings (C07D519/00), each condensed system is shown as complementary information. The appropriate marks are found in Tables F and G and are determined by considering each condensed system in turn (however for Ergot and Vinca (= dimeric indole) alkaloids in C07D519/02 and C07D519/04, no complementary information is to be used)
- 3) Compounds containing in addition to a condensed system for which a specific group is provided (Table F), at least one further condensed relevant hetero ring, are to be classified according to the whole molecule, the complementary information showing all the relevant hetero rings present in the molecule according to Table H, e.g.



= C07D471/18 and NOT: C07D453/..

- 4) Group C07D521/00 is to be used only for its specified subgroups, but not for the classification of any other document; this implies the complete classification of all the examples of any document (cf. 6.b.1).

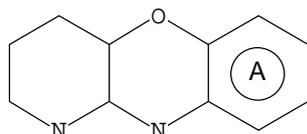
c. Classification and notations:

1) Classification of the condensed system

- a) Specific groups: (Table F) these are subdivided according to structure or substituents (however cfr. Rule 7.b.3), no complementary information on the individual component relevant hetero rings is given
- b) No specific groups are provided: (Table G) these groups are always subdivided according to the same system, indicating the number of relevant hetero rings of the molecule, and the type of condensation of the whole molecule; the notations are found in Table J
- c) Whenever relevant "variable" hetero rings are or may be present, a complete classification for any of the exemplified values of these rings is to be given.

2) Complementary information (showing the individual relevant hetero ring of the compound)

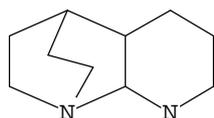
- a) Each relevant hetero ring is shown by a mark of Table H
- b) This notation is followed by a letter indicating how this hetero ring is condensed: Table K
- c) When a relevant hetero ring - either a "well defined" or a "variable" - may be present in the formula, (i.e. a facultative hetero ring), the complete classification of the formula requires thus at least a double classification, e.g.



A = "carbocycle": C07D498/04...

A = "a hetero ring": C07D498/14... (ex. of 5 types)

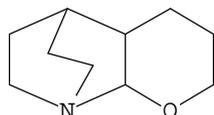
- d) For compounds containing as relevant hetero rings only the same hetero ring more than once, these hetero rings being directly condensed among themselves - and not provided for by Table F - the total number of relevant rings - i.e. carbocyclic and hetero-cyclic - is given after the enumeration of all the relevant hetero ring, (e.g. +2 for two relevant rings, 3 for three relevant rings ...)



(pyridine) (pyridine) (pyridine)

C07D471/18 + 221C + 221C + 221B + 3

- e) The notation will not be written in the official IPC manner, e.g.

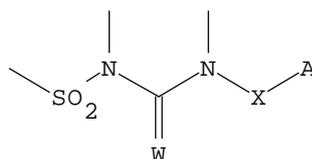


C07D491/18 // (C07D491/18, C07D311/00, C07D221/00, C07D221/00) but only as the part after the double stroke. The symbols /00 are not used, but are replaced by the notations according to 7.c.2 (indication of the mode of condensation of the individual relevant hetero rings: table K).

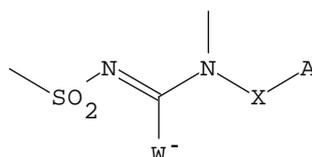
The complete notations of the individual relevant hetero rings are written according to the last place rule in Table H.

Thus the notation for this example becomes: C07D491/18 + 311B + 221C + 221C

- f) Heterocyclic compounds containing the group



or isomers thereof, e.g.



wherein A, which is attached through a ring carbon atom, is a hetero ring or a condensed hetero ring system, X is a direct or indirect link and W is a hetero atom, are classified in C07D521/00S and subgroups]

TABLE A:

the hetero rings contain as hetero atoms:

C07D401/	only N, at least one of them being a C5N ring
C07D403/	only N, not provided for by C07D401/,
C07D405/	only O, and at least one ring with only N
C07D407/	only O
C07D409/	only S
C07D411/	only O+S
C07D413/	only N+O
C07D417/	only N+S
C07D419/	only N+O+S
C07D421/	Se/Te; halogen; (+O) (+S) (+N)
C07D415/00	containing the THIAMINE skeleton, or its open chain analogs

TABLE B:

standard subdivision of main groups of Table A (EXCEPT for C07D415/00), mainly based on the number of relevant rings and on the chain between the hetero rings

/02	(NOT TO BE USED) containing two hetero rings
/04	directly linked by a ring-member to a ring-member bond, the whole hetero ring system being considered, e.g. 7-(3-pyridyl)-quinoline
/06	linked by a carbon chain containing only aliphatic carbon atoms, i.e. the chain is not interrupted by a cyclic radical
/08	linked by a carbon chain containing alicyclic rings, i.e. the chain is (or is interrupted by) such rings
/10	linked by a carbon chain containing aromatic rings, i.e. the chain is (or is interrupted by) such rings
/12	linked by a chain containing hetero atoms as chain links (thus the chain can, e.g. be a single hetero atom)
/14	Containing three or more hetero rings

USED BEFORE 01.07.2005

/14R	[N: containing four or more hetero rings, at least two of which are covered by the same main group C07D203/00 to C07D347/00, see Note 6c.3]
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TABLE C: individual notations of component hetero rings (used before 01.07.2005)

Only N:			
203	1N		2C
205	1N		3C
207	1N		4C
209		condensed pyrroles	
209C		indoles	
211	1N	hydrogenated	5C
211N	1N	dihydropyridines having acido carbon atoms directly linked to ring-C	5C
213	1N	aromatic	5C
215		quinolines	
217		isoquinolines	
219		acridines	
221		other condensed pyridines	C5N
223	1N		6C
225	1N		> 6C
229	2N		1C,2C
231	2N	(1,2)	3C
233	2N	(1,3)	3C
235		condensed imidazoles	
235C		benzimidazoles	
237	2N	(1,2)	4C
237B		pyridazines	
239	2N	(1,3)	4C
239B		pyrimidines	
241	2N	(1,4)	4C
241B		pyrazines	
243	2N		5C
245	2N		> 5C
249	3N	(1,2,3)	2C
249B		(1,2,4)	
251	3N	(1,3,5)	3C
253	3N	(1,2,4), (1,2,3)	3C
255	3N	• 251-253	
257	4N		
259	> 4N		

Only N+O:			
261	1N+1O	(1,2)	3C
263	1N+1O	(1,3)	3C
263B		oxazoles	
265	1N+1O		4C
265D		1,4-oxazines + condensed	
267	1N+1O		>4C
271	2N+1O		2C
273	N+O	• 261 to 271	
Only N+S:			
275	1N+1S	(1,2)	3C
277	1N+1S	(1,3)	3C
277B		Thiazoles	3C
279	1N+1S		4C
281	1N+1S		>4C
285	N+S	• 275-281	
285B		thiadiazoles + condensed	
285D		thiadiazines + condensed	
Only N+O+S: N+Se/Te(+O) (+S)			
291	N+O+S		
293	N+Se/Te(+O) (+S)		
Only O; O+S; O+Se/Te (+S):			
303	1O		2C
305	1O		3C
307	1O		4C
307B		furans	
309	1O		5C
311		condensed pyrans	
311C		benzo[b]pyrans	
313	1O		> 5C
317	2O		3C
319	2O		4C
321	2O		>4 C
323	> 2O		
327	O+S		

329	O+Se/Te(+S)		
Only S; S+Se/Te:			
331	1S		2C,3C
333	1S		4C
333B		thiophenes	
335	1S		5C
337	1S		> 5C
339	2S		
341	> 2S		
343	S+Se/Te		
Only Se/Te:			
345	Se, Te; Se+Te		
Containing halogen:			
347		containing halogen	

NOTES to table C

1. condensed derivatives are together with the parent hetero ring, unless a SPECIFIC name is provided
2. hydrogenated derivatives are together with the parent hetero ring, with the exception of 211, 213
3. the relative position of the hetero atoms in the hetero ring is given between brackets
4. acido carbon atoms are carbon atoms having three bonds to hetero atoms with at the most one bond to halogen, e.g. ester or nitrile radicals

TABLE F:

No complementary information is to be used in these groups; however see 7.b.3

C07D451/00	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)
C07D453/00	Quinuclidine; Isoquinuclidine; Alkylenedioxy-derivatives of C07D453/04 (quinine derivatives)
C07D455/00	Quinolizine; Alkylenedioxy derivatives of C07D455/02B (berberine derivatives), of C07D455/08 (emetine derivatives)
C07D457/00	Indolo[4,3-f,g]quinoline, (e.g. Ergot alkaloids)
C07D459/00	Benz[g]indolo[2,3-a]quinolizine (yohimbane) and lactones (reserpilic acid lactone)
C07D461/00	Indolo [3,2,1-d,e]pyrido [3,2,1-i,j][1,5]-naphthyridine ring systems, e.g. vincamine (dimeric indolo alkaloids C07D519/04)
C07D463/00	Carbacephalosporins
C07D473/00	Purine
C07D475/00	Pteridine
C07D477/00	Thienamycins (Carbapenicillins)
C07D489/00	4aH-8,9c-Iminoethanophenanthro[4,5-b,c,d]furan ring systems, (e.g. morphine) and 6,14-carbon bridged derivatives (oripavines)
C07D499/00	Penicillin
C07D501/00	Cephalosporin
C07D503/00	Oxadethiapenicillins
C07D505/00	Oxadethiacephalosporins
C07D519/02 and C07D519/04	Ergot and Vinca alkaloids containing two or more condensed systems in the molecule

TABLE G:

Complementary information to be used in these groups; however see 7.b.1 in fine.

In the condensed system, relevant hetero rings containing:

C07D471/00	only nitrogen atoms, with at least one (hydro) pyridine, not provided for by Table F; (cfr. 7.b.3)
C07D487/00	only nitrogen atoms, not provided for by Table F and by C07D471/00
C07D491/00	at least one ring containing only oxygen atoms and at least one ring containing only nitrogen atoms, not provided for by C07D451/00 (scopolamine); alkylendioxy derivatives of C07D453/04 (quininine derivatives), of C07D455/02B (berberine derivatives), and of C07D455/08 (emetine derivatives); lactones of C07D459/00 (reserpilic acid lactones) and C07D489/00 (morphine)
C07D493/00	only oxygen atoms
C07D495/00	at least one ring containing only sulfur atoms
C07D497/00	at least one ring containing only oxygen and sulfur atoms
C07D498/00	at least one ring containing only nitrogen and oxygen atoms
C07D513/00	at least one ring containing only nitrogen and sulfur atoms (penicillin C07D499/00; cephalosporin C07D501/00)
C07D515/00	at least one ring containing only nitrogen, oxygen and sulfur atoms
C07D517/00	at least one ring containing selenium, tellurium or halogen atoms, with or without other hetero atoms
C07D519/00	two or more condensed systems in the molecule not provided for by C07D519/02 and C07D519/04
C07D521/00	unspecified hetero rings; (cfr. 7.b.4)

TABLE H:

Complementary information marks for individual relevant hetero rings

Only N:			
203	1N		2C
205	1N		3C
209	1N		4C
221	1N		5C
223	1N		6C
225	1N		> 6C
229	1N		1C,2C
231	2N	(1,2)	3C
235	2N	(1,3)	3C
237	2N	(1,2)	4C
239	2N	(1,3)	4C
241	2N	(1,4)	4C
243	2N		5C
245	2N		> 5C
249	3N		2C
251	3N	(1,3,5)	3C
253	3N	• 251	3C
255	3N	• 251-253	
257			4N
259			> 4N
Only N+O:			
261	1N+1O	(1,2)	3C
263	1N+1O	(1,3)	3C
265	1N+1O		4C
267	1N+1O		> 4C
271	2N+1O		2C
273	N+O	• 261-271	
Only N+S:			
275	1N+1S	(1,2)	3C
277	1N+1S	(1,3)	3C
279	1N+1S		4C
281	1N+1S		> 4C
285	N+S	• 275-281	

Only N+O+S: N+Se/Te(+O) (+S)			
291	N+O+S		
293	N+Se/Te(+O) (+S)		
Only O; O+S; O+Se/Te (+S):			
303	1O		2C
305	1O		3C
307	1O		4C
311	1O		5C
313	1O		> 5C
317	2O		3C
319	2O		4C
321	2O	• 317-319	
323	> 2O		
327	O+S		
329	O+Se/Te (+S)		
Only S; S+Se/Te:			
331	1S		2C, 3C
333	1S		4C
335	1S		5C
337	1S		> 5C
339	2S		
341	> 2S		
343	S+Se/Te		
Only Se/Te:			
345	Se; Te; Se+Te		
Containing halogen:			
347	Halogen (+N,O,S,Se,Te)		

TABLE J:

Type of condensation of the whole molecule; number of relevant hetero rings:

/02 . TWO hetero rings

/04 .. ortho-condensed systems

/06 .. peri-condensed systems

/08 .. bridged systems

/10 .. spiro-condensed systems

/12 . THREE hetero rings

/14 .. ortho-condensed systems

/16 .. peri-condensed systems

/18 .. bridged systems

/20 .. spiro-condensed systems

/22 . MORE THAN THREE hetero rings

TABLE K:

The relevant hetero ring is (not) directly condensed with other relevant hetero rings and it shares (n) hetero atoms with them

Notation:	Type of condensation:	(n)
A	not directly	/
B	directly	0
C	directly	1
D	directly	2
E	directly	3 or more