


# 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 $K$, $\Lambda$ 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 |

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|---|---|---|
| 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 |

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|---|---|---|
| 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 |

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|---|---|---|
| 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 |

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| 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 |

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|---|---|---|
| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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| 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 |

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|---|---|---|
| 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 |