SMILES: [13C-]#[O+]

Molecular Formula of Main Isotopologue: CO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 18.315 ± 2.417

## **Molecule 2**

SMILES: [13CH3]0

Molecular Formula of Main Isotopologue: CH4O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.911 ± 2.311

# **Molecule 3**

SMILES: [H]OC([H])([H])OC([H])([H])[2H]

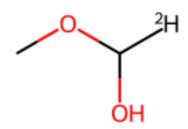
Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.578 ± 2.400

SMILES: [H]OC([H])([2H])OC([H])([H])[H]

Molecular Formula of Main Isotopologue:  $C_2H_6O_2$ 

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.542 ± 2.786

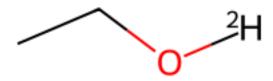


# **Molecule 5**

SMILES: [H]C([H])([H])C([H])([H])O[2H]

Molecular Formula of Main Isotopologue:  $C_2H_6O$ 

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.333 ± 2.251

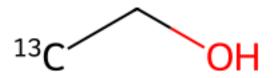


# **Molecule 6**

SMILES: [13CH3]CO

Molecular Formula of Main Isotopologue: C2H6O

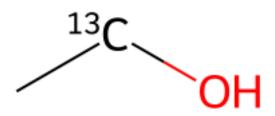
Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.124 ± 2.471



SMILES: C[13CH2]O

Molecular Formula of Main Isotopologue: C2H6O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.072 ± 2.390



# **Molecule 8**

SMILES: [H]C([H])([H])OC([H])([H])O[2H]

Molecular Formula of Main Isotopologue:  $C_2H_6O_2$ 

Predicted Column Density ( $log_{10} cm^{-2}$ ): 16.045 ± 2.665



# **Molecule 9**

SMILES: [2H]C#N

Molecular Formula of Main Isotopologue: CHN

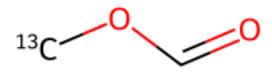
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.904 ± 2.160



SMILES: [13CH3]OC=0

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.833 ± 2.374

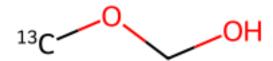


### **Molecule 11**

SMILES: [13CH3]OCO

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.784 ± 2.779



# **Molecule 12**

SMILES: CO[13CH2]O

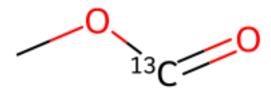
Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.732 ± 3.212

SMILES: CO[13CH]=0

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.714 ± 2.247

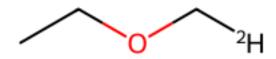


## **Molecule 14**

SMILES: [H]C([H])([2H])OC([H])([H])C([H])([H])[H]

Molecular Formula of Main Isotopologue: C₃H<sub>8</sub>O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.600 ± 2.218

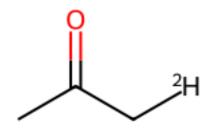


# **Molecule 15**

SMILES: [H]C([H])([H])C(=O)C([H])([H])[2H]

Molecular Formula of Main Isotopologue:  $C_3H_6O$ 

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.380 ± 2.578



SMILES: [H]SC([H])([H])[2H]

Molecular Formula of Main Isotopologue: CH<sub>4</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.262 ± 2.258



## **Molecule 17**

SMILES: [H]C([H])=C([H])C([H])([H])[2H]

Molecular Formula of Main Isotopologue: C₃H<sub>6</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.209 ± 2.307

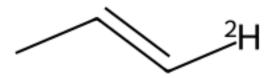


# **Molecule 18**

SMILES: [H]C([2H])=C([H])C([H])([H])[H]

Molecular Formula of Main Isotopologue:  $C_3H_6$ 

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.209 ± 2.307



SMILES: [H]C([H])([H])OC([H])([H])C([H])([H])[2H]

Molecular Formula of Main Isotopologue: C₃H8O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.129 ± 2.315

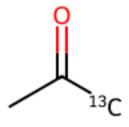


### **Molecule 20**

SMILES: CC([13CH3])=O

Molecular Formula of Main Isotopologue: C₃H6O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.110 ± 2.973

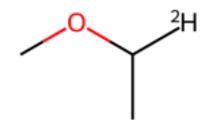


# **Molecule 21**

SMILES: [H]C([H])([H])OC([H])([2H])C([H])([H])[H]

Molecular Formula of Main Isotopologue: C₃H8O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.093 ± 2.354



SMILES: [13CH]#N

Molecular Formula of Main Isotopologue: CHN

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.073 ± 2.561

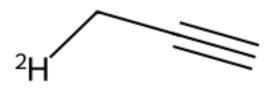


## **Molecule 23**

SMILES: [H]C#CC([H])([H])[2H]

Molecular Formula of Main Isotopologue:  $C_3H_4$ 

Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.001 ± 6.286

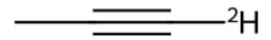


# **Molecule 24**

SMILES: [H]C([H])([H])C#C[2H]

Molecular Formula of Main Isotopologue:  $C_3H_4$ 

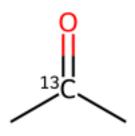
Predicted Column Density ( $log_{10} cm^{-2}$ ): 15.001 ± 6.286



SMILES: C[13C](C)=0

Molecular Formula of Main Isotopologue: C₃H6O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.991 ± 2.607

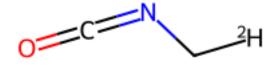


# **Molecule 26**

SMILES: [H]C([H])([2H])N=C=O

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>3</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.956 ± 2.451

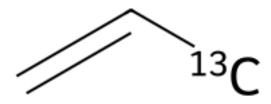


# **Molecule 27**

SMILES: C=C[13CH3]

Molecular Formula of Main Isotopologue: C₃H<sub>6</sub>

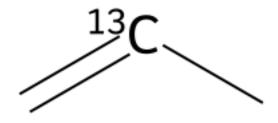
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.939 ± 2.762



SMILES: C=[13CH]C

Molecular Formula of Main Isotopologue: C₃H<sub>6</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.873 ± 2.608

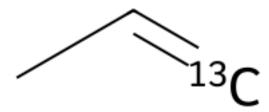


## **Molecule 29**

SMILES: CC=[13CH2]

Molecular Formula of Main Isotopologue: C₃H<sub>6</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.873 ± 2.608

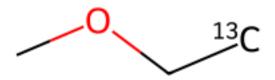


# **Molecule 30**

SMILES: COC[13CH3]

Molecular Formula of Main Isotopologue:  $C_3H_8O$ 

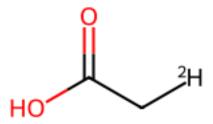
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.859 ± 2.782



SMILES: [H]OC(=O)C([H])([H])[2H]

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.821 ± 4.300

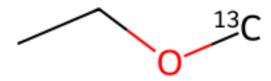


## **Molecule 32**

SMILES: CCO[13CH3]

Molecular Formula of Main Isotopologue: C₃H8O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.806 ± 2.713

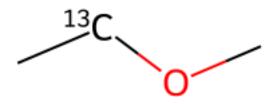


# **Molecule 33**

SMILES: C[13CH2]OC

Molecular Formula of Main Isotopologue: C₃H8O

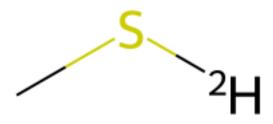
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.806 ± 2.713



SMILES: [H]C([H])([H])S[2H]

Molecular Formula of Main Isotopologue: CH<sub>4</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.804 ± 2.570

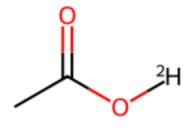


## **Molecule 35**

SMILES: [H]C([H])([H])C(=O)O[2H]

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.760 ± 4.317



# **Molecule 36**

SMILES: C#C[13CH3]

Molecular Formula of Main Isotopologue: C₃H₄

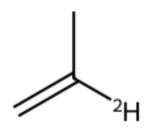
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.732 ± 6.421

<sup>13</sup>C———

SMILES: [H]C([H])=C([2H])C([H])([H])[H]

Molecular Formula of Main Isotopologue: C₃H<sub>6</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.702 ± 2.842

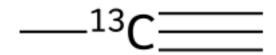


## **Molecule 38**

SMILES: C#[13C]C

Molecular Formula of Main Isotopologue: C₃H₄

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.677 ± 6.383



# **Molecule 39**

SMILES: CC#[13CH]

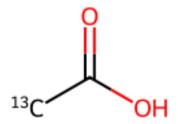
Molecular Formula of Main Isotopologue: C₃H₄

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.677 ± 6.383

SMILES: [13CH3]C(=0)0

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.551 ± 4.601

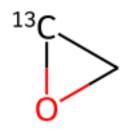


## **Molecule 41**

SMILES: C1[13CH2]01

Molecular Formula of Main Isotopologue: C2H4O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.546 ± 2.431

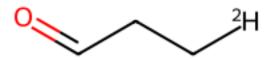


# **Molecule 42**

SMILES: [H]C(=O)C([H])([H])C([H])([H])[2H]

Molecular Formula of Main Isotopologue: C₃H6O

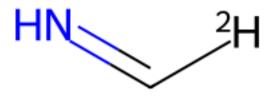
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.546 ± 3.158



SMILES: [H]N=C([H])[2H]

Molecular Formula of Main Isotopologue: CH₃N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.528 ± 3.329

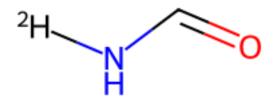


### **Molecule 44**

SMILES: [H]C(=O)N([H])[2H]

Molecular Formula of Main Isotopologue: CH₃NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.515 ± 2.280



# **Molecule 45**

SMILES: [13CH3]S

Molecular Formula of Main Isotopologue: CH<sub>4</sub>S

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.485 ± 2.845

<sup>13</sup>C----SH

SMILES: [13C-]#[S+]

Molecular Formula of Main Isotopologue: CS

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.429 ± 2.661

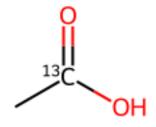


## **Molecule 47**

SMILES: C[13C](=0)0

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.380 ± 4.343

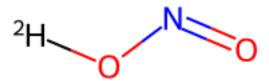


# **Molecule 48**

SMILES: [2H]ON=O

Molecular Formula of Main Isotopologue: HNO2

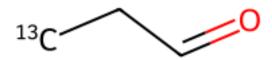
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.318 ± 3.005



SMILES: [13CH3]CC=0

Molecular Formula of Main Isotopologue: C₃H6O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.276 ± 3.469

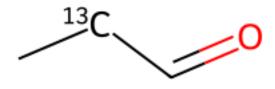


## **Molecule 50**

SMILES: C[13CH2]C=0

Molecular Formula of Main Isotopologue: C₃H6O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.276 ± 3.469

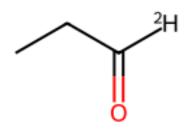


# **Molecule 51**

SMILES: [H]C([H])([H])C([H])([H])C([2H])=0

Molecular Formula of Main Isotopologue:  $C_3H_6O$ 

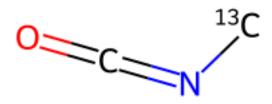
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.219 ± 3.120



SMILES: [13CH3]N=C=O

Molecular Formula of Main Isotopologue: C2H3NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.179 ± 2.971

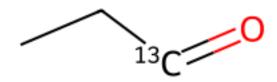


### **Molecule 53**

SMILES: CC[13CH]=0

Molecular Formula of Main Isotopologue: C₃H6O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.157 ± 3.109

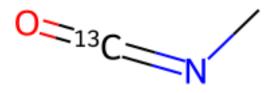


# **Molecule 54**

SMILES: CN=[13C]=0

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>3</sub>NO

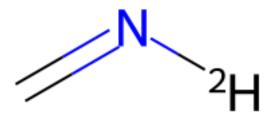
Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.072 ± 2.684



SMILES: [H]C([H])=N[2H]

Molecular Formula of Main Isotopologue: CH<sub>3</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.070 ± 3.448

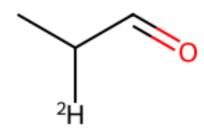


### **Molecule 56**

SMILES: [H]C(=O)C([H])([2H])C([H])([H])[H]

Molecular Formula of Main Isotopologue: C₃H6O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 14.039 ± 3.495

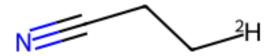


# **Molecule 57**

SMILES: [H]C([H])([2H])C([H])([H])C#N

Molecular Formula of Main Isotopologue: C₃H₅N

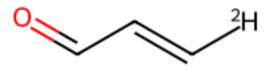
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.941 ± 2.488



SMILES: [H]C(=O)C([H])=C([H])[2H]

Molecular Formula of Main Isotopologue: C₃H₄O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.882 ± 2.395

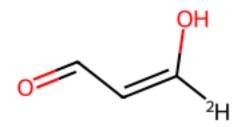


### **Molecule 59**

SMILES: [H]OC([2H])=C([H])C([H])=O

Molecular Formula of Main Isotopologue: C₃H₄O₂

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.821 ± 2.523

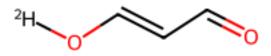


# **Molecule 60**

SMILES: [H]C(=O)C([H])=C([H])O[2H]

Molecular Formula of Main Isotopologue: C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.795 ± 2.674



SMILES: [13CH2]=N

Molecular Formula of Main Isotopologue: CH<sub>3</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.686 ± 3.661

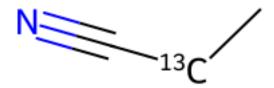


### **Molecule 62**

SMILES: C[13CH2]C#N

Molecular Formula of Main Isotopologue: C₃H₅N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.671 ± 2.882



# **Molecule 63**

SMILES: [13CH3]CC#N

Molecular Formula of Main Isotopologue: C<sub>3</sub>H<sub>5</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.671 ± 2.882



SMILES: [H]N([2H])C(=O)C([H])([H])[H]

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>5</sub>NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.669 ± 2.582

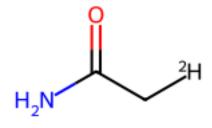


### **Molecule 65**

SMILES: [H]N([H])C(=O)C([H])([H])[2H]

Molecular Formula of Main Isotopologue: C2H5NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.620 ± 2.408

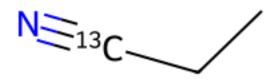


# **Molecule 66**

SMILES: CC[13C]#N

Molecular Formula of Main Isotopologue:  $C_3H_5N$ 

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.617 ± 2.819



SMILES: [2H]C#CC#N

Molecular Formula of Main Isotopologue: C₃HN

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.604 ± 5.809

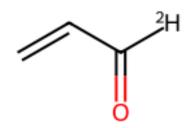


## **Molecule 68**

SMILES: [H]C([H])=C([H])C([2H])=O

Molecular Formula of Main Isotopologue: C₃H₄O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.556 ± 2.463

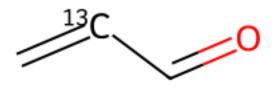


# **Molecule 69**

SMILES: C=[13CH]C=0

Molecular Formula of Main Isotopologue: C₃H₄O

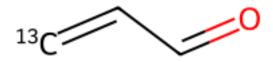
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.546 ± 2.670



SMILES: [13CH2]=CC=O

Molecular Formula of Main Isotopologue: C₃H₄O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.546 ± 2.670

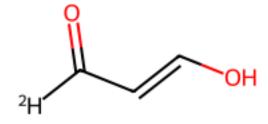


## **Molecule 71**

SMILES: [H]OC([H])=C([H])C([2H])=O

Molecular Formula of Main Isotopologue: C₃H₄O₂

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.530 ± 2.566

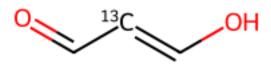


# **Molecule 72**

SMILES: O=C[13CH]=CO

Molecular Formula of Main Isotopologue: C₃H₄O₂

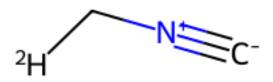
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.520 ± 2.783



SMILES: [H]C([H])([2H])[N+]#[C-]

Molecular Formula of Main Isotopologue: C2H3N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.513 ± 2.332

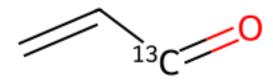


### **Molecule 74**

SMILES: C=C[13CH]=0

Molecular Formula of Main Isotopologue: C₃H₄O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.494 ± 2.397

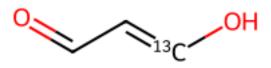


# **Molecule 75**

SMILES: O=CC=[13CH]O

Molecular Formula of Main Isotopologue: C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>

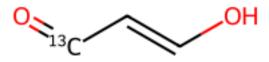
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.468 ± 2.486



SMILES: O=[13CH]C=CO

Molecular Formula of Main Isotopologue: C₃H₄O₂

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.468 ± 2.486



## **Molecule 77**

SMILES: [13CH2]=S

Molecular Formula of Main Isotopologue: CH<sub>2</sub>S

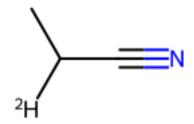
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.436 ± 2.342

# **Molecule 78**

SMILES: [H]C([H])([H])C([H])([2H])C#N

Molecular Formula of Main Isotopologue: C₃H₅N

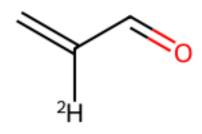
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.434 ± 2.880



SMILES: [H]C(=O)C([2H])=C([H])[H]

Molecular Formula of Main Isotopologue: C₃H₄O

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.375 ± 2.911

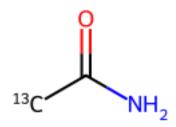


# **Molecule 80**

SMILES: [13CH3]C(N)=O

Molecular Formula of Main Isotopologue: C2H5NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.350 ± 2.843

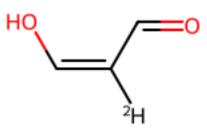


# **Molecule 81**

SMILES: [H]OC([H])=C([2H])C([H])=O

Molecular Formula of Main Isotopologue: C<sub>3</sub>H<sub>4</sub>O<sub>2</sub>

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.350 ± 2.998



SMILES: C#C[13C]#N

Molecular Formula of Main Isotopologue: C₃HN

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.279 ± 5.874

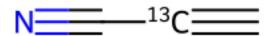


## **Molecule 83**

SMILES: C#[13C]C#N

Molecular Formula of Main Isotopologue: C₃HN

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.279 ± 5.874



# **Molecule 84**

SMILES: [13CH]#CC#N

Molecular Formula of Main Isotopologue: C₃HN

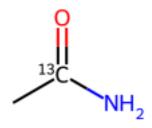
Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.279 ± 5.874



SMILES: C[13C](N)=O

Molecular Formula of Main Isotopologue: C2H5NO

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.231 ± 2.417

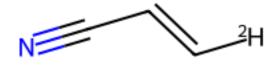


### **Molecule 86**

SMILES: [H]C([2H])=C([H])C#N

Molecular Formula of Main Isotopologue: C₃H₃N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 13.098 ± 4.765

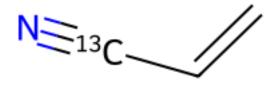


# **Molecule 87**

SMILES: C=C[13C]#N

Molecular Formula of Main Isotopologue:  $C_3H_3N$ 

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.773 ± 4.891



SMILES: [13CH2]=CC#N

Molecular Formula of Main Isotopologue: C₃H₃N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.762 ± 4.913

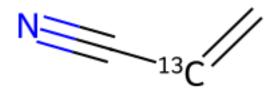


## **Molecule 89**

SMILES: C=[13CH]C#N

Molecular Formula of Main Isotopologue: C₃H₃N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.762 ± 4.913



# **Molecule 90**

SMILES: [C-]#[N+][13CH3]

Molecular Formula of Main Isotopologue: C2H3N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.737 ± 2.881

SMILES: C[N+]#[13C-]

Molecular Formula of Main Isotopologue: C<sub>2</sub>H<sub>3</sub>N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.682 ± 2.789

$$---N^{+}=^{13}C^{-}$$

# **Molecule 92**

SMILES: [H]C([H])=C([2H])C#N

Molecular Formula of Main Isotopologue: C₃H₃N

Predicted Column Density ( $log_{10} cm^{-2}$ ): 12.591 ± 5.008

