

MOLECULES INDEX

Molecules are grouped according to the number of constituent atoms. Within each group they are listed alphabetically (CH appears ahead of CN). Subscripts are used to differentiate between alphabetically identical molecules. The smallest subscript is ranked first, and precedence is given in order from the left (CH₂ appears ahead of C₂H). Molecular ions are listed immediately following the equivalent molecule (CH₂ appears ahead of CH₂⁺) and are given precedence over isotopes (CH₂⁺ appears ahead of ¹³CH₂). Isotopes are listed following the parent molecule and are given precedence in the order in which the molecule is written (¹³CH₂ appears ahead of CDH). Thus the molecules CH₂, CH₂⁺, CDH, CD₂, C₂H, C₂H⁺, C¹³CH, C₂D would appear in that order.

Molecules containing 6 atoms or less are written in their commonly-used form e.g. CH₃OH is not rearranged to be CH₄O as is the practice in some indices. However the editor, to preserve his sanity and disguise his ignorance, has wantonly destroyed the chemical identity of molecules having more than 6 atoms, except in the case of the easily recognisable cyanopolyne series which was frequently discussed at the Symposium.

Page numbers refer to the title page of the article in which the listed molecule is mentioned.

1 atom

| | |
|------------------------------|---|
| Ar | 367, 373, 389 |
| B | 373 |
| C | 165, 177, 183, 209, 239, 257, 281, 283, 325, 337, 341, 355, 373, 309, 397, 411, 423, 427, 445, 471, 479, 627 |
| C ⁺ | 67, 77, 81, 177, 263, 273, 281, 283, 291, 297, 307. 311, 317, 323, 331, 337, 341, 423, 427, 445 |
| ¹³ C | 209, 397, 423, 427, |
| ¹³ C ⁺ | 341, 423, 427 |
| Ca | 261, 341 |
| Cd | 367 |
| Cl | 247, 257, 271, 273 |
| Cl ⁺ | 271, 273 |
| Co | 367 |
| Cu | 367 |
| e | 77, 339 |
| ¹⁷ F | 427 |
| ¹⁸ F | 427 |
| Fe | 367 |

H 1, 77, 137, 159, 177, 189, 209, 213, 231, 261, 263, 271,
273, 281, 283, 289, 291, 297, 325, 337, 341, 355, 367,
397, 427, 439, 445, 479, 551, 559, 583, 611, 627, 637
 H^+ 77, 273, 283, 291, 297, 337, 427
 H^- 273
 D 273, 341, 427
 D^+ 273, 291, 427
 He 1, 221, 261, 289, 291, 317, 323, 341, 367, 373, 397, 427,
583, 589, 627
 He^* 299
 He^+ 77, 81, 331, 337, 341
 ${}^3\text{He}$ 427
 ${}^3\text{He}^+$ 427
 Li 427
 Li^+ 291
 Mg 257, 337, 471
 Mg^+ 337
 Mn 367
 N 77, 261, 273, 281, 311, 325, 331, 337, 341, 355, 373,
389, 397, 423, 427, 479
 N^+ 311, 331
 ${}^{13}\text{N}$ 427
 ${}^{15}\text{N}$ 397, 427, 479
 Na 341
 Ne 373, 389
 Ni 367
 O 77, 165, 239, 273, 281, 291, 297, 325, 331, 337, 341,
355, 373, 389, 397, 423, 427, 439, 445, 455, 479
 O^+ 273, 311
 O^- 389
 ${}^{14}\text{O}$ 427
 ${}^{15}\text{O}$ 427
 ${}^{17}\text{O}$ 397, 427
 ${}^{18}\text{O}$ 397, 427
 S 183, 257, 297, 337, 373, 397, 445
 S^+ 291, 297, 337, 427
 S^- 297
 ${}^{33}\text{S}$ 397, 427
 ${}^{34}\text{S}$ 397, 427
 ${}^{34}\text{S}^+$ 427
 Si 261, 337, 341, 397, 427, 445
 Si^+ 337
 ${}^{29}\text{Si}$ 427
 ${}^{30}\text{Si}$ 427

2 atoms

| | |
|---|--|
| A1H | 247 |
| C ₂ | 177, 231, 247, 257, 261, 263, 273, 325, 337, 367, 613 |
| C ₂ ⁺ | 291, 307 |
| CC1 ⁺ | 273 |
| CF | 239 367, 613 |
| CH | 71, 177, 231, 239, 247, 257, 261, 263, 273, 325, 337, |
| CH ⁺ | 247, 257, 261, 263, 273, 283, 291, 311, 317, 331, 445 |
| ¹³ CH | 247 |
| CD | 583 |
| CN | 59, 67, 77, 231, 247, 273, 307, 325, 331, 337, 395, 423, 479, 497, 515 |
| CN ⁺ | 247, 307, 331 |
| CO | 1, 21, 31, 33, 41, 47, 81, 83, 85, 89, 103, 111, 113, 115, 123, 125, 127, 129, 135, 137, 151, 157, 159, 163, 165, 173, 175, 177, 183, 185, 187, 189, 197, 205, 209, 213, 239, 247, 257, 261, 273, 281, 289, 297, 307, 311, 317, 323, 331, 337, 339, 341, 355, 365, 373, 381, 387, 395, 409, 411, 417, 421, 423, 427, 439, 445, 455, 465, 471, 473, 479, 487, 495, 497, 503, 509, 515, 537, 545, 551, 591, 611, 613, 619, 625, 637 |
| CO ⁺ | 247, 291, 311 |
| ¹³ CO | 1, 31, 33, 113, 115, 117, 127, 135, 137, 157, 159, 185, 187, 196, 247, 341, 397, 411, 417, 421, 423, 427, 487, ¹⁷ O 397, 417, 427 509, 515 |
| ¹⁸ O | 71, 397, 411, 417, 421, 427 |
| ¹³ C ¹⁸ O | 397, 417 |
| CS | 1, 47, 117, 157, 247, 297, 307, 337, 397, 421, 427, 479, 497, 613 |
| ¹³ CS | 397 |
| C ³³ S | 397 |
| C ³⁴ S | 397 |
| CaH | 247 |
| CaO | 389 |
| ClO | 239 |
| FeH | 367 |
| FeH ⁺ | 273 |
| H ₂ | 1, 21, 33, 41, 47, 59, 67, 71, 77, 83, 85, 89, 91, 101, 117, 127, 137, 151, 159, 163, 165, 175, 177, 185, 187, 189, 209, 221, 231, 247, 263, 271, 273, 283, 291, 297, 307, 311, 317, 323, 325, 331, 339, 341, 365, 367, 423, 427, 439, 445, 455, 465, 469, 471, 479, 495, 503, 549, 551, 565, 583, 589, 591, 611, 613 |
| H ₂ ⁺ | 231, 291 |
| HD | 231, 247, 273, 341, 427, 439, 613, 637 |
| D ₂ | 231 |
| H ⁷ ⁹ Br ⁺ | 239 |
| D ⁷ ⁹ Br ⁺ | 239 |
| HCl | 247, 257, 269, 271, 273 |
| HCl ⁺ | 271, 273 |
| HeAr ⁺ | 231 |

| | |
|---------------------------------|--|
| HeH ⁺ | 231 |
| HeNe ⁺ | 231 |
| ³ HeNe ⁺ | 231 |
| MgH | 247 |
| MgH ⁺ | 247, 273 |
| MgO | 389 |
| N ₂ | 59, 247, 323, 325, 331, 337, 341, 365, 427, 613 |
| N ₂ ⁺ | 231, 291, 311 |
| ¹⁴ N ¹⁵ N | 427 |
| NH | 239, 247, 281, 331, 337 |
| NH ⁺ | 247, 311, 331, 583 |
| NO | 239, 247, 289, 311, 337, 373 |
| NO ⁺ | 231, 311, 337 |
| NS | 261, 337 |
| NaH | 247 |
| NaH ⁺ | 273 |
| O ₂ | 77, 177, 239, 247, 291, 297, 311, 323, 325, 331, 337 |
| O ₂ ⁺ | 231, 291, 311 |
| OH | 1, 103, 111, 125, 129, 177, 189, 231, 239, 247, 257, 273, 281, 289, 337, 341, 397, 427, 445, 455, 473, 479, 487, 503, 515, 525, 537, 539, 549, 551, 559, 565, 579, 581, 583, 589, 613, 627 |
| OH ⁺ | 341 |
| OH ⁻ | 281 |
| ¹⁸ OH | 397 |
| OD | 583 |
| PH | 239 |
| S ₂ | 337 |
| SH | 247, 273, 297, 337, 445 |
| SH ⁺ | 337 |
| SO | 1, 31, 69, 71, 117, 297, 337 |
| SO ⁺ | 291, 337 |
| ³⁴ SO | 71 |
| Si ₂ | 337 |
| Si ₂ ⁺ | 337 |
| SiC | 337, 479, 497 |
| SiC ⁺ | 337 |
| SiH | 247, 337 |
| SiH ⁺ | 273, 337, |
| SiO | 31, 33, 39, 247, 337, 341, 397, 445, 479, 487, 497, 503, 515, 525, 535, 537, 539, 541, 543, 545, 551, 565, 613, 619, 625 |
| SiO ⁺ | 337 |
| ²⁹ SiO | 397 |
| SiS | 297, 479, 497 |
| TiO | 479, 515 |

3 atoms

| | |
|---|--|
| C ₃ | 247, 307, 337 |
| CH ₂ | 177, 231, 239, 247, 257, 289, 331, 337, 381, 423, 613 |
| CH ₂ ⁺ | 283, 291, 311, 317, 323, 331, 341 |
| (CH ₂ ⁺)* | 323 |
| CD ₂ | 231 |
| C ₂ H | 47, 81, 239, 299, 307, 311, 331, 337, 341, 427, 479, 497 |
| C ₂ H ⁺ | 81, 263, 291, 307, 423 |
| CN ₂ | 337 |
| C ₂ N | 337 |
| C ₂ N ⁺ | 307, 311, 331, 337, 341 |
| CNO | 411, |
| CO ₂ | 247, 311, 323, 337, 355, 365, 633 |
| C ₂ O | 337 |
| CS ₂ | 337 |
| FeF ₂ | 367 |
| FeH ₂ | 367 |
| H ₃ | 231, |
| H ₃ ⁺ | 77, 231, 291, 297, 311, 331, 339, 337, 341, 427, 439 |
| H ₂ D ⁺ | 427, 439 |
| D ₃ | 231 |
| D ₃ ⁺ | 231 |
| HCN | 1, 25, 31, 39, 47, 59, 67, 77, 83, 103, 109, 157, 209, 299, 305, 307, 325, 331, 337, 341, 365, 397, 423, 427, 479, 497, 509, 545 |
| HCN ⁺ | 59, 291, 299, 307, 311, 331 |
| DCN | 307, 427 |
| H ¹ ³ CN | 39, 59, 397, 427 |
| HC ¹ ⁵ N | 397, 427 |
| HCO | 177, 231, 239, 281, 331, 337, 355, 439 |
| HCO ⁺ | 1, 25, 31, 39, 81, 109, 177, 231, 297, 311, 323, 331, 337, 339, 341, 427, 439, 479 |
| DCO ⁺ | 1, 341, 427, 439 |
| H ¹ ³ CO ⁺ | 341, 397, 427 |
| HC ¹ ⁸ O ⁺ | 397, 427 |
| HCS ⁺ | 297, 337 |
| HNC | 1, 25, 77, 337, 341, 427, 439, 479, 497 |
| HNO | 231, 289, 311, 337 |
| HNO ⁺ | 311 |
| HO ₂ | 239, 337 |
| H ₂ O | 1, 21, 31, 41, 129, 175, 177, 239, 247, 257, 269, 289, 307, 311, 317, 323, 331, 337, 341, 355, 365, 373, 387, 445, 479, 487, 515, 525, 545, 551, 565, 579, 591, 593, 599, 603, 613, 627, 637 |
| H ₂ O [*] | 289 |
| H ₂ O ⁺ | 231, 291 |
| H ₂ ¹⁸ O | 21 |
| H ₂ S | 31, 297, 307, 337, 365 |
| H ₂ S ⁺ | 297 |
| NCO | 337 |

| | |
|---------------------------------|---|
| NCO ⁺ | 77 |
| NCS | 337 |
| NH ₂ | 59, 231, 239, 289, 307, 311, 331, 337, 355, 583 |
| NH ₂ ⁺ | 311, 331 |
| ND ₂ | 307 |
| N ₂ H ⁺ | 25, 31, 71, 231, 341, 427, 479 |
| N ¹⁵ NH ⁺ | 427 |
| N ₂ D ⁺ | 71, 341 |
| NO ₂ | 239 |
| N ₂ O | 337 |
| OCS | 31, 297, 337, 341, 365, 397, 445 |
| O ¹³ CS | 397 |
| PH ₂ | 239 |
| SO ₂ | 1, 21, 25, 31, 297, 365 |
| SiH ₂ | 337 |

4 atoms

| | |
|--|--|
| C ₄ | 337 |
| CH ₃ | 59, 231, 289, 331, 337, 341, 381, 439 |
| CH ₃ ⁺ | 67, 291, 305, 307, 311, 317, 323, 331, 337, 341, 427 |
| CH ₂ D | 439 |
| CH ₂ D ⁺ | 439 |
| CD ₃ | 307 |
| CD ₃ ⁺ | 307 |
| C ₂ H ₂ | 59, 291, 299, 307, 311, 317, 325, 331, 337, 365, 367, 373, 427, 479, 497, 509 |
| C ₂ H ₂ ⁺ | 77, 291, 299, 307, 311, 323, 337 |
| C ₃ H | 337 |
| C ₃ H ⁺ | 337 |
| CHCO ⁺ | 337 |
| CH ₂ F | 239 |
| C ₂ N ₂ | 307, 325 |
| C ₃ N | 47, 337, 479, 497 |
| C ₂ O ₂ ⁺ | 337 |
| COOH | 337 |
| COOH ⁺ | 337 |
| HCCN | 59 |
| H ₂ CN ⁺ | 77, 299, 307, 311, 317, 331, 337, 341 |
| HCNH ⁺ | 307, 337, 341 |
| DCND ⁺ | 307 |
| HCO ₂ | 355 |
| H ₂ CO | 1, 25, 71, 81, 85, 89, 95, 99, 101, 103, 113, 117, 123, 177, 221, 281, 323, 331, 337, 341, 355, 365, 397, 405, 409, 427, 439, 473, 627 |
| H ₂ CO ⁺ | 337 |
| HDCO | 341, 427, 439 |
| H ₂ ¹³ CO | 397, 405, 409, 439 |
| H ₂ C ¹⁸ O | 397, 405, 409 |
| H ₂ CS | 25, 297, 365 |
| H ₂ CS ⁺ | 337 |
| HNCO | 317, 337 |
| HNCS | 337 |
| H ₂ NO ⁺ | 311 |
| H ₂ O ₂ | 337 |
| H ₃ O ⁺ | 177, 337, 341, |
| NH ₃ | 1, 39, 59, 67, 69, 71, 77, 83, 85, 89, 91, 93, 175, 221, 231, 289, 307, 311, 317, 323, 325, 331, 337, 341, 355, 365, 373, 387, 427, 479, 495, 497, 503, 565, 603, 627, 633 |
| ¹⁵ NH ₃ ⁺ | 47, 231, 291, 311, 317, 331, 341 |
| NH ₃ | 427 |
| NH ₂ D | 427 |
| N ₂ H ₂ | 355 |
| NOCN | 45 |

5 atoms

| | |
|---|--|
| CH ₄ | 41, 77, 283, 289, 291, 307, 311, 317, 323, 325, 337, 341, 355, 365, 367, 373, 387, 479, 497, 509, 591 |
| CD ₄ | 307 |
| C ₂ H ₃ | 337 |
| C ₂ H ₃ ⁺ | 67, 299, 307, 311, 323 |
| C ₂ D ₂ H ⁺ | 307 |
| C ₃ H ₂ | 337 |
| C ₄ H | 47, 479, 497 |
| CH ₂ CN | 59, 337 |
| CH ₂ CO | 317, 337 |
| CH ₃ I | 59 |
| CH ₂ N ₂ | 337 |
| CH ₂ NH | 311, 337 |
| CH ₂ OH | 337 |
| C ₄ N | 45 |
| C ₄ O | 45 |
| HC ₃ N | 1, 25, 47, 59, 71, 77, 81, 91, 299, 307, 317, 325, 331, 337, 397, 427, 479, 497 |
| HC ₃ N ⁺ | 307 |
| H ¹ ³ CC ₂ N | 397 |
| HC ¹ ³ CCN | 59 |
| HC ₂ ¹ ³ CN | 59 |
| H ₃ CO | 239, 337 |
| H ₃ CO ⁺ | 323, 439 |
| H ₂ DCO ⁺ | 439 |
| HCOOH | 337, 355, 365, 627 |
| H ₃ CS | 337 |
| NH ₄ ⁺ | 291, 307, 311, 323, 331, 341 |
| NH ₂ CN | 365 |

6 atoms

| | |
|--|--|
| CH ₅ ⁺ | 291, 311, 317, 323, 337 |
| C ₂ H ₄ | 291, 311, 337, 367, 497 |
| C ₂ H ₄ ⁺ | 323 |
| C ₄ H ₂ | 325, 337 |
| CH ₂ C ₂ H | 337 |
| CH ₃ CN | 307, 325, 365, 479 |
| CH ₃ CO | 337 |
| CH ₃ CO ⁺ | 317, 337 |
| CH ₂ NH ₂ | 311 |
| CH ₂ NH ₂ ⁺ | 311, 337 |
| CH ₃ OH | 1, 117, 317, 323, 337, 365, 373, 524, 525, 565 |
| C ₅ N | 45 |
| H ₂ C ₃ N | 59 |
| H ₂ C ₃ N ⁺ | 299, 307 |

| | |
|-----------------------------------|--------------------|
| H ₄ CN ⁺ | 311 |
| (HCO) ₂ | 45, 337 |
| HCONH ₂ | 337, 355, 365, 397 |
| H ¹³ CONH ₂ | 397 |
| NH ₅ ⁺ | 291, 317, 341 |
| NH ₃ CO ⁺ | 317 |

7 atoms

| | |
|--|--|
| C ₂ H ₅ | 337 |
| C ₃ H ₄ | 59, 325, 331, 337, 365 |
| C ₄ H ₃ | 337 |
| C ₄ H ₃ ⁺ | 67 |
| CH ₅ N | 325, 337, 365 |
| C ₂ H ₄ N ⁺ | 305, 307 |
| C ₃ H ₃ N | 307, 331, 337 |
| C ₃ H ₃ N ⁺ | 77, 299, 307, 331 |
| CH ₅ O ⁺ | 317, 323, 337 |
| C ₂ H ₂ O ₃ | 45 |
| C ₂ H ₄ O | 331, 337, 365 |
| C ₅ O ₂ | 45 |
| HC ₅ N | 41, 47, 59, 67, 69, 71, 77, 81, 325, 331, 479, 497 |
| HC ₄ ¹³ CN | 59 |

8 atoms

| | |
|--|---------------|
| C ₂ H ₆ | 337, 367, 497 |
| C ₃ H ₅ | 337 |
| C ₃ H ₅ ⁺ | 77 |
| C ₆ H ₂ | 325 |
| CH ₆ N ⁺ | 311, 317 |
| C ₂ H ₅ N ⁺ | 311 |
| C ₃ H ₄ N ⁺ | 299, 317, 331 |
| C ₄ H ₃ N | 45, 325 |
| C ₅ H ₂ N ⁺ | 331 |
| C ₂ H ₄ O ₂ | 45, 331, 365 |
| C ₃ H ₄ O | 337 |

9 atoms

| | |
|--|---|
| C ₃ H ₆ | 337 |
| C ₃ H ₅ N | 45, 331, 337, 365 |
| C ₂ H ₆ O | 307, 323, 331, 365 |
| C ₃ H ₄ O ₂ | 45 |
| HC ₇ N | 47, 59, 69, 71, 325, 331, 479, 495, 497 |

10 atoms

| | |
|--|----------|
| C ₄ H ₆ | 337 |
| C ₅ H ₅ | 325 |
| C ₈ H ₂ | 325 |
| C ₃ H ₆ N | 331 |
| C ₄ H ₅ N | 45, 325 |
| C ₅ H ₄ N | 331 |
| C ₂ H ₇ O ⁺ | 307, 323 |
| C ₃ H ₆ O | 45 |

More than 10 atoms

| | |
|--|---------------|
| C ₅ H ₆ | 45 |
| C ₆ H ₆ | 291, 325, 497 |
| C ₇ H ₈ | 325 |
| C ₈ H ₆ | 325 |
| C ₉ H ₈ | 325 |
| C ₁₀ H ₂ | 325 |
| C ₁₀ H ₈ | 325 |
| C ₄ H ₇ N | 45 |
| C ₇ H ₅ N | 325 |
| C ₈ H ₆ N | 325 |
| C ₈ H ₆ N ₂ | 389 |
| C ₄ H ₆ O | 45 |
| HC ₉ N | 47, 325, 331 |