

IRAM Memo 2014-?
LINEDB

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Abstract

TO BE FILLED

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1 Test

2 Providing your own database

LINEDB accepts building a local database with a custom list of lines. This can be achieved through two ASCII files:

1. the line "catalog" *e.g.*

```
  29005   NNH+
93171.8800   .0400 -2.7844 2    0.0000  9 -29005 102 1 1         0 1
93173.7000   .0400 -2.5625 2    0.0000 15 -29005 102 1 2         0 1
93176.1300   .2200 -3.2614 2    0.0000  3 -29005 102 1 0         0 1
  30002   HC-13-O+
86754.2884  0.0046 -2.2835 2    0.0000  3 -30002 101 1           0
```

   This catalog must follow the JPL convention (in particular, column alignment) described in Appendix A. The lines must be gathered by species. Each group is identified by a first line providing the tag value and the species name. The latter should be limited to 32 characters because of internal limitations of the **LINEDB** databases. There can be no blank nor comment lines in this file.

2. the *partition function* file. It must be named `partfunc.cat` and must use the following format *e.g.*:

```
species      NNH+      29005
temperatures 300.   225.   150.   75.    37.5   18.75  9.375
qpart        3.0831 2.9586 2.7832 2.4842 2.1875 1.8952 1.6116

species      HC-13-O+  30002
temperatures 300.   225.   150.   75.    37.5   18.75  9.375
qpart        2.1599 2.0353 1.8598 1.5607 1.2637 0.9707 0.6859
```

   The tag and species name should match the catalog ones. The number of temperatures/qpart pairs are free. Those three lines must be consecutive in the file, with one set of lines per species. There can be a custom number of blank and comment (!) lines between each set of lines.

Given those files, importing them in **LINEDB** is as easy as:

```
SIC> use in mybase.dat
I-USE,  mybase.dat (offline) selected with /(partfunc.json|partfunc.cat) for partition functions
SIC> select
I-SELECT,  4 lines found in the frequency range 0 to infinity MHz
SIC> list
  # Species        Freq[MHz] Err[MHz] Eup[K]  Gup  Aij[s-1]    Upper level -- Lower level    Origin
  1 HC-13-O+       86754.288   0.005     4.2    3  1.21e-05             1 -- 0              mybase.dat
  2 NNH+           93171.880   0.040     4.5    9  3.63e-05           1 1 -- 0 1            mybase.dat
  3 NNH+           93173.700   0.040     4.5   15  2.18e-05           1 2 -- 0 1            mybase.dat
  4 NNH+           93176.130   0.220     4.5    3  1.09e-04           1 0 -- 0 1            mybase.dat
```

It is advised to save this catalog in the **LINEDB** binary format, *i.e.* after the previous steps:

```
SIC> use out mybase.db
SIC> insert
```

3 Interfacing the CDMS via VAMDC

As of 2016, February 24th, the Cologne Database for Molecular Spectroscopy (CDMS) is in the process of moving its database to the Virtual Atomic and Molecular Data Centre (VAMDC). For external users (like LINEDB programmers and users), this implies several changes exposed hereafter.

3.1 Changes for end-users

To first order, using the new protocol to query the CDMS database should be transparent to the end user. This is one of the purpose of **LINEDB**. However, it seems that the database behind the new protocol is not same as before. The user should be aware that:

- as of today, the request takes more time and more bandwidth than before (48 minutes to download the database in the range 100-400 MHz, 893 MB in return),
- the species name/formula may be different between the old and new database (e.g. "Methanol" vs "CH3OH", "CCH, v=0" vs "CCH"),
- the vibrational state has been removed from the formulas (see e.g. "CCH" above),
- querying a formula may return the same molecule under different formulas (e.g. you ask for "HC-CCN" and **LINEDB** returns "HCCCN" and "HC3N"),
- some lines seem to have disappeared in the new database

3.2 Queries

The new server supports TAP-VAMDC queries using VSS1 or VSS2 languages. The query may be as simple as:

```
select *
```

to retrieve the whole database, or for example

```
select * where
(RadTransFrequency >= 9.671000e+04 and RadTransFrequency <= 9.677000e+04) and
RadTransProbabilityA >= 3.000000e-06 and
InChiKey in ('TXKMVPPZCYKFAC-UHFFFAOYSA-N','OKKJLVBELUTLKV-UHFFFAOYSA-N')
```

to retrieve the S2O and CH3OH lines (`InChIKey`), between 96710 and 96770 MHz (`RadTransFrequency`), which have an Einstein coefficient above 3e-6 (`RadTransProbabilityA`). Once the query command is built, it is encoded in the whole HTTP url.

The list of supported restrictables (i.e. the parameters which can be used for filtering) can be found in the VAMDC documentation[1]. For interfacing with the command `SELECT`, **LINEDB** uses the restrictables shown in the Table 1. `RadTransFrequency` and `RadTransProbabilityA` are direct equivalent of the `SELECT` filters. There is no restrictable for selecting a line by its upper level energy (`/ENERGY`), so the filtering is performed internally in **LINEDB** afterwards.

The `/SPECIES` case is a more complex issue. **LINEDB** uses the molecule formula or name to identify a species. The equivalent in the XSAMS format is the `OrdinaryStructuralFormula` (see subsection 3.3 for details). However, because this property can be an ambiguous reference to a species (e.g. "Methanol" and "CH3OH", "HCCCN" and "HC3N"), it can not be used as a filter. VAMDC offers instead the InChI (*IUPAC International Chemical Identifier*[2]) or the InChIKey (hashed InChI) as non-ambiguous

[1] See `http://www.vamdc.eu/documents/standards/dictionary/restrictables.html`
[2] See `www.iupac.org/inchi/`

identifier. In practice, **LINEDB** has to know how to translate the formula as an InChIKey. This is done by downloading and parsing the full `Species` table (and only this one) once at the beginning of the session. As of today this table provides 734 species; they are listed in the Appendix C.

Table 1: Look-up-table between the **LINEDB** `SELECT` options and the VAMDC restrictables.

`SELECT` option	Restrictable	Comments
`/SPECIES`	`InChIkey`	Translation needed
`/FREQUENCY`	`RadTransFrequency`	[MHz]
`/ENERGY`	N/A	Done internally in **LINEDB**
`/AIJ`	`RadTransProbabilityA`	$[s^{-1}]$
`/ORIGIN`	(not relevant)	
`/SORTBY`	(not relevant)	
`/EPSILON`	(not relevant)	

3.3 Parsing

In return of the VAMDC query, the server returns the filtered database under the VADMC-XSAMS format (modified version of the *XML Schema for Atoms, Molecules and Solids*[3]). This is basically an XML file providing several tables. **LINEDB** is interested in the `<Species><Molecules>` table (which provides a collection of `<Molecule>` blocks) and the `<Processes><Radiative>` table (which provide a collection of `<RadiativeTransition>` blocks.

3.3.1 Molecule description

A typical example of a `<Molecule>` is (truncated for clarity):

```
<Molecule speciesID="XCDMS-132">

  <MolecularChemicalSpecies>
    <OrdinaryStructuralFormula>
      <Value>C-13-O-18</Value>
    </OrdinaryStructuralFormula>
    <StoichiometricFormula>CO</StoichiometricFormula>
    <ChemicalName>
      <Value>Carbon Monoxide</Value>
    </ChemicalName>
    <InChI>1S/CO/c1-2/i1+1,2+2</InChI>
    <InChIKey>UGFAIRIUMAVXCW-RGIGPVFXSA-N</InChIKey>
    <VAMDCSpeciesID>UGFAIRIUMAVXCW-RGIGPVFXSA-N</VAMDCSpeciesID>
    <PartitionFunction>
      <T units="K">
        <DataList>1.072 1.148 (truncated) 1000.0</DataList>
      </T>
      <Q>
        <DataList>2.05524705685 2.07536036351 (truncated) 798.466964704</DataList>
      </Q>
    </PartitionFunction>
  </MolecularChemicalSpecies>

  <MolecularState stateID="SCDMS-9240238">
    <MolecularStateCharacterisation>
      <StateEnergy methodRef="MCDMS-6647" energyOrigin="SCDMS-9240238-origin-132">
        <Value units="1/cm">0.0</Value>
      </StateEnergy>
      <TotalStatisticalWeight>2</TotalStatisticalWeight>
```

[3]See `http://vamdc.eu/documents/standards/dataModel/vamdcxsams/introduction.html`

```
      <NuclearStatisticalWeight>2</NuclearStatisticalWeight>
    </MolecularStateCharacterisation>
    <Case>
      <dcs:QNs>
        <dcs:ElecStateLabel>X</dcs:ElecStateLabel>
        <dcs:v>0</dcs:v>
        <dcs:J>0</dcs:J>
        <dcs:F nuclearSpinRef="C-13">0.5</dcs:F>
      </dcs:QNs>
    </Case>
  </MolecularState>

  <MolecularState stateID="SCDMS-9240239">
    <MolecularStateCharacterisation>
      <StateEnergy methodRef="MCDMS-6647" energyOrigin="SCDMS-9240238-origin-132">
        <Value units="1/cm">3.492795</Value>
      </StateEnergy>
      <TotalStatisticalWeight>2</TotalStatisticalWeight>
      <NuclearStatisticalWeight>1</NuclearStatisticalWeight>
    </MolecularStateCharacterisation>
    <Case>
      <dcs:QNs>
        <dcs:ElecStateLabel>X</dcs:ElecStateLabel>
        <dcs:v>0</dcs:v>
        <dcs:J>1</dcs:J>
        <dcs:F nuclearSpinRef="C-13">0.5</dcs:F>
      </dcs:QNs>
    </Case>
  </MolecularState>

</Molecule>
```

LINEDB uses the `OrdinaryStructuralFormula` as the species name, but its `InChIKey` is used for database queries. The partition function is taken from the `PartitionFunction` block. It can provide any number of temperatures, it can also be absent. Each energy level of the molecule (energy, quantum numbers, statistical weight) is described in a separated `<MolecularState>` block.

3.3.2 Radiative transition description

A single transition is described in the `<Processes><Radiative>` table as a `<RadiativeTransition>` block. For example (truncated for clarity):

```
<RadiativeTransition id="PCDMS-R7452690" process="excitation">
  <EnergyWavelength>
    <Frequency methodRef="MCDMS-6648">
      <SourceRef>BCDMS-344</SourceRef>
      <Value units="MHz">104711.4035</Value>
      <Accuracy>0.0057</Accuracy>
    </Frequency>
    <Frequency methodRef="MCDMS-6646">
      <Value units="MHz">104711.3656</Value>
      <Accuracy>0.0003</Accuracy>
    </Frequency>
  </EnergyWavelength>
  <UpperStateRef>SCDMS-9240239</UpperStateRef>
  <LowerStateRef>SCDMS-9240238</LowerStateRef>
  <SpeciesRef>XCDMS-132</SpeciesRef>
  <Probability>
    <TransitionProbabilityA>
      <Value units="1/cm">5.45485286998e-08</Value>
    </TransitionProbabilityA>
  </Probability>
</RadiativeTransition>
```

Note that the species (`SpeciesRef`), the lower level (`LowerStateRef`), and the upper level (`UpperStateRef`) are identified by their unique identifiers which backpoint to the given species in the `<Molecules>` table. The measured frequency is described in a `<Frequency>` block. There can be several frequencies for a single transition, measured by several sources.

4 LINEDB Language Internal Help

4.1 Language

```
          LINEDB\ Command Language Summary
This language is an interface to on-line and off-line line catalogs.

USE       Define the atomic and molecular line database(s) used as input and
SELECT    Select lines in the input database(s) according to user defined fi
LIST      List lines from the current line index
INSERT    Insert lines from the current line index into the output database
REMOVE    Remove lines from the current line index from the output database
```

4.2 USE

```
   LINEDB\USE  IN|OUT|BOTH  dbname1  [[dbname2]  [dbname3...]] [/ASTRO]
[/OVERWRITE]

Define the atomic and molecular line database(s) used  as  input  and/or
output.

Input databases can be either an existing filenames or a database avail-
able through internet. Recognized internet databases are
   JPL    the JPL molecular spectroscopy database
   CDMS   the Cologne Database for Molecular Spectrocopy
These names can thus not be used as database filenames.

The input file is tested to determine whether it is a valid SQLITE data-
base.  If  not, it is assumed to be an ASCII file following the JPL data
format, see e.g.
    https://spec.jpl.nasa.gov/ftp/pub/catalog/README, and
    https://spec.jpl.nasa.gov/ftp/pub/catalog/catdir.html
for reference and examples. In this case, the  log10  of  the  partition
functions of all the referenced species must be provided in a file named
"partfunc.cat",  with  at  least  the  300K  value.  See  ker-
nel/python/linedb/demo/demo-53001.cat  and  kernel/python/linedb/de-
mo/partfunc.cat in the Gildas sources for a complete example.

Multiple input databases can be used together. However, only one  output
database  can  be defined at a given time. The OUT and BOTH keywords ap-
plies only to SQLITE databases. The /OVERWRITE option implies  that  the
output database is first removed. The absence of the option implies that
any subsequent call to the INSERT command will append lines to  the  al-
ready existing output database.

After execution of the command, the name of the input databases is saved
in the list LINEDB%DBIN. For symmetry, the name of the  output  database
is saved in the list LINEDB%DBOUT (with a single element in this case).
```

4.2.1 USE /ASTRO

```
   [LINEDB\]USE OUT dbname /ASTRO [/OVERWRITE]
```

Create an output catalog using the Astro format, i.e. an ASCII table with frequencies (GHz) in first column and species name in second column, plus possibly comment lines and trailing comments.

This output kind can only be used to export (USE OUT + INSERT) lines. USE IN is forbidden.

When INSERT is invoked several times (in the same session, or when reopening an output catalog), it does NOT CHECK FOR DUPLICATES. REMOVE is not available.

4.3 SELECT

LINEDB\SELECT [/ORIGIN Originname] [/SPECIES Name1 Name2 ...] [/FREQ Fmin Fmax] [/ENERGY Emax] [/AIJ Amin] [/SORTBY Order] [/EPSILON Eps]

Select lines available from the input database. An index containing the line information is formed and a SIC structure mapping these information is defined.

The index can be sorted by increasing frequency or energy. One or more species name can be provided. In offline catalogs, the search is case-insensitive and wildcards '*' can be used, while online catalogs do not implement this possibility. A possible workaround of this limitation is to make a local copy of an online database (with all filters enabled except species name) and search in it:

```
SIC> use in cdms
SIC> select /freq 123000 124000
SIC> use out tmp.db
SIC> insert
SIC> use in tmp.db
SIC> select /spec ch3o*
```

The initial origin of the line (e.g. JPL, CDMS or private catalog), the name of the species, a frequency range, the maximum energy of the upper level and the maximum Einstein coefficient Amin can be used as filters in the line selection process. By default, Amin defaults to 1e-10, i.e. lines with a smaller Einstein coefficient are filtered out.

As an output, the LINES SIC structure will contain the content of the current index, i.e.,

```
   LINES%          Global structure
   LINES%N         Integer scalar      [---] Number of lines in current inde
   LINES%SPECIES   Character[LINES%N]  [---] Species names
   LINES%FREQUENCY Double[LINES%N]     [MHz] Frequencies
   LINES%UNCERTAINTY Real[LINES%N]     [MHz] Uncertainty of the line frequen
   LINES%AIJ       Double[LINES%N]     [s-1] Einstein coefficient
   LINES%EUP       Real[LINES%N]       [  K] Upper level energy
   LINES%GUP       Real[LINES%N]       [---] Upper level degeneracy
   LINES%QNUP      Character[LINES%N]  [---] Upper level quantum numbers
   LINES%ELOW      Real[LINES%N]       [  K] Lower level energy
   LINES%GLOW      Real[LINES%N]       [---] Lower level degeneracy
```

```
   LINES%QNLOW     Character[LINES%N]  [---] Lower level quantum numbers
```

The lines will be sorted according to Order, which can be any combination of "frequency", "energy" and "aij", and all the subsequent permutations. Default is frequency. If sortby is ["energy", "aij"] and if epsilon is specified, aij will be used as a criterion when the difference in energy is less than epsilon.

4.4 LIST

```
LINEDB\LIST [/FULL] [/TOC]
```

List a set of columns for all lines found in the current index built during the last SELECT command. The option /FULL lists all the columns available in the database.

The /TOC option partitions the lines by equivalence class (species name) and gives a count of each class.

4.5 INSERT

```
LINEDB\INSERT
```

Insert the entries (lines properties and partition functions) of the current line index (result of the last SELECT command) into the output database.

4.6 REMOVE

```
LINEDB\REMOVE
```

Remove the entries (lines properties and partition functions) of the current line index (result of the last SELECT command) into the output database. The partition function is erased only if no other line of the same species remains in the database.

A JPL convention

The JPL convention, as of March 24th 2014, is reproduced here. This is the expected format for ASCII local databases supported by **LINEDB**. See the online version of the document at: http://spec.jpl.nasa.gov/ftp/pub/catalog/REA

```
The catalog data files are composed of 80-character card images, with one card
image per spectral line.  The format of each card image is:
  FREQ, ERR, LGINT, DR,  ELO, GUP, TAG, QNFMT,  QN',  QN"
(F13.4,F8.4, F8.4,  I2,F10.4,  I3,  I7,    I4,  6I2,  6I2)

FREQ:  Frequency of the line in MHz.
ERR:   Estimated or experimental error of FREQ in MHz.
LGINT: Base 10 logarithm of the integrated intensity in units of nm^2 MHz at
       300 K.
DR:    Degrees of freedom in the rotational partition function (0 for atoms,
       2 for linear molecules, and 3 for nonlinear molecules).
ELO:   Lower state energy in cm^{-1} relative to the ground state.
GUP:   Upper state degeneracy.
TAG:   Species tag or molecular identifier.
       A negative value flags that the line frequency has
       been measured in the laboratory.  The absolute value of TAG is then the
       species tag and ERR is the reported experimental error.  The three most
       significant digits of the species tag are coded as the mass number of
       the species.
QNFMT: Identifies the format of the quantum numbers
QN':   Quantum numbers for the upper state.
QN":   Quantum numbers for the lower state.

The on-line version of the catalog contains individual files for each
molecular species.  Line files are designated as cttttttt.cat, where tttttt
is the zero-filled catalog tag number. For example,
the H atom line list is in file c001001.cat.

A directory of the catalog is found in a file called 'catdir.cat.'
Each element of this directory is an 80-character record with the following
format:
TAG,  NAME, NLINE,  QLOG,  VER
(I6,X, A13,    I6, 7F7.4,  I2)

TAG:   The species tag or molecular identifier.
NAME:  An ASCII name for the species.
NLINE: The number of lines in the catalog.
QLOG:  A seven-element vector containing the base 10 logorithm of the partition
       function for temperatures of 300 K, 225 K, 150 K, 75 K, 37.5 K, 18.75 K,
       and 9.375 K, respectively.
VER:   The version of the calculation for this species in the catalog.
       The version number is followed by * if the entry is newer than the
       last edition of the catalog.
```

B Coding the quantum numbers

In the **LINEDB** offline databases, as well as in JPL and "old" (non-VAMDC) CDMS, the quantum numbers of the lower and upper transition levels are encoded in a character string. This appendix describes the recipe to be used for encoding. It duplicates the pages `https://www.astro.uni-koeln.de/cdms/catalog` and `https://www.astro.uni-koeln.de/node/475` for memory.

B.1 Quantum numbers

The quantum numbers are given in the following order:
J (or N); K_a and K_c (or $\pm$; K); v; F_1 ... F
for the upper state followed immediately by those for the lower state (see also below).

- N is the total rotational angular momentum excluding electron and nuclear spins. For singlet molecules, J, the total rotational angular momentum including electron spin, is equal to N.
- K_a and K_c are the projections of N onto the A and C inertial axes, respectively. For symmetric top molecules, only K is needed (instead of K_a and K_c) along with + or −, which designate the parity; if redundant, the latter might be omitted. Instead of K, Λ or l may be used for linear molecules.
- v is a *state number*! It specifies different vibrational or electronic states. It may also be used to distinguish between different species that have been fit simultaneously. Details on the meaning of the state numbers are given in the documentation! Note: More than one state number may be needed to designate one vibrational state - this is the case, for example, for a degenerate (e.g. bending) state of a symmetric top molecule!
- F_1 ... F designate spin quanta. In general, the electron spin S is coupled to the rotational angular momentum first, followed by nuclear spins. In this case $F_1 = J$

Very Important:

Exactly two characters are available for each quantum number. Therefore, half integer quanta are rounded up! In addition, capital letters are used to indicate quantum numbers larger than 99. E.g. A0 is 100, Z9 is 359. Small types are used to signal corresponding negative quantum numbers.

Since the program was written for asymmetric top molecules, some of the quantum numbers may be redundant.

Six quantum numbers are available at most to describe the upper and lower state, respectively. In case more quantum numbers are needed, even if some of them are redundant, the only spin designating quantum numbers are n, F, were n is an aggregate spin number (see below).

B.2 Aggregate spin number

The aggregate spin number is used in the SPFIT and SPCAT programs whenever more than six quantum numbers are needed to descibe a state - even if some of the quantum numbers are redundant. It can be decoded using information provided in the .fit file or the .out file after the list of parameters in both cases. The NH2 example is used, in which $S = 1/2$, $I_N = 1$, and $I_H = 1/2$ for both H nuclei and $N + S = J$; $J + I_N = F_1$; $I_{H1} + I_{H2} = I_{tot}$; and $F_1 + I_{tot} = F$.

Please note: The coding will be the same for equivalent spin combinations, meaning one spin of 1/2, one spin of 1, and two equivalent spins of 1/2. The coding will be different for other spin combinations, e.g. two spins of 1/2 and two equivalent spins of 1/2 with PH2 as an example or one spin of 1, one spin of 1/2 and two equivalent spins of 1/2 with 13CH2 as an example.

```
BLOCK - WT - SYM - V - TSP - N  -  other quanta  (rel. to F=0 )
    1    1    0    0    0  -2.5  -2.0  -1.0   1.0
```

TSP is the aggregate spin number, here 0. Subsequently, N and the other quanta (J, F_1, and I_{tot}) are given relative to $F = 0$.

If we take, for example, line number 12:

```
 3  3  1  0  0  6  4  1  3  0  0  7   11686.80
```

we see that for the upper state we have $N = 3$, hence $F = 3 + 2.5 = 6–0.5 = 5.5$, $J = 3.5$, $F_1 = 4.5$, and finally $I_{tot} = 1.0$ is redundant. Similarly for the upper state: $N = 4$, hence $F = 6.5$, $J = 4.5$, $F_1 = 5.5$, and finally $I_{tot} = 1.0$ is again redundant. For TSP = 1 we find:

```
   2    1    1    0    1  -1.5  -1.0   0.0   0.0
```

For example in line 21 there is TSP = 1 twice:

```
 5  2  3  0  1  7  6  1  6  0  1  8    8749.68
```

For the upper and lower state, respectively:
$N = 5$, $N = 5.5$, $F_1 = 6.5$, $I_{tot} = 0.0$, and $F = 6.5$.
$N = 6$, $N = 6.5$, $F_1 = 7.5$, $I_{tot} = 0.0$, and $F = 7.5$.

C CDMS Species

List of the 734 CDMS species and their InChI as of 2016, February 24th.

OrdinaryStructuralFormula	InChI	InChIKey
aa-(C2H5)2O	1S/C4H10O/c6-1(7,3(10,11)12)5-2(8,9)4(13,14)15	QCLHONSZGNPZDF-UHFFFAOYSA-N
AA-n-C4H9CN	1S/C5H9N/c1-2-3-4-5-6/h2-4H2,1H3	RFFFKMOABOFIDF-UHFFFAOYSA-N
a-C-13-H3CH2OH	1S/C2H6O/c1-2-3/h3H,2H2,1H3/i1+1	LFQSCWFLJHTTHZ-OUBTZVSYSA-N
a-CH3C-13-H2OH	1S/C2H6O/c1-2-3/h3H,2H2,1H3/i2+1	LFQSCWFLJHTTHZ-VQEHIDDOSA-N
a-CH3CH2OD	1S/C2H6O/c1-2-3/h3H,2H2,1H3/i3D	LFQSCWFLJHTTHZ-WFVSFCRTSA-N
a-CH3CHDOH	1S/C2H6O/c1-2-3/h3H,2H2,1H3/i2D	LFQSCWFLJHTTHZ-VMNATFBRSA-N
ag-(C2H5)2O	1S/C4H10O/c1-3-5-4-2/h3-4H2,1-2H3	RTZKZFJDLAIYFH-UHFFFAOYSA-N
aGg'-(CH2OH)2	1S/C2H6O2/c3-1-2-4/h3-4H,1-2H2	LYCAIKOWRPUZTN-UHFFFAOYSA-N
a'GG'g-CH2OHCH2CH2OH	1S/C3H8O2/c4-2-1-3-5/h4-5H,1-3H2	YPFDHNVEDLHUCE-UHFFFAOYSA-N
AG-n-C4H9CN	1S/C5H7N.2H/c1-2-3-4-5-6;;/h2-3H2,1H3;;	WZUGPCNHUZMJNU-UHFFFAOYSA-N
a-H2CCHOH	1S/C2H4O/c1-2-3/h2-3H,1H2	IMROMDMJAWUWLK-UHFFFAOYSA-N
AlC3N	1/C3N.Al/c1-2-3-4;/rC3AlN/c4-2-1-3-5	WSWSAUVPURRARL-OFWOWBOUNA-N
AlCCH	1/C2H.Al/c1-2;/h1H;/rC2HAl/c1-2-3/h1H	NPKICPBOXPXYSD-OKROMESVNA-N
AlCN	1/CN.Al/c1-2;/rCAlN/c2-1-3	HWKFKJIIRKPLHF-ZZXBCICDNA-N
AlH	1/Al.H/rAlH/h1H	SPRIOUNJHPCKPV-OBKUDOBONA-N
AlNC	1/CN.Al/c1-2;/rCAlN/c1-3-2	HWKFKJIIRKPLHF-FRUVTJLNNA-N
AlS	1/Al.S/rAlS/c1-2	SLWLWUJHXQUDJS-DRDSLJIGNA-N
Ar-36-H+	1S/ArH/h1H/q+1/i1-4	TVQSUVFYDVJWLI-AHCXROLUSA-N
Ar-38-H+	1S/ArH/h1H/q+1/i1-2	TVQSUVFYDVJWLI-YPZZEJLDSA-N
ArD+	1S/ArH/h1H/q+1/i1D	TVQSUVFYDVJWLI-MICDWDOJSA-N
ArH+	1S/ArH/h1H/q+1	TVQSUVFYDVJWLI-UHFFFAOYSA-N
B-10-O	1S/BO/c1-2/i1-1	MOWNZPNSYMGTMD-BJUDXGSMSA-N
BH	1S/BH/h1H	UWBOAQKPEXKXSU-UHFFFAOYSA-N
BO	1S/BO/c1-2	MOWNZPNSYMGTMD-UHFFFAOYSA-N
C10H	1S/C10H/c1-3-5-7-9-10-8-6-4-2/h1H	OGPUWCLRWVYODD-UHFFFAOYSA-N
C-13-C4H	1S/C5H/c1-3-5-4-2/h1H/i2+1	FKHSYQQNHVRJIA-VQEHIDDOSA-N
C-13-C4S	1S/C5S/c1-2-3-4-5-6/i1+1	OSDVLXAJVSEOND-OUBTZVSYSA-N
C-13-C5H	1S/C6H/c1-3-5-6-4-2/h1H/i1+1	MGBKUZLTRVWILP-OUBTZVSYSA-N
C-13-CC-13-S	1S/C3S/c1-2-3-4/i1+1,3+1	DYOPWGBKIHJGRG-ZKDXJZICSA-N
C-13-CCCH	1S/C4H/c1-3-4-2/h1H/i2+1	GRADOOOISCPIDG-VQEHIDDOSA-N
C-13-CCH	1S/C3H/c1-3-2/h1H/i2+1	WWDRUPNDOSDMRD-VQEHIDDOSA-N
C-13-CCN	1S/C3N/c1-2-3-4/i1+1	URBHYAWCGWIELS-OUBTZVSYSA-N
C-13-CCO	1S/C3O/c1-2-3-4/i1+1	ZCNKODXATWVMAO-OUBTZVSYSA-N
C-13-CCS	1S/C3S/c1-2-3-4/i1+1	DYOPWGBKIHJGRG-OUBTZVSYSA-N
C-13-CCS-34	1S/C3S/c1-2-3-4/i1+1,4+2	DYOPWGBKIHJGRG-URHJBJCFSA-N
C-13-CH	1S/C2H/c1-2/h1H/i2+1	XEHVFKKSDRMODV-VQEHIDDOSA-N
C-13-CP	1S/C2P/c1-2-3/i1+1	UWBINSNTTNXVNB-OUBTZVSYSA-N
C-13-D+	1S/CH/h1H/q+1/i1+1D	WVVLBIYUCXYYEU-VVKOMZTBSA-N
C-13-F+	1S/CF/c1-2/q+1/i1+1	LDIFHDJQDDMHHQ-OUBTZVSYSA-N
C-13-H+	1S/CH/h1H/q+1/i1+1	WVVLBIYUCXYYEU-OUBTZVSYSA-N
C-13-H+	1S/CH/h1H/q+1/i1+1	WVVLBIYUCXYYEU-OUBTZVSYSA-N
C-13-H2(OH)CHO	1S/C2H4O2/c3-1-2-4/h1,4H,2H2/i2+1	WGCNASOHLSPBMP-VQEHIDDOSA-N
C-13-H3C-13-N	1S/C2H3N/c1-2-3/h1H3/i1+1,2+1	WEVYAHXRMPXWCK-ZDOIIHCHSA-N
C-13-H3CH2CN	1S/C3H5N/c1-2-3-4/h2H2,1H3/i1+1	FVSKHRXBFJPNKK-OUBTZVSYSA-N
C-13-H3CN	1S/C2H3N/c1-2-3/h1H3/i1+1	WEVYAHXRMPXWCK-OUBTZVSYSA-N
C-13-H3D	1S/CH4/h1H4/i1+1D	VNWKTOKETHGBQD-VVKOMZTBSA-N
C-13-H3OH	1S/CH4O/c1-2/h2H,1H3/i1+1	OKKJLVBELUTLKV-OUBTZVSYSA-N
C-13-N-15	1S/CN/c1-2/i1+1,2+1	JEVCWSUVFOYBFI-ZDOIIHCHSA-N
C-13-N	1S/CN/c1-2/i1+1	JEVCWSUVFOYBFI-OUBTZVSYSA-N
C-13-O-17	1S/CO/c1-2/i1+1,2+1	UGFAIRIUMAVXCW-ZDOIIHCHSA-N
C-13-O-18	1S/CO/c1-2/i1+1,2+2	UGFAIRIUMAVXCW-RGIGPVFXSA-N
C-13-O-18+	1S/CO/c1-2/q+1/i1+1,2+2	BOJPITGAFFYFJK-RGIGPVFXSA-N
C-13-O	1S/CO/c1-2/i1+1	UGFAIRIUMAVXCW-OUBTZVSYSA-N
C-13-O+	1S/CO/c1-2/q+1/i1+1	BOJPITGAFFYFJK-OUBTZVSYSA-N
C-13-S	1S/CS/c1-2/i1+1	DXHPZXWIPWDXHJ-OUBTZVSYSA-N
C-13-S	1S/CS/c1-2/i1+1	DXHPZXWIPWDXHJ-OUBTZVSYSA-N
C-13-S-33	1S/CS/c1-2/i1+1,2+1	DXHPZXWIPWDXHJ-ZDOIIHCHSA-N
C-13-S-34	1S/CS/c1-2/i1+1,2+2	DXHPZXWIPWDXHJ-RGIGPVFXSA-N
C-13-S-36	1S/CS/c1-2/i1+1,2+4	DXHPZXWIPWDXHJ-JOTDZXCOSA-N
C-14-H+	1S/CH/h1H/q+1/i1+2	WVVLBIYUCXYYEU-NJFSPNSNSA-N
C2C-13-C2H	1S/C5H/c1-3-5-4-2/h1H/i5+1	FKHSYQQNHVRJIA-HOSYLAQJSA-N
C2C-13-C2S	1S/C5S/c1-2-3-4-5-6/i3+1	OSDVLXAJVSEOND-LBPDFUHNSA-N
C2C-13-C3H	1S/C6H/c1-3-5-6-4-2/h1H/i5+1	MGBKUZLTRVWILP-HOSYLAQJSA-N
C2Cl	1S/C2Cl/c1-2-3	KSTABLGHYDHWIX-UHFFFAOYSA-N

C2Cl-37	1S/C2Cl/c1-2-3/i3+2	KSTABLGHYDHWIX-YZRHJBSPSA-N
C2H-	1S/C2H/c1-2/h1H/q-1	BLRXYTIIKIPJQL-UHFFFAOYSA-N
C2H2	1S/C2H2/c1-2/h1-2H	HSFWRNGVRCDJHI-UHFFFAOYSA-N
C2H3+	1S/C2H3/c1-2/h1H,2H2/q+1	QLLSNXSJBAXPLZ-UHFFFAOYSA-N
C2H3C3N	1S/C5H2N.H/c6-3-1-2-5-4-7-5;/h4H;	MBRISWRVJUODEA-UHFFFAOYSA-N
C2H3CN	1S/C3H3N/c1-2-3-4/h2H,1H2	NLHHRLWOUZZQLW-UHFFFAOYSA-N
C2H3NH2	1S/C2H5N/c1-2-3/h2H,1,3H2	UYMKPFRHYYNDTL-UHFFFAOYSA-N
C2H3NH2	1S/C2H5N/c1-2-3/h2H,1,3H2	UYMKPFRHYYNDTL-UHFFFAOYSA-N
C2H5C-13-N	1S/C3H5N/c1-2-3-4/h2H2,1H3/i3+1	FVSKHRXBFJPNKK-LBPDFUHNSA-N
C2H5CN-15	1S/C3H5N/c1-2-3-4/h2H2,1H3/i4+1	FVSKHRXBFJPNKK-AZXPZELESA-N
C2H5CN	1S/C3H5N/c1-2-3-4/h2H2,1H3	FVSKHRXBFJPNKK-UHFFFAOYSA-N
C2H5NH2	1S/C2H7N/c1-2-3/h2-3H2,1H3	QUSNBJAOOMFDIB-UHFFFAOYSA-N
C2H5OCHO	1S/C3H6O2/c1-2-5-3-4/h3H,2H2,1H3	WBJINCZRORDGAQ-UHFFFAOYSA-N
C3	1S/C3/c1-3-2	NVLRFXKSQQPKAD-UHFFFAOYSA-N
C-34-S	1S/CS/c1-2/i2+2	DXHPZXWIPWDXHJ-HQMMCQRPSA-N
C3C-13-C2H	1S/C6H/c1-3-5-6-4-2/h1H/i6+1	MGBKUZLTRVWILP-PTQBSOBMSA-N
C3C-13-CH	1S/C5H/c1-3-5-4-2/h1H/i3+1	FKHSYQQNHVRJIA-LBPDFUHNSA-N
C3C-13-CS	1S/C5S/c1-2-3-4-5-6/i4+1	OSDVLXAJVSEOND-AZXPZELESA-N
C3Cl	1S/C3Cl/c1-2-3-4	GGJNGOJODQFACZ-UHFFFAOYSA-N
C3D	1S/C3H/c1-3-2/h1H/i1D	WWDRUPNDOSDMRD-MICDWDOJSA-N
C3F	1S/C3F/c1-2-3-4	MLLIJOISDYNGEI-UHFFFAOYSA-N
C3H+	1S/C3H/c1-3-2/h1H/q+1	CVRLLNGNDQSJON-UHFFFAOYSA-N
C3H	1S/C3H/c1-3-2/h1H	WWDRUPNDOSDMRD-UHFFFAOYSA-N
C3N-	1S/C3N/c1-2-3-4/q-1	LBEHQPQVLRPOSM-UHFFFAOYSA-N
C3O2	1S/C3O2/c4-2-1-3-5	GNEVIACKFGQMHB-UHFFFAOYSA-N
C3S	1S/C3S/c1-2-3-4	DYOPWGBKIHJGRG-UHFFFAOYSA-N
C4C-13-CH	1S/C6H/c1-3-5-6-4-2/h1H/i4+1	MGBKUZLTRVWILP-AZXPZELESA-N
C4C-13-H	1S/C5H/c1-3-5-4-2/h1H/i1+1	FKHSYQQNHVRJIA-OUBTZVSYSA-N
C4C-13-S	1S/C5S/c1-2-3-4-5-6/i5+1	OSDVLXAJVSEOND-HOSYLAQJSA-N
C4D-	1S/C4H/c1-3-4-2/h1H/q-1/i1D	PQJAELMLZABTNY-MICDWDOJSA-N
C4H-	1S/C4H/c1-3-4-2/h1H/q-1	PQJAELMLZABTNY-UHFFFAOYSA-N
C4N	1S/C4N/c1-2-3-4-5	MSPUUAZNBIERMN-UHFFFAOYSA-N
C4S	1S/C4S/c1-2-3-4-5	LRHZPSDGDVTJIL-UHFFFAOYSA-N
C5C-13-H	1S/C6H/c1-3-5-6-4-2/h1H/i2+1	MGBKUZLTRVWILP-VQEHIDDOSA-N
C5D	1S/C5H/c1-3-5-4-2/h1H/i1D	FKHSYQQNHVRJIA-MICDWDOJSA-N
C5H	1S/C5H/c1-3-5-4-2/h1H	FKHSYQQNHVRJIA-UHFFFAOYSA-N
C5N-	1S/C5N/c1-2-3-4-5-6/q-1	YCHYXZIXNMKBQL-UHFFFAOYSA-N
C5N	1S/C5N/c1-2-3-4-5-6	WJKMMAVZCWXFGT-UHFFFAOYSA-N
C5S	1S/C5S/c1-2-3-4-5-6	OSDVLXAJVSEOND-UHFFFAOYSA-N
C5S-34	1S/C5S/c1-2-3-4-5-6/i6+2	OSDVLXAJVSEOND-ZQBYOMGUSA-N
C6D	1S/C6H/c1-3-5-6-4-2/h1H/i1D	MGBKUZLTRVWILP-MICDWDOJSA-N
C6H	1S/C6H/c1-3-5-6-4-2/h1H	MGBKUZLTRVWILP-UHFFFAOYSA-N
C6H-	1S/C6H/c1-3-5-6-4-2/h1H/q-1	OOJJGCKLCPCQKV-UHFFFAOYSA-N
C7H	1S/C7H/c1-3-5-7-6-4-2/h1H	GBSBUWYWLDNSHO-UHFFFAOYSA-N
C7S	1S/C7S/c1-2-3-4-5-6-7-8	JQAUHVAGVJHYPO-UHFFFAOYSA-N
C8H	1S/C8H/c1-3-5-7-8-6-4-2/h1H	GTEOCQSGHJLKQX-UHFFFAOYSA-N
C8H-	1S/C8H/c1-3-5-7-8-6-4-2/h1H/q-1	JPYHXIJMECKQLV-UHFFFAOYSA-N
C9H	1S/C9H/c1-3-5-7-9-8-6-4-2/h1H	UQBWJKSYXDXINQ-UHFFFAOYSA-N
CaC	1S/C.Ca	JETSKDPKURDVNI-UHFFFAOYSA-N
CaCCH	1S/C2H.Ca/c1-2;/h1H;	WOIRITHJTJCTGG-UHFFFAOYSA-N
CaCl	1S/Ca.ClH/h;1H/q+1;/p-1	WGPMOVAPQPJDDK-UHFFFAOYSA-M
CaF	1S/Ca.FH/h;1H/q+1;/p-1	PMJVACMPRFHIPZ-UHFFFAOYSA-M
CaNC	1S/CN.Ca/c1-2;	GSWCPZCFMKGRDZ-UHFFFAOYSA-N
CaO	1S/Ca.O	ODINCKMPIJJUCX-UHFFFAOYSA-N
CaOH	1S/Ca.H2O/h;1H2/q+1;/p-1	KIZFHUJKFSNWKO-UHFFFAOYSA-M
CaS	1S/Ca.S	JGIATAMCQXIDNZ-UHFFFAOYSA-N
CC-13-C-13-S	1S/C3S/c1-2-3-4/i2+1,3+1	DYOPWGBKIHJGRG-SUEIGJEOSA-N
c-C-13-C2H2	1S/C3H2/c1-2-3-1/h1-2H/i3+1	VVLPCWSYZYKZKR-LBPDFUHNSA-N
CC-13-C3H	1S/C5H/c1-3-5-4-2/h1H/i4+1	FKHSYQQNHVRJIA-AZXPZELESA-N
CC-13-C3S	1S/C5S/c1-2-3-4-5-6/i2+1	OSDVLXAJVSEOND-VQEHIDDOSA-N
CC-13-C4H	1S/C6H/c1-3-5-6-4-2/h1H/i3+1	MGBKUZLTRVWILP-LBPDFUHNSA-N
CC-13-CCH	1S/C4H/c1-3-4-2/h1H/i4+1	GRADOOOISCPIDG-AZXPZELESA-N
CC-13-CH	1S/C3H/c1-3-2/h1H/i3+1	WWDRUPNDOSDMRD-LBPDFUHNSA-N
CC-13-CN	1S/C3N/c1-2-3-4/i2+1	URBHYAWCGWIELS-VQEHIDDOSA-N
CC-13-CO	1S/C3O/c1-2-3-4/i2+1	ZCNKODXATWVMAO-VQEHIDDOSA-N

CC-13CS	1S/C3S/c1-2-3-4/i2+1	DYOPWGBKIHJGRG-VQEHIDDOSA-N
CC-13-CS-34	1S/C3S/c1-2-3-4/i2+1,4+2	DYOPWGBKIHJGRG-KUTBYDBQSA-N
CC-13-H	1S/C2H/c1-2/h1H/i1+1	XEHVFKKSDRMODV-OUBTZVSYSA-N
CC-13-P	1S/C2P/c1-2-3/i2+1	UWBINSNTTNXVNB-VQEHIDDOSA-N
c-C2H4NH	1S/C2H5N/c1-2-3-1/h3H,1-2H2	NOWKCMXCCJGMRR-UHFFFAOYSA-N
c-C2H4O-18	1S/C2H4O/c1-2-3-1/h1-2H2/i3+2	IAYPIBMASNFSPL-YZRHJBSPSA-N
c-C2H4O	1S/C2H4O/c1-2-3-1/h1-2H2	IAYPIBMASNFSPL-UHFFFAOYSA-N
c-C2H4S	1S/C2H4S/c1-2-3-1/h1-2H2	VOVUARRWDCVURC-UHFFFAOYSA-N
c-C3D2	1S/C3H2/c1-2-3-1/h1-2H/i1D,2D	VVLPCWSYZYKZKR-QDNHWIQGSA-N
c-C3H2	1S/C3H2/c1-2-3-1/h1-2H	VVLPCWSYZYKZKR-UHFFFAOYSA-N
(c-C3H2)CH2	1S/C4H4/c1-4-2-3-4/h2-3H,1H2	GOSMMPKSWSOPRZ-UHFFFAOYSA-N
c-C3H4	1S/C3H4/c1-2-3-1/h1-2H,3H2	OOXWYYGXTJLWHA-UHFFFAOYSA-N
c-C3H5CN	1S/C4H5N/c5-3-4-1-2-4/h4H,1-2H2	AUQDITHEDVOTCU-UHFFFAOYSA-N
c-C3HCN	1S/C4HN/c5-3-4-1-2-4/h1H	RRSLKEZTFAPRQW-UHFFFAOYSA-N
c-C3HD	1S/C3H2/c1-2-3-1/h1-2H/i1D	VVLPCWSYZYKZKR-MICDWDOJSA-N
c-C4H4NH	1S/C4H5N/c1-2-4-5-3-1/h1-5H	KAESVJOAVNADME-UHFFFAOYSA-N
c-C4H4O	1S/C4H4O/c1-2-4-5-3-1/h1-4H	YLQBMQCUIZJEEH-UHFFFAOYSA-N
c-C6H4	1S/C6H4/c1-2-4-6-5-3-1/h1-4H	KLYCPFXDDDMZNQ-UHFFFAOYSA-N
c-C6H5CN	1S/C7H5N/c8-6-7-4-2-1-3-5-7/h1-5H	JFDZBHWFFUWGJE-UHFFFAOYSA-N
c-C6H5OH	1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H	ISWSIDIOOBJBQZ-UHFFFAOYSA-N
CCC-13-CH	1S/C4H/c1-3-4-2/h1H/i3+1	GRADOOOISCPIDG-LBPDFUHNSA-N
CCC-13-H	1S/C3H/c1-3-2/h1H/i1+1	WWDRUPNDOSDMRD-OUBTZVSYSA-N
c-CC-13-H4O	1S/C2H4O/c1-2-3-1/h1-2H2/i1+1	IAYPIBMASNFSPL-OUBTZVSYSA-N
CCC-13-N	1S/C3N/c1-2-3-4/i3+1	URBHYAWCGWIELS-LBPDFUHNSA-N
CCC-13-O	1S/C3O/c1-2-3-4/i3+1	ZCNKODXATWVMAO-LBPDFUHNSA-N
CCC-13-S	1S/C3S/c1-2-3-4/i3+1	DYOPWGBKIHJGRG-LBPDFUHNSA-N
CCC-13-S-34	1S/C3S/c1-2-3-4/i3+1,4+2	DYOPWGBKIHJGRG-XWRVAIBUSA-N
CCCC-13-H	1S/C4H/c1-3-4-2/h1H/i1+1	GRADOOOISCPIDG-OUBTZVSYSA-N
c-CCC-13-H2	1S/C3H2/c1-2-3-1/h1-2H/i1+1	VVLPCWSYZYKZKR-OUBTZVSYSA-N
CCCCD	1S/C4H/c1-3-4-2/h1H/i1D	GRADOOOISCPIDG-MICDWDOJSA-N
CCCCH	1S/C4H/c1-3-4-2/h1H	GRADOOOISCPIDG-UHFFFAOYSA-N
CCCCH	1S/C4H/c1-3-4-2/h1H	GRADOOOISCPIDG-UHFFFAOYSA-N
CCCCH	1S/C4H/c1-3-4-2/h1H	GRADOOOISCPIDG-UHFFFAOYSA-N
CCCCH	1S/C4H/c1-3-4-2/h1H	GRADOOOISCPIDG-UHFFFAOYSA-N
CCCN-15	1S/C3N/c1-2-3-4/i4+1	URBHYAWCGWIELS-AZXPZELESA-N
CCCN	1S/C3N/c1-2-3-4	URBHYAWCGWIELS-UHFFFAOYSA-N
CCCN	1S/C3N/c1-2-3-4	URBHYAWCGWIELS-UHFFFAOYSA-N
CCCO-18	1S/C3O/c1-2-3-4/i4+2	ZCNKODXATWVMAO-DOMIDYPGSA-N
CCCO	1S/C3O/c1-2-3-4	ZCNKODXATWVMAO-UHFFFAOYSA-N
CCCO	1S/C3O/c1-2-3-4	ZCNKODXATWVMAO-UHFFFAOYSA-N
CCCS	1S/C3S/c1-2-3-4	DYOPWGBKIHJGRG-UHFFFAOYSA-N
CCCS-34	1S/C3S/c1-2-3-4/i4+2	DYOPWGBKIHJGRG-DOMIDYPGSA-N
CCD	1S/C2H/c1-2/h1H/i1D	XEHVFKKSDRMODV-MICDWDOJSA-N
CCH	1S/C2H/c1-2/h1H	XEHVFKKSDRMODV-UHFFFAOYSA-N
CCH	1S/C2H/c1-2/h1H	XEHVFKKSDRMODV-UHFFFAOYSA-N
CCH	1S/C2H/c1-2/h1H	XEHVFKKSDRMODV-UHFFFAOYSA-N
CCH	1S/C2H/c1-2/h1H	XEHVFKKSDRMODV-UHFFFAOYSA-N
CCH	1S/C2H/c1-2/h1H	XEHVFKKSDRMODV-UHFFFAOYSA-N
CCH	1S/C2H/c1-2/h1H	XEHVFKKSDRMODV-UHFFFAOYSA-N
CCH	1S/C2H/c1-2/h1H	XEHVFKKSDRMODV-UHFFFAOYSA-N
CCP	1S/C2P/c1-2-3	UWBINSNTTNXVNB-UHFFFAOYSA-N
CCS	1S/C2S/c1-2-3	NELREAXCVQVNGC-UHFFFAOYSA-N
CD+	1S/CH/h1H/q+1/i1D	WVVLBIYUCXYYEU-MICDWDOJSA-N
CD+	1S/CH/h1H/q+1/i1D	WVVLBIYUCXYYEU-MICDWDOJSA-N
CF	1S/CF/c1-2	ISOSXCFSIDVNNC-UHFFFAOYSA-N
CF+	1S/CF/c1-2/q+1	LDIFHDJQDDMHHQ-UHFFFAOYSA-N
CH+	1S/CH/h1H/q+1	WVVLBIYUCXYYEU-UHFFFAOYSA-N
CH+	1S/CH/h1H/q+1	WVVLBIYUCXYYEU-UHFFFAOYSA-N
CH+	1S/CH/h1H/q+1	WVVLBIYUCXYYEU-UHFFFAOYSA-N
CH	1S/CH/h1H	VRLIPUYDFBXWCH-UHFFFAOYSA-N
CH2	1S/CH2/h1H2	HZVOZRGWRWCICA-UHFFFAOYSA-N
c-H2C3O	1S/C3H2O/c4-3-1-2-3/h1-2H	GGRQLKPIJPFWEZ-UHFFFAOYSA-N
CH2D+	1S/CH3/h1H3/q+1/i1D	JUHDUIDUEUEQND-MICDWDOJSA-N
CH2DCCH	1S/C3H4/c1-3-2/h1H,2H3/i2D	MWWATHDPGQKSAR-VMNATFBRSA-N

CH2DCN	1S/C2H3N/c1-2-3/h1H3/i1D	WEVYAHXRMPXWCK-MICDWDOJSA-N
CH2DipCH2CN	1S/C3H5N/c1-2-3-4/h2H2,1H3/i1D	FVSKHRXBFJPNKK-MICDWDOJSA-N
CH2DoopCH2CN	1S/C3H5N/c1-2-3-4/h2H2,1H3/i1D	FVSKHRXBFJPNKK-MICDWDOJSA-N
CH2(OH)C-13-HO	1S/C2H4O2/c3-1-2-4/h1,4H,2H2/i1+1	WGCNASOHLSPBMP-OUBTZVSYSA-N
CH2(OH)CHO	1S/C2H4O2/c3-1-2-4/h1,4H,2H2	WGCNASOHLSPBMP-UHFFFAOYSA-N
CH2OHCOOH	1S/C2H4O3/c3-1-2(4)5/h3H,1H2,(H,4,5)	AEMRFAOFKBGASW-UHFFFAOYSA-N
CH3C-13-H2CN	1S/C3H5N/c1-2-3-4/h2H2,1H3/i2+1	FVSKHRXBFJPNKK-VQEHIDDOSA-N
CH3C-13-N	1S/C2H3N/c1-2-3/h1H3/i2+1	WEVYAHXRMPXWCK-VQEHIDDOSA-N
CH3C3N	1S/C4H3N/c1-2-3-4-5/h1H3	WNXDCVVDPKHWMW-UHFFFAOYSA-N
CH3C4H	1S/C5H4/c1-3-5-4-2/h1H,2H3	VNMDYSSJFJFEQI-UHFFFAOYSA-N
CH3C5N	1S/C6H3N/c1-2-3-4-5-6-7/h1H3	KPEAXUODRYGJCC-UHFFFAOYSA-N
CH3C6H	1S/C7H4/c1-3-5-7-6-4-2/h1H,2H3	RZZZNMYNZMTPRN-UHFFFAOYSA-N
CH3C7N	1S/C8H3N/c1-2-3-4-5-6-7-8-9/h1H3	DHPXVNMVXDJNGW-UHFFFAOYSA-N
CH3C8H	1S/C9H4/c1-3-5-7-9-8-6-4-2/h1H,2H3	WZZXZKDJDUNZAG-UHFFFAOYSA-N
CH3C9N	1S/C10H3N/c1-2-3-4-5-6-7-8-9-10-11/h1H3	JAZGYQZPDOXVLO-UHFFFAOYSA-N
CH3CCD	1S/C3H4/c1-3-2/h1H,2H3/i1D	MWWATHDPGQKSAR-MICDWDOJSA-N
CH3CCH	1S/C3H4/c1-3-2/h1H,2H3	MWWATHDPGQKSAR-UHFFFAOYSA-N
CH3CCH	1S/C3H4/c1-3-2/h1H,2H3	MWWATHDPGQKSAR-UHFFFAOYSA-N
CH3CCH	1S/C3H4/c1-3-2/h1H,2H3	MWWATHDPGQKSAR-UHFFFAOYSA-N
CH3CCH	1S/C3H4/c1-3-2/h1H,2H3	MWWATHDPGQKSAR-UHFFFAOYSA-N
CH3CCNC	1S/C4H3N/c1-3-4-5-2/h1H3	QRJFDECOKMVIKS-UHFFFAOYSA-N
CH3CHDCN	1S/C3H5N/c1-2-3-4/h2H2,1H3/i2D	FVSKHRXBFJPNKK-VMNATFBRSA-N
CH3CH(NH2)CN	1S/C3H6N2/c1-3(5)2-4/h3H,5H2,1H3	UAMZETBJZRERCQ-UHFFFAOYSA-N
CH3CHNH2COOH	1S/C3H7NO2/c1-2(4)3(5)6/h2H,4H2,1H3,(H,5,6)	QNAYBMKLOCPYGJ-UHFFFAOYSA-N
CH3CHNH2COOH	1S/C3H7NO2/c1-2(4)3(5)6/h2H,4H2,1H3,(H,5,6)	QNAYBMKLOCPYGJ-UHFFFAOYSA-N
CH3CN-15	1S/C2H3N/c1-2-3/h1H3/i3+1	WEVYAHXRMPXWCK-LBPDFUHNSA-N
CH3CN	1S/C2H3N/c1-2-3/h1H3	WEVYAHXRMPXWCK-UHFFFAOYSA-N
CH3CNH+	1S/C2H3N/c1-2-3/h1H3/p+1	WEVYAHXRMPXWCK-UHFFFAOYSA-O
CH3CP	1S/C2H3P/c1-2-3/h1H3	KECHNHGPNWSPDK-UHFFFAOYSA-N
CH3D	1S/CH4/h1H4/i1D	VNWKTOKETHGBQD-MICDWDOJSA-N
CH3O-18-H	1S/CH4O/c1-2/h2H,1H3/i2+2	OKKJLVBELUTLKV-HQMMCQRPSA-N
CH3OC-13-HO	1S/C2H4O2/c1-4-2-3/h2H,1H3/i2+1	TZIHFWKZFHZASV-VQEHIDDOSA-N
CH3OCH3	1S/C2H6O/c1-3-2/h1-2H3	LCGLNKUTAGEVQW-UHFFFAOYSA-N
CH3OH	1S/CH4O/c1-2/h2H,1H3	OKKJLVBELUTLKV-UHFFFAOYSA-N
CH3SH	1S/CH4S/c1-2/h2H,1H3	LSDPWZHWYPCBBB-UHFFFAOYSA-N
c-HCOOH	1S/CH2O2/c1-3-2/h1-2H	RXIZGRWAJVLEHT-UHFFFAOYSA-N
c-HC(O)SH	1S/CH2OS/c2-1-3/h1H,(H,2,3)	AWIJRPNMLHPLNC-UHFFFAOYSA-N
CHD2CN	1S/C2H3N/c1-2-3/h1H3/i1D2	WEVYAHXRMPXWCK-DICFDUPASA-N
CHOCHOHCH2OH	1S/C3H6O3/c4-1-3(6)2-5/h1,3,5-6H,2H2	MNQZXJOMYWMBOU-UHFFFAOYSA-N
CHOCOOH	1S/C2H2O3/c3-1-2(4)5/h1H,(H,4,5)	HHLFWLYXYJOTON-UHFFFAOYSA-N
cis-HC(O)NHD	1S/CH3NO/c2-1-3/h1H,(H2,2,3)/i/hD	ZHNUHDYFZUAESO-DYCDLGHISA-N
cis-HOCO	1S/CHO2/c2-1-3/h(H,2,3)	ORTFAQDWJHRMNX-UHFFFAOYSA-N
cis-HOSO+	1S/O2S/c1-3-2/p+1	RAHZWNYVWXNFOC-UHFFFAOYSA-O
CN-15	1S/CN/c1-2/i2+1	JEVCWSUVFOYBFI-VQEHIDDOSA-N
CN	1S/CN/c1-2	JEVCWSUVFOYBFI-UHFFFAOYSA-N
CN-	1S/CN/c1-2/q-1	XFXPMWWXUTWYJX-UHFFFAOYSA-N
CO-17	1S/CO/c1-2/i2+1	UGFAIRIUMAVXCW-VQEHIDDOSA-N
CO-18	1S/CO/c1-2/i2+2	UGFAIRIUMAVXCW-HQMMCQRPSA-N
CO-18+	1S/CO/c1-2/q+1/i2+2	BOJPITGAFFYFJK-HQMMCQRPSA-N
CO+	1S/CO/c1-2/q+1	BOJPITGAFFYFJK-UHFFFAOYSA-N
CO+	1S/CO/c1-2/q+1	BOJPITGAFFYFJK-UHFFFAOYSA-N
CO	1S/CO/c1-2	UGFAIRIUMAVXCW-UHFFFAOYSA-N
CO	1S/CO/c1-2	UGFAIRIUMAVXCW-UHFFFAOYSA-N
CoC	1S/C.Co	CODVACFVSVNQPY-UHFFFAOYSA-N
CP	1S/CP/c1-2	GDPLAAHPHNAIGW-UHFFFAOYSA-N
CS	1S/CS/c1-2	DXHPZXWIPWDXHJ-UHFFFAOYSA-N
CS	1S/CS/c1-2	DXHPZXWIPWDXHJ-UHFFFAOYSA-N
CS	1S/CS/c1-2	DXHPZXWIPWDXHJ-UHFFFAOYSA-N
CS+	1S/CS/c1-2/q+1	ITHBHNXWPWSYRD-UHFFFAOYSA-N
CS-33	1S/CS/c1-2/i2+1	DXHPZXWIPWDXHJ-VQEHIDDOSA-N
CS-34	1S/CS/c1-2/i2+2	DXHPZXWIPWDXHJ-HQMMCQRPSA-N
CS-36	1S/CS/c1-2/i2+4	DXHPZXWIPWDXHJ-XKBLRHCCSA-N
CT+	1S/CH/h1H/q+1/i1T	WVVLBIYUCXYYEU-CNRUNOGKSA-N
Cu-63-H	1S/Cu.H/i1-1;	JJFLDSOAQUJVBF-ULWFUOSBSA-N
Cu-65-H	1S/Cu.H/i1+1;	JJFLDSOAQUJVBF-YTBWXGASSA-N

D2C-13-O	1S/CH2O/c1-2/h1H2/i1+1D2	WSFSSNUMVMOOMR-WGVGGRBOSA-N
D2CCO	1S/C2H2O/c1-2-3/h1H2/i1D2	CCGKOQOJPYTBIH-DICFDUPASA-N
D2CO	1S/CH2O/c1-2/h1H2/i1D2	WSFSSNUMVMOOMR-DICFDUPASA-N
D2CS	1S/CH2S/c1-2/h1H2/i1D2	DBTDEFJAFBUGPP-DICFDUPASA-N
D2NCH2CN	1S/C2H4N2/c3-1-2-4/h1,3H2/i/hD2	DFNYGALUNNFWKJ-ZSJDYOACSA-N
D2O	1S/H2O/h1H2/i/hD2	XLYOFNOQVPJJNP-ZSJDYOACSA-N
D2S	1S/H2S/h1H2/i/hD2	RWSOTUBLDIXVET-ZSJDYOACSA-N
D2S-34	1S/H2S/h1H2/i1+2/hD2	RWSOTUBLDIXVET-LAPWFLRPSA-N
DC-13-CCN	1S/C3HN/c1-2-3-4/h1H/i1+1D	LNDJVIYUJOJFSO-VVKOMZTBSA-N
DC-13-N-15	1S/CHN/c1-2/h1H/i1+1D,2+1	LELOWRISYMNNSU-JWZNKSNFSA-N
DC-13-N	1S/CHN/c1-2/h1H/i1+1D	LELOWRISYMNNSU-VVKOMZTBSA-N
DC-13-O+	1S/CHO/c1-2/h1H/q+1/i1+1D	XPRMKTHGXOVKEH-VVKOMZTBSA-N
DCC-13-CN	1S/C3HN/c1-2-3-4/h1H/i1D,2+1	LNDJVIYUJOJFSO-UBIWUTSMSA-N
DCCC-13-N	1S/C3HN/c1-2-3-4/h1H/i1D,3+1	LNDJVIYUJOJFSO-DOVDSDCISA-N
DCCCCCCCN	1S/C7HN/c1-2-3-4-5-6-7-8/h1H/i1D	XRJCSTPFBZTAPK-MICDWDOJSA-N
DCCCCCN	1S/C5HN/c1-2-3-4-5-6/h1H/i1D	WRARULQOSOCOQD-MICDWDOJSA-N
DCCCN-15	1S/C3HN/c1-2-3-4/h1H/i1D,4+1	LNDJVIYUJOJFSO-WLZVQDDYSA-N
DCCCN	1S/C3HN/c1-2-3-4/h1H/i1D	LNDJVIYUJOJFSO-MICDWDOJSA-N
DCCCN	1S/C3HN/c1-2-3-4/h1H/i1D	LNDJVIYUJOJFSO-MICDWDOJSA-N
DCCN	1S/C2HN/c1-2-3/h1H/i1D	SZICEGNEOSKVLO-MICDWDOJSA-N
DCN-15	1S/CHN/c1-2/h1H/i1D,2+1	LELOWRISYMNNSU-UBIWUTSMSA-N
DCN	1S/CHN/c1-2/h1H/i1D	LELOWRISYMNNSU-MICDWDOJSA-N
DCN	1S/CHN/c1-2/h1H/i1D	LELOWRISYMNNSU-MICDWDOJSA-N
DCNO	1S/CHNO/c1-2-3/h1H/i1D	UXKUODQYLDZXDL-MICDWDOJSA-N
DCO-18+	1S/CHO/c1-2/h1H/q+1/i1D,2+2	XPRMKTHGXOVKEH-YLRDUFTQSA-N
DCO+	1S/CHO/c1-2/h1H/q+1/i1D	XPRMKTHGXOVKEH-MICDWDOJSA-N
DC(O)NH2	1S/CH3NO/c2-1-3/h1H,(H2,2,3)/i1D	ZHNUHDYFZUAESO-MICDWDOJSA-N
DCP	1S/CHP/c1-2/h1H/i1D	DPYPSJGRRFKXBE-MICDWDOJSA-N
DCS+	1S/CHS/c1-2/h1H/q+1/i1D	YOFNWWZZELAVRX-MICDWDOJSA-N
DN2+	1S/N2/c1-2/p+1/i/hD	IJGRMHOSHXDMSA-DYCDLGHISA-O
DNC	1S/CHN/c1-2/h2H/i2D	QIUBLANJVAOHHY-VMNATFBRSA-N
DOC+	1S/CHO/c1-2/h2H/q+1/i2D	FIRPXVMETWVPCB-VMNATFBRSA-N
E-HC2CHCHCN	1S/C5H3N/c1-2-3-4-5-6/h1,3-4H	ZXFTWPNQZKQCAL-UHFFFAOYSA-N
E-HNCHCN	1S/C2H2N2/c3-1-2-4/h1,3H	LAVVSPWGGHZKLI-UHFFFAOYSA-N
Fe-56-C	1/C.Fe/rCFe/c1-2	QMQXDJATSGGYDR-WGUWINONNA-N
FeCO	1/CO.Fe/c1-2;/rCFeO/c2-1-3	SVMGVNXXUVNGRK-IVCKVGOVNA-N
Ga-n-C3H7OH	1S/C3H8O/c1-2-3-4/h4H,2-3H2,1H3	BDERNNFJNOPAEC-UHFFFAOYSA-N
GA-n-C4H9CN	1S/C5H9N/c1-2-3-4-5-6/h2-4H2,1H3	RFFFKMOABOFIDF-UHFFFAOYSA-N
gGg'-(CH2OH)2	1S/C2H6O2/c3-1-2-4/h3-4H,1-2H2	LYCAIKOWRPUZTN-UHFFFAOYSA-N
H2C-13-CHCN	1S/C3H3N/c1-2-3-4/h2H,1H2/i1+1	NLHHRLWOUZZQLW-OUBTZVSYSA-N
H2C-13-CO	1S/C2H2O/c1-2-3/h1H2/i1+1	CCGKOQOJPYTBIH-OUBTZVSYSA-N
H2C-13-NH	1S/CH3N/c1-2/h2H,1H2/i1+1	WDWDWGRYHDPSDS-OUBTZVSYSA-N
H2C-13-O	1S/CH2O/c1-2/h1H2/i1+1	WSFSSNUMVMOOMR-OUBTZVSYSA-N
H2C-13-OH+	1S/CH3O/c1-2/h2H,1H2/q+1/i1+1	NRCYHMDIJIIHBJ-OUBTZVSYSA-N
H2C-13-S	1S/CH2S/c1-2/h1H2/i1+1	DBTDEFJAFBUGPP-OUBTZVSYSA-N
H2C2S	1S/C2H2S/c1-2-3/h1H2	CWMKZYCJCZVSHO-UHFFFAOYSA-N
H2C3H	1S/C3H3/c1-3-2/h1H,2H2	DITHIFQMPPCBCU-UHFFFAOYSA-N
H2C3S	1S/C3H2S/c1-2-3-4/h1H2	YUYXFAJNLSCPNK-UHFFFAOYSA-N
H2C4N	1S/C4H2N/c1-2-3-4-5/h1H2	VWBZDMRGJAHYJU-UHFFFAOYSA-N
H2CC-13-HCN	1S/C3H3N/c1-2-3-4/h2H,1H2/i2+1	NLHHRLWOUZZQLW-VQEHIDDOSA-N
H2CC-13-O	1S/C2H2O/c1-2-3/h1H2/i2+1	CCGKOQOJPYTBIH-VQEHIDDOSA-N
H2CCCHCN	1S/C4H3N/c1-2-3-4-5/h3H,1H2	IRLQAJPIHBZROB-UHFFFAOYSA-N
H2CCHC-13-N	1S/C3H3N/c1-2-3-4/h2H,1H2/i3+1	NLHHRLWOUZZQLW-LBPDFUHNSA-N
H2CCHCCH	1S/C4H4/c1-3-4-2/h1,4H,2H2	WFYPICNXBKQZGB-UHFFFAOYSA-N
H2CCHCN-15	1S/C3H3N/c1-2-3-4/h2H,1H2/i4+1	NLHHRLWOUZZQLW-AZXPZELESA-N
H2CCN	1S/C2H2N/c1-2-3/h1H2	XSTKDMFTWATIQP-UHFFFAOYSA-N
H2C(CN)2	1S/C3H2N2/c4-2-1-3-5/h1H2	CUONGYYJJVDODC-UHFFFAOYSA-N
H2CCNH	1S/C2H3N/c1-2-3/h3H,1H2	ZUKSLMGYYPZZJD-UHFFFAOYSA-N
H2CCO-18	1S/C2H2O/c1-2-3/h1H2/i3+2	CCGKOQOJPYTBIH-YZRHJBSPSA-N
H2CCO	1S/C2H2O/c1-2-3/h1H2	CCGKOQOJPYTBIH-UHFFFAOYSA-N
H2Cl+	1S/ClH2/h1H2/q+1/i1+2	IGJWHVUMEJASKV-NJFSPNSNSA-N
H2Cl+	1S/ClH2/h1H2/q+1	IGJWHVUMEJASKV-UHFFFAOYSA-N
H2CN-15-H	1S/CH3N/c1-2/h2H,1H2/i2+1	WDWDWGRYHDPSDS-VQEHIDDOSA-N
H2CN	1S/CH2N/c1-2/h1H2	PZIDJKOIMRBQLL-UHFFFAOYSA-N
H2CNCN	1S/C2H2N2/c1-4-2-3/h1H2	DJJGJRBOTPORBZ-UHFFFAOYSA-N

H2CND	1S/CH3N/c1-2/h2H,1H2/i/hD	WDWDWGRYHDPSDS-DYCDLGHISA-N
H2CNH	1S/CH3N/c1-2/h2H,1H2	WDWDWGRYHDPSDS-UHFFFAOYSA-N
H2CO-18	1S/CH2O/c1-2/h1H2/i2+2	WSFSSNUMVMOOMR-HQMMCQRPSA-N
H2CO	1S/CH2O/c1-2/h1H2	WSFSSNUMVMOOMR-UHFFFAOYSA-N
H2COH+	1S/CH3O/c1-2/h2H,1H2/q+1	NRCYHMDIJIIHBJ-UHFFFAOYSA-N
H2CP	1S/CH2P/c1-2/h1H2	IOPIMTCNBFTMDS-UHFFFAOYSA-N
H2CS	1S/CH2S/c1-2/h1H2	DBTDEFJAFBUGPP-UHFFFAOYSA-N
H2CS-33	1S/CH2S/c1-2/h1H2/i2+1	DBTDEFJAFBUGPP-VQEHIDDOSA-N
H2CS-34	1S/CH2S/c1-2/h1H2/i2+2	DBTDEFJAFBUGPP-HQMMCQRPSA-N
H2D+	1S/H3/c1-2-3-1/q+1/i1+1	RQZCXKHVAUFVMF-OUBTZVSYSA-N
H2DO+	1S/H2O/h1H2/p+1/i/hD	XLYOFNOQVPJJNP-DYCDLGHISA-O
H2F+	1S/FH2/h1H2/q+1	YNESUKSMQODWNS-UHFFFAOYSA-N
H2NC-13-N	1S/CH2N2/c2-1-3/h2H2/i1+1	XZMCDFZZKTWFGF-OUBTZVSYSA-N
H2NCH2CN	1S/C2H4N2/c3-1-2-4/h1,3H2	DFNYGALUNNFWKJ-UHFFFAOYSA-N
H2NCH2COOH	1S/C2H5NO2/c3-1-2(4)5/h1,3H2,(H,4,5)	DHMQDGOQFOQNFH-UHFFFAOYSA-N
H2NCH2COOH, II	1S/C2H5NO2/c3-1-2(4)5/h1,3H2,(H,4,5)	DHMQDGOQFOQNFH-UHFFFAOYSA-N
H2NCO+	1S/CH2NO/c1-2-3/h1-2H/q+1	BHYKZJBRVXPIMH-UHFFFAOYSA-N
H2O+	1S/H2O/h1H2/q+1	RECVMTHOQWMYFX-UHFFFAOYSA-N
H2S	1S/H2S/h1H2	RWSOTUBLDIXVET-UHFFFAOYSA-N
H2S-33	1S/H2S/h1H2/i1+1	RWSOTUBLDIXVET-OUBTZVSYSA-N
H2S-34	1S/H2S/h1H2/i1+2	RWSOTUBLDIXVET-NJFSPNSNSA-N
H2SiO	1S/H2OSi/c1-2/h2H2	HZBAVWLZSLOCFR-UHFFFAOYSA-N
H2SiS	1S/H2SSi/c1-2/h2H2	CXVUPNQQVSTPBQ-UHFFFAOYSA-N
H3O+	1S/H2O/h1H2/p+1	XLYOFNOQVPJJNP-UHFFFAOYSA-O
HB-10-O	1S/BHO/c1-2/h1H/i1-1	UXUFOKFTFHRQTE-BJUDXGSMSA-N
HBO	1S/BHO/c1-2/h1H	UXUFOKFTFHRQTE-UHFFFAOYSA-N
HC11N	1S/C11HN/c1-2-3-4-5-6-7-8-9-10-11-12/h1H	VSPOLSIHZRDJDD-UHFFFAOYSA-N
HC-13-C-13-CN	1S/C3HN/c1-2-3-4/h1H/i1+1,2+1	LNDJVIYUJOJFSO-ZDOIIHCHSA-N
HC-13-CC-13-N	1S/C3HN/c1-2-3-4/h1H/i1+1,3+1	LNDJVIYUJOJFSO-ZKDXJZICSA-N
HC-13-CCCCCCN	1S/C7HN/c1-2-3-4-5-6-7-8/h1H/i1+1	XRJCSTPFBZTAPK-OUBTZVSYSA-N
HC-13-CCCCN	1S/C5HN/c1-2-3-4-5-6/h1H/i1+1	WRARULQOSOCOQD-OUBTZVSYSA-N
HC-13-CCN	1S/C3HN/c1-2-3-4/h1H/i1+1	LNDJVIYUJOJFSO-OUBTZVSYSA-N
HC-13-CCN	1S/C3HN/c1-2-3-4/h1H/i1+1	LNDJVIYUJOJFSO-OUBTZVSYSA-N
HC-13-CCN	1S/C3HN/c1-2-3-4/h1H/i1+1	LNDJVIYUJOJFSO-OUBTZVSYSA-N
HC-13-CCN	1S/C3HN/c1-2-3-4/h1H/i1+1	LNDJVIYUJOJFSO-OUBTZVSYSA-N
HC-13-CCN	1S/C3HN/c1-2-3-4/h1H/i1+1	LNDJVIYUJOJFSO-OUBTZVSYSA-N
HC-13-CCN	1S/C3HN/c1-2-3-4/h1H/i1+1	LNDJVIYUJOJFSO-OUBTZVSYSA-N
HC-13-CN	1S/C2HN/c1-2-3/h1H/i1+1	SZICEGNEOSKVLO-OUBTZVSYSA-N
HC-13-N-15	1S/CHN/c1-2/h1H/i1+1,2+1	LELOWRISYMNNSU-ZDOIIHCHSA-N
HC-13-N-15	1S/CHN/c1-2/h1H/i1+1,2+1	LELOWRISYMNNSU-ZDOIIHCHSA-N
HC13N	1S/C13HN/c1-2-3-4-5-6-7-8-9-10-11-12-13-14/h1H	OROZKPLETKDYMP-UHFFFAOYSA-N
HC-13-N	1S/CHN/c1-2/h1H/i1+1	LELOWRISYMNNSU-OUBTZVSYSA-N
HC-13-NH+	1S/CHN/c1-2/h1H/p+1/i1+1	LELOWRISYMNNSU-OUBTZVSYSA-O
HC-13-NO	1S/CHNO/c1-2-3/h1H/i1+1	UXKUODQYLDZXDL-OUBTZVSYSA-N
HC-13-O+	1S/CHO/c1-2/h1H/q+1/i1+1	XPRMKTHGXOVKEH-OUBTZVSYSA-N
HC-13-(O)NH2	1S/CH3NO/c2-1-3/h1H,(H2,2,3)/i1+1	ZHNUHDYFZUAESO-OUBTZVSYSA-N
HC-13-P	1S/CHP/c1-2/h1H/i1+1	DPYPSJGRRFKXBE-OUBTZVSYSA-N
HC-13-S+	1S/CHS/c1-2/h1H/q+1/i1+1	YOFNWWZZELAVRX-OUBTZVSYSA-N
HC15N-15-O	1S/CHNO/c1-2-3/h1H/i2+1	UXKUODQYLDZXDL-VQEHIDDOSA-N
HC3N	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HC3N	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HC3N	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HC3N	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HC3N	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HC3NH+	1S/C3HN/c1-2-3-4/h1H/p+1	LNDJVIYUJOJFSO-UHFFFAOYSA-O
HC3P	1S/C3HP/c1-2-3-4/h1H	QFYONCMOBIGBSA-UHFFFAOYSA-N
HC4NC	1S/C5HN/c1-3-4-5-6-2/h1H	STBDUUJTODBNPI-UHFFFAOYSA-N
HC5N	1S/C5HN/c1-2-3-4-5-6/h1H	WRARULQOSOCOQD-UHFFFAOYSA-N
HC5N	1S/C5HN/c1-2-3-4-5-6/h1H	WRARULQOSOCOQD-UHFFFAOYSA-N
HC9N	1S/C9HN/c1-2-3-4-5-6-7-8-9-10/h1H	XBYCNIKNUFWLQZ-UHFFFAOYSA-N
HCC-13-C-13-N	1S/C3HN/c1-2-3-4/h1H/i2+1,3+1	LNDJVIYUJOJFSO-SUEIGJEOSA-N
HCC-13-CCCCCN	1S/C7HN/c1-2-3-4-5-6-7-8/h1H/i2+1	XRJCSTPFBZTAPK-VQEHIDDOSA-N
HCC-13-CCCN	1S/C5HN/c1-2-3-4-5-6/h1H/i2+1	WRARULQOSOCOQD-VQEHIDDOSA-N
HCC-13-CN-15	1S/C3HN/c1-2-3-4/h1H/i2+1,4+1	LNDJVIYUJOJFSO-NDLBAUGKSA-N
HCC-13-CN	1S/C3HN/c1-2-3-4/h1H/i2+1	LNDJVIYUJOJFSO-VQEHIDDOSA-N

HCC-13-CN	1S/C3HN/c1-2-3-4/h1H/i2+1	LNDJVIYUJOJFSO-VQEHIDDOSA-N
HCC-13-CN	1S/C3HN/c1-2-3-4/h1H/i2+1	LNDJVIYUJOJFSO-VQEHIDDOSA-N
HCC-13-CN	1S/C3HN/c1-2-3-4/h1H/i2+1	LNDJVIYUJOJFSO-VQEHIDDOSA-N
HCC-13-CN	1S/C3HN/c1-2-3-4/h1H/i2+1	LNDJVIYUJOJFSO-VQEHIDDOSA-N
HCC-13-CN	1S/C3HN/c1-2-3-4/h1H/i2+1	LNDJVIYUJOJFSO-VQEHIDDOSA-N
HCC-13-N	1S/C2HN/c1-2-3/h1H/i2+1	SZICEGNEOSKVLO-VQEHIDDOSA-N
HCCC-13-CCCCN	1S/C7HN/c1-2-3-4-5-6-7-8/h1H/i3+1	XRJCSTPFBZTAPK-LBPDFUHNSA-N
HCCC-13-CCN	1S/C5HN/c1-2-3-4-5-6/h1H/i3+1	WRARULQOSOCOQD-LBPDFUHNSA-N
HCCC-13-N	1S/C3HN/c1-2-3-4/h1H/i3+1	LNDJVIYUJOJFSO-LBPDFUHNSA-N
HCCC-13-N	1S/C3HN/c1-2-3-4/h1H/i3+1	LNDJVIYUJOJFSO-LBPDFUHNSA-N
HCCC-13-N	1S/C3HN/c1-2-3-4/h1H/i3+1	LNDJVIYUJOJFSO-LBPDFUHNSA-N
HCCC-13-N	1S/C3HN/c1-2-3-4/h1H/i3+1	LNDJVIYUJOJFSO-LBPDFUHNSA-N
HCCC-13-N	1S/C3HN/c1-2-3-4/h1H/i3+1	LNDJVIYUJOJFSO-LBPDFUHNSA-N
HCCC-13-N	1S/C3HN/c1-2-3-4/h1H/i3+1	LNDJVIYUJOJFSO-LBPDFUHNSA-N
HCCC-13-N	1S/C3HN/c1-2-3-4/h1H/i3+1	LNDJVIYUJOJFSO-LBPDFUHNSA-N
HCCC-13-N	1S/C3HN/c1-2-3-4/h1H/i3+1	LNDJVIYUJOJFSO-LBPDFUHNSA-N
HCCCC-13-CCCN	1S/C7HN/c1-2-3-4-5-6-7-8/h1H/i4+1	XRJCSTPFBZTAPK-AZXPZELESA-N
HCCCC-13-CN	1S/C5HN/c1-2-3-4-5-6/h1H/i4+1	WRARULQOSOCOQD-AZXPZELESA-N
HCCCCC-13-CCN	1S/C7HN/c1-2-3-4-5-6-7-8/h1H/i5+1	XRJCSTPFBZTAPK-HOSYLAQJSA-N
HCCCCC-13-N	1S/C5HN/c1-2-3-4-5-6/h1H/i5+1	WRARULQOSOCOQD-HOSYLAQJSA-N
HCCCCCC-13-CN	1S/C7HN/c1-2-3-4-5-6-7-8/h1H/i6+1	XRJCSTPFBZTAPK-PTQBSOBMSA-N
HCCCCCCC-13-N	1S/C7HN/c1-2-3-4-5-6-7-8/h1H/i7+1	XRJCSTPFBZTAPK-CDYZYAPPSA-N
HCCCCCCCN-15	1S/C7HN/c1-2-3-4-5-6-7-8/h1H/i8+1	XRJCSTPFBZTAPK-VJJZLTLGSA-N
HCCCCCCCN	1S/C7HN/c1-2-3-4-5-6-7-8/h1H	XRJCSTPFBZTAPK-UHFFFAOYSA-N
HCCCCCCCN	1S/C7HN/c1-2-3-4-5-6-7-8/h1H	XRJCSTPFBZTAPK-UHFFFAOYSA-N
HCCCCCCCN	1S/C7HN/c1-2-3-4-5-6-7-8/h1H	XRJCSTPFBZTAPK-UHFFFAOYSA-N
HCCCCCN-15	1S/C5HN/c1-2-3-4-5-6/h1H/i6+1	WRARULQOSOCOQD-PTQBSOBMSA-N
HCCCCCN	1S/C5HN/c1-2-3-4-5-6/h1H	WRARULQOSOCOQD-UHFFFAOYSA-N
HCCCCCN	1S/C5HN/c1-2-3-4-5-6/h1H	WRARULQOSOCOQD-UHFFFAOYSA-N
HCCCCCN	1S/C5HN/c1-2-3-4-5-6/h1H	WRARULQOSOCOQD-UHFFFAOYSA-N
HCCCCCN	1S/C5HN/c1-2-3-4-5-6/h1H	WRARULQOSOCOQD-UHFFFAOYSA-N
HCCCCCN	1S/C5HN/c1-2-3-4-5-6/h1H	WRARULQOSOCOQD-UHFFFAOYSA-N
HCCCCCN	1S/C5HN/c1-2-3-4-5-6/h1H	WRARULQOSOCOQD-UHFFFAOYSA-N
HCCCCCN	1S/C5HN/c1-2-3-4-5-6/h1H	WRARULQOSOCOQD-UHFFFAOYSA-N
HCCCHO	1S/C3H2O/c1-2-3-4/h1,3H	IJNJLGFTSIAHEA-UHFFFAOYSA-N
HCCCN-15	1S/C3HN/c1-2-3-4/h1H/i4+1	LNDJVIYUJOJFSO-AZXPZELESA-N
HCCCN-15	1S/C3HN/c1-2-3-4/h1H/i4+1	LNDJVIYUJOJFSO-AZXPZELESA-N
HCCCN	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HCCCN	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HCCCN	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HCCCN	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HCCCN	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HCCCN	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HCCCN	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HCCCN	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HCCCN	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HCCCN	1S/C3HN/c1-2-3-4/h1H	LNDJVIYUJOJFSO-UHFFFAOYSA-N
HCCD	1S/C2H2/c1-2/h1-2H/i1D	HSFWRNGVRCDJHI-MICDWDOJSA-N
HCCN-15	1S/C2HN/c1-2-3/h1H/i3+1	SZICEGNEOSKVLO-LBPDFUHNSA-N
HCCN	1S/C2HN/c1-2-3/h1H	SZICEGNEOSKVLO-UHFFFAOYSA-N
HCCO	1S/C2HO/c1-2-3/h1H	QEJQAPYSVNHDJF-UHFFFAOYSA-N
HCCP	1S/C2HP/c1-2-3/h1H	WQCRITLCZNJTQF-UHFFFAOYSA-N
HCN-15	1S/CHN/c1-2/h1H/i2+1	LELOWRISYMNNSU-VQEHIDDOSA-N
HCN-15	1S/CHN/c1-2/h1H/i2+1	LELOWRISYMNNSU-VQEHIDDOSA-N
HCN	1S/CHN/c1-2/h1H	LELOWRISYMNNSU-UHFFFAOYSA-N
HCN	1S/CHN/c1-2/h1H	LELOWRISYMNNSU-UHFFFAOYSA-N
HCN	1S/CHN/c1-2/h1H	LELOWRISYMNNSU-UHFFFAOYSA-N
HCN	1S/CHN/c1-2/h1H	LELOWRISYMNNSU-UHFFFAOYSA-N
HCN	1S/CHN/c1-2/h1H	LELOWRISYMNNSU-UHFFFAOYSA-N
HCN	1S/CHN/c1-2/h1H	LELOWRISYMNNSU-UHFFFAOYSA-N
HCND+	1S/CHN/c1-2/h1H/p+1/i/hD	LELOWRISYMNNSU-DYCDLGHISA-O
HCNH+	1S/CHN/c1-2/h1H/p+1	LELOWRISYMNNSU-UHFFFAOYSA-O
HCNO	1S/CHNO/c1-2-3/h1H	UXKUODQYLDZXDL-UHFFFAOYSA-N

HCO-17+	1S/CHO/c1-2/h1H/q+1/i2+1	XPRMKTHGXOVKEH-VQEHIDDOSA-N
HCO-18+	1S/CHO/c1-2/h1H/q+1/i2+2	XPRMKTHGXOVKEH-HQMMCQRPSA-N
HC(O-18)NH2	1S/CH3NO/c2-1-3/h1H,(H2,2,3)/i3+2	ZHNUHDYFZUAESO-YZRHJBSPSA-N
HCO+	1S/CHO/c1-2/h1H/q+1	XPRMKTHGXOVKEH-UHFFFAOYSA-N
HCO+	1S/CHO/c1-2/h1H/q+1	XPRMKTHGXOVKEH-UHFFFAOYSA-N
HCO+	1S/CHO/c1-2/h1H/q+1	XPRMKTHGXOVKEH-UHFFFAOYSA-N
HC(O)CN	1S/C2HNO/c1-4-2-3/h1H	GROIQSCNHYLOLC-UHFFFAOYSA-N
HC(O)N-15-H2	1S/CH3NO/c2-1-3/h1H,(H2,2,3)/i2+1	ZHNUHDYFZUAESO-VQEHIDDOSA-N
HC(O)NH2	1S/CH3NO/c2-1-3/h1H,(H2,2,3)	ZHNUHDYFZUAESO-UHFFFAOYSA-N
HC(O)NH2	1S/CH3NO/c2-1-3/h1H,(H2,2,3)	ZHNUHDYFZUAESO-UHFFFAOYSA-N
HCP	1S/CHP/c1-2/h1H	DPYPSJGRRFKXBE-UHFFFAOYSA-N
HCP	1S/CHP/c1-2/h1H	DPYPSJGRRFKXBE-UHFFFAOYSA-N
HCS+	1S/CHS/c1-2/h1H/q+1	YOFNWWZZELAVRX-UHFFFAOYSA-N
HCS	1S/CHS/c1-2/h1H	RIFHJAODNHLCBH-UHFFFAOYSA-N
HCS-34+	1S/CHS/c1-2/h1H/q+1/i2+2	YOFNWWZZELAVRX-HQMMCQRPSA-N
HD	1S/H2/h1H/i1+1	UFHFLCQGNIYNRP-OUBTZVSYSA-N
HD2+	1S/H3/c1-2-3-1/q+1/i1+1,2+1	RQZCXKHVAUFVMF-ZDOIIHCHSA-N
HDC-13-O	1S/CH2O/c1-2/h1H2/i1+1D	WSFSSNUMVMOOMR-VVKOMZTBSA-N
HDCCO	1S/C2H2O/c1-2-3/h1H2/i1D	CCGKOQOJPYTBIH-MICDWDOJSA-N
HDCO	1S/CH2O/c1-2/h1H2/i1D	WSFSSNUMVMOOMR-MICDWDOJSA-N
HDCS	1S/CH2S/c1-2/h1H2/i1D	DBTDEFJAFBUGPP-MICDWDOJSA-N
HDNCH2CN	1S/C2H4N2/c3-1-2-4/h1,3H2/i/hD	DFNYGALUNNFWKJ-DYCDLGHISA-N
HDS	1S/H2S/h1H2/i/hD	RWSOTUBLDIXVET-DYCDLGHISA-N
HDS-34	1S/H2S/h1H2/i1+2/hD	RWSOTUBLDIXVET-DQGQKLTASA-N
HeH+	1S/HHe/h1H/q+1	HSFAAVLNFOAYQX-UHFFFAOYSA-N
HMgNC	1S/CN.Mg.H/c1-2;;/q-1;+1;	KBZWQHRUEURBTO-UHFFFAOYSA-N
HNC-13	1S/CHN/c1-2/h2H/i1+1	QIUBLANJVAOHHY-OUBTZVSYSA-N
HNC	1S/CHN/c1-2/h2H	QIUBLANJVAOHHY-UHFFFAOYSA-N
HNC	1S/CHN/c1-2/h2H	QIUBLANJVAOHHY-UHFFFAOYSA-N
HNCN	1S/CHN2/c2-1-3/h2H	RCDKZYGELCBJTH-UHFFFAOYSA-N
HNCNH	1S/CH2N2/c2-1-3/h2-3H	VPKDCDLSJZCGKE-UHFFFAOYSA-N
HNCO	1S/CHNO/c2-1-3/h2H	OWIKHYCFFJSOEH-UHFFFAOYSA-N
HNCS	1S/CHNS/c2-1-3/h2H	GRHBQAYDJPGGLF-UHFFFAOYSA-N
HNCS	1S/CHNS/c2-1-3/h2H	GRHBQAYDJPGGLF-UHFFFAOYSA-N
HNSi	1S/HNSi/c1-2/h1H	PMXLLFCEIKHJCZ-UHFFFAOYSA-N
HOC+	1S/CHO/c1-2/h2H/q+1	FIRPXVMETWVPCB-UHFFFAOYSA-N
HOC+	1S/CHO/c1-2/h2H/q+1	FIRPXVMETWVPCB-UHFFFAOYSA-N
HOCN	1S/CHNO/c2-1-3/h3H	XLJMAIOERFSOGZ-UHFFFAOYSA-N
HOCS+	1S/COS/c2-1-3/p+1	JJWKPURADFRFRB-UHFFFAOYSA-O
HONC	1S/CHNO/c1-2-3/h3H	OTXBWGUYZNKPMG-UHFFFAOYSA-N
HPO	1S/HOP/c1-2/h2H	AUONHKJOIZSQGR-UHFFFAOYSA-N
HS2	1S/HS2/c1-2/h1H	PYPQFOINVKFSJD-UHFFFAOYSA-N
HSC	1S/CHS/c1-2/h2H	BJTXGIFVDOPDDI-UHFFFAOYSA-N
HSCN	1S/CHNS/c2-1-3/h3H	ZMZDMBWJUHKJPS-UHFFFAOYSA-N
HSCO+	1S/COS/c2-1-3/p+1	JJWKPURADFRFRB-UHFFFAOYSA-O
HSiCN	1S/CHNSi/c2-1-3/h3H	FFABTTOEXXTIQH-UHFFFAOYSA-N
HSiNC	1S/CHNSi/c1-2-3/h3H	GMUJPAYAWSUYJU-UHFFFAOYSA-N
HSiO	1S/HOSi/c1-2/h2H	WILDNFAEIHTQPM-UHFFFAOYSA-N
HSiS	1S/HSSi/c1-2/h1H	WTGIOQMHIHCSPZ-UHFFFAOYSA-N
HSO	1S/HOS/c1-2/h2H	CKIBMZIMKMUBPA-UHFFFAOYSA-N
i-C3H7CN	1S/C4H7N/c1-4(2)3-5/h4H,1-2H3	LRDFRRGEGBBSRN-UHFFFAOYSA-N
K-41-Cl	1S/ClH.K/h1H;/q;+1/p-1/i;1+2	WCUXLLCKKVVCTQ-NLQOEHMXSA-M
K-41-OH	1S/K.H2O/h;1H2/q+1;/p-1/i1+2;	KWYUFKZDYYNOTN-DEQYMQKBSA-M
KC	1S/C.K	CIAXFBVXQWOYPA-UHFFFAOYSA-N
KCCH	1S/C2H.K/c1-2;/h1H;	XNFJTMFUDFBRKP-UHFFFAOYSA-N
KCH	1S/CH.K/h1H;	NQQQKRVLTKUEHH-UHFFFAOYSA-N
KCl-35	1S/ClH.K/h1H;/q;+1/p-1	WCUXLLCKKVVCTQ-UHFFFAOYSA-M
KCl-37	1S/ClH.K/h1H;/q;+1/p-1/i1+2;	WCUXLLCKKVVCTQ-DEQYMQKBSA-M
KCN, KNC	1S/CN.K/c1-2;	YUZRZFQHUCKACF-UHFFFAOYSA-N
KF	1S/FH.K/h1H;/q;+1/p-1	NROKBHXJSPEDAR-UHFFFAOYSA-M
KH	1S/K.H	NTTOTNSKUYCDAV-UHFFFAOYSA-N
KOH	1S/K.H2O/h;1H2/q+1;/p-1	KWYUFKZDYYNOTN-UHFFFAOYSA-M
l-C-13-C2H2	1S/C3H2/c1-3-2/h1H2/i2+1	LPUFMQSFYARLPQ-VQEHIDDOSA-N
l-C-13-C3H2	1S/C4H2/c1-3-4-2/h1H2/i2+1	MRJFCQHWODZEPM-VQEHIDDOSA-N
l-C2C-13-CH2	1S/C4H2/c1-3-4-2/h1H2/i3+1	MRJFCQHWODZEPM-LBPDFUHNSA-N

l-C2C-13-H2	1S/C3H2/c1-3-2/h1H2/i1+1	LPUFMQSFYARLPQ-OUBTZVSYSA-N
l-C3C-13-H2	1S/C4H2/c1-3-4-2/h1H2/i1+1	MRJFCQHWODZEPM-OUBTZVSYSA-N
l-C3H2	1S/C3H2/c1-3-2/h1H2	LPUFMQSFYARLPQ-UHFFFAOYSA-N
l-C3HD	1S/C3H2/c1-3-2/h1H2/i1D	LPUFMQSFYARLPQ-MICDWDOJSA-N
l-C4H2	1S/C4H2/c1-3-4-2/h1H2	MRJFCQHWODZEPM-UHFFFAOYSA-N
l-C4HD	1S/C4H2/c1-3-4-2/h1H2/i1D	MRJFCQHWODZEPM-MICDWDOJSA-N
l-C5H2	1S/C5H2/c1-3-5-4-2/h1H2	RKOOMBNWEBDZSV-UHFFFAOYSA-N
l-C6H2	1S/C6H2/c1-3-5-6-4-2/h1H2	GVNATLAZZSCGHN-UHFFFAOYSA-N
l-C7H2	1S/C7H2/c1-3-5-7-6-4-2/h1H2	CAURLQMRZVHOKK-UHFFFAOYSA-N
l-CC-13-C2H2	1S/C4H2/c1-3-4-2/h1H2/i4+1	MRJFCQHWODZEPM-AZXPZELESA-N
l-CC-13-CH2	1S/C3H2/c1-3-2/h1H2/i3+1	LPUFMQSFYARLPQ-LBPDFUHNSA-N
l-H2C3O	1S/C3H2O/c1-2-3-4/h1H2	TURAMGVWNUTQKH-UHFFFAOYSA-N
l-HC4N	1S/C4HN/c1-2-3-4-5/h1H	ODQBXVVTGHKNBU-UHFFFAOYSA-N
l-HC6N	1S/C6HN/c1-2-3-4-5-6-7/h1H	ALKJBUGWBIRQRO-UHFFFAOYSA-N
LiCCH	1/C2H.Li/c1-2;/h1H;/rC2HLi/c1-2-3/h1H	AGUDKYVAXRDJLV-AQMOIWIONA-N
LiOH	1/Li.H2O/h;1H2/q+1;/p-1/rHLiO/c1-2/h2H	WMFOQBRAJBCJND-OFPRHQIINA-M
l-SiCCC	1S/C3Si/c1-2-3-4	LTOFVVKLWCONTO-UHFFFAOYSA-N
MgCCH	1S/C2H.Mg/c1-2;/h1H;	BJYBJVMTVQAASG-UHFFFAOYSA-N
MgCl	1S/ClH.Mg/h1H;/q;+1/p-1	FOSCDBCOYQJHPN-UHFFFAOYSA-M
MgF	1S/FH.Mg/h1H;/q;+1/p-1	WSXHQDSJUJYQDO-UHFFFAOYSA-M
MgH	1S/Mg.H	RZCHRULKKYOSQS-UHFFFAOYSA-N
MgNC	1S/CN.Mg/c1-2;/q-1;+1	SPFFMFQAAOAXRY-UHFFFAOYSA-N
MgNC	1S/CN.Mg/c1-2;/q-1;+1	SPFFMFQAAOAXRY-UHFFFAOYSA-N
MgOH	1S/Mg.H2O/h;1H2/q+1;/p-1	UNYOJUYSNFGNDV-UHFFFAOYSA-M
N-15-H2D	1S/H3N/h1H3/i1+1/hD	QGZKDVFQNNGYKY-XKYOGGAFSA-N
N-15-H3	1S/H3N/h1H3/i1+1	QGZKDVFQNNGYKY-OUBTZVSYSA-N
N-15-HD2	1S/H3N/h1H3/i1+1/hD2	QGZKDVFQNNGYKY-OCMDEUDMSA-N
N-15-ND+	1S/N2/c1-2/p+1/i1+1/hD	IJGRMHOSHXDMSA-XKYOGGAFSA-O
N-15-NH+	1S/N2/c1-2/p+1/i1+1	IJGRMHOSHXDMSA-OUBTZVSYSA-O
N-15-O-17	1S/NO/c1-2/i1+1,2+1	MWUXSHHQAYIFBG-ZDOIIHCHSA-N
N-15-O	1S/NO/c1-2/i1+1	MWUXSHHQAYIFBG-OUBTZVSYSA-N
N-15-S	1S/NS/c1-2/i1+1	QXTCFDCJXWLNAP-OUBTZVSYSA-N
N-15-S-34	1S/NS/c1-2/i1+1,2+2	QXTCFDCJXWLNAP-RGIGPVFXSA-N
N2H+	1S/N2/c1-2/p+1	IJGRMHOSHXDMSA-UHFFFAOYSA-O
N2H+	1S/N2/c1-2/p+1	IJGRMHOSHXDMSA-UHFFFAOYSA-O
N-36-S	1S/NS/c1-2/i2+4	QXTCFDCJXWLNAP-XKBLRHCCSA-N
NaC-13-N, NaNC-13	1S/CN.Na/c1-2;/i1+1;	RTVFYQXEHKQMKO-YTBWXGASSA-N
NaC	1S/C.Na	GWBWGPRZOYDADH-UHFFFAOYSA-N
NaCCH	1S/C2H.Na/c1-2;/h1H;	SLBNQJAGYKQCKI-UHFFFAOYSA-N
NaCH	1S/CH.Na/h1H;	XXZMUPQTBRAJCE-UHFFFAOYSA-N
NaCl	1S/ClH.Na/h1H;/q;+1/p-1	FAPWRFPIFSIZLT-UHFFFAOYSA-M
NaCl-37	1S/ClH.Na/h1H;/q;+1/p-1/i1+2;	FAPWRFPIFSIZLT-DEQYMQKBSA-M
NaCN, NaNC	1S/CN.Na/c1-2;	RTVFYQXEHKQMKO-UHFFFAOYSA-N
NaF	1S/FH.Na/h1H;/q;+1/p-1	PUZPDOWCWNUUKD-UHFFFAOYSA-M
NaH	1S/Na.H	MPMYQQHEHYDOCL-UHFFFAOYSA-N
NaOH	1S/Na.H2O/h;1H2/q+1;/p-1	HEMHJVSKTPXQMS-UHFFFAOYSA-M
NC2P	1S/C2NP/c3-1-2-4	ZDTBSGXXDJXYMT-UHFFFAOYSA-N
NC3NC	1S/C4N2/c1-6-4-2-3-5	TVONEOQDFYTJQQ-UHFFFAOYSA-N
NCC(O)NH2	1S/C2H2N2O/c3-1-2(4)5/h(H2,4,5)	YDVJBLJCSLVMSY-UHFFFAOYSA-N
NCHCCO	1S/C3HNO/c4-2-1-3-5/h1H	JVTCKUMKUIZLIA-UHFFFAOYSA-N
NCO-	1S/CHNO/c2-1-3/h3H/p-1	XLJMAIOERFSOGZ-UHFFFAOYSA-M
NCO	1S/CNO/c2-1-3	HKKDKUMUWRTAIA-UHFFFAOYSA-N
NCS	1S/CNS/c2-1-3	NYAZXHASVIWIRJ-UHFFFAOYSA-N
ND	1S/HN/h1H/i1D	PDCKRJPYJMCOFO-MICDWDOJSA-N
ND3	1S/H3N/h1H3/i/hD3	QGZKDVFQNNGYKY-ZRLBSURWSA-N
Ne-22-H+	1S/HNe/h1H/q+1/i1+2	QJGKDYDFCAGVLL-NJFSPNSNSA-N
NeD+	1S/HNe/h1H/q+1/i1D	QJGKDYDFCAGVLL-MICDWDOJSA-N
NeH+	1S/HNe/h1H/q+1	QJGKDYDFCAGVLL-UHFFFAOYSA-N
NH	1S/HN/h1H	PDCKRJPYJMCOFO-UHFFFAOYSA-N
NH2	1S/H2N/h1H2	MDFFNEOEWAXZRQ-UHFFFAOYSA-N
NH2D	1S/H3N/h1H3/i/hD	QGZKDVFQNNGYKY-DYCDLGHISA-N
NH2OH	1S/H3NO/c1-2/h2H,1H2	AVXURJPOCDRRFD-UHFFFAOYSA-N
NH3D+	1S/H3N/h1H3/p+1/i/hD	QGZKDVFQNNGYKY-DYCDLGHISA-O
NHD2	1S/H3N/h1H3/i/hD2	QGZKDVFQNNGYKY-ZSJDYOACSA-N
Ni-58-C	1S/C.Ni/i;1-1	VMWYVTOHEQQZHQ-HCMAANCNSA-N

Ni-58-O	1S/Ni.O/i1-1;	GNRSAWUEBMWBQH-ULWFUOSBSA-N
NiCO	1S/CO.Ni/c1-2;/i;1-1	ZVHVRQOGCXCNDC-HCMAANCNSA-N
NN-15-D+	1S/N2/c1-2/p+1/i1+1/hD	IJGRMHOSHXDMSA-XKYOGGAFSA-O
NN-15-H+	1S/N2/c1-2/p+1/i1+1	IJGRMHOSHXDMSA-OUBTZVSYSA-O
NO-17	1S/NO/c1-2/i2+1	MWUXSHHQAYIFBG-VQEHIDDOSA-N
NO-18	1S/NO/c1-2/i2+2	MWUXSHHQAYIFBG-HQMMCQRPSA-N
NO	1S/NO/c1-2	MWUXSHHQAYIFBG-UHFFFAOYSA-N
NO	1S/NO/c1-2	MWUXSHHQAYIFBG-UHFFFAOYSA-N
NO+	1S/NO/c1-2/q+1	KEJOCWOXCDWNID-UHFFFAOYSA-N
NS	1S/NS/c1-2	QXTCFDCJXWLNAP-UHFFFAOYSA-N
NS	1S/NS/c1-2	QXTCFDCJXWLNAP-UHFFFAOYSA-N
NS	1S/NS/c1-2	QXTCFDCJXWLNAP-UHFFFAOYSA-N
NS-33	1S/NS/c1-2/i2+1	QXTCFDCJXWLNAP-VQEHIDDOSA-N
NS-34	1S/NS/c1-2/i2+2	QXTCFDCJXWLNAP-HQMMCQRPSA-N
O-17-CS	1S/COS/c2-1-3/i2+1	JJWKPURADFRFRB-VQEHIDDOSA-N
(O-18)2	1S/O2/c1-2/i1+2,2+2	MYMOFIZGZYHOMD-XPULMUKRSA-N
O-18-C-13-S	1S/COS/c2-1-3/i1+1,2+2	JJWKPURADFRFRB-RGIGPVFXSA-N
O-18-CS	1S/COS/c2-1-3/i2+2	JJWKPURADFRFRB-HQMMCQRPSA-N
O-18-CS-34	1S/COS/c2-1-3/i2+2,3+2	JJWKPURADFRFRB-FTOQCNSHSA-N
O-18-H-	1S/H2O/h1H2/p-1/i1+2	XLYOFNOQVPJJNP-NJFSPNSNSA-M
O-18-H+	1S/HO/h1H/q+1/i1+2	MSCUNRCIQGLERU-NJFSPNSNSA-N
O2	1S/O2/c1-2	MYMOFIZGZYHOMD-UHFFFAOYSA-N
O2	1S/O2/c1-2	MYMOFIZGZYHOMD-UHFFFAOYSA-N
OC-13-S	1S/COS/c2-1-3/i1+1	JJWKPURADFRFRB-OUBTZVSYSA-N
OC-13-S-33	1S/COS/c2-1-3/i1+1,3+1	JJWKPURADFRFRB-ZKDXJZICSA-N
OC-13-S-34	1S/COS/c2-1-3/i1+1,3+2	JJWKPURADFRFRB-VVLWLDGLSA-N
OC3S	1S/C3OS/c4-2-1-3-5	RHUZNLULDNYSIW-UHFFFAOYSA-N
OCS	1S/COS/c2-1-3	JJWKPURADFRFRB-UHFFFAOYSA-N
OCS	1S/COS/c2-1-3	JJWKPURADFRFRB-UHFFFAOYSA-N
OCS-33	1S/COS/c2-1-3/i3+1	JJWKPURADFRFRB-LBPDFUHNSA-N
OCS-34	1S/COS/c2-1-3/i3+2	JJWKPURADFRFRB-YZRHJBSPSA-N
OCS-36	1S/COS/c2-1-3/i3+4	JJWKPURADFRFRB-UDGUOMFESA-N
o-c-SiCCC	1S/C3Si/c1-3-2-4(1)3	DPHAGGUAZDWEDA-UHFFFAOYSA-N
OD-	1S/H2O/h1H2/p-1/i/hD	XLYOFNOQVPJJNP-DYCDLGHISA-M
OD+	1S/HO/h1H/q+1/i1D	MSCUNRCIQGLERU-MICDWDOJSA-N
OH-	1S/H2O/h1H2/p-1	XLYOFNOQVPJJNP-UHFFFAOYSA-M
OH+	1S/HO/h1H/q+1	MSCUNRCIQGLERU-UHFFFAOYSA-N
ONCN	1S/CN2O/c2-1-3-4	CAMRHYBKQTWSCM-UHFFFAOYSA-N
OO-18	1S/O2/c1-2/i1+2	MYMOFIZGZYHOMD-NJFSPNSNSA-N
OSiS	1S/OSSi/c1-3-2	AQOINVOFBYVPKZ-UHFFFAOYSA-N
p-c-SiCCC	1S/C3Si/c1-2-3(1)4-2	HDUIMCUTPCUDIB-UHFFFAOYSA-N
PH	1S/HP/h1H	BHEPBYXIRTUNPN-UHFFFAOYSA-N
PH2	1S/H2P/h1H2	FVZVCSNXTFCBQU-UHFFFAOYSA-N
PH3	1S/H3P/h1H3	XYFCBTPGUUZFHI-UHFFFAOYSA-N
PN-15	1S/NP/c1-2/i1+1	AOPJVJYWEDDOBI-OUBTZVSYSA-N
PN	1S/NP/c1-2	AOPJVJYWEDDOBI-UHFFFAOYSA-N
PNO	1S/NOP/c2-1-3	XISXEABRPCPPBM-UHFFFAOYSA-N
PO	1S/OP/c1-2	LFGREXWGYUGZLY-UHFFFAOYSA-N
S2O	1S/OS2/c1-3-2	TXKMVPPZCYKFAC-UHFFFAOYSA-N
S-33-O	1S/OS/c1-2/i2+1	XTQHKBHJIVJGKJ-VQEHIDDOSA-N
S-33-O2	1S/O2S/c1-3-2/i3+1	RAHZWNYVWXNFOC-LBPDFUHNSA-N
S-34-O	1S/OS/c1-2/i2+2	XTQHKBHJIVJGKJ-HQMMCQRPSA-N
S-34-O2	1S/O2S/c1-3-2/i3+2	RAHZWNYVWXNFOC-YZRHJBSPSA-N
S-36-O	1S/OS/c1-2/i2+4	XTQHKBHJIVJGKJ-XKBLRHCCSA-N
s-C2H5CHO	1S/C3H6O/c1-2-3-4/h3H,2H2,1H3	NBBJYMSMWIIQGU-UHFFFAOYSA-N
ScCl	1S/ClH.Sc/h1H;/q;+1/p-1	TXKISLDZNJFQBN-UHFFFAOYSA-M
ScCl-37	1S/ClH.Sc/h1H;/q;+1/p-1/i1+2;	TXKISLDZNJFQBN-DEQYMQKBSA-M
ScF	1S/FH.Sc/h1H;/q;+1/p-1	IASCHBSZTVAFET-UHFFFAOYSA-M
s-cis-H2CCHCOOH	1S/C3H4O2/c1-2-3(4)5/h2H,1H2,(H,4,5)	NIXOWILDQLNWCW-UHFFFAOYSA-N
ScS	1S/S.Sc	SWQYMBDZKRJOCX-UHFFFAOYSA-N
SH-	1S/H2S/h1H2/p-1	RWSOTUBLDIXVET-UHFFFAOYSA-M
SH	1S/HS/h1H	PXQLVRUNWNTZOS-UHFFFAOYSA-N
SH	1S/HS/h1H	PXQLVRUNWNTZOS-UHFFFAOYSA-N
s-H2CCHOH	1S/C2H4O/c1-2-3/h2-3H,1H2	IMROMDMJAWUWLK-UHFFFAOYSA-N
Si-29-C4	1S/C4Si/c1-2-3-4-5/i5+1	GPTYCJIDZIAMDI-HOSYLAQJSA-N

Si-29-CC	1S/C2Si/c1-2-3/i3+1	BMBSCNAKKVJFQF-LBPDFUHNSA-N
Si-29-H3CN	1S/CH3NSi/c2-1-3/h3H3/i3+1	LCHWKMAWSZDQRD-LBPDFUHNSA-N
Si-29-O-17	1S/OSi/c1-2/i1+1,2+1	LIVNPJMFVYWSIS-ZDOIIHCHSA-N
Si-29-O-18	1S/OSi/c1-2/i1+2,2+1	LIVNPJMFVYWSIS-WWQQEUHZSA-N
Si-29-O	1S/OSi/c1-2/i2+1	LIVNPJMFVYWSIS-VQEHIDDOSA-N
Si-29-S	1S/SSi/c1-2/i2+1	DWFFKGPZNGKUPH-VQEHIDDOSA-N
Si-29-S	1S/SSi/c1-2/i2+1	DWFFKGPZNGKUPH-VQEHIDDOSA-N
Si-29-S-33	1S/SSi/c1-2/i1+1,2+1	DWFFKGPZNGKUPH-ZDOIIHCHSA-N
Si-29-S-34	1S/SSi/c1-2/i1+2,2+1	DWFFKGPZNGKUPH-WWQQEUHZSA-N
Si-29-S-36	1S/SSi/c1-2/i1+4,2+1	DWFFKGPZNGKUPH-DYHRWIPISA-N
Si2H2	1S/H2Si2/c1-3-2/h1H	KMJYJNWJAVVEFQ-UHFFFAOYSA-N
Si2H2	1S/H2Si2/c1-3-4-2	CFIGCZGLYCTLBI-UHFFFAOYSA-N
Si-30-C4	1S/C4Si/c1-2-3-4-5/i5+2	GPTYCJIDZIAMDI-RHRFEJLCSA-N
Si-30-CC	1S/C2Si/c1-2-3/i3+2	BMBSCNAKKVJFQF-YZRHJBSPSA-N
Si-30-H3CN	1S/CH3NSi/c2-1-3/h3H3/i3+2	LCHWKMAWSZDQRD-YZRHJBSPSA-N
Si-30-O-17	1S/OSi/c1-2/i1+1,2+2	LIVNPJMFVYWSIS-RGIGPVFXSA-N
Si-30-O	1S/OSi/c1-2/i2+2	LIVNPJMFVYWSIS-HQMMCQRPSA-N
Si-30-S	1S/SSi/c1-2/i2+2	DWFFKGPZNGKUPH-HQMMCQRPSA-N
Si-30-S	1S/SSi/c1-2/i2+2	DWFFKGPZNGKUPH-HQMMCQRPSA-N
Si-30-S-33	1S/SSi/c1-2/i1+1,2+2	DWFFKGPZNGKUPH-RGIGPVFXSA-N
Si-30-S-34	1S/SSi/c1-2/i1+2,2+2	DWFFKGPZNGKUPH-XPULMUKRSA-N
Si-30-S-36	1S/SSi/c1-2/i1+4,2+2	DWFFKGPZNGKUPH-OIYXHDJBSA-N
SiC-13-C	1S/C2Si/c1-2-3/i2+1	BMBSCNAKKVJFQF-VQEHIDDOSA-N
SiC-13-C3	1S/C4Si/c1-2-3-4-5/i1+1	GPTYCJIDZIAMDI-OUBTZVSYSA-N
SiC	1S/CSi/c1-2	HBMJWWWQQXIZIP-UHFFFAOYSA-N
SiC2C-13-C	1S/C4Si/c1-2-3-4-5/i3+1	GPTYCJIDZIAMDI-LBPDFUHNSA-N
SiC2N	1S/C2NSi/c3-1-2-4	CUSPLGSOPAWJJL-UHFFFAOYSA-N
SiC3C-13	1S/C4Si/c1-2-3-4-5/i4+1	GPTYCJIDZIAMDI-AZXPZELESA-N
SiC3H	1S/C3HSi/c1-2-3-4/h1H	DIVDZESDUHQUNI-UHFFFAOYSA-N
SiC4	1S/C4Si/c1-2-3-4-5	GPTYCJIDZIAMDI-UHFFFAOYSA-N
SiC5	1S/C5Si/c1-2-3-4-5-6	DLOOFNODOVOVLW-UHFFFAOYSA-N
SiC6	1S/C6Si/c1-2-3-4-5-6-7	YAZTXTUOWISWIF-UHFFFAOYSA-N
SiCC-13-C2	1S/C4Si/c1-2-3-4-5/i2+1	GPTYCJIDZIAMDI-VQEHIDDOSA-N
SiCC	1S/C2Si/c1-2-3	BMBSCNAKKVJFQF-UHFFFAOYSA-N
SiCC	1S/C2Si/c1-2-3	BMBSCNAKKVJFQF-UHFFFAOYSA-N
SiCC	1S/C2Si/c1-2-3	BMBSCNAKKVJFQF-UHFFFAOYSA-N
SiCCH	1S/C2HSi/c1-2-3/h1H	KUFWTXSQQKDMAI-UHFFFAOYSA-N
SiCN	1S/CNSi/c2-1-3	HNQXCHVZYRDHJN-UHFFFAOYSA-N
SiH	1S/HSi/h1H	QHGSGZLLHBKSAH-UHFFFAOYSA-N
SiH3C-13-N	1S/CH3NSi/c2-1-3/h3H3/i1+1	LCHWKMAWSZDQRD-OUBTZVSYSA-N
SiH3CCH	1S/C2H4Si/c1-2-3/h1H,3H3	SRNLFSKWPCUYHC-UHFFFAOYSA-N
SiH3CN	1S/CH3NSi/c2-1-3/h3H3	LCHWKMAWSZDQRD-UHFFFAOYSA-N
SiN	1S/NSi/c1-2	NCLWWTWAYQTPBU-UHFFFAOYSA-N
SiNC	1S/CNSi/c1-2-3	GCFWXKMKTHYVTQ-UHFFFAOYSA-N
SiO-17	1S/OSi/c1-2/i1+1	LIVNPJMFVYWSIS-OUBTZVSYSA-N
SiO-18	1S/OSi/c1-2/i1+2	LIVNPJMFVYWSIS-NJFSPNSNSA-N
SiO	1S/OSi/c1-2	LIVNPJMFVYWSIS-UHFFFAOYSA-N
SiS	1S/SSi/c1-2	DWFFKGPZNGKUPH-UHFFFAOYSA-N
SiS	1S/SSi/c1-2	DWFFKGPZNGKUPH-UHFFFAOYSA-N
SiS	1S/SSi/c1-2	DWFFKGPZNGKUPH-UHFFFAOYSA-N
SiS-33	1S/SSi/c1-2/i1+1	DWFFKGPZNGKUPH-OUBTZVSYSA-N
SiS-34	1S/SSi/c1-2/i1+2	DWFFKGPZNGKUPH-NJFSPNSNSA-N
SiS-34	1S/SSi/c1-2/i1+2	DWFFKGPZNGKUPH-NJFSPNSNSA-N
SiS-36	1S/SSi/c1-2/i1+4	DWFFKGPZNGKUPH-RNFDNDRNSA-N
SO-16-O-18	1S/O2S/c1-3-2/i1+2	RAHZWNYVWXNFOC-NJFSPNSNSA-N
SO-17	1S/OS/c1-2/i1+1	XTQHKBHJIVJGKJ-OUBTZVSYSA-N
SO-18	1S/OS/c1-2/i1+2	XTQHKBHJIVJGKJ-NJFSPNSNSA-N
SO	1S/OS/c1-2	XTQHKBHJIVJGKJ-UHFFFAOYSA-N
SO	1S/OS/c1-2	XTQHKBHJIVJGKJ-UHFFFAOYSA-N
SO	1S/OS/c1-2	XTQHKBHJIVJGKJ-UHFFFAOYSA-N
SO2	1S/O2S/c1-3-2	RAHZWNYVWXNFOC-UHFFFAOYSA-N
SO2	1S/O2S/c1-3-2	RAHZWNYVWXNFOC-UHFFFAOYSA-N
SO2	1S/O2S/c1-3-2	RAHZWNYVWXNFOC-UHFFFAOYSA-N
SOO-17	1S/O2S/c1-3-2/i1+1	RAHZWNYVWXNFOC-OUBTZVSYSA-N
s-trans-H2CCHCOOH	1S/C3H4O2/c1-2-3(4)5/h2H,1H2,(H,4,5)	NIXOWILDQLNWCW-UHFFFAOYSA-N

t-HC-13-OOH	1S/CH2O2/c1-3-2/h1-2H/i1+1	RXIZGRWAJVLEHT-OUBTZVSYSA-N
t-HC3O	1S/C3HO/c1-2-3-4/h1H	NONQAKWUTFTDMS-UHFFFAOYSA-N
t-HCOOH	1S/CH2O2/c1-3-2/h1-2H	RXIZGRWAJVLEHT-UHFFFAOYSA-N
t-HC(O)SH	1S/CH2OS/c2-1-3/h1H,(H,2,3)	AWIJRPNMLHPLNC-UHFFFAOYSA-N
Ti-46-O2	1S/2O.Ti/i;;1-2	GWEVSGVZZGPLCZ-HPBINRSPSA-N
Ti-46-S	1S/S.Ti/i;1-2	RCYJPSGNXVLIBO-ZQSXMSGHSA-N
Ti-48-N	1S/N.Ti	NRTOMJZYCJJWKI-UHFFFAOYSA-N
Ti-48-O	1S/O.Ti	OGIDPMRJRNCKJF-UHFFFAOYSA-N
Ti-48-S	1S/S.Ti	RCYJPSGNXVLIBO-UHFFFAOYSA-N
Ti-50-O2	1S/2O.Ti/i;;1+2	GWEVSGVZZGPLCZ-NGAFWABFSA-N
Ti-50-S	1S/S.Ti/i;1+2	RCYJPSGNXVLIBO-NLQOEHMXSA-N
TiO2	1S/2O.Ti	GWEVSGVZZGPLCZ-UHFFFAOYSA-N
trans-HC(O)NHD	1S/CH3NO/c2-1-3/h1H,(H2,2,3)/i/hD	ZHNUHDYFZUAESO-DYCDLGHISA-N
YO	1S/O.Y	APUGIHICMSAKGR-UHFFFAOYSA-N
YS	1S/S.Y	NVLRWXFPPTWZMX-UHFFFAOYSA-N
(Z)-HC2CHCHCN	1S/C5H3N/c1-2-3-4-5-6/h1,3-4H	ZXFTWPNQZKQCAL-UHFFFAOYSA-N
Z-HNCHCN	1S/C2H2N2/c3-1-2-4/h1,3H	LAVVSPWGGHZKLI-UHFFFAOYSA-N
Zn-64-H	1S/Zn.H/i1-1;	FLVYKYVLYPYTAY-ULWFUOSBSA-N
Zn-66-H	1S/Zn.H/i1+1;	FLVYKYVLYPYTAY-YTBWXGASSA-N
Zn-68-H	1S/Zn.H/i1+3;	FLVYKYVLYPYTAY-YBECMJGWSA-N