

INDEX OF CHEMICAL SPECIES

1 atom

Ag	469	<sup>107</sup> Ag 469, 485	<sup>109</sup> Ag 485
Al	485, 497, 559, 565	<sup>26</sup> Al 469, 485	
Ar	47, 77, 93, 469, 565	Ar <sup>+29</sup>	<sup>40</sup> Ar 469
B	461		
Ba	469	(130, 132, 134, 135, 136, 137, 138)Ba	485
Be	461		
C	25, 123, 137, 171, 217, 227, 235, 253, 257, 259, 273, 275, 305, 327, 341, 345, 357, 369, 379, 393, 395, 407, 409, 417, 431, 455, 461, 469, 485, 501, 539, 547, 557, 565, 577		
C <sup>+</sup>	1, 25, 109, 123, 137, 217, 235, 259, 273, 275, 305, 357, 393, 417, 539, 545, 547		
C <sup>++</sup>	393	C <sup>+++</sup> 393	
<sup>13</sup> C	123, 311, 407, 461, 469, 547, 577		<sup>13</sup> C <sup>+</sup> 1, 547
Ca	395, 469, 485, 495, 565	Ca <sup>+</sup> 395	
<sup>42</sup> Ca	485	(43, 44, 46, 48)Ca	485
Cl	93, 217, 327, 559	Cl <sup>+</sup> 93	
Co	495, 565		
Cr	391, 469, 565		
Cu	565		
e <sup>-</sup>	1, 31, 109, 121, 235, 305, 395, 485, 501, 545		e <sup>+</sup> 485
Eu	391, 497		
F	559		
Fe	227, 461, 469, 497, 559, 565	Fe <sup>+</sup> 395	
H	1, 25, 29, 31, 67, 75, 77, 109, 121, 123, 167, 205, 217, 227, 235, 245, 253, 259, 275, 295, 297, 305, 323, 357, 393, 395, 409, 431, 447, 455, 461, 501, 525, 531, 545, 557, 565, 577		
H <sup>+</sup>	1, 25, 31, 109, 137, 153, 185, 217, 245, 275, 323, 345, 379, 395, 485		
H <sup>-</sup>	109, 121, 395		
D	1, 109, 217, 227, 235, 461, 469, 493, 577		
D <sup>+</sup>	1, 109, 217, 227, 311		
He	1, 29, 31, 43, 47, 93, 109, 227, 235, 253, 305, 339, 393, 565		
He <sup>+</sup>	19, 29, 235, 305, 393, 443		
<sup>3</sup> He	109, 493		
Hf	497		
Hg	495	(196, 202)Hg	495
I	485	<sup>129</sup> I 469, 485	
Ir	497		
K	469, 565	<sup>40</sup> K	469

Kr	469, 485	Kr <sup>+</sup> 27	Kr <sup>++</sup> 27
<sup>85</sup> Kr	493	(78, 80, 82, 83, 86)Kr	485
La	497		
Li	109, 461, 565	Li <sup>+</sup> 109	<sup>6</sup> Li 109, 461
Lu	497		
Mg	227, 469, 485, 559, 565	Mg <sup>+</sup> 395	
<sup>25</sup> Mg	461, 485	<sup>26</sup> Mg	461, 469, 485
Mn	565		
N	1, 137, 171, 217, 227, 235, 253, 257, 275, 293, 305, 311, 327, 339, 393, 409, 417, 455, 461, 469, 501, 531, 565		
N <sup>+</sup>	1, 19, 29, 137, 305	<sup>15</sup> N	461, 469
Na	395, 495, 565	<sup>22</sup> Na	485
Nd	469, 485	<sup>143</sup> Nd	469, 485
<sup>148</sup> Nd	485, 493	(143, 144, 145, 148, 150)Nd	485
Ne	93, 469, 565	<sup>22</sup> Ne	469, 485
Ni	469, 497, 565		
O	1, 29, 67, 137, 217, 227, 235, 253, 257, 259, 273, 275, 293, 295, 297, 311, 327, 341, 345, 357, 369, 379, 393, 395, 407, 409, 417, 431, 447, 455, 461, 469, 485, 501, 531, 539, 545, 559, 565		
O <sup>+</sup>	19, 217	O <sup>++</sup>	137
<sup>17</sup> O	1, 469, 485	<sup>18</sup> O	461, 469, 485
Os	495	<sup>184</sup> Os	485
P	409, 469		
<sup>107</sup> Pd	469, 485	<sup>108</sup> Pd	485
<sup>148</sup> Pm	493		
<sup>244</sup> Pu	485		
S	67, 171, 275, 357, 395, 409, 417, 455, 531, 559		
S <sup>+</sup>	455		
Sc	495		
Se	497		
Si	137, 171, 227, 327, 341, 357, 391, 395, 409, 461, 485, 559, 565	(29, 30)Si	327, 485
Sm	469, 497	(144, 148, 150, 152, 154)Sm	485
<sup>147</sup> Sm	469, 485	<sup>149</sup> Sm	485, 493
Sr	391, 469, 485	(84, 86)Sr	485
Th	469		
Ti	469, 485, 559, 565	(46, 47, 49, 50)Ti	485
<sup>204</sup> Tl	493		
U	469, 485		
V	469, 565		
<sup>185</sup> W	493		
Xe	469, 495	(124, 126)Xe	485, 495
<sup>128</sup> Xe	485	<sup>129</sup> Xe	469, 485
	(130, 131, 132, 134, 136)Xe	485	
Yb	497		
Zr	559		

2 atoms

AlH	95, 395	AlCl	559	AlO	91
ArD <sup>+</sup>	77				
C <sub>2</sub>	51, 67, 95, 103, 123, 133, 217, 227, 245, 357, 395, 407, 417, 431, 447, 461	C <sub>2</sub> <sup>-</sup>	395		
CH	51, 95, 123, 133, 137, 217, 227, 235, 245, 273, 275, 289, 297, 305, 327, 395, 417, 431, 447, 461, 559, 577				
CH <sup>+</sup>	1, 25, 51, 95, 109, 123, 133, 217, 227, 273, 275, 577				
<sup>13</sup> CH <sup>+</sup>	123	CD <sup>+</sup>	95		
CN	51, 67, 95, 123, 133, 171, 217, 227, 245, 275, 293, 305, 311, 357, 395, 407, 417, 429, 447, 455, 531, 547				
CN <sup>-</sup>	395				
CO	1, 19, 31, 47, 51, 67, 75, 77, 91, 95, 123, 133, 137, 153, 171, 217, 227, 235, 257, 259, 273, 275, 293, 303, 311, 323, 327, 345, 357, 369, 379, 395, 409, 417, 431, 461, 501, 525, 531, 539, 547, 557, 559, 565				
CO <sup>+</sup>	77, 95, 275, 311, 417, 447, 577				
<sup>13</sup> CO	1, 51, 133, 171, 205, 259, 311, 327, 369, 547				
<sup>17</sup> O	171, 259	<sup>18</sup> O	51, 171, 201, 245		
<sup>13</sup> C <sup>18</sup> O	171				
CS	1, 31, 67, 95, 153, 187, 235, 245, 275, 327, 357, 395, 417, 447, 455, 559, 565, 577				
CaH	95	CaO	469		
CrO	91				
FeO	565	FeS	559, 565		
H <sub>2</sub>	1, 19, 27, 29, 31, 43, 47, 49, 51, 67, 75, 77, 95, 109, 121, 123, 133, 137, 153, 167, 171, 185, 187, 217, 227, 235, 245, 253, 259, 273, 275, 295, 297, 305, 311, 323, 327, 339, 341, 345, 357, 369, 395, 409, 417, 431, 525, 531, 539, 547, 557, 565, 577				
H <sub>2</sub> <sup>+</sup>	27, 109, 253, 255, 273	H <sub>2</sub> <sup>-</sup>	395		
HD	1, 31, 95, 109, 171, 217, 227, 255, 311				
HD <sup>+</sup>	109	D <sub>2</sub>	43, 77		
HCl	1, 19, 47, 51, 77, 95, 133, 171, 327, 559, 577				
HF	559				
HeH <sup>+</sup>	109				
LiH	109	LiH <sup>+</sup>	109		
MgH	51, 95, 395	MgH <sup>+</sup>	95, 133		
MgO	95, 205, 395				
N <sub>2</sub>	19, 51, 95, 167, 171, 257, 293, 311, 409, 431, 501, 525, 531, 565				
N <sub>2</sub> <sup>+</sup>	19, 29, 49, 95, 305, 311, 417, 455				
NH	51, 95, 217, 227, 275, 293, 327, 417, 455				
NH <sup>+</sup>	1, 91, 95, 305				
NO	51, 75, 95, 227, 273, 275, 305, 417				
NO <sup>+</sup>	77, 95				
NaH	51, 95				
O <sub>2</sub>	1, 19, 51, 95, 167, 171, 227, 235, 257, 259, 275, 293, 295, 345, 431, 501, 525, 531, 565				

$O_2^+$	19, 431	$O^{18}O$	171, 345
OH	29, 31, 51, 67, 91, 95, 109, 123, 133, 137, 185, 217, 227, 235, 245, 255, 259, 273, 275, 293, 295, 297, 303, 327, 345, 357, 369, 379, 395, 409, 417, 429, 431, 447, 455, 461, 501, 547, 559, 577		
$OH^+$	51, 77, 217, 273, 275, 431		
$OH^-$	531	OD	235, 461
$P_2$	409	PN	171, 409
$S_2$	409, 417, 455, 461	$S_2^-$	395
SH	95, 275, 357, 395, 409, 455, 559	$SH^-$	531
SO	171, 235, 245, 275, 345, 357, 417, 559		
$SO^+$	77, 577		
ScO	327		
SiC	369, 395, 469		
SiH	51, 395, 409	$SiH^+$	51
SiN	387, 395		
SiO	31, 95, 171, 245, 275, 289, 327, 341, 345, 357, 369, 379, 395, 409, 559		
SiS	91, 171, 327, 341, 345, 357, 395, 409, 547, 559		
$Si^{33}S$	577		
TiO	327, 395		
VO	327, 395		
ZrO	395		

3 atoms

$C_3$	51, 95, 123, 275, 395, 417, 431
$CH_2$	51, 95, 217, 227, 259, 273, 275, 305, 327, 501
$CH_2^+$	217, 273, 275
$C_2H$	51, 67, 171, 227, 245, 259, 275, 311, 327, 357, 395, 409, 431
$^{13}CCH$	171
	$C_2D$ 87, 311
$CHO^+$	431
$C_2N$	171
$CO_2$	31, 259, 275, 327, 409, 417, 431, 443, 447, 461, 501, 525, 531, 559, 565
	$CO_2^+$ 95
$C_2O$	245
$COH^+$	205
$CS_2$	67, 75, 417, 455, 565
$H_3^+$	1, 51, 77, 171, 217, 235, 255, 259, 273, 305, 311
$H_2D^+$	1, 77, 171, 217, 305, 311
HCH	289
HCN	1, 19, 31, 43, 47, 51, 67, 75, 77, 171, 187, 199, 203, 245, 253, 275, 289, 305, 327, 345, 357, 369, 379, 395, 407, 429, 431, 547, 557, 559, 565
$HCN^+$	305
	DCN 107, 199, 311, 577
$H^{13}CN$	357, 547
	$HC^{15}N$ 43
HCO	67, 273, 311, 461, 501, 525, 559, 565
$HCO^+$	1, 31, 51, 77, 171, 203, 205, 217, 227, 235, 245, 255, 259, 275, 289, 311, 345, 357, 531

DCO <sup>+</sup>	1, 171, 255, 311, 531	H <sup>13</sup> CO <sup>+</sup>	201, 311
HCS <sup>+</sup>	1, 31, 77, 171, 205, 235, 245		
HNC	67, 77, 171, 203, 245, 253, 305, 311, 357, 431		
HNO	205, 577		
HO <sub>2</sub>	275		
H <sub>2</sub> O	1, 19, 31, 51, 67, 75, 95, 123, 137, 167, 171, 187, 217, 227, 255, 259, 275, 295, 297, 303, 305, 311, 327, 343, 345, 357, 369, 379, 395, 409, 417, 425, 427, 431, 441, 447, 455, 461, 469, 501, 525, 531, 539, 547, 559, 565, 577		
H <sub>2</sub> O <sup>+</sup>	29, 95, 123, 273, 275, 417, 431		
HDO	205, 311, 461, 531		
HOC <sup>+</sup>	77, 203, 577	DOC <sup>+</sup>	77
HO <sup>13</sup> C <sup>+</sup>	77	H <sup>18</sup> O <sup>13</sup> C <sup>+</sup>	77
H <sub>2</sub> S	67, 275, 293, 345, 357, 369, 395, 409, 455, 501, 559, 565		
H <sub>2</sub> S <sup>+</sup>	565		
Kr <sup>+</sup> H <sub>2</sub> <sup>+</sup>	27	Kr <sup>+</sup> H <sub>2</sub> <sup>+</sup>	27
NCS	67	NCSi	171
NH <sub>2</sub>	51, 67, 205, 275, 417, 431, 501		
NH <sub>2</sub> <sup>+</sup>	51, 77, 217, 305		
N <sub>2</sub> H <sup>+</sup>	1, 77, 171, 245, 259, 289, 305	N <sub>2</sub> D <sup>+</sup>	1, 311
NO <sub>2</sub>	75		
NaOH	205		
OCS	31, 47, 67, 75, 245, 275, 501		
O <sub>2</sub> H <sup>+</sup>	1		
SO <sub>2</sub>	75, 171, 205, 235, 245, 275, 345, 357, 369, 417		
<sup>33</sup> SO <sub>2</sub>	205		
SiC <sub>2</sub>	171, 187, 345, 357, 395, 409, 559		
<sup>29</sup> SiC <sub>2</sub>	171	<sup>30</sup> SiC <sub>2</sub>	171
Si <sub>2</sub> C	409		

4 atoms

CH <sub>3</sub>	67, 95, 273, 275, 431, 531		
CH <sub>3</sub> <sup>+</sup>	1, 203, 273, 275, 305, 311, 431, 577		
CH <sub>2</sub> D	311	CH <sub>2</sub> D <sup>+</sup>	311
CH <sub>2</sub> S	245		
C <sub>2</sub> H <sub>2</sub>	51, 67, 75, 87, 257, 259, 275, 327, 357, 379, 395, 407, 409, 431, 559, 565		
C <sub>2</sub> H <sub>2</sub> <sup>+</sup>	1, 357	<sup>12</sup> C <sup>13</sup> CH <sub>2</sub>	327
C <sub>3</sub> H	87, 171, 187, 205, 245, 259, 357, 409		
C <sub>3</sub> H <sup>+</sup>	1		
C <sub>3</sub> O	171, 187		
CHCO <sup>+</sup>	431		
C <sub>2</sub> N <sub>2</sub>	67		
C <sub>3</sub> N	171, 187, 245, 357	CCNC	171
C <sub>3</sub> O	171, 187, 245, 577		
HC <sub>2</sub> H	187		
HCCN	187, 245		
H <sub>2</sub> CN <sup>+</sup>	1, 305, 357, 431		

HCNH <sup>+</sup>	1, 77, 171, 289, 311, 577	DCNH <sup>+</sup> 311
HCO <sub>2</sub> <sup>‡</sup>	171	
H <sub>2</sub> CO	31, 67, 95, 185, 187, 257, 275, 293, 305, 311, 431, 443, 461, 501, 525, 539, 557, 559, 565	
H <sub>2</sub> CO <sup>+</sup>	431	HDCO 311
H <sub>2</sub> CS	67, 275	
HNCO	245	H <sup>15</sup> HCO 205      HNC <sup>18</sup> O 205
HNCS	67	
HOCN	77	
HOCO	501	HOCO <sup>+</sup> 77, 171, 577
H <sub>2</sub> O <sub>2</sub>	75, 275	
H <sub>3</sub> O <sup>+</sup>	77, 123, 259, 273, 431	
HSC <sub>2</sub>	171	HSiC <sub>2</sub> 171
N <sub>4</sub> <sup>‡</sup>	19	
NH <sub>3</sub>	1, 19, 31, 51, 67, 75, 89, 95, 137, 167, 171, 187, 199, 201, 245, 275, 293, 305, 327, 345, 357, 417, 425, 427, 431, 455, 501, 525, 531, 539, 547, 565	
NH <sub>3</sub> <sup>‡</sup>	1, 67, 305	NH <sub>2</sub> D 205, 305
O <sub>4</sub> <sup>‡</sup>	19	
Si <sub>2</sub> C <sub>2</sub>	409	

5 atoms

Al <sub>2</sub> O <sub>3</sub>	469, 485, 559, 565	
CH <sub>4</sub>	1, 19, 51, 75, 167, 257, 275, 327, 357, 409, 417, 425, 427, 431, 501, 525, 531, 559, 565, 577	
CH <sub>4</sub> <sup>‡</sup>	1, 431	
C <sub>2</sub> H <sub>3</sub>	431	C <sub>2</sub> H <sub>3</sub> <sup>‡</sup> 1, 77, 357
C <sub>3</sub> H <sub>2</sub>	87, 171, 187, 203, 205, 245, 259, 345, 357, 577	
C <sub>3</sub> H <sub>2</sub> <sup>+</sup>	1, 187	<sup>13</sup> CC <sub>2</sub> H <sub>2</sub> 171      C <sub>2</sub> <sup>13</sup> CH <sub>2</sub> 171
C <sub>4</sub> H	171, 187, 199, 205, 245, 357	
CH <sub>3</sub> Cl	327	
CH <sub>2</sub> CN	67	
C <sub>4</sub> N	171	
CaTiO <sub>3</sub>	485, 565	
Cr <sub>2</sub> O <sub>3</sub>	469	
Fe(OH) <sub>2</sub>	409	
HC <sub>3</sub> N	1, 31, 43, 51, 67, 171, 187, 199, 235, 245, 257, 289, 311, 345, 357, 565	DC <sub>3</sub> N 199, 311
H <sub>2</sub> CCO	205, 245	
H <sub>3</sub> CO <sup>+</sup>	311, 431	H <sub>2</sub> D <sup>13</sup> CO <sup>+</sup> 311
HCOOH	431, 565	H <sup>13</sup> COOH 205
Mg(OH) <sub>2</sub>	409	MgSiO <sub>3</sub> 565
NC <sub>3</sub> N	199	
NH <sub>4</sub> <sup>+</sup>	1, 305, 431	
OCCCS	205	
SiH <sub>4</sub>	171, 327, 357, 387	

6 atoms

$\text{CH}_5^+$	1	$\text{CH}_4\text{D}^+$	311
$\text{C}_2\text{H}_4$	275, 327, 357, 387, 409, 431, 565	$\text{C}_2\text{H}_4^+$	1
$\text{C}_3\text{H}_3^+$	1, 235, 431		
$\text{C}_4\text{H}_2$	187, 357		
$\text{C}_5\text{H}$	171		
$\text{CH}_3\text{CN}$	1, 51, 67, 187, 203, 245, 259, 289, 357, 431, 501, 565		
$\text{CH}_3\text{NC}$	203, 245		
$\text{CH}_3\text{OH}$	1, 201, 245, 259, 293, 501, 531, 565		
$^{13}\text{CH}_3\text{OH}$	205, 431		
$\text{CH}_3\text{SH}$	205		
$\text{H}_2\text{C}_3\text{N}^+$	1, 235		
$\text{H}_2\text{C}_2\text{NH}$	245		
$\text{H}_2\text{COOH}^+$	19		
$\text{N}_2\text{H}_4$	67, 327		
$\text{NH}_2\text{CHO}$	205	$\text{NH}_2^{13}\text{CHO}$	205

7 atoms

$\text{C}_2\text{H}_5$	275	$\text{C}_2\text{H}_5^+$	431
$\text{C}_3\text{H}_4$	187, 201, 245, 431, 565		
$\text{CH}_3\text{NH}_2$	431		
$\text{C}_3\text{H}_3\text{N}$	205, 245		
$\text{CH}_3\text{CNH}^+$	203		
$\text{CH}_3\text{HCN}^+$	1		
$\text{CH}_3\text{NCH}^+$	203		
$\text{CH}_3\text{CHO}$	201, 245, 259		
$\text{Fe}_3\text{O}_4$	565		
$\text{MgAl}_2\text{O}_4$	485		
$\text{Mg}_2\text{SiO}_4$	469, 485, 565		
$\text{NH}_3\cdot\text{H}_2\text{O}$	565		

8 atoms

$\text{C}_2\text{H}_6$	327, 387
$\text{C}_3\text{H}_5^+$	431
$\text{CH}_3\text{C}_3\text{N}$	187, 245, 577
$\text{CH}_3\text{OCHO}$	205
$\text{CH}_2\text{CH}\cdot\text{HCO}$	205
$\text{CH}_2\text{CH}\cdot\text{NCO}$	205
$\text{CH}_3\text{CONC}$	525

9 atoms

CH <sub>3</sub> C <sub>4</sub> H	187, 245
C <sub>2</sub> H <sub>5</sub> CN	205
CH <sub>3</sub> C <sub>4</sub> N	577
C <sub>2</sub> H <sub>2</sub> <sup>+</sup> .HC <sub>3</sub> N	1
C <sub>2</sub> H <sub>5</sub> OH	205, 293
(CH <sub>3</sub> ) <sub>2</sub> O	205
CuCl <sub>2</sub> .2H <sub>2</sub> O	93
HC <sub>7</sub> N	187, 245, 357, 547

10 atoms

C <sub>4</sub> H <sub>6</sub>	245
C <sub>4</sub> H <sub>5</sub> N	205
C <sub>6</sub> H <sub>3</sub> N	187, 245
C <sub>3</sub> H <sub>6</sub> O	205

Above 10 atoms

C <sub>6</sub> H <sub>6</sub>	95
C <sub>3</sub> H <sub>7</sub> N	205
C <sub>4</sub> H <sub>7</sub> N	205
C <sub>4</sub> H <sub>4</sub> N <sub>4</sub>	253
CH <sub>4</sub> .6H <sub>2</sub> O	565
CaAl <sub>12</sub> O <sub>18</sub>	469
CaAl <sub>12</sub> O <sub>19</sub>	485
CaAl <sub>2</sub> Si <sub>8</sub>	485
CaAl <sub>2</sub> Si <sub>2</sub> O <sub>8</sub>	485
CaMgSi <sub>2</sub> O <sub>6</sub>	485
Ca <sub>2</sub> MgSi <sub>2</sub> O <sub>7</sub>	469
HC <sub>9</sub> N	187, 205, 245
HC <sub>11</sub> N	187, 245, 357, 557, 577