**Extended Third Millennium Ideal Gas and Condensed Phase Thermochemical Database  
 for Combustion with Updates from “Active Thermochemical Tables”**

**Authors: Elke Goos, Alexander Burcat and Branko Ruscic.**

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Update of

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Alexander Burcat and Branko Ruscic

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<http://burcat.technion.ac.il>; quote date.

mirrored at <http://garfield.chem.elte.hu/Burcat/burcat.html>; quote date.

or received from Elke Goos, date.

Table 6. Enthalpy of formation, **Δ***fH298* and **Δ***fH0,* heat capacity and entropy at 298 K, and ***H298-H0***  fromtheoriginal calculation Last addition *January 1 2023****.***

| **Compound** | | **Mol. Wgt.** | **Δf*H298* kJ/mol** | **Δf*H0* kJ/mol** | **± kJ/mol** | | ***Cp298* J/mol K** | | **S*298* J/mol K** | | ***H298-H0* kJ/mol** | |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ag (cr) REFERENCE ELEMENT | | 107.86820 | 0. | 0. |  | | 25.350 | | 42.55 | | 5.745 | | † |
| Ag | | 107.86820 | 284.9 | 284.448 | ±0.8 | | 20.786 | | 172.998 | | 6.197 | | † |
| Ag+ | | 107.86765 | 1022.1 | 1015.444 |  | | 20.792 | | 167.236 | | 6.198 | | † |
| Ag- | | 107.86875 | 153.08 | 158.83 |  | | 20.792 | | 167.236 | | 6.198 | | † |
| AgN3 Silver Azide (Solid) | | 149.88842 | 310.3 | 315.0 |  | | 59.482 | | 259.274 | | 13.993 | | X |
| Air (standard mixture) | | 28.96518 | -0.126 | -0.125 |  | | 29.104 | | 198.824 | | 8.649 | | † |
| AL(cr) REFERENCE ELEMENT | | 26.98154 | 0. | 0. |  | | 24.2 | | 28.3 | | 4.540 | | † |
| AL | | 26.98154 | 330. | 327.621 | ±4.2 | | 21.391 | | 164.555 | | 6.919 | | † |
| AlB2 (S) Aluminum Diboride (S) | | 48.60354 | -150.996 |  |  | | 43.644 | | 34.727 | |  | |  |
| AlB2 g | | 48.60354 | ??834.269 | 830.209 | ±8. | | 44.331 | | 253.948 | | 11.028 | | # |
| ALBr | | 106.88554 | 14.325 | 21.554 |  | | 35.618 | | 239.635 | | 9.571 | | † |
| ALBr2 | | 186.78954 | -140.662 | -125. | ±50. | | 53.256 | | 312.236 | | 13.398 | | † |
| ALBr3 | | 266.69354 | -410.477 | -387.1 | ±5.1 | | 75.372 | | 348.026 | | 17.943 | | † |
| ALCL <&> | | 62.43424 | -51.007 | -51.2 | ±3. | | 34.661 | | 227.961 | | 9.323 | | † |
| ALCL+ | | 62.43369 | 861.849 | 855.286 | ±42. | | 33.794 | | 232.190 | | 9.154 | | † |
| ALCL2 | | 97.88694 | -240.874 | -240. | ±40. | | 51.566 | | 290.374 | | 12.847 | | † |
| ALCL3 <&> | | 133.33964 | -584.679 | -582.768 | ±5. | | 71.537 | | 313.089 | | 16.401 | | † |
| ALF <&> | | 45.97994 | -264.060 | -264. | ±3. | | 31.937 | | 215.162 | | 8.892 | | † |
| ALF+ | | 45.97939 | 692.234 | 686.176 | ±25. | | 31.155 | | 220.068 | | 8.813 | | † |
| ALF2 | | 64.97834 | -631.764 | -630. | ±30. | | 45.418 | | 264.924 | | 11.601 | | † |
| ALF2- | | 64.97889 | -853.231 | -845. | ±20. | | 44.746 | | 257.272 | | 11.332 | | † |
| ALF3 <&> | | 83.97675 | -1209.28 | -1205.54 | ±3.1 | | 62.199 | | 276.674 | | 14.044 | | † |
| ALH | | 27.98948 | 249.250 | 249.356 | ±20 | | 29.371 | | 187.863 | | 8.668 | | † |
| ALH2 | | 28.99742 | 276.774 | 279.691 | ±20. | | 35.773 | | 213.316 | | 10.091 | | † |
| ALH3 solid alpha, hexagonal | | 30.00536 | -11.4 | +0.402 |  | | 40.210 | | 30.040 | | 5.440 | | † |
| ALH3 | | 30.00536 | 128.896 | 135.728 | ±20. | | 40.057 | | 206.579 | | 10.411 | | † |
| ALO <&> | | 42.98094 | 67.319 | 67.411 | ±8 | | 30.884 | | 218.389 | | 8.788 | | † |
| ALO+ | | 42.98039 | 992.993 | 986.586 |  | | 33.135 | | 230.978 | | 9.090 | | † |
| ALO- | | 42.98149 | -272.972 | -266.589 | ±11 | | 30.335 | | 211.945 | | 8.745 | | † |
| ALOH | | 43.98888 | -192.762 | -190. | ±13 | | 43.512 | | 222.643 | | 10.352 | | † |
| HALO | | 43.98888 | 1.821 | 5. | ±50. | | 40.996 | | 219.696 | | 9.935 | | † |
| ALO2 | | 58.98034 | -38.658 | -38.799 | ±32 | | 51.661 | | 269.637 | | 13.362 | | † |
| ALO2- | | 58.98089 | -452.572 | -443.799 | ±60 | | 46.063 | | 229.783 | | 10.645 | | † |
| ALO2H (HALO2) | | 59.98828 | -355.472 | -350. | ±50 | | 51.256 | | 254.826 | | 11.981 | | † |
| AL(OH)2 | | 60.99622 | -507.661 | -500. | ±50 | | 62.980 | | 284.406 | | 14.028 | | † |
| AL(OH)3 | | 78.00356 | -1016.67 | -1000. |  | | 87.249 | | 301.541 | | 17.596 | | † |
| AL2 <&> | | 53.96308 | 501.302 | 500.243 | ±20 | | 37.055 | | 243.842 | | 10.139 | | † |
| AL2O | | 69.96248 | -148.611 | -147.968 | ±20 | | 51.978 | | 253.135 | | 12.777 | | † |
| AL2O+ | | 69.96193 | 648.97 | 643.212 |  | | 52.898 | | 260.663 | | 12.981 | | † |
| AL2O2 | | 85.96188 | -403.096 | -401.178 | ±40. | | 68.122 | | 288.044 | | 15.843 | | † |
| AL2O2+ | | 85.96133 | 557.439 | 554.026 |  | | 68.924 | | 289.704 | | 14.975 | | † |
| AL2O3(S) | | 101.96128 | -1675.70 | -1663.62 |  | | 79.033 | | 50.920 | | 10.016 | | † |
| AL2O3(G) | | 101.96128 | -546.891 | -544.39 | ±100. | | 86.990 | | 316.662 | | 19.598 | | † |
| Ar REFERENCE ELEMENT<^!> | | 39.948 | 0 | 0 |  | | 20.786 | | 154.847 | | 6.197 | | † |
| 166.406 | | 39.94745 | 1526.778 | 1520.6 | ±0.001 | | 20.984 | |  | | 6.206 | | † |
| ArH Radical | | 40.95594 | 211.75 | 210.447 | ±8. | | 44.036 | | 235.028 | | 11.737 | | # |
| ArH+ 3L84 | | 40.95539 | 1165.2 | 1160.7 |  | | 29.105 | | 188.478 | | 8.676 | | # |
| Ar2g | | 79.8960 | -6.346 | -1.012 | ±0.009 | | 48.156 | | 270.235 | | 12.606 | | # |
| Au (s) Gold Reference Element | | 196.96657 | 0. | 0. |  | | 25.420 | | 47.400 | | 6/009 | | # |
| Au (g) Aurum | | 196.96657 | 360.500 | 360.312 |  | | 20.786 | | 180.396 | | 6.197 | | # |
| Au+ Aurum cation | | 196.96602 | 1264.825 | 1258.440 |  | | 20.786 | | 174.633 | | 6.197 | | # |
| Au- Aurum anion | | 196.96710 | 139.566 | 145.565 |  | | 20.786 | | 174.633 | | 6.197 | | # |
| AuCl | |  | -34.727 |  | ±4.2 | |  | | 92.885 | |  | | X |
| AuCl3 | |  | -115.060 |  | ±4.2 | |  | | 148.114 | |  | | X |
| AuF3 | |  | -363.590 |  | ±9.2 | |  | |  | |  | | X |
| B(S) REFERENCE ELEMENT | | 10.811 | 0. | 0.000 |  | | 11.315 | | 5.834 | | 1.214 | | † |
| B <&> | | 10.811 | 575.699 | 559.898 | ±12 | | 20.797 | | 153.438 | | 6.316 | | † |
| B+ cation | | 10.81045 | 1382.315 | 1360.536 |  | | 20.786 | | 138.545 | | 6.197 | | † |
| B- anion | | 10.81155 | 542.631 | 533.132 |  | | 20.788 | | 156.814 | | 6.273 | | † |
| BBr | | 90.715 | 240.952 | 245.429 |  | | 32.787 | | 224.992 | | 8.997 | | † |
| BBr2 | | 170.619 | 97.829 | 111.362 | ±25. | | 48.451 | | 294.539 | | 12.201 | | † |
| BBr3 | | 250.523 | -205.3 | -183. | ±3.0 | | 67.777 | | 324.505 | | 15.703 | | † |
| BCL <&> | | 46.2637 | 183.173 | 180.117 | ±20. | | 31.656 | | 213.244 | | 8.861 | | † |
| BCL+ | | 46.26315 | 1234.28 | 1225.027 | ±42. | | 31.644 | | 219.133 | | 8.860 | | † |
| BCLF | | 65.26210 | -279.184 | -280. | ±10 | | 42.820 | | 264.941 | | 11.033 | | † |
| BCLF2 | | 84.26050 | -888. | -885.694 | ±5. | | 54.473 | | 275.115 | | 12.324 | | † |
| BCL2 <&> | | 81.7164 | -60.881 | -62. | ±10. | | 45.746 | | 271.202 | | 11.514 | | † |
| BCL2+ | | 81.71585 | 672.315 | 663.664 | ±20. | | 52.975 | | 257.809 | | 12.849 | | † |
| BCL2F | | 100.71480 | -643. | -641.423 | ±5. | | 58.911 | | 287.581 | | 13.231 | | † |
| BCL3 <^> | | 117.1691 | -404.5 | -403.485 | ±1.3 | | 62.556 | | 289.468 | | 13.971 | | † |
| BF <&> | | 29.80940 | -106.932 | -110. | ±10. | | 29.594 | | 200.453 | | 8.695 | | † |
| BF2 <&> | | 48.80781 | -499.427 | -500. | ±10. | | 40.055 | | 247.133 | | 10.612 | | † |
| BF2+ | | 48.80726 | 322.6 | 315.816 | ±2.5 | | 44.291 | | 225.151 | | 10.612 | | † |
| BF2- | | 48.80355 | -733.803 | -728. | ±14. | | 39.436 | | 240.589 | | 10.434 | | † |
| BF3 <^> | | 67.80621 | -1136.0 | -1133.2 | ±0.8 | | 50.462 | | 254.429 | | 11.651 | | † |
| BF4- | | 86.80516 | -1761.27 | -1750. | ±40. | | 67.794 | | 268.855 | | 13.796 | | † |
| BH | | 11.81894 | 448.727 | 445.536 | ±2. | | 29.181 | | 171.836 | | 8.639 | | † |
| BHF2 | | 49.81575 | -739.614 | -736.000 | ±3.3 | | 42.230 | | 244.323 | | 10.659 | | † |
| BH2 | | 12.82688 | 328.909 | 328.568 | ±10 | | 34.975 | | 193.675 | | 10.024 | | † |
| BH3 | | 13.83482 | 104.747 | 108.603 |  | | 36.018 | | 188.251 | | 10.060 | | † |
| BH4 | | 14.84276 | 255.210 | 262.560 |  | | 44.277 | | 211.994 | | 10.771 | | † |
| BH4Na Solid | | 37.83253 | -191.840 |  |  | | 86.560 | | 101.400 | |  | | # |
| BH5 | | 15.85070 | 77.387 | 87.199 |  | | 52.616 | | 229.580 | | 12.572 | | † |
| BI Mono Iodo Boron | | 137.71547 | 325.988 | 324.657 | ±12 | | 33.731 | | 233.319 | | 9.142 | | † |
| BI2 | | 264.61994 | 238.036 | 239.810 | ±10 | | 50.294 | | 311.115 | | 12.688 | | † |
| BI3 BoronTriIodide | | 391.52441 | 21.400 | 25.475 | ±4. | | 71.027 | | 350.427 | | 16.933 | | † |
| BO <&> | | 26.81040 | 20.406 | 17.286 | ±10 | | 29.196 | | 203.468 | | 8.674 | | † |
| BO- | | 26.81095 | -277.791 | -274.714 | ±5. | | 29.197 | | 197.683 | | 8.674 | | † |
| BOCL OBCl | | 62.2631 | -318.537 | -319. | ±10 | | 45.079 | | 237.306 | | 10.608 | | † |
| BOCL2 | | 97.7158 | -361.566 | -360 | ±60 | | 58.826 | | 292.296 | | 13.170 | | † |
| BOF OBF | | 45.80880 | -592.978 | -593. | ±10 | | 41.653 | | 224.981 | | 9.988 | | † |
| BOF2 OBF2 | | 64.80721 | -832.768 | -830. | ±50 | | 50.491 | | 268.239 | | 11.611 | | † |
| BO2 | | 42.80980 | -309.122 | -310. |  | | 43.285 | | 230.138 | | 10.772 | | † |
| BO2- | | 42.81035 | -714.494 | -708. | ±20. | | 39.147 | | 215.734 | | 9.598 | | † |
| B2 <&> | | 21.62200 | 857.371 | 850.993 | ±15. | | 31.503 | | 202.064 | | 8.805 | | † |
| B2CL4 | | 163.4328 | -490. | -490.798 | ±10. | | 97.997 | | 371.268 | | 21.588 | | † |
| B2F4 | | 97.61561 | -1438. | -1435.6 | ±7. | | 80.629 | | 326.206 | | 17.681 | | † |
| B2H | | 22.62994 | 796.270 | 792.816 |  | | 42.328 | | 214.282 | | 10.116 | | † |
| B2H2 | | 23.63788 | 454.475 | 455.001 | ±8.4 | | 46.880 | | 213.225 | | 10.371 | | † |
| B2H6 | | 27.66964 | 36.6 | 52.5 | ±2. | | 56.643 | | 232.027 | | 11.932 | | † |
| B2Mg(S) see MgB2 | | 45.9270 | -92.0 | -91.3 | ±8.4 | |  | |  | |  | | # |
| B2Mg g see MgB2 | | 45.9270 | 834.5 | 830.6 | ±8. | |  | |  | |  | | # |
| B2O | | 37.6214 | 192.798 | 187.783 | ±100. | | 47.247 | | 226.244 | | 11.783 | | † |
| B2O2 (BO)2 | | 53.6208 | -457.711 | -460. | ±10. | | 60.269 | | 249.669 | | 13.397 | | † |
| B2O3(S) | | 69.6182 | -1273.5 | -1267.35 | ±1.4 | | 62.761 | | 53.97 | | 9.301 | | †X |
| B2O3 <&> | | 69.6202 | -835.382 | -834.353 | ±8. | | 64.917 | | 285.902 | | 14.419 | | † |
| B3O3CL3 (BOCl)3 | | 186.7893 | -1635.98 | -1630. | ±15 | | 124.123 | | 380.039 | | 24.452 | | † |
| B3O3F3 (BOF)3 | | 137.42641 | -2382.7 | -2374. | ±12 | | 110.653 | | 343.946 | | 21.201 | | † |
| B3O3H3 BOROXIN | | 83.45502 | -1203.76 | -1190. | ±20 | | 80.615 | | 286.152 | | 15.603 | | † |
| H3B3O6 BORIC ACID | | 131.45322 | -2263.69 | -2245. | ±20 | | 133.912 | | 359.908 | | 23.697 | | † |
| BaO | | 153.32640 | -117.95 |  |  | | 32.898 | | 235.460 | | 9.014 | | † |
| Bi(s) REFERENCE ELEMENT | | 208.98040 | 0. | 0. |  | | 25.5 | | 56.7 | | 6.43 | | # |
| Bi | | 208.98040 | 207. |  |  | | 20.786 | | 187.090 | | 6.200 | | # |
| Bi+ | | 208.97983 | 918.233 | 912.300 |  | | 20.786 | | 175.481 | | 6.197 | | # |
| Bi- | |  | 116.2 |  |  | |  | |  | |  | | X |
| BiCl | | 244.43308 | 74.30 |  |  | | 36.134 | | 255.753 | | 9.767 | | # |
| BiCl2 BiChloroBismuth | | 279.88587 | -93.692 |  |  | | 56.839 | | 322.337 | | 14.850 | | # |
| BiCl3 TrichloroBismuth | | 315.33848 | -265.266 |  |  | | 81.609 | | 373.383 | | 20.878 | | # |
| BiF MonofluoroBismuth | | 227.97878 | -29.384 |  |  | | 34.309 | | 250.982 | | 9.255 | | # |
| BiF2 BiFluoroBismuth | | 246.97719 | -200.359 |  |  | | 48.723 | | 289.057 | | 12.176 | | # |
| BiF3 TrifluoroBismuth | | 265.97559 | -707.933 |  |  | | 67.996 | | 312.818 | | 15.565 | | # |
| BiH3 Bismuthine | | 212.00420 | 278. |  |  | | 43.070 | | 241.539 | | 10.691 | | # |
| BiI MonoIodoBismuth | | 335.88485 | 102.80 |  |  | | 37.155 | | 280.376 | | 10.327 | | # |
| Bi(OH)3 | | 260.00240 | -198.234 |  |  | | 99.223 | | 351.516 | | 18.607 | | # |
| BiO | | 244.97978 | 121.3 |  | ±12.6 | | 32.765 | | 246.171 | | 8.994 | | # |
| BiO- | |  | -33.2. |  | ±7.1 | |  | |  | |  | | X |
| BiO2- | |  | -187. |  | ±10. | |  | |  | |  | | X |
| Bi2 | | 417.96080 | 220.0 |  |  | | 36.942 | | 273.743 | | 10.287 | | # |
| Bi2- | |  | 97.07 |  | ±0.88 | |  | |  | |  | | X |
| Bi2O3 /O\  Bi-O-Bi  \O/ | | 465.95896 | 376.807 |  |  | | 83.662 | | 341.171 | | 16.786 | | # |
| Bi2O3 O=Bi-O-Bi=O | | 465.95896 | 636.679 |  |  | | 93.274 | | 373.903 | | 20.518 | | # |
| Br <~> | | 79.904 | 111.852 | 117.915 | ±0.06 | | 20.786 | | 175.019 | | 6.197 | | #† |
| Br+ | | 79.90345 | 1257.917 | 1257.782 | ±0.055 | | 20.787 | | 176.874 | | 6.197 | | † |
| Br- | | 79.90455 | -218.874 | -206.614 | ±0.055 | | 20.786 | | 163.493 | | 6.197 | | † |
| BrCl | | 115.35670 | 14.789 | 22.233 | ±0.082 | | 35.011 | | 240.049 | | 9.407 | | † |
| DBr | | 81.91810 | -37.036 | -29.160 |  | | 29.228 | | 204.484 | | 8.668 | | † |
| DOBr | | 97.91750 | -65.898 | -55.487 | ±10.5 | | 39.755 | | 251.976 | | 10.474 | | # |
| BrF | | 98.90240 | -58.851 | -51.200 | ±1.0 | | 32.959 | | 228.988 | | 9.021 | | † |
| BrF3 | | 136.89921 | -255.6 | -244.81 | ±3.0 | | 67.354 | | 295.775 | | 14.712 | | † |
| BrF5 | | 174.89602 | -428.8 | -413.65 | ±2.0 | | 101.335 | | 323.253 | | 19.175 | | † |
| HBr <^~> | | 80.91194 | -35.851 | -28.005 | ±0.15 | | 29.141 | | 198.700 | | 8.648 | | † |
| H81Br+ | | 80.91139 | 1096. | 1097.64 | ±0.15 | | 29.153 | | 204.873 | | 8.651 | | # |
| HOBr Hypobromic acid <~> | | 96.91134 | -61.78 | -47.8 | ±0.54 | | 38.362 | | 247.786 | | 10.359 | | # |
| HOBr+ | | 96.91079 | 970.8 | 975.227 | ±0.6 | | 37.205 | | 252.202 | | 10.210 | | # |
| HBrH+ Bromonium | | 81.91933 | 920.5d | 925.0d | ±1.7d | | 34.332 | | 219.069 | | 9.974 | | # |
| BrNH2 (see NBrH2} | | 95.92662 |  |  |  | |  | |  | |  | | # |
| BrI Iodine Monobromide | | 206.80847 | 40.775d | 49.725 | ±0.066 | | 36.490 | | 258.718 | | 9.908 | | # |
| BrONO | | 125.90954 | 84.140 | 96.529 | ±8. | | 55.405 | | 288.760 | | 12.887 | | # |
| BrONO2 | | 141.90894 | 36.066 | 50.479 | ±8. | | 69.272 | | 313.457 | | 15.202 | | # |
| BRO <~> | | 95.9034 | 123.61 | 131.149 | ±0.29 | | 34.141 | | 232.898 | | 9.062 | | # |
| BrO+ | | 95.90285 | 1138.3 | 1139.9 | ±1.2 | | 31.081 | | 231.165 | | 8.807 | | # |
| BrO- Hypobromite | | 95.90395 | -113.997d | -100.006 | ±1.5d | | 31.066 | | 225.387 | | 8.806 | | # |
| BrO2 Br-O-O <~> | | 111.9028 | 110.2 | 119.251 | ±3.9 | | 46.577 | | 283.389 | | 11.859 | | #† |
| BrO2 O-Br-O | | 111.9028 | 158.18 | 167.78 | ±2.7 | | 45.243 | | 270.659 | | 11.340 | | #† |
| BrO3 | | 127.9022 | 221 | 233.180 | ±50 | | 59.995 | | 284.507 | | 13.101 | | # |
| BrS` | | 111.9700 | 148.5 | 155.8 | ±2.2 | | 34.740 | | 244.706 | | 9.353 | | # |
| TBr Tritium Bromide | | 82.920 | -40.29 | -32.51 | ±8. | | 29.435 | | 207.829 | | 8.683 | | # |
| Br2 (L) REFERENCE ELEMENT | | 159.8080 | 0 | 0 |  | | 75.680 | | 152.210 | | 24.520 | | † |
| Br2 gas <^~> | | 159.8080 | 30.881 | 45.676 | ±0.11 | | 36.057 | | 245.469 | | 9.725 | | † |
| Br2+ | | 159.80745 | 1051.573 | 1060.99 | ±0.22 | | 37.266 | | 213.233 | | 9.797 | | # |
| Br2- | | 159.80855 | -220.4 | -201.3 | ±1.9 | | 45.038 | | 231.861 | | 11.614 | | # |
| Br2NH (see NBr2H) | | 174.8227 |  |  |  | |  | |  | |  | | # |
| Br2O BrBrO | | 175.8074 | 164.9 | 180.701 | ±2.2 | | 51.296 | | 302.173 | | 13.059 | | #† |
| Br2O Br-O-Br | | 175.8074 | 104.61 | 121.095 | ±1.2 | | 50.051 | | 290.488 | | 12.375 | | #† |
| Br2S | | 191.87400 | 55.647 | 71.26 | ±4.2 | | 53.492 | | 305.867 | | 13.322 | | # |
| Br3N (see NBr3 ) | | 253.71874 |  |  |  | |  | |  | |  | | # |
| Br3P Phosphorus TriBromide | | 270.68576 | -124.26 | -100.031 | ±8. | | 76.086 | | 344.685 | | 17.906 | | # |
| Br3P+ Phosphorus Tribromide catio | | 270.68521 | 800.36 | 818.73 | ±10. | | 74.918 | | 354.034 | | 17.577 | | # |
| Br3P- Phosphorus Tribromide anion | |  | -293.w |  | ±17. | |  | |  | |  | | X |
| C(GR) REF ELEMENT <!> | | 12.0107 | 0 | 0 |  | | 8.528 | | 5.734 | | 1.054 | | † |
| C(diamond) (cr) | | 12.0107 | 1.849 | 2.380 | ±0.043 | | 6.109 ±2.2411 | | 2.364 | | 0.523 | | # |
| C <^!> | | 12.01070 | 716.67 | 711.198 | ±0.45 | | 20.839 | | 158.102 | | 6.536 | | † |
| C singlet (excited) c | | 12.01070 | 838.466 | 833.31d | ±0.055 | |  | |  | |  | | X |
| C triplet only (excited) d | | 12.01070 | 716.87 | 711.384 | ±0.58 | | 20.839 | | 158.101 | | 5.536 | |  |
| C+ | | 12.01045 | 1809.444 | 1804.034 | ±0.8 | | 20.974 | | 154.664 | | 6.649 | | † |
| C- | | 12.01125 | 588.55 | 589.785 | ±0.06 | | 20.787 | | 159.004 | | 6.219 | | † |
| ALC | | 38.99224 | 682.28 | 678.815 | ±50. | | 33.218 | | 225.918 | | 9.058 | | † |
| CBr | | 91.91470 | 495.85 | 500.2 |  | | 32.370 | | 230.888 | | 8.946 | | #† |
| CBrClF2 <~> | | 165.36421 | -442.19 | -430.989 | ±5.4 | | 74.650 | | 318.724 | | 15.528 | | #† |
| CBrCl2F FC-11B2 | | 181.81850 | -239.97 | -229.79 | ±5.4 | | 80.108 | | 330.773 | | 16.731 | | #† |
| CBrCl3 BromoTrichloroMethane | | 198.27280 | -42.07 | -32.92 | ±0.71d | | 85.307 | | 320.288 | | 17.934 | | # |
| CBrF3 Freon 1301 <~> | | 148.90991 | -652.26d | -640.14d | ±0.64d | | 69.270 | | 297.695 | | 14.444 | | #† |
| BrCN Cyanogen Bromide | | 105.92144 | 180.75 | 187.74 | ±0.76 | | 45.842 | | 246.185 | | 10.732 | | # |
| BrCN+ | | 105.92089 | 1330.2 | 1330.81 | ±1.1 | | 45.956 | | 252.500 | | 10.841 | | # |
| BrNC Isocyanogen Bromided | | 105.92144 | 338.53 | 344.396 | ±3.55 | | 45.636 | | 234.516 | | 11.782 | | # |
| CBr2 | | 171.81870 | 343.51 | 356.89 |  | | 49.273 | | 288.706 | | 12.192 | | #† |
| CBr2CLF FC-11B3 | | 226.26980 | -187.44 | -170.36 | ±5.4 | | 82.338 | | 343.087 | | 17.498 | | #† |
| CBr2CL2 | | 242.72410 | 3.39 | 19.34 | ±1.43 | | 88.011 | | 354.873 | | 18.804 | | # |
| CBr2F2 | | 209.81551 | -384.5 | -366.38 | ±1.33 | | 77.000 | | 325.413 | | 16.280 | | #† |
| Br2C=Oa liq. | | 187.81810 | -144.45d |  | ±0.96d | |  | |  | |  | | X |
| Br2C=O Dibromophosgene | | 187.81810 | -113.53 | -97.593 | ±0.45 | | 61.823 | | 307.931 | | 13.976 | | # |
| CBr3 | | 251.72270 | 232.212 | 254.030 | ±4.2 | | 69.174 | | 331.466 | | 16.015 | | #† |
| CBr3Cl | | 287.1754 | 53.03 | 76.6d | ±1.5 | | 89.848 | | 357.394 | | 19.581 | | #† |
| CBr3F | | 270.72110 | -132.3 | -108.463 | ±1.5 | | 85.042 | | 346.866 | | 18.409 | | #† |
| CBr4 cr monoclinic | | 331.6267 | 48.1d |  | ±1.3d | |  | |  | |  | | X |
| CBr4 | | 331.62670 | 102.01 | 132.3d | ±1.05 | | 91.162 | | 317.516 | | 20.396 | | # |
| CCL <~> | | 47.46340 | 432.611 | 428.860 |  | | 32.268 | | 224.556 | | 9.395 | | † |
| CCL+ cation | | 47.46285 | 1288.2 | 1279.4 | ±8. | | 30.261 | | 212.119 | | 8.753 | | # |
| CCL- anion | | 47.46395 | 425.88 | 428.197 | ±8. | | 35.817 | | 219.918 | | 9.525 | | # |
| CClD3 | | 53.50571 | -103.901 | -96.273 | ±8. | | 46.211 | | 241.760 | | 10.869 | | # |
| CCLF | | 66.46180 | 25.846 | 25.0 | ±30. | | 42.962 | | 259.150 | | 10.902 | | † |
| COClF Carbonic Chloride Fluoride | | 82.46120 | -412.791 | -410.054 | ±8. | | 52.397 | | 276.926 | | 11.904 | | †# |
| CCLF2 <~> | | 85.46021 | -275. | -272.96 | ±25. | | 55.172 | | 287.353 | | 12.432 | | † |
| CCLF3 FC-13 <^> | | 104.45861 | -710.02 | -704.93 | ±1.0d | | 66.887 | | 285.424 | | 13.791 | | † |
| CLCN Cyanogen Chloride <&> | | 61.47014 | 134.200 | 133.510 | ±0.45d | | 44.960 | | 236.144 | | 10.669 | | † |
| CLCN+ | | 61.46959 | 1333.33 | 1326.3 | ±0.95 | | 45.016 | | 242.867 | | 10.813 | | # |
| CLNC | | 61.47014 | 316.59 | 315.0 | ±2.4 | | 44.244 | | 264.563 | | 11.539 | | # |
| COCL Carbonyl Chloride <~> | | 63.46280 | -16.000 | -17.567 | ±10. | | 45.073 | | 265.195 | | 11.551 | | † |
| CCL2 <&> | | 82.91670 | 231.7 | 230.5 | ±1.7 | | 51.028 | | 266.112 | | 11.728 | | # |
| CCL2+ | | 82.91555 | 1226.42 | 1119.31 | ±8. | | 43.744 | | 266.132 | | 11.148 | | # |
| CCL2F | | 101.91450 | -105. | -103.57 | ±20. | | 59.121 | | 298.917 | | 13.217 | | † |
| CCL2F2 FREON-12 <^~> | | 120.91291 | -495.81 | -491.63 | ±1.4d | | 72.477 | | 300.908 | | 14.881 | | #† |
| COCl2 liq Phosgen liq | | 98.9155 | -242.62d | -255.32d | ±0.28d | |  | | 192.80 | |  | | X |
| COCL2 PHOSGEN | | 98.9158 | -219.5 | -217.80 | ±0.28d | | 57.761 | | 283.752 | | 12.879 | | † |
| CCL3 <&> | | 118.3697 | 71.128 | 71.553 | ±2.5 | | 63.500 | | 303.100 | | 14.400 | | † |
| CCL3F FC-11 <^> | | 137.36720 | -290.67 | -287.496 | ±1.12 | | 78.071 | | 309.785 | | 16.064 | | #† |
| CCL3NO2 Chloropicrin | | 164.37434 | -72.019 | -65.324 | ±8. | | 104.209 | | 355.281 | | 21.145 | | # |
| CCL3O\* | | 134.36820 | -18.41 | -18.12 |  | | 90.154 | | 332.520 | | 18.768 | | # |
| CCL3OO\* | | 150.36760 | -20.744 | -16.634 | ±8. | | 95.677 | | 341.828 | | 19.396 | | # |
| CCL4 liquid c | | 153.82150 | -128.22d | -108.81d | ±0.49d | | 133.888 | | 216.187 | |  | |  |
| CCL4 <^> | | 153.82150 | -95.6 | -93.343 | ±2.5 | | 82.890 | | 309.467 | | 17.159 | | † |
| CD <&> | | 14.0251 | 599.700 | 596.251 |  | | 29.206 | | 192.997 | | 8.795 | | # |
| CD A 4Σ-  (Excited state only) | | 14.02480 | 670.477 | 667.158 |  | | 29.176 | | 189.887 | | 8.657 | | # |
| CDCLO Formyl-d-Chloride | | 65.47690 | -190.678 | -187.627 |  | | 47.008 | | 261.854 | | 11.218 | | # |
| CDCL3 Chloroform-d | | 120.38290 | -107.946 | -103.221 | ±8. | | 68.295 | | 297.051 | | 14.385 | | # |
| CDH3 | | 17.04862 | -78.45 | -70.49 |  | | 36.573 | | 200.068 | | 10.08 | | # |
| DCN | | 28.03154 | 128.220 | 128.407 | ±6.7 | | 37.590 | | 205.168 | | 9.487 | | # |
| DN=C=O Isocyanic acid-D | | 44.03094 | -128.415 | -125.852 | ±8. | | 48.136 | | 244.244 | | 11.450 | | # |
| CDO Formyl – D Radical | | 30.0245 | 40.945 | 40.0 |  | | 35.920 | | 228.610 | |  | | # |
| CD2 | | 16.0389 | 382.59 | 382.063 |  | | 36.262 | | 204.294 | | 10.150 | | # |
| CD2O Methanal-D2 | | 32.0383 | -114.893 | -111.141 |  | | 38.137 | | 225.076 | | 10.211 | | # |
| CD3 | | 18.05301 | 138.69 | 141.841 |  | | 41.807 | | 207.024 | | 10.756 | | # |
| CD3F MethylFluoride-D3 | | 37.05141 | -261.115 | -253.236 | ±8. | | 41.909 | | 229.852 | | 10.440 | | # |
| O=CD-ND2 Formamide-D3 | | 48.05915 | -212.970 | -203.549 | ±8. | | 60.306 | | 290.056 | | 13.162 | | # |
| CD3NO2 | | 64.05885 | -61.789 | -48.423 |  | | 63.166 | | 291.669 | | 13.556 | | # |
| CD4 RRHO | | 20.0671 | -89.010 | -81.166 |  | | 40.536 | | 199.014 | | 10.348 | |  |
| CD4 ANHARMONIC | | 20.0671 | -89.010 | -81.161 |  | | 40.582 | | 199.023 | | 10.343 | | # |
| CD4O CD3OD Methanol-d4 | | 36.06651 | -217.670 | -207.07 |  | | 49.478 | | 249.248 | | 11.932 | | # |
| CD5N CD3ND2 MethylAmine-d5 | | 36.08795 | -41.973 | -27.405 | ±0.6 | | 57.167 | | 251.355 | | 12.244 | | # |
| CF <~> | | 31.00910 | 246.932 | 243.333 | ±0.15d | | 30.056 | | 213.034 | | 9.065 | | † |
| CF+ Fluoromethyliumylidened | | 31.00855 | 1132.d | 1122.66d | ±0.55 | | 29.642 | | 201.509 | | 8.697 | | #† |
| CF- | | 31.00965 | 197.9d | 200.6d | ±2.1d | | 31.858 | | 199.919 | | 8.880 | | # |
| FCN <&> | | 45.01584 | 8.141 | 8.132 | ±0.72 | | 41.757 | | 224.607 | | 10.129 | | #† |
| FCN+c | | 45.01529 | 1300.66 | 1293.847 | ±1.1 | | 42.557 | | 232.192 | | 10.417 | | # |
| FNC d | | 45.01584 | 301.1 | 299.19 | ±2.24 | | 43.166 | | 268.604 | | 11.713 | | # |
| COF (FCO/CFO) <~> | | 47.00850 | -176.305 | -176.887 | ±0.5 | | 38.880 | | 248.992 | | 10.388 | | #† |
| COF Fluoroisoformyl 1871-24-5 | | 47.00850 | -33.8 | -39.2 | ±1.2 | |  | |  | |  | | X |
| COF+ c CAS # 1871-25-6d | | 47.00795 | 1355.1d | 1347.4d | ±2.2d | |  | |  | |  | | X |
| FCO+ c 38264-00-5 | | 47.00795 | 730.1d | 724.2d | ±1.5d | | 39.388 | | 222.810 | | 9.703 | | # |
| FCO-c,d | | 47.00905 | -410.14 | -405.352 | ±1.66 | | 43.822 | | 251.940 | | 11.216 | | # |
| CF2(s) (polymer C2F4 Teflon)/2 | | 50.00751 | -12.850 | -2.971 |  | | 51.282 | | 59.679 | | 11.373 | | # |
| CF2 singlet <~> | | 50.00751 | -193.36d | -193.84d | ±0.57d | | 38.915 | | 240.831 | | 10.351 | | #† |
| CF2 Difluoromethylene triplet | | 50.00751 | 44.07d | 43.35d | ±0.57d | | 40.031 | | 251.177 | | 10.576 | | # |
| CF2+ | | 50.00696 | 917.03 | 910.37 | ±1.6 | | 38.541 | | 246.731 | | 10.342 | | † |
| CF2- c | | 50.00805 | -216.096 | -211.019 | ±0.73d | | 44.228 | | 258.428 | | 10.999 | | # |
| COF2 <~> | | 66.00721 | -606.65 | -603.57 | ±0.5 | | 47.365 | | 258.971 | | 11.134 | | #† |
| COF2+ | | 66.00636 | 656.82 | 653.379 | ±0.6 | | 48.745 | | 260.659 | | 11.463 | | # |
| COF2- | | 66.00746 | -611.6 | -603.345 | ±2.77 | | 54.339 | | 265.677 | | 12.161 | | # |
| FCOF *trans* Fluoro(fluorooxy) Methylene | | 66.00691 | -40.2d | -38.7d | ±2.0d | | 54.686 | | 270.473 | | 12.543 | | # |
| FCOF *cis* | | 66.00691 | -136.7d | -135.5d | ±2.1 | | 56.177 | | 276.481 | | 12.919 | | # |
| CF3 <~> | | 69.00591 | -467.4a | -464.6 | ±1.97 | | 49.642 | | 264.521 | | 11.491 | | † |
| CF3+ Trifluoromethylium | | 69.00536 | 411.627 | 408.179 | ±0.7d | | 49.339 | | 254.540 | | 11.541 | | † |
| CF3- | | 69.00645 | -646.7d | -638.57 | ±1.9d | | 56.614 | | 263.934 | | 12.358 | | # |
| CF3I <~> | | 195.91038 | -590.5 | -584.62 | ±0.68 | | 70.941 | | 307.633 | | 15.008 | | # |
| CF3O Radical <~> | | 85.00531 | -630.696 | -625.69 | ±8. | | 64.550 | | 283.750 | | 13.622 | | # |
| CF3OO RADICAL | | 101.00471 | -637.290 | -630.602 | ±8. | | 80.004 | | 317.945 | | 16.283 | | # |
| CF4 FC-14 <^~> | | 88.00461 | -933.4 | -927.15 | ±0.53 | | 61.052 | | 261.459 | | 12.730 | | † |
| CH new 2022 <!> | | 13.01864 | 596.171 | 592.857 | ±0.1 | | 29.175 | | 183.037 | | 8.625 | | # |
| CH A 4Σ-  (Excited state only) | | 13.01864 | 667.919 | 664.583 | ±0.68d | | 29.151 | | 182.626 | | 8.624 | | # |
| CH A 2Δ (Excited state only) | | 13.01864 | 876.167 | 872.829 |  | | 29.156 | | 177.109 | | 8.626 | | # |
| CH B 2Σ- (Excited state only) | | 13.01864 | 909.012 | 905.656 |  | | 29.298 | | 178.364 | | 8.643 | | # |
| CH+ ion | | 13.01809 | 1630.571 | 1620.15d | ±0.28d | | 29.159 | | 171.673 | | 8.628 | | † |
| CH- | | 13.01919 | 471.085 | 474.07d | ±0.65d | | 35.329 | | 178.546 | | 9.552 | | # |
| CHBr | | 92.92264 | 377.857 | 384.99 | ±2. | | 39.789 | | 252.872 | | 10.416 | | # |
| CHBrClF | | 137.37374 | -231.8d | -219.3d | ±5.5d | | 62.869 | | 310.691 | | 13.787 | | #† |
| CHBrCl2 FC-20B1 | | 163.82804 | -51.48 | -39.48 | ±5.4 | | 67.395 | | 316.478 | | 14.730 | | #† |
| CHBrF2 HBFC-22B1 | | 130.91975 | -425.46 | -412.26 | ±1.07 | | 58.767 | | 295.230 | | 13.170 | | † |
| CHBr2 | | 172.82664 | 198.489 | 215.446 |  | | 54.834 | | 298.588 | | 12.851 | | # |
| CHBr2CL | | 208.27934 | -2.95 | +16.16 | ±5.4 | | 69.149 | | 328.026 | | 15.291 | | #† |
| CHBr2F FC-21B2 or FC-23 | | 191.82504 | -179.5 | -159.639 | ±5.4 | | 64.915 | | 316.925 | | 14.360 | | #† |
| CHBr3 (liq) Bromoform d | | 252.73064 | 1.6d |  | ±1.3d | |  | |  | |  | | X |
| CHBr3 Bromoform | | 252.73064 | 47.38 | 73.53 | ±1.24 | | 71.026 | | 330.864 | | 15.915 | | # |
| CHBr3O CBr3OH | | 268.73004 | -121.043 | -92.633 | ±10. | | 92.739 | | 353.385 | | 19.534 | | # |
| CHBr3O+ CBr3OH+ | | 268.72949 | 883..188 | 883.159 | ±12. | | 94.293 | | 364.593 | | 20.196 | | # |
| CHCL | | 48.47134 | 320.7 | 320.362 | ±8. | | 37.854 | | 235.136 | | 10.216 | | #† |
| CHCLF | | 67.46974 | -83.490 | -80.0 | ±25. | | 43.662 | | 266.544 | | 10.801 | | † |
| CHCLF2 HCFC-22 | | 86.46815 | -489.8d | -483.8d | ±2.0d | | 55.851 | | 280.895 | | 12.362 | | #† |
| CHCLO Formyl Chloride | | 64.47074 | -180.573 | -177.363 |  | | 44.687 | | 259.282 | | 11.008 | | # |
| CHCL2 | | 83.92487 | 95.8 | 97.469 |  | | 53.900 | | 285.500 | | 12.800 | | † |
| CHCL2F FC-21 <^> | | 102.92244 | -284.900 | -279.305 | ±5.5d | | 60.987 | | 293.173 | | 13.286 | | † |
| CHCL2O \*CCl2OH | | 99.92344 | -83.554 | -79.082 | ±8. | | 67.834 | | 312.822 | | 14.337 | | # |
| CHCL3 liquid Chloroform c | | 119.37674 | -134.04d |  | ±0.63 | | 114.35 | |  | |  | | X |
| CHCL3 CHLOROFORM <^> | | 119.37674 | -103.259 | -98.353 | ±0.67d | | 65.384 | | 295.875 | | 14.153 | | #† |
| CHCL3O CCl3OH | | 135.37614 | -275.977 | -270.06 | ±3.2 | | 86.644 | | 323.540 | | 17.008 | | # |
| CHD2NO2 | | 63.05268 | -57.716 | -44.135 |  | | 60.806 | | 289.264 | | 13.290 | | # |
| CHD3 | | 19.06095 | -85.290 | -77.391 |  | | 39.005 | | 208.610 | | 10.243 | | # |
| CHF RADICAL singlet <~> | | 32.01734 | 148.614 | 148.333 | ±0.58d | | 34.588 | | 223.342 | | 9.981 | | #† |
| CHF triplet | | 32.01704 | 210.51 | 210.205 | 0.71d | | 34.972 | | 231.423 | | 10.005 | | # |
| CHF + c Fluoromethyliumyld | | 32.01649 | 1123.37 | 1116.891 | ±2.0 | | 34.519 | | 226.609 | | 9.982 | | # |
| CHF – c | | 32.01759 | 90.275 | 95.994 | ±0.62 | | 36.879 | | 232.444 | | 10.179 | | # |
| CHFO HFCO | | 48.01644 | -382.529 | -378.903 | ±0.55d | | 40.019 | | 246.727 | | 10.414 | | # |
| CHFO+ HFCO+ | | 48.01589 | 819.23 | 816.377 | ±1.25 | | 41.856 | | 253.771 | | 10.695 | | # |
| CHF2 <~> | | 51.01544 | -238.9 | -235.707 |  | | 43.062 | | 258.000 | | 10.920 | | † |
| CHF3(liq) Fluoroform HFC-23 c | | 70.01385 | -704.32d |  | ±0.65d | |  | |  | |  | | X |
| CHF3 Fluoroform HFC-23 <^~> | | 70.01385 | -693.289 | -686.34 | ±0.63d | | 51.139 | | 259.375 | | 11.573 | | †# |
| CHF3O CF3OH | | 86.01325 | -911.392 | -903.074 | ±8. | | 70.162 | | 281.858 | | 14.268 | | # |
| CF3OH- anion | | 86.01380 | *-861.997* | -850.595 | ±8. | | 86,917 | | 310.365 | | 17.466 | | # |
| CHI2 DiIodoMethyl Radical | | 266.82758 | 290.4 | 294.943 | ±6. | | 58.519 | | 293.206 | | 13.940 | | # |
| CHI3 IODOFORM | | 393.73205 | 210.874 | 218.799 | ±4.2 | | 75.072 | | 355.672 | | 17.157 | | † |
| HCN anharmonica <^~> | | 27.02568 | 129.799 | 129.676d | ±0.1d | | 35.857 | | 201.824 | | 9.235 | | † |
| HCN+ | | 27.02483 | 1448.748 | 1442.676 | ±0.21d | | 37.399 | | 209.919 | | 9.497 | | # |
| HCN-c | | 27.02593 | 123.31 | 129.51d | ±0.1R | | 35.383 | | 225.915 | | 10.046 | | # |
| HNC Hydrogen isocyanide | | 27.02568 | 191.908 | 191.530 | ±0.57d | | 40.271 | | 205.511 | | 10.001 | | † |
| HNC+ | | 27.02483 | 1359.05 | 1352.891 | ±1.4d | | 38.160 | | 208.755 | | 9.584 | | # |
| HNC- | | 27.02593 | 185.543 | 191.56 | ±0.38R | |  | |  | |  | | X |
| HNCO Isocyanic acid <~> | | 43.02478 | -118.600 | -119.05d | ±0.37d | | 45.078 | | 238.265 | | 10.966 | | † |
| HNCO+ Isocyanic acid cation | | 43.02423 | 1006.582 | 1002.939 | ±0.54 | | 47.690 | | 234.205 | | 11.406 | | # |
| HOCN Cyanic acid <~> | | 43.02478 | -15.456 | -12.76 | ±20. | | 46.047 | | 241.244 | | 11.268 | | # |
| HCNO IsoFulminic acid <~> | | 43.02478 | 167.603 | 171.042 | ±1.2 | | 48.395 | | 225.025 | | 10.623 | | # |
| HCNO+ IsoFulminic acid cation | | 43.02423 | 1218.89 | 1215.822 | ±1.53 | | 49.864 | | 232.192 | | 10.834 | | # |
| HONC Fulminic acid d | | 43.02478 | 233.15d | 234.68d | ±1.02d | | 49.654 | | 248.364 | | 12.400 | | # |
| CHN2 HN\*-CN Cyanamide Rad. | | 41.03212 | 315.838 | 318.414 | ±8. | | 46.657 | | 247.283 | | 11.381 | | # |
| CHN2 cy H(-C-N=N-) Diazirinyl | | 41.03212 | 556.179 | 559.612 | ±8. | | 41.497 | | 242.076 | | 10.525 | | # |
| CH(O)N3 Formil Azide | | 71.03826 | 163.586 | 171.997 | ±8. | | 64.977 | | 289.428 | | 14.221 | | # |
| CH(NO2)3 | | 151.03526 | -13.389 | +5.042 |  | | 134.09 | | 435.569 | | 25.902 | | # |
| CHO FORMYL RADICAL <!> | | 29.01804 | 42.3 | 41.928 | ±0.3 | | 34.680 | | 224.28 | | 10.000 | | # |
| CHO+ Oxomethylium <~> | | 29.01749 | 833.940 | 827.4 | ±0.26 | | 34.172 | | 201.764 | | 9.046 | | #† |
| CHO- Formyl anion | | 29.01859 | 5.958 | 11.747 | ±0.44d | | 35.462 | | 222.237 | | 10.036 | | # |
| COH Isoformyl | | 29.01804 | 218.10  217.69g | 217.72 | ±0.83  0.67g | | 34.970 | | 225.030 | | 10.008 | | # |
| COH- Isoformyl anion | | 29.01859 | 47.2d | 50.8d | ±2.7d | | 47.273 | | 239.129 | | 12.136 | | # |
| COH+ c  Hydroxymethylimuylidene | | 29.01749 | 993.859d | 992.33d | ±0.8 | |  | |  | |  | | X |
| CHOS\* O=CH-S\* | | 61.08404 | 27.121 | 29.536 | ±8. | | 46.428 | | 268.37 | | 11.625 | | # |
| COOH equilibrium HOCO <~> *trans-cis* | | 45.01744 | -183.97d | -181.39 | ±0.55 | | 43.610 | | 251.736 | | 10.813 | | #† |
| HOCO *trans* Hydroxyformil | | 45.01744 | -184.36d | -181.95 | ±0.55 | | 44.134 | | 251.607 | | 10.909 | | # |
| HOCO *cis* | | 45.01744 | -177.06d | -173.26d | ±0.62 | | 43.696 | | 251.739 | | 10.843 | | # |
| COOH+ HOCO+ c | | 45.01689 | 604.166 | 600.905 | ±0.472 | | 44.976 | | 240.172 | | 11.031 | | # |
| HOCO- *cis* | | 45.01799 | -329.5d | -320.44 | ±1.2 | | 46.240 | | 249.307 | | 11.101 | | # |
| HCOO\* Formyloxydanyl Radical | | 45.01744 | -125.059  -127.23h | -122.350 | ±0.6  0.56h | | 41.985 | | 255.230 | | 11.258 | | # |
| HCOO+ 54375-27-8 | | 45.01689 | 1018.1 | 1015.3 | ±1.63 | | 44.992 | | 240.181 | | 11.033 | | X |
| HC(O)O- Formyloxy anion | | 45.01799 | -472.05 | -462.152 | ±0.75 | | 38.528 | | 244.166 | | 10.267 | | # |
| HOCO- *equil*  Hydroxyformyl anion | | 45.01799 | -327.630g | -317.695 | ±058g | | 50.522 | | 254.138 | | 11.885 | | # |
| HCOO *trans* Dioxymethylened | | 45.01744 | 356.6 | 359.0 | ±5.9d | |  | |  | |  | | X |
| HCOO equil Dioxymethylened | | 45.01744 | 329.9d | 332.1d | ±5.9d | | 49.044 | | 258.230 | | 11.641 | | # |
| HC\*(O-O) Cyclo Dioxiranyl | | 45.01744 | 212.75 | 216.252 | ±1.97 | | 40.689 | | 245.442 | | 10.465 | | # |
| HCO3- Bicarbonate anion (gas) | | 61.01738 | -737.57 | -724.8 | ±8. | | 53.316 | | 266.488 | | 11.732 | | # |
| CHO3 O=CHOO\* formylperoxy | | 61.01684 | -108.972  -105.52h | -103.640 | ±8.  ±0.93h | | 56.205 | | 278.620 | | 12.975 | | # |
| HCP HC≡P Methinphosphide | | 43.99240 | 216.363 | 217.790 | ±8. | | 36.018 | | 214.407 | | 9.221 | | # |
| HCS | | 45.08464 | 282.47 | 282.053 | ±8. | | 36.376 | | 236.044 | | 10.117 | | # |
| CSi see SiC Siliconcarbide | |  |  |  |  | |  | |  | |  | |  |
| CH2 Methylene Equilibrium <!> | | 14.02658 | 391.2 | 390.7 | ±0.14d | | 35.130 | | 194.436 | | 10.032 | | # |
| CH2 Methylene SINGLET <!> | | 14.02658 | 428.8 | 428.3 | ±0.15d | | 33.781 | | 189.220 | | 9.940 | | # |
| CH2 Methylene Triplet only <!> | | 14.02658 | 391.2 | 390.7 | ±1.6 | | 35.014 | | 194.418 | | 10.027 | | # |
| CH2+ | | 14.02603 | 1399.825 | 1393.114 | ±0.15d | | 35.109 | | 191.690 | | 10.036 | | # |
| CH2- | | 14.02713 | 322.326 | 328.113 | ±0.56d | | 33.653 | | 196.021 | | 9.933 | | # |
| CH2BrCL HALON101 | | 129.38358 | -43.471 | -30.7d | ±5.5d | | 52.663 | | 287.768 | | 12.206 | | †# |
| CH2BrF | | 112.92898 | -212.42 | -197.85 | ±5.5d | | 49.089 | | 276.282 | | 11.623 | | #† |
| CH2BrI BromoIodoMethane | | 220.83505 | 56.8 | 72.199 | ±6. | | 56.338 | | 307.845 | | 12.980 | | # |
| CH2Br2 | | 173.83458 | 3.10 | 24.527 | ±1.15 | | 54.552 | | 293.391 | | 12.614 | | # |
| CH2CL <~> | | 49.47928 | 119.2 | 122.332 |  | | 43.173 | | 242.634 | | 10.980 | | † |
| CH2CLF GC-31 | | 68.47768 | -262.546 | -256.4d | ±5.5d | | 47.046 | | 264.426 | | 11.252 | | † |
| CH2CL2 (liq)a | | 84.93198 | -123.46d |  | ±0.66d | |  | |  | |  | | X |
| CH2CL2 <^> | | 84.93198 | -95.396 | -88.547 | ±0.74 | | 50.951 | | 270.365 | | 11.854 | | † |
| CH2DNO2 | | 62.04652 | -52.532 | -38.81 |  | | 58.983 | | 286.942 | | 13.098 | | # |
| CH2D2 | | 18.05478 | -81.750 | -73.81 |  | | 37.663 | | 207.948 | | 10.152 | | # |
| CH2F <~> | | 33.02498 | -32.077 | -28.572 | ±8. | | 39.568 | | 229.665 | | 10.429 | | † |
| CH2F2 (liq) FC-32 | | 52.02339 | -467.45d |  | ±0.55d | |  | |  | |  | | X |
| CH2F2 FC-32 <~> | | 52.02339 | -452.709 | -444.65 | ±0.53d | | 42.869 | | 246.347 | | 10.693 | | † |
| H2CN\* Methyleneamidogen <~> | | 28.03332 | 238.569 | 242.229 | ±0.93 | | 37.768 | | 224.307 | | 10.197 | | # |
| H2CN+ triplet | | 28.03277 | 1459.8d | 1457.2d | ±2.5d | | 38.062 | | 234.863 | | 10.207 | | # |
| H2CN- Methyleneamidogen | | 28.03387 | 183.1d | 193.1d | ±1.2d | | 36.164 | | 218.240 | | 10.075 | | # |
| HCNH *trans* E-Iminomethyl | | 28.03332 | 272.59 | 276.24 | ±1.31 | | 38.072 | | 229.017 | | 10.211 | | # |
| HCNH *cis* Z-Iminomethyl | | 28.03332 | 291.11 | 294.689 | ±1.31 | | 38.892 | | 229.493 | | 10.278 | | # |
| HCNH+ c | | 28.03277 | 955.58d | 953.4d | ±1.6d | | 42.379 | | 206.208 | | 9.802 | | # |
| HCNH- *trans* c Iminomethyld | | 28.03387 | 229.05 | 239.072 | ±1.88 | | 35.673 | | 224.378 | | 10.032 | | # |
| HCNH- *cis* | | 28.03387 | 244.32 | 254.317 | ±1.88 | | 36.048 | | 224.618 | | 10.057 | | # |
| CNH2d Aminomethylidyne | | 28.03332 | 368.80 | 372.353 | ±1.45 | | 38.606 | | 224.280 | | 10.303 | | # |
| CNH2+ triradical cation c | | 28.03277 | 1171.87 | 1168.99 | ±2.46 | | 40.770 | | 219.260 | | 10.537 | | # |
| H2NCO | | 44.03272 | -13.493 | -7.670 | ±8 | | 52.145 | | 261.635 | | 12.373 | | # |
| CH2NO CH2=N-O\* | | 44.03272 | 154.574 | 161.568 | ±8. | | 47.206 | | 253.626 | | 11.203 | | # |
| H2CNO H2C\*N=O⬄CH2=N-O\* !! | | 44.03302 | 223.928 |  | ±8.4 | | 42.388 | | 244.644 | |  | |  |
| CH2NO2 NITRO-METHYL RAD | | 60.03242 | 128.399 | 137.818 | ±8. | | 58.673 | | 288.583 | | 13.118 | | # |
| CH2NO2- NITRO-METHYL anion | | 60.03267 | -119.144 | -103.776 | ±8. | | 60.608 | | 269.244 | | 13.158 | | # |
| CH2NO3 Methyl Nitrate Radical | | 76.03152 | 75.186 | 85.027 | ±8. | | 82.224 | | 310.849 | | 17.037 | | # |
| CH2NO3+Methylene Nitrate cation | | 76.03097 | 781.538 | 785.042 | ±8. | | 78.918 | | 292.703 | | 16.903 | | # |
| CH2N2 (cr) Cyanamide cr | | 42.04006 | 58.84d |  | ±0.55d | |  | |  | |  | | X |
| CH2N2 CYANAMIDE H2N-CN | | 42.04006 | 134.553 | 140.881 | ±8 | | 51.224 | | 242.169 | | 11.864 | | # |
| H2CN2 HN=C=NH | | 42.04006 | 146.478 | 153.138 | ±8 | | 50.808 | | 237.172 | | 11.532 | | # |
| CH2N2 H2C=N=N | | 42.04006 | 268.425 | 274.647 | ±8 | | 51.781 | | 242.272 | | 11.969 | | # |
| H2CN2 Cy 3H-Diazirine | | 42.04006 | 315.365 | 323.136 | ±8. | | 41.463 | | 237.580 | | 10.420 | | # |
| H2CN2 Cy 1H-Diazirine | | 42.04006 | 398.062 | 406.387 | ±8. | | 45.208 | | 246.252 | | 10.866 | | # |
| CH2N2O H2C=N-N=O | | 58.03946 | 229.589 | 238.224 | ±8. | | 61.025 | | 275.259 | | 13.897 | | # |
| CH2N2O2 H2C=N-NO2 | | 74.03886 | 129.273 | 141.310 | ±8. | | 70.391 | | 293.002 | | 14.835 | | # |
| CH2(NO2)2 H2C(NO2)2 | | 106.03796 | -52.421 | -34.338 | ±8. | | 84.334 | | 356.676 | | 17.469 | | # |
| CH2(NO2)2- H2C(NO2)2 anion | | 106.03820 | -173.306 | -151.498 | ±8. | | 96.526 | | 362.801 | | 20.395 | | # |
| CH2N4 Cy 1H-Tetrazole CH2N4 | | 70.05354 | 320.000 | 335.232 | ±3. | | 55.908 | | 269.008 | | 11.629 | | # |
| CH2O polyoxymethylene Solid c | | 30.02598 | -170.875d |  | ±0.21d | |  | |  | |  | | X |
| CH2O Paraformaldehyde Cr c | | 30.02598 | -179.2 |  | ±1.6d | |  | |  | |  | | X |
| CH2O FORMALDEHYDE <!> | | 30.02598 | -109.16 | -105.322 | ±0.11 | | 35.388 | | 218.764 | | 10.020 | | #† |
| H2CO+ Formaldehyde cationed | | 30.02543 | 948.386 | 945.814 | ±0.13d | | 38.241 | | 225.544 | | 10.237 | | # |
| H2CO- Formaldehyde anion | | 30.02653 | -33.9d | -24.0d | ±2.2d | | 37.190 | | 232.186 | | 10.155 | | # |
| HCOH *trans* HydroxyMethylene | | 30.02598 | 108.16d | 111.93 | ±0.43 | | 36.066 | | 225.212 | | 10.059 | | # |
| HCOH *cis* HydroxyMethylene | | 30.02598 | 126.63 | 130.37 | ±0.44 | | 36.260 | | 225.393 | | 10.075 | | # |
| HCOH triplet d | | 30.02598 | 216.0d | 219.1d | ±1.4d | | 39.242 | | 236.235 | | 10.316 | | # |
| HCOH+ equil. | | 30.02543 | 974.79 | 972.268 | ±1.48 | | 37.716 | | 229.514 | | 10.186 | | # |
| HCOH- equilc HydroxyMethylene | | 30.02653 | 139.19 | 148.443 | ±1.71 | | 43.163 | | 236.846 | | 10.806 | | # |
| HCOH- *trans* d | | 30.02653 | 151.5d | 153.4d | ±1.8d | |  | |  | |  | | X |
| HCOH+ *cis*d | | 30.02543 | 989.5d | 986.9d | ±1.8d | |  | |  | |  | | X |
| HCOH- *cis* c | | 30.02653 | 153.47 | 161.6d | ±1.9d | |  | |  | |  | | X |
| H2OC singlet Aquacarbon | | 30.02598 | 467.5d | 470.2d | ±2.4d | |  | |  | |  | | X |
| H2OC triplet Aquacarbon | | 30.02598 | 439.5d | 441.4d | ±2.1d | |  | |  | |  | | X |
| CH2OS O=CH-SH | | 62.09198 | -123.54 | -117.365 | ±8. | | 53.189 | | 270.982 | | 12.102 | | # |
| CH2SO S=CH-OH | | 62.09198 | -95.977 | -89.118 | ±8. | | 49.121 | | 260.825 | | 11.415 | | # |
| HCOOH (liq) c | | 46.02538 | -425.29d | -432.13d | ±0.24d | | 99.161 | | 128.951 | |  | |  |
| HCOOH FORMIC ACID equil. | | 46.02538 | -378.49 | -371.196 | ±0.25 | | 41.305 | | 247.148 | | 10.928 | | † |
| HCOOH FORMIC ACID syn | | 46.02538 | -378.51 | -371.19 | ±0.25 | | 44.156 | | 248.287 | | 10.764 | | # |
| HCOOH FORMIC ACID anti | | 46.02538 | -362.10 | -354.86 | ±0.41 | | 45.523 | | 249.035 | | 10.974 | | # |
| HCOOH+ FORMIC ACID anti | | 46.0248 | 722.5d | 723.3d | ±1.4d | |  | |  | |  | | X |
| HCOOH- FORMIC ACID syn | | 46.02593 | -267.1d | -254.7d | ±2.3d | | 52.768 | | 264.607 | | 12.322 | | # |
| H2COO Dioxymethyl | | 46.02538 | 106.3d | 113.4d | ±1.2d | | 47.169 | | 249.361 | | 11.090 | | # |
| H2COO+d | | 46.02483 | 1075.2d | 1075.8d | ±1.9d | | 47.660 | | 256.228 | | 11.271 | | # |
| H2COO- c | | 46.02593 | 45.03 | 57.1d | ±2.4 | | 43.256 | | 255.365 | | 10.695 | | 0# |
| H2C(O-O) Dioxirane (cyclo) | | 46.02538 | 1.61 [1.3]d | 9.362 [9.0]d | ±1.14 | | 41.778 | | 240.562 | | 10.450 | | # |
| H2C(O-O)+ Dioxirane cation (cycl) | | 46.02483 | 1049.93 | 1051.367 | ±2.13 | | 42.799 | | 246.502 | | 10.567 | | # |
| H2C(O-O)- Dioxirane anion (cy) | | 46.02593 | -184.12 | -170.416 | ±3.8 | | 43.256 | | 249.601 | | 10.695 | | # |
| CH2OOH Hydroperoxymethyl | | 47.03332 | 65.6 | 74.027 | ±1.4 | | 72.279 | | 275.931 | | 14.008 | | # |
| O=C(OH)2 Carbonic acid g tr-tr | | 62.02480 | -570.55 | -561.70 | ±0.98 | | 60.466 | | 296.791 | | 14.140 | | # |
| O=C(OH)2+ Carbonic acid cation | | 62.02423 | 503.80 | 506.32 | ±8. | | 61.804 | | 303.481 | | 14.372 | | # |
| O=C(OH)2- Carbonic acid anion | | 62.02533 | -501.74 | -488.10 | ±8. | | 67.887 | | 308.371 | | 15.126 | | # |
| H2CS | | 46.09258 | 114.951 | 118.676 | ±8. | | 38.196 | | 231.186 | | 10.209 | | # |
| H2CS2 S=CH-SH | | 78.15858 | 113.817 | 119.588 | ±8. | | 56.137 | | 276.474 | | 12.575 | | # |
| CH2S3 S=CH-S-SH | | 110.22458 | 136.783 | 142.721 | ±8. | | 78.199 | | 319.963 | | 16.820 | | # |
| CH2S3+ S=CH-S-SH+ cation | | 110.22403 | 1008.93 | 1008.17 | ±8. | | 79.729 | | 326.736 | | 17.041 | | # |
| CH2Si HSi≡CH | | 42.11208 | 452.424 | 453.661 | ±8. | | 47.841 | | 241.991 | | 11.503 | | # |
| CH2Si- HSi≡CH anion | | 42.11263 | 338.644 | 346.284 | ±8. | | 47.098 | | 248.026 | | 11.170 | | # |
| CH3 <!> | | 15.03452 | 146.7 | 150.0 | ±0.08d | | 38.417 | | 194.008 | | 10.366 | | # |
| CH3+ | | 15.03397 | 1101.792 | 1099.37 | ±0.077 | | 34.749 | | 186.827 | | 9.983 | | # |
| CH3- | | 15.03507 | 144.4d | 154.354 | ±1.11 | | 34.938 | | 193.515 | | 9.999 | | # |
| CH3Brc (liq) | | 94.93852 | -59.78 | -56.77d | ±0.187 | |  | |  | |  | | X |
| CH3Br <~> | | 94.93852 | -36.443 | -21.034 | ±0.18d | | 42.312 | | 245.954 | | 10.607 | | # |
| CH3Br+ | | 94.93797 | 987.41 | 995.72 | ±0.2 | | 48.635 | | 250.568 | | 11.508 | | # |
| CH3Cl (liq)dd | | 50.48722 | -102.38d | -106.35d | ±0.2 | |  | |  | |  | | X |
| CH3CL <^~> | | 50.48722 | -81.87 | -73.94 | ±0.6 | | 40.741 | | 234.396 | | 10.416 | | † |
| CH3Cl+c | | 50.48667 | 1012.6 | 1014.15 | ±0.2 | | 42.293 | | 240.874 | | 10.599 | | # |
| CH3F FC-41 (liq)c | | 34.03292 | -246.78d |  | ±0.51d | |  | |  | |  | | X |
| CH3F FC-41 <~> | | 34.03292 | -236.577 | -228.544 | ±0.3 | | 37.505 | | 222.826 | | 10.135 | | #† |
| CH3F+ | | 34.03237 | 979.4 | 980.8 | ±0.64 | | 42.408 | | 229.921 | | 10.563 | | # |
| CH3PF2=O | | 100.00448 | -984.9 | -969.55 | ±8. | | 86.928 | | 305.191 | | 16.917 | | # |
| CH3PF2=O+ (5 elements – e+) | | 100.00394 | 128.332 | 142.7 | ±8. | | 90.369 | | 317.498 | | 17.856 | | X |
| CH3Hg Methyl Mercury | | 215.62452 | 188.28 | 200.21 | ±8.4 | | 46.073 | | 260.58 | | 11.165 | | # |
| CH3Ia (liq) | | 141.93899 | -12.220d |  | ±0.19 | |  | |  | |  | | X |
| CH3I Methyl Iodide <~> | | 141.93899 | 14.30 | 24.46d | ±0.17d | | 44.084 | | 253.007 | | 10.816 | | †# |
| CH3I+ | | 141.93844 | 941.1d | 944.75d | ±0.17 | | 44.946 | | 260.267 | | 10.952 | | # |
| CH3N (H2C=NH)Methyleneimine | | 29.04126 | 88.701 | 96.616 | ±1. | | 38.084 | | 221.565 | | 10.176 | | # |
| CH3N+ (H2C=NH)+ | | 29.04071 | 1055.02 | 1055.988 | ±2.06 | | 45.222 | | 235.558 | | 10.925 | | # |
| CH3N- (H2C=NH)- c | | 29.04181 | 215.20d | 228.7d | ±2.5d | |  | |  | |  | | X |
| HCNH2 Aminomethylene | | 29.04126 | 238.9d | 246.6d | ±1.7d | | 45.152 | | 240.492 | | 10.960 | | # |
| HCNH2+ | | 29.04071 | 1039.34 | 1040.83 | ±2.6d | | 40.741 | | 233.121 | | 10.399 | | # |
| HCNH2- radical anion | | 29.04181 | 343.96 | 357.252 | ±2.6d | | 45.799 | | 239.141 | | 10.996 | | # |
| CH3N Methyl-N Radical | | 29.04126 | 316.0d | 323.8d | ±1.6d | | 39.990 | | 226.694 | | 10.330 | | # |
| H3CN+ Methylaminyliumyl quartet | | 29.04071 | 1477.4d | 1478.4d | ±2.6d | | 43.922 | | 236.484 | | 10.835 | | # |
| H3CN- | | 29.04181 | 308.4d | 322.3d | ±1.8d | | 40.459 | | 226.984 | | 10.394 | | # |
| CH3NO NITROSOMETHYL | | 45.04096 | 70.760 | 80.677 | ±8. | | 50.807 | | 261.418 | | 12.514 | | # |
| OCHNH2 FORMAMIDE | | 45.04066 | -189.598 | -178.241 | ±8. | | 47.623 | | 247.737 | | 11.073 | | # |
| CH2=NOH Formaldehyde Oxime | | 45.04096 | 18.648 | 30.00 | ±8. | | 47.876 | | 253.486 | | 11.072 | | # |
| NCH3O FORMIMIDIC ACID | | 45.04096 | -121.537 | -109.866 | ±8. | | 45.004 | | 257.645 | | 10.760 | | # |
| H3CNO CH2-NH=O | | 45.04096 | 66.421 | 78.102 | ±8. | | 45.193 | | 251.503 | | 10.750 | | # |
| CH3NO2 NITRO-METHANE | | 61.04036 | -74.76 | -60.599 | ±0.47f | | 55.528 | | 273.718 | | 12.610 | | # |
| CH3NO2- NitroMethane anion | | 61.04061 | -98.479 | -79.426 | ±8. | | 65.869 | | 279.946 | | 13.915 | | # |
| CH3NO2 Methyl Nitrite CH3ONO | | 61.04036 | -65.44 | -54.015 | ±1. | | 64.891 | | 302.910 | | 15.345 | | # |
| CH3NO3 METHYL-NITRATE | | 77.03976 | -122.005 | -107.13 | ±4.2 | | 76.597 | | 305.793 | | 16.234 | | # |
| CH3N2 CH3N=N\* | | 43.04800 | 236.216 | 246.971 | ±8 | | 51.182 | | 258.278 | | 11.671 | | # |
| CH3N2 CH2\*-N=NH | | 43.04800 | 332.448 | 343.709 | ±8. | | 47.988 | | 263.640 | | 11.165 | | # |
| CH3N2 cy(-CH\*-NH-NH-) | | 43.04800 | 461.257 | 472.900 | ±8. | | 46.303 | | 247.027 | | 10.782 | | # |
| CH3N2 cy(-CH2-NH-N\*-) | | 43.04800 | 383.158 | 394.889 | ±8. | | 45.450 | | 252.246 | | 10.695 | | # |
| CH3N2O3 H2C(OH)-N\*-NO2 rad | | 91.04620 | 40.715 | 58.170 | ±8. | | 87.965 | | 343.096 | | 17.991 | | # |
| CH3N3 CH3-N=N=N MethylAzide | | 57.05474 | 297.29 | 309.93 | ±8. | | 63.015 | | 279.531 | | 14.118 | | # |
| CH3N3O4 CH3N(NO2)2 | | 121.05234 | 95.793 | 117.605 | ±8. | | 109.685 | | 376.477 | | 22.309 | | # |
| CH3O MethylOxide <!> | | 31.03392 | 21.0 | 28.4 | ±0.36d | | 42.541 | | 234.278 | | 10.719 | | # |
| CH3O+ MethylOxide cation triplet | | 31.03337 | 1061.18 | 1062.60 | ±0.7 | | 40.994 | | 230.786 | | 10.391 | | # |
| CHOH2+d Methylideneoxonium | | 31.03337 | 1042.05 | 1043.19 | ±8. | | 43.951 | | 231.894 | | 10.760 | | # |
| CH3O- | | 31.03446 | -136.44 | -122.213 | ±0.35 | | 36.469 | | 220.494 | | 10.066 | | # |
| CH2OH <!> | | 31.03392 | -17.0 | -10.7 | ±0.44d | | 47.401 | | 244.170 | | 11.781 | | † |
| CH2OH+ | | 31.03337 | 716.400 | 718.00d | ±0.24d | | 37.835 | | 228.047 | | 10.149 | | † |
| CH2OH- c | | 31.03447 | -3.0d | 9.8d | ±1.8 | | 46.672 | | 237.897 | | 11.420 | | # |
| CH3OD | | 33.04832 | -205.331 | -194.49 |  | | 44.142 | | 242.751 | | 11.543 | | # |
| CH3OS HO-CH2-S\* radical | | 63.09992 | -33.849 | -23.935 | ±8. | | 56.778 | | 276.313 | | 12.594 | | # |
| CH3O2 Peroxymethyl Rad <~> | | 47.03332 | 11.941 | 21.801 | ±0.90d | | 52.238 | | 259.572 | | 12.576 | | # |
| CH3OO+ | | 47.03277 | 1008.7d | 1010.9 | ±2.4d | | 53.523 | | 259.738 | | 12.422 | | # |
| CH3OO- MethylPeroxy anion | | 47.03387 | -106.6d | -90.27d | ±1. | | 52.620 | | 258.906 | | 12.156 | | # |
| CH3P CH2=PH | | 46.00828 | 118.478 | 126.954 | ±8. | | 43.847 | | 242.533 | | 10.640 | | # |
| CH3S Thiomethoxy Radical | | 47.10052 | 121.470 | 128.518 | ±8. | | 46.635 | | 242.040 | | 11.120 | | # |
| CH3SS | | 79.16652 | 80.00 | 88.839 | ±8. | | 62.225 | | 291.673 | | 13.743 | | # |
| CH3Si Methyl Silicon radical | | 43.12002 | 304.419 | 301.137 | ±8. | | 47.653 | | 242.582 | | 11.255 | | # |
| CH3Si- Methyl Silicon anion | | 43.12057 | 276.445 | 288.244 | ±8. | | 47.394 | | 237.369 | | 11.245 | | # |
| CH3Zn MethylZinc radical | | 80.42452 | 190.000 | 198.044 | ±17. | | 48.393 | | 253.131 | | 11.369 | | # |
| CH4 RRHO <^!> | | 16.04246 | -74.6 | -66.633 | ±0.3 | | 35.613 | | 186.314 | | 10.023 | |  |
| CH4 ANHARMONIC <^!> | | 16.04246 | -74.6 | -66.626 | ±0.057 | | 35.691 | | 186.371 | | 10.016 | | † |
| CH4+ Methane cation | | 16.04191 | 1150.0d | 1150.86 | ±0.26 | | 44.371 | | 196.529 | | 10.925 | | # |
| CH4- Methane anion | | 16.04301 | -3.09 | +10.497 | ±4.2d | | 42.817 | | 195.995 | | 10.600 | | # |
| CH4N CH3NH\* Methylamidogen | | 30.0492 | 178.556 | 189.498 | ±0.89d | | 46.408 | | 234.833 | | 11.383 | | # |
| CH4N+ CH3NH\*+ c | | 30.04865 | 1131.42 | 1135.2d | ±2.42 | |  | |  | |  | | X |
| CH4N- CH3NH\*- | | 30.04975 | 128.601 | 146.257 | ±0.78 | | 44.039 | | 235.077 | | 10.866 | | # |
| CH4N \*CH2NH2 Aminomethyl | | 30.0492 | 148.743 | 159.755 | ±1.01 | | 48.813 | | 242.801 | | 11.313 | | # |
| \*CH2NH2+ | | 30.04865 | 758.317 | 764.123 | ±1.75 | | 40.290 | | 230.359 | | 10.322 | | # |
| \*CH2NH2- c | | 30.04975 | 194.92 | 212.1d | ±2.8d | | 49.495 | | 244.185 | | 12.053 | | # |
| CH4N2 AminMethenImine NH=CH-NH2 | | 44.05594 | 49.764 | 64.424 | ±8. | | 55.783 | | 258.454 | | 12.000 | | # |
| CH4N2 Diaziridine -H2CNHNH- | | 44.05594 | 239.505 | 255.450 | ±8. | | 46.098 | | 242.397 | | 10.714 | | # |
| (NH2)2C=O Solid UreaW | | 60.05534 | -333.11 |  | ±0.7 | | 92.79 | | 104.26 | |  | | X |
| (NH2)2C=O Urea | | 60.05534 | -231.999 | -215.617 | ±8. | | 77.445 | | 299.707 | | 14.618 | | # |
| CH4N4O2 (s) Nitroguanidine, Picrite solid | | 104.06822 | -95. |  |  | |  | |  | |  | | X |
| CH4N4O2 Nitroguanidine, Picrite | | 104.06822 | 89.295 | 113.750 | ±8. | | 106.201 | | 358.208 | | 19.555 | |  |
| CH4N4O2 NG (NH2)2C=N-NO2 | | 104.06822 | 48.162 | 73.401 | ±8. | | 106.906 | | 348.642 | | 18.762 | | # |
| CH3OH(L) Methanol liq | | 32.04186 | -238.398 | -235.063 | ±0.17 | | 81.080 | | 127.269 | | 18.995 | | #† |
| CH3OH <^!> | | 32.04186 | -200.94 | -190.11 | ±0.18 | | 44.039 | | 239.81 | | 11.444 | | #† |
| CH3OH+ c | | 32.04131 | 852.493 | 856.98d | ±0.33 | | 45.702 | | 254.808 | | 11.546 | | # |
| CH3OH – | | 32.04240 | 39.37 | 52.909 | ±2.94 | | 60.480 | | 310.882 | | 14.988 | | # |
| CH2OH2 Methyleneoxoniumrad | | 32.04186 | 149.2 | 158.2 | ±4.1 | | 58.337 | | 259.615 | | 13.329 | | # |
| CH2OH2+ " cation | | 32.04131 | 825.9d | 830.046 | ±4.5d | | 52.353 | | 247.500 | | 11.987 | | # |
| CH4OS HO-CH2-SH | | 64.10786 | -177.816 | -164.620 | ±8. | | 64.058 | | 276.592 | | 13.546 | | # |
| CH4O2 (CH3OOH) <~> | | 48.04126 | -126.733 | -114.22 | ±0.91d | | 66.753 | | 275.904 | | 14.160 | | # |
| CH3OOH+ | | 48.0407 | 828.3d | 834.7d | ±5.7d | |  | |  | |  | | X |
| CH4O2 CH2(OH)2 Methanediol | | 48.04126 | -392.61d | -379.21d | ±1.d | | 56.171 | | 254.327 | | 12.269 | | # |
| CH4S (CH3SH) MethylMercaptan | | 48.10846 | -20.426 | -9.927 | ±8. | | 50.185 | | 253.190 | | 11.903 | | # |
| CH4S2 CH2(SH)2 Methane dithyol | | 80.17446 | 23.18 | 34.99 | ±8. | | 70.897 | | 288.644 | | 15.001 | | # |
| CH4S3 CH(SH)3 Methane trithyol | | 112.24046 | 58.07 | 70.6 | ±8. | | 94.990 | | 320.990 | | 18.728 | | # |
| CH4Si H2C=SiH2 | | 44.12796 | 187.276 | 196.311 | ±8. | | 56.872 | | 245.568 | | 12.168 | | # |
| CH4Si+ H2C=SiH2+ cation | | 44.12741 | 1051.435 | 1053.766 | ±8. | | 58.636 | | 253.837 | | 12.464 | | # |
| CH4Si- H2C=SiH2- anion | | 44.12851 | 177.426 | 191.439 | ±8. | | 62.287 | | 264.645 | | 13.165 | | # |
| CH5+ Methonium | | 17.04985 | 917.22 | 922.482 | ±0.5 | | 40.147 | | 214.892 | | 10.764 | | # |
| CH5N liq CH3-NH2 liq | | 31.05714 | -44.69d |  | ±0.58 | |  | |  | |  | | X |
| CH5N CH3-NH2 MethylAmine | | 31.05714 | -20.91d | -5.83d | ±0.53d | | 48.831 | | 235.325 | | 11.570 | | # |
| CH5N+ CH3-NH2+ c | | 31.05659 | 859.387d | 867.473 | ±2.28 | | 48.751 | | 255.530 | | 12.275 | | # |
| CH5N- CH3NH2- c | | 31.05769 | 48.65d | 69.366 | ±3.85 | | 52.338 | | 250.270 | | 12.040 | | # |
| CH5N2 CH3N\*NH2 | | 45.06388 | 211.300 | 228.491 | ±8. | | 64.884 | | 276.081 | | 13.703 | | # |
| CH5N2 CH2\*NHNH2 | | 45.06388 | 269.236 | 236.059 | ±8. | | 68.327 | | 287.002 | | 14.071 | | # |
| CH5N3 GUANIDINE | | 59.07062 | 27.952 | 48.939 | ±8. | | 75.796 | | 297.900 | | 14.223 | | # |
| CH5O+ CH3-OH2+ Rydberg Cation | | 33.04925 | 583.706 | 585.97 | ±8. | | 51.102 | | 244.423 | | 11.902 | | # |
| CH5OP CH3-O-PH2 | | 64.02356 | -168.448 | -151.345 | ±8. | | 68.507 | | 285.470 | | 14.821 | | # |
| CH5OP+ CH3-O-PH2+ cation | | 64.02301 | 696.657 | 706.740 | ±8. | | 70.932 | | 284.522 | | 14.959 | | # |
| CH5OP- CH3-O-PH2- anion | | 64.02411 | -84.960 | -66.203 | ±8. | | 82.619 | | 318.170 | | 18.760 | | # |
| CH5P CH3-PH2 MePhosphine | | 48.02416 | -14.104 | +1.321 | ±8. | | 55.974 | | 257.454 | | 12.158 | | # |
| CH5P+ CH3-PH2+ | | 48.02361 | 863.971 | 872.221 | ±8. | | 58.612 | | 262.287 | | 12.463 | | # |
| CH5P- CH3-PH2- | | 48.02471 | 137.615 | 158.218 | ±8. | | 61.613 | | 258.030 | | 12.946 | | # |
| CH5Si\* CH3-SH2\* | | 45.13590 | 141.879 | 154.470 | ±8. | | 61.598 | | 258.522 | | 12.851 | | # |
| CH5Si\*+ CH3-SH2\*+ cation | | 45.13535 | 864.938 | 869.895 | ±8. | | 58.975 | | 263.859 | | 13.358 | | # |
| CH5Si\*- CH3-SH2\*- anion | | 45.13645 | 22.434 | 40.694 | ±8. | | 61.340 | | 256.661 | | 12.773 | | # |
| CH6N+ CH3NH3+c | | 32.06453 | 615.9d | 628.572 | ±2.44 | | 50.770 | | 245.598 | | 11.923 | | # |
| CH6N2 MethylHydrazine | | 46.07182 | 109.41 | 130.443 | ±8. | | 68.911 | | 274.188 | | 14.081 | | # |
| CH6P CH3PH3 | | 49.03210 | 174.590 | 192.28 | ±8. | | 67.736 | | 265.889 | | 14.119 | | # |
| CH6P+ CH3PH3+ | | 49.03155 | 672.499 | 685.029 | ±8. | | 60.604 | | 257.771 | | 12.864 | | # |
| CH6P- CH3PH3- | | 49.03265 | 94.080 | 116.926 | ±8. | | 71.972 | | 271.554 | | 14.892 | | # |
| CH6P2 H2P-CH2-PH2 | | 80.00586 | 39.108 | 59.514 | ±8. | | 81.963 | | 303.156 | | 16.772 | | # |
| CH6P2+ H2P-CH2-PH2+ | | 80.00531 | 940.830 | 953.683 | ±8. | | 88.248 | | 313.678 | | 17.765 | | # |
| CH3SiH3 CH3SiH3 | | 46.14384 | -27.420 | -11.579 | ±8. | | 66.009 | | 267.332 | | 13.827 | | # |
| CH3SiH3+ CH3SiH3+ MethylSilane | | 46.14329 | 1001.110 | 1007.766 | ±8. | | 81.219 | | 285.168 | | 16.670 | | # |
| CH6SiO CH3Si2OH | | 62.14324 | -350.243 | -333.021 | ±8 | | 82.779 | | 286.412 | | 16.449 | | # |
| CH6SiO SiH3CH2OH | | 62.14324 | -148.042 | -130.461 | ±8 | | 80.141 | | 284.692 | | 16.104 | | # |
| CH6Si2+ CH3SiH2SiH cation | | 74.22879 | 1038.277 | 1045.198 | ±8. | | 95.143 | | 343.868 | | 18.756 | | # |
| CH6Si2- CH3SiH2SiH anion | | 74.22989 | 82.365 | 108.692 | ±8. | | 92.630 | | 338.515 | | 18.053 | | # |
| CH6Sn CH3SnH3 | | 136.76834 | 118.407 | 136.091 | ±4.2 | | 73.750 | | 285.712 | | 15.907 | | # |
| CH12Si4 C(SiH3)4 | | 136.44798 | 42.472 | 75.417 | ±8. | | 191.403 | | 443.308 | | 36.601 | | # |
| CH12Si4+ C(SiH3)4+ | | 136.44743 | 1008.409 | 1033.197 | ±8. | | 183.774 | | 416.273 | | 32.831 | | # |
| CI Carbon Iodide | | 138.91517 | 570.201 | 568.358 | ±60. | | 36.908 | | 241.318 | | 9.494 | | † |
| ICN | | 152.92191 | 222.1 | 222.6 | ±1. | | 48.420 | | 257.340 | | 11.470 | | # |
| CI2 DiIodoCarbene | | 265.81964 | 468.394 | 470. | ±60. | | 50.945 | | 304.324 | | 12.643 | | † |
| CI3 Triiodomethyl Radical | | 392.72411 | 405.984 | 410.000 | ±60. | | 70.550 | | 361.033 | | 16.831 | | # |
| CI4 (cr) Tetraiodomethane monocli | | 519.62858 | 392.5 |  | ±8.0d | |  | |  | |  | | X |
| CI4 TetraIodoMethane | | 519.62858 | 336.09  326.9h | 340.7d | ±1.32  4.1h | | 95.819 | | 391.347 | | 22.327 | | # |
| CN <~> | | 26.01774 | 438.68 | 435.4 | ±2 | | 29.156 | | 202.643 | | 8.672 | | #† |
| CN+ | | 26.01689 | 1788.9 | 1779.2d | ±1.5 | | 29.463 | | 196.935 | | 8.682 | | #† |
| CN- | | 26.01799 | 61.06 | 63.972d | ±0.1d | | 29.151 | | 196.576 | | 8.671 | | #† |
| NaCN (cr,l) | | 49.00721 | -90.709 | -98.283 |  | | 69.036 | | 118.457 | | 19.422 | | † |
| CNO Nitrosomethylidyne | | 42.01684 | 390.02 | 389.161 | ±1.60 | | 43.004 | | 231.132 | | 10.587 | | # |
| CNO+ c 67197-19-7 Cyanato Fulminato rad + | | 42.01629 | 1517.94 | 1509.5d | ±2.1d | | 42.452 | | 258.382 | | 11.780 | | # |
| CNO- c  Fulminated | | 42.01739 | 53.39d | 59.4d | ±1.95 | | 40.179 | | 221.186 | | 9.850 | | # |
| CNO (NCO) | | 42.01684 | 128.040 | 127.57 | ±0.39d | | 39.989 | | 232.229 | | 10.198 | | †# |
| NCO+ Cyanato Cation | | 42.01629 | 1268.52 | 1261.69 | ±0.58 | | 42.256 | | 224.660 | | 10.357 | | # |
| NCO- Isocyanate Anion | | 42.01739 | -227.578 | -221.177 | ±0.56 | | 38.296 | | 219.928 | | 9.525 | | # |
| C(NO) cyclo radical Oxazirinyl | | 42.01684 | 451.47 | 450.681 | ±1.64 | | 40.008 | | 247.713 | | 10.518 | | # |
| C(NO)+ cyclo radical cation | | 42.01629 | 1573.6 | 1566.84 | ±2.74 | | 38.442 | | 240.676 | | 10.291 | | # |
| C(NO)- cyclo radical anion | | 42.01739 | 444.38 | 449.54 | ±2.71 | | 41.769 | | 244.214 | | 10.765 | | # |
| CNN C=N≡N <~> | | 40.02418 | 573.47 | 572.816 | ±3.2d | | 42.656 | | 232.398 | | 10.378 | | #† |
| CNN+ Diazomethyliumyl | | 40.02363 | 1644.52 | 1636.647 | ±5.95 | | 46.292 | | 235.933 | | 11.399 | | # |
| CNN- | | 40.02473 | 395.66 | 401.777 | ±3.15 | | 39.970 | | 219.837 | | 9.804 | | # |
| NCN (NCN) <~> Methanetetraylbisamidogen | | 40.02418 | 445.7d | 445.3d | ±1.8d | | 41.946 | | 225.814 | | 10.180 | | #† |
| NCN+ Cyanoaminyliumyl | | 40.02363 | 1668.52 | 1661.023 | ±5.86 | | 43.990 | | 228.261 | | 11.023 | | # |
| NCN- | | 40.02473 | 199.52 | 205.784 | ±1.75 | | 39.121 | | 219.761 | | 9.657 | | # |
| C(NN) cyclo | | 40.02418 | 580.58 | 580.23 | ±4.31 | | 36.072 | | 232.352 | | 10.076 | | # |
| \*C(O)N3 Formil Azide Radical | | 70.03032 | 352.1 | 356.1 | ±3.3 | | 64.612 | | 296.398 | | 14.435 | | # |
| CN4 N≡C-N=N-N Cyanogen azide | | 68.03766 | 498.251 | 502.746 | ±8. | | 63.652 | | 284.193 | | 13.899 | | # |
| C(NO2)4 TetraNitroMethane | | 196.03286 | 82.383 | 101.687 |  | | 176.076 | | 503.712 | | 33.810 | | # |
| CO <^!> | | 28.0104 | -110.53 | -113.813 | ±0.17 | | 29.141 | | 197.657 | | 8.671 | | † |
| CO+ d | | 28.00955 | 1247.812 | 1238.337 | ±0.025 | | 19.137 | | 203.230 | | 8.671 | | † |
| CO- c | | 28.01065 | 36.2d | 39.1d | ±3.1d | | 29.284 | | 205.007 | | 8.679 | | # |
| COS Anharmonic <^> | | 60.07610 | -141.700 | -141.836 | ±2. | | 41.549 | | 231.650 | | 9.942 | | † |
| CO2 <^!> | | 44.00980 | -393.51 | -393.142 | ±0.13 | | 37.135 | | 213.787 | | 9.365 | | † |
| CO2 triplet | | 44.00950 | 49.6d | 48.9d | ±2.4 | | 37.135 | | 222.922 | | 9.365 | | # |
| CO2+ | | 44.00895 | 943.137 | 936.107 | ±0.023 | | 41.799 | | 228.017 | | 10.566 | | † |
| CO2+ quartet | | 44.00895 | 1334.2d | 1327.1d | ±3.2d | | 40.390 | | 249.543 | | 10.550 | | # |
| CO2- c | | 44.01005 | -345.88 | -339.561 | ±2.4d | | 38.598 | | 221.010 | | 9.612 | | # |
| COO Dioxymethylidyne | | 44.00950 | 296.3d | 295.1d | ±2.1 | | 39.823 | | 242.861 | | 10.452 | | # |
| COO+ doublet | | 44.00951 | 1444.d | 1434.5d | ±3.7d | | 43.809 | | 262.383 | | 12.047 | | # |
| COO- doublet | | 44.01005 | -114.49 | -108.829 | ±8. | | 37.335 | | 243.341 | | 10.234 | | # |
| C(OO) Cyclo Dioxyranilydene | | 44.00950 | 189.78 | 189.062 | ±1.71 | | 39.823 | | 237.099 | | 10.452 | | # |
| C(OO)+ Cyclo cation | | 44.00895 | 1417.9d | 1409.3d | ±6.d | | 43.810 | | 256.619 | | 12.047 | | # |
| CO3- gas Carbonate anion | | 60.00945 | -580.74 | -572.53 | ±8. | | 51.134 | | 273.431 | | 12.059 | | # |
| CO3Ca see CaCO3 | |  |  |  |  | |  | |  | |  | | # |
| CO3Na2 see Na2CO3 | |  |  |  |  | |  | |  | |  | | † |
| CP <&> | | 42.98446 | 508.486 | 506.183 | ±8. | | 29.890 | | 216.242 | | 8.716 | | #† |
| CP+ cation | | 42.98391 | 1633.2 | 1624.69 | ±8. | | 29.836 | | 210.377 | | 8.713 | | # |
| CP- anion | | 42.98446 | 218.166 | 222.040 | ±8. | | 29.998 | | 210.999 | | 8.723 | | # |
| CS <&> | | 44.0767 | 278.550 | 275.307 | ±3.8 | | 29.799 | | 210.559 | | 8.708 | | † |
| CS2 Anharmonic <^> | | 76.143 | 116.70 | 115.913 | ±1. | | 45.482 | | 237.889 | | 10.664 | | † |
| CT (C3H) Tritium Carbon | | 15.02675 | 583.827 | 588.876 |  | | 29.290 | | 192.044 | | 8.706 | | # |
| CT3 (C3H3) Methyl T-3 | | 21.05885 | 115.725 | 118.338 | ±8. | | 44.704 | | 220.760 | | 11.294 | | # |
| CT4 (C3H4) Methane T-4 | | 24.0749 | -117.612 | -110.05 | ±8. | | 43.945 | | 205.285 | | 10.630 | | # |
| CW Tungsten Carbide | | 195.8507 | -40.54 |  |  | | 35.378 | | 32.374 | |  | | † |
| ZrC Zirconium Carbide | | 103.23470 | -196.648 | -195.960 | ±13. | | 37.899 | | 33.321 | | 5.862 | | † |
| C2 singlet 1Σ+g  <!> | | 24.0214 | 826.799 | 820.31d | ±[0.3]d | | 29.214 | | 190.673 | | 8.675 | | #† |
| C2 triplet 3Πu <!> | | 24.0214 | 842.402 | 827.260 | ±8. | | 29.326 | | 200.552 | | 17.248 | | # |
| C2+ cation | | 24.02085 | 1980.05 | 1968.3d | ±2.5d | | 29.400 | | 204.179 | | 8.685 | | † |
| C2- anion | | 24.02195 | 505.3 | 504.928 | ±0.5 | | 29.241 | | 196.599 | | 8.676 | | #† |
| ALC2 | | 51.00294 | 675.616 | 670. | ±35. | | 47.818 | | 252.941 | | 12.263 | | † |
| C2Br | | 103.9260 | 623.667 | 626.39 | ±2. | | 45.103 | | 295.017 | | 11.648 | | # |
| C2Br2 DiBromoAcetylene | | 183.8294 | 322.05 | 333.250 | ±3.45 | | 68.067 | | 294.448 | | 15.427 | | # |
| C2Br2F4 HALON 2402 (114B2) | | 259.82301 | -823.076 | -802.65 | ±8. | | 119.972 | | 386.278 | | 23.851 | | # |
| C2Br3 | | 263.7340 | 385.388 | 405.674 |  | | 83.269 | | 369.892 | | 18.602 | | # |
| C2Br4 | | 343.638 | 215.584 | 218.816 |  | | 102.196 | | 387.413 | | 22.410 | | # |
| C2Br5 | | 423.54200 | 283.257 | 318.915 |  | | 126.162 | | 444.694 | | 27.749 | | # |
| C2Br6 | | 503.44600 | 165.480 | 209.480 |  | | 146.665 | | 459.134 | | 31.667 | | # |
| C2CL | | 59.47410 | 534.083 | 530. | ±50. | | 45.046 | | 241.948 | | 10.781 | | † |
| C2CL2 DiChloroAcetylene | | 94.92680 | 233.78 | 230.475 | ±1.81 | | 65.374 | | 272.112 | | 14.593 | | #† |
| C2CL2F2 CCLF=CFCL E(trans) | | 132.92361 | -341.486 | -339.3 | ±8. | | 87.333 | | 327.192 | | 17.925 | | # |
| C2CL2F2 CCLF=CCLF Z(cis) | | 132.92361 | -339.548 | -337.37 | ±8. | | 87.632 | | 327.213 | | 17.934 | | # |
| C2CL2F4 FC-114 CClF2-CClF2 | | 170.92041 | -931.777 | -925.136 | ±8. | | 116.051 | | 369.953 | | 22.298 | | # |
| C2CL2F4 FC-114 A CCl2F-CF3 | | 170.92041 | -943.71 | -937.085 | ±8. | | 115.786 | | 367.373 | | 22.314 | | # |
| C2CL3 | | 130.3795 | 237.68 | 237.680 | ±8. | | 77.713 | | 333.469 | | 16.736 | | #† |
| CCl2F-CCLF2 FC-113 | | 187.37471 | -732.186 | -726.543 | ±8. | | 121.956 | | 377.803 | | 23.463 | | # |
| C2CL3F3 FC-113A | | 187.37471 | -759.145 | -753.330 | ±8. | | 120.576 | | 376.459 | | 23.301 | | # |
| C2CL3O CCL3C=O | | 146.37890 | -23.543 | -23.237 | ±8. | | 96.241 | | 348.965 | | 19.913 | | # |
| C2CL4 | | 165.8322 | -21.064 | -20.159 | ±8.0 | | 94.781 | | 341.211 | | 19.564 | | #† |
| C2CL4+ | | 165.83165 | 876.418 | 871.506 | ±8. | | 92.415 | | 346.756 | | 19.184 | | # |
| C2CL5 | | 201.2849 | 21.983 | 23.108 | ±8. | | 115.214 | | 404.117 | | 23.935 | | # |
| C2CL5F CFC-111 | | 220.28330 | -348.473 | -374.119 | ±8. | | 128.537 | | 408.602 | | 25.646 | | # |
| C2CL6 | | 236.7376 | -162.110 | -159.69 | ±8 | | 136.326 | | 407.696 | | 27.235 | | #† |
| C2D ETHYNYL-D | | 26.03550 | 565.940 | 561.364 |  | | 43.432 | | 218.821 | | 10.967 | | # |
| C2D2 | | 28.04960 | 222.672 | 222.470 |  | | 49.378 | | 208.869 | | 10.879 | | # |
| C2D2O | | 44.04900 | 39.915 | 42.544 |  | | 55.516 | | 249.581 | | 12.387 | | # |
| C2D4 | | 32.07780 | 30.270 | 38.111 |  | | 52.950 | | 230.655 | | 11.404 | | # |
| C2OD4 | | 48.07721 | -180.581 | -170.731 |  | | 66.931 | | 270.623 | | 13.735 | | # |
| C2D6 | | 36.10601 | -110.60 | -94.786 |  | | 59.774 | | 236.691 | | 12.001 | | # |
| C2D6N2 Azomethane-D6 | | 64.11949 | 119.248 | 138.518 |  | | 92.278 | | 296.225 | | 17.210 | | # |
| C2D6O DimethylEther-D6 | | 52.10541 | -208.406 | -192.046 |  | | 77.652 | | 282.381 | | 15.794 | | # |
| C2F <~> | | 43.01980 | 353.847 | 350.00 | ±50. | | 42.6 | | 231.036 | | 10.367 | | † |
| CFCN | | 57.02654 | 291.130 | 288.886 | ±8. | | 55.158 | | 272.234 | | 13.099 | | # |
| C2F2 FCCF <~> | | 62.01821 | 2.86 | -0.375 | ±1.55 | | 61.987 | | 256.504 | | 14.167 | | #† |
| C2F2+ FCCF+ | | 62.0177 | 1087.9d | 1078.7d | ±2.d | |  | |  | |  | | X |
| C2F3 <~> | | 81.01661 | -228.175 | -227.0 | ±20. | | 66.178 | | 297.643 | | 14.164 | | † |
| CF3CN | | 95.02335 | -499.250 | -495.505 |  | | 78.189 | | 299.006 | | 15.934 | | # |
| CF3CN- anion | | 95.02390 | -505.892 | -497.185 | ±8. | | 83.305 | | 324.994 | | 17.083 | | # |
| CF3C=O radical | | 97.01601 | -608.253 | -605.414 | ±8. | | 80.364 | | 316.924 | | 16.846 | | # |
| C2F4(s) PTFE (CF2)x x2 | | 100.01501 | -25.700 | -5.942 |  | | 102.564 | | 119.358 | |  | |  |
| (C2F4)n gas (teflon) PTFE | | 100.01501 | -829.53d |  | ±0.6 | | 42.671 | | 96.148 | |  | | # |
| C2F4 FC-1114 <~> | | 100.01501 | -675.34 | -671.91 | ±0.77d | | 80.459 | | 300.128 | | 16.331 | | †# |
| C2F5 <~> | | 119.01316 | -901.924 | -896.557 | ±8. | | 94.231 | | 340.995 | | 18.803 | | # |
| C2F6 FC-116 <~> | | 138.01182 | -1350.52 | -1342.167 | ±1.63 | | 106.294 | | 341.033 | | 20.229 | | †# |
| CF3-O-O-CF3 | | 170.01062 | -1464.6 | -1454.5 | ±8 | | 137.210 | | 455.396 | | 27.159 | | # |
| C2H ETHYNYL <!> | | 25.02934 | 568.056 | 563.945 | ±0.3 | | 41.992 | | 213.290 | | 10.452 | | †# |
| C2H+ Ethynylium | | 25.02879 | 1697.10 | 1687.566 | ±0.18d | | 38.746 | | 203.063 | | 9.677 | | # |
| C2H - Ethynide | | 25.02989 | 274.776 | 277.476 | ±0.41d | | 39.587 | | 204.389 | | 9.838 | | # |
| C2HBr Bromoacetylene | | 104.93334 | 275.88 | 282.38 | ±2.1 | | 55.696 | | 253.676 | | 12.101 | | # |
| C2HBr2 | | 184.83734 | 333.590 | 348.909 |  | | 68.272 | | 326.691 | | 15.342 | | # |
| C2HBr3 | | 264.74134 | 144.181 | 168.884 |  | | 85.590 | | 359.979 | | 18.418 | | # |
| C2HBr4 1,1,2,2-CHBr2CBr2 | | 344.64534 | 218.823 | 250.685 | ±8.4 | | 107.701 | | 425.045 | | 23.519 | | # |
| C2HBr4 1,1,1,2-CBr3CHBr | | 344.64534 | 243.634 | 274.593 | ±8.4 | | 113.967 | | 417.090 | | 24.422 | | # |
| C2HBr5 | | 424.54934 | 113.094 | 153.466 |  | | 126.628 | | 439.579 | | 27.268 | | # |
| C2HCL | | 60.48204 | 228.99 | 228.134 | ±1.1d | | 54.32 | | 241.955 | | 11.788 | | #† |
| C2HCLF 1,1-CLF Radical | | 79.48074 | 101.87 | 103.90 | ±8. | | 63.592 | | 289.422 | | 13.317 | | # |
| C2HCLF2-1,1 FC-1122 | | 98.47885 | -333.654 | -329.16 |  | | 76.650 | | 304.242 | | 15.263 | | † |
| C2HCLF2 cis FC-1131 | | 98.47885 | -323.569 | -319.158 |  | | 75.394 | | 304.601 | | 15.346 | | # |
| C2HCLF2 trans | | 98.47885 | -323.103 | -318.531 |  | | 75.149 | | 303.573 | | 15.184 | | # |
| CF2H-CCLF2 FC-124A | | 136.47563 | -908.397 | -899.425 | ±8 | | 99.463 | | 343.448 | | 19.610 | | # |
| CF3-CHCLF HCFC124 | | 136.47563 | -930.714 | -921.556 | ±8 | | 98.642 | | 343.304 | | 19.424 | | # |
| C2HCL2F 1,1+*cis+trans* FC-1121 | | 114.93314 | -168.648 | -164.97 |  | | 77.324 | | 320.190 | | 16.259 | | † |
| CF3-CHCL2 HCFC123 | | 152.92995 | -757.45 | -748.879 | ±8 | | 102.625 | | 352.494 | | 20.189 | | # |
| CF2CL-CHFCL FC123A | | 152.92995 | -719.414 | -711.363 | ±8 | | 104.631 | | 366.615 | | 20.710 | | # |
| CFCL2-CHF2 | | 152.92995 | -709.983 | -701.888 | ±8 | | 104.481 | | 363.468 | | 20.665 | | # |
| C2HCL3 liq TriChloroEthylene | | 131.3874 | -48.3 |  | ±1.5 | |  | |  | |  | | X |
| C2HCL3 <~> | | 131.3874 | -14.700 | -11.143 | ±1.5 | | 79.734 | | 324.837 | | 16.555 | | #† |
| C2HCl3+ cation | | 131.38689 | 907.411 | 904.574 | ±8. | | 78.317 | | 325.026 | | 16.484 | | # |
| C2HCL4 | | 166.84014 | 21.824 | 26.108 | ±8. | | 100.608 | | 375.159 | | 20.419 | | # |
| C2HCL5 | | 202.29284 | -160.410 | -153.83 | ±8. | | 113.348 | | 379.920 | | 22.716 | | # |
| C2HD Acetylene-D-1 | | 27.04344 | 225.434 | 225.632 |  | | 46.615 | | 210.682 | | 10.428 | | # |
| C2HF | | 44.02774 | 104.419 | 103.727 | ±0.93 | | 52.268 | | 231.573 | | 11.446 | | #† |
| C2HF+ cation Fluoroacetylen | | 44.02719 | 1195.77 | 1188.99 | ±8. | | 51.366 | | 236.805 | | 11.334 | | # |
| C2HF2 | | 63.02615 | -42.5 | -40.52 | ±17.9 | | 59.249 | | 279.393 | | 13.183 | | # |
| C2HF3 <~> | | 82.02455 | -487.84 | -482.59 | ±8.4d | | 69.191 | | 292.665 | | 14.328 | | #† |
| C2HF5 FC-125 | | 120.02136 | -1120.00 | -1110.4 | ±8. | | 95.808 | | 334.635 | | 18.776 | | # |
| HCCN singlet HC\*\*-CN | | 39.03608 | 526.552 | 524.380 | ±8. | | 50.901 | | 252.653 | | 12.848 | | # |
| HCCN triplet HC\*=C=N\* | | 39.03608 | 476.541 | 475.094 | ±8. | | 51.486 | | 247.916 | | 12.848 | | # |
| C2HNO NC-CHO | | 55.03548 | 44.120 | 46.152 | ±8. | | 55.793 | | 270.935 | | 12.123 | | # |
| C2HNO2 HCC-NO2 | | 71.03488 | 278.654 | 283.597 | ±8. | | 69.580 | | 289.604 | | 14.414 | | # |
| C2H(NO2)2 NO2-CH=C\*NO2 | | 117.04042 | 328.398 | 339.383 | ±8. | | 107.603 | | 339.383 | | 21.386 | | # |
| C2HN3 (CN)2NH | | 67.04956 | 354.130 | 357.904 | ±8. | | 72.613 | | 290.126 | | 15.751 | | # |
| C2HN3+ (CN)2NH+ | | 67.04901 | 1452. | 1449.957 | ±8. | | 71.115 | | 293.348 | | 15.192 | | # |
| C2HN7O2 Cy 5-Azido-2nitrotriazole | | 155.07532 | 508.722 | 528.410 | ±12.5 | | 134.619 | | 406.367 | | 25.731 | | # |
| HCCO Ketyl Radical Oxoethenyl <!> | | 41.02874 | 178.3  178.15h | 177.258  176.85 | ±1.5  0.58h | | 49.975 | | 246.408 | | 11.665 | | #† |
| HCCO+ | | 41.02819 | 1147.93 | 1138.9d | ±2.5d | | 50.317 | | 244.396 | | 11.865 | | # |
| HCCO- Ethynol aniond | | 41.02989 | -53.565 | -48.07 | ±0.85 | | 47.880 | | 239.169 | | 11.380 | | # |
| C2HO3 KethylPeroxy \*OOCH=C=O | | 73.02754 | 77.161 | 80.506 | ±8. | | 71.005 | | 313.210 | | 16.016 | | # |
| C2HS\* HC≡CS\* radical | | 57.09534 | 360.724 | 359.337 | ±8. | | 55.711 | | 248.858 | | 12.139 | | # |
| H2C2 VINYLIDENE <!> | | 26.03728 | 412.272 | 411.973 | ±0.61 | | 42.614 | | 221.021 | | 10.874 | | #† |
| CCH2+ c | | 26.0367 | 1515.16 | 1508.6d | ±2.56 | |  | |  | |  | | X |
| CCH2- Vinylidene anion | | 26.03783 | 359.01 | 364.3d | ±0.82d | | 39.330 | | 224.438 | | 10.341 | | # |
| C2H2 ACETYLENE <^!> | | 26.03728 | 228.20 | 228.769 | ±0.15d | | 44.001 | | 200.917 | | 10.006 | | † |
| HCCH+ | | 26.03673 | 1333.918 | 1328.441 | ±0.193 | | 42.839 | | 206.479 | | 9.854 | | # |
| HCCH- | | 26.0378 | 353.07d | 359.5d | ±3.0d | |  | |  | |  | | X |
| HCCH- *cis* | | 26.0378 | 377.1d | 383.0d | ±3.2d | |  | |  | |  | | X |
| C2H2Br2 1,2-DiBromoEthylene | | 185.84528 | 99.286 | 119.008 | ±8. | | 69.704 | | 313.877 | | 15.373 | | # |
| C2H2Br4 CHBr2CHBr2 | | 345.6532 | 32.719 | 69.245 | ±8. | | 107.898 | | 398.858 | | 23.089 | | # |
| C2H2CL CHCL=CH\* Radical | | 61.48998 | 274.767 | 277.937 | ±8 | | 53.700 | | 270.153 | | 11.996 | | # |
| C2H2CLF | | 80.48868 | -165.393 | -159.0 | ±15 | | 64.216 | | 283.339 | | 13.469 | | † |
| C2H2CL2 CCL2=CH2 | | 96.94268 | 2.2 | 8.084 | ±1.4 | | 67.725 | | 288.353 | | 13.872 | | # |
| C2H2CL2 1,1+*cis+trans* equilib. | | 96.94268 | 3.410 | 8.284 |  | | 68.847 | | 297.020 | | 14.882 | | † |
| C2H2Cl2 1,2 CHCl=CHCl trans | | 96.94268 | 0.120 | +5.300 | ±0.54 | | 66.220 | | 296.356 | | 14.381 | | # |
| 1,2 CHCl=CHCl cis | | 96.94268 | -2.530 | +3.47 | ±0.54 | | 64.396 | | 289.691 | | 13.700 | | # |
| C2H2CL3 CH2-CCL3 | | 132.39538 | 71.864 | 77.770 | ±8. | | 95.682 | | 331.217 | | 18.441 | | # |
| C2H2F2 1,1+*cis*+*trans* equilib. | | 64.03409 | -336.4 | -329.48 | ±4 | | 60.237 | | 266.054 | | 12.480 | | † |
| C2H2F2 1,1 FC-1132A <~> | | 64.03409 | -332.93 | -326.00 | ±2.31 | | 60.237 | | 266.054 | | 12.480 | | # |
| H2C2F2 *cis* | | 64.03409 | -306.5 | -299.80 | ±5. | | 58.349 | | 268.723 | | 12.701 | | # |
| F2C2H2 *trans* FC-1132 <~> | | 64.03409 | -303.73 | -297.15 | ±5. | | 60.074 | | 267.847 | | 12.955 | | # |
| C2F3H2 CF3CH2\* Radical <~> | | 83.03249 | -517.142 | -508.946 |  | | 77.092 | | 298.883 | | 15.616 | | # |
| CF3-CFH2 <~> | | 102.03089 | -913.3 | -902.01 | ±17.5 | | 86.273 | | 315.752 | | 16.937 | | # |
| CHF2-CHF2 HFC-134 | | 102.03089 | -883.3 | -872.21 | ±5.5 | | 84.129 | | 313.143 | | 17.130 | | # |
| C2H2I2 *trans & cis*d | | 279.84622 | 207.430 | 215.116 | ±0.43 | | 71.559 | | 266.264 | | 16.085 | | # |
| C2H2N CH2CN Methyl-Cyanide | | 40.04402 | 257.78 | 260.54 |  | | 54.345 | | 255.826 | | 12.356 | | # |
| C2H2N CH2NC MethylIsocyanate | | 40.04402 | 358.23 | 360.59 | ±8. | | 53.971 | | 256.71 | | 12.550 | | # |
| C2H2NO NC-CH2-O\* | | 56.04342 | 175.619 | 181.426 | ±8. | | 61.512 | | 281.028 | | 13.444 | | # |
| C2H2NO2 NC-CH2-O-O\* | | 72.04282 | 177.987 | 185.371 | ±8. | | 74.150 | | 312.514 | | 16.207 | | # |
| 1,2-C2H2(NO2)2 *trans* | | 118.04896 | 40.953 | 56.131 | ±8. | | 108.234 | | 360.962 | | 21.428 | | # |
| 1,2-C2H2(NO2)2- *trans anion* | | 118.04891 | -184.297 | -162.624 | ±8. | | 104.884 | | 377.889 | | 21.592 | | # |
| CH2CO Ketene singlet <!> | | 42.03668 | -48.579 | -45.460 | ±0.15d | | 51.740 | | 251.442 | | 11.796 | | † |
| CH2CO Ketene triplet | | 42.03668 | 179.5d | 182.6d | ±1.3d | | 44.014 | | 253.826 | | 10.608 | | # |
| CH2CO+ c | | 42.03613 | 885.29 | 882.19 | ±0.15d | | 51.239 | | 248.303 | | 11.814 | | # |
| CH2CO- c | | 42.0372 | -23.9d | -14.7d | ±2.4d | |  | |  | |  | | X |
| HCCOH ETHYNOL <!> | | 42.03668 | 93.3 | 95.408 | ±1.4d | | 57.592 | | 249.544 | | 12.810 | | # |
| HCCOH+ c | | 42.03613 | 1067.0 | 1063.22 | ±2.6d | | 55.952 | | 291.819 | | 12.495 | | # |
| (CH=CH)O Oxirene singlet | | 42.03668 | 275.93 | 276.6d | ±3.1d | | 54.213 | | 245.56 | | 11.925 | | # |
| (CH=CH)O Oxirene triplet | | 42.03668 | 387.7d | 391.9d | ±2.8d | | 44.014 | | 248.063 | | 10.608 | | # |
| O(CH=CH)+ Oxirene cationd | | 42.03613 | 1112.34 | 1109.7d | ±5.3d | | 48.719 | | 247.073 | | 11.188 | | # |
| C2H2O2 HOCH=C=O | | 58.03608 | -155.16 | -149.807 | ±8. | | 61.975 | | 288.151 | | 13.902 | | # |
| C2H2O2 HOC≡COH Ethyndiol | | 58.03608 | -27.953 | -24.487 | ±8. | | 69.504 | | 325.406 | | 15.789 | | # |
| C2H2O2 *trans* & *cis* GLYOXAL | | 58.03608 | -212.08 | -206.51 | ±0.6d | | 60.409 | | 272.483 | | 13.682 | | † |
| C2H2O2 *cis* GLYOXAL | | 58.03668 | -193.86d | -188.42d | ±0.73d | |  | |  | |  | | X |
| C2H2O2 Oxiranone | | 58.03608 | -177.92 | -170.37 | ±8. | | 53.635 | | 263.960 | | 11.713 | | # |
| C2H2O3 Glioxalic/Glioxylyc acid  O=COH-CH=O | | 74.03548 | -477.56 | -468.578 | ±8. | | 70.634 | | 292.297 | | 14.601 | | # |
| (COOH)2 Oxalic Acid cristal c | | 90.03488 | -819.28 |  | ±0.451 | |  | |  | |  | | X |
| C2H2O4 Oxalic Acid | | 90.03488 | -721.37 | -710.756 | ±2.1 | | 86.178 | | 320.649 | | 17.322 | | # |
| C2H2S HC≡CSH Ethynethio | | 58.10328 | 257.764 | 259.376 | ±8. | | 60.982 | | 259.376 | | 13.375 | | # |
| C2H2S3 S=CH-S-CH=S | | 122.23528 | 234.551 | 240.230 | ±8 | | 85.859 | | 330.750 | | 18.132 | | # |
| C2H3 VINYL RADICAL <!> | | 27.04522 | 296.580 | 300.867 | ±0.45d | | 42.071 | | 233.663 | | 10.522 | | †# |
| C2H3+ Vinylium Ion | | 27.04467 | 1122.34 | 1119.2 | ±0.67d | | 50.714 | | 225.350 | | 11.780 | | # |
| C2H3- | | 27.04577 | 226.583 | 237.256 | ±1.00 | | 40.011 | | 227.870 | | 10.334 | | # |
| C2H3 CH3C doublet Ethylidyne | | 27.04522 | 508.63 | 512.743 | ±1.31 | | 42.923 | | 227.225 | | 10.696 | | # |
| C2H3 CH3C quartet Ethylidyne | | 27.04522 | 637.5d | 642.0d | ±2.3d | | 38.876 | | 231.294 | | 10.235 | | # |
| C2H3+ CH3C+ cation | | 27.04467 | 1332.93 | 1329.88 | ±2.8d | | 48.451 | | 225.885 | | 11.661 | | # |
| C2H3- CH3C- anion | | 27.04577 | 448.65 | 458.95 | ±2.8d | | 42.996 | | 221.440 | | 10.706 | | # |
| C2H3Br Bromoethylene <~> | | 106.94922 | 74.070 | 89.049 | ±0.68d | | 54.824 | | 275.474 | | 12.090 | | # |
| C2H3BrO2 Bromoacetic Acid | | 138.94802 | -383.5 | -364.61 | ±3.1 | | 80.542 | | 337.015 | | 16.862 | | †# |
| CH3CBr3 1,1,1-Tribromoethane | | 266.75722 | 3.18 | 34.718 | ±8. | | 97.982 | | 355.210 | | 20.051 | | # |
| CBr3CH2OH 2,2,2- tribromoethanol | | 282.75662 | -150.959 | -118.238 | ±12. | | 111.721 | | 377.126 | | 22.778 | | # |
| CBr3CH2OH+ 2,2,2- tribromoethanol cation | | 282.75607 | 825.800 | 850.984 | ±12. | | 115.414 | | 392.641 | | 24.113 | | # |
| CBr3CH2OH- 2,2,2- tribromoethanol anion | | 282.75717 | -257.572 | -222.170 | ±12. | | 119.012 | | 427.521 | | 26,355 | | # |
| C2H3CL Vinyl Chloride | | 62.49792 | 22.1 | 29.68 | ±1.02d | | 53.681 | | 264.024 | | 11.820 | | # |
| CH3C(O)Cl liq Acetyl Chloride | | 78.49732 | -272.69d |  | ±0.33d | |  | |  | |  | | X |
| CH3C(O)CL Acetyl Chloridel | | 78.49732 | -241.46 | -232.448 | ±033d | | 66.868 | | 289.950 | | 14.728 | | # |
| C2H3CLO2 Chloroacetic Acid | | 94.49672 | -427.6 | -416.0 | ±1.0 | | 78.839 | | 325.918 | | 16.514 | | # |
| C2H3CL3 CH3-CCL3 | | 133.40332 | -144.6 | -133.98 | ±2.0 | | 92.410 | | 320.413 | | 18.025 | | # |
| CH3CD3 1,1,1-Ethane-D3 | | 33.08753 | -107.57 | -92.313 | ±3.3 | | 57.385 | | 241.997 | | 12.406 | | # |
| C2H3F Vinyl Fluoride <~> | | 46.04362 | -140.1 | -134.7d | ±2.5 | | 50.407 | | 252.674 | | 11.336 | | # |
| C2H3F2 <~> | | 65.04203 | -302.50 | -293.172 |  | | 67.256 | | 288.291 | | 14.304 | | # |
| CH3CF3 FC-143A <~> | | 84.04043 | -755.66 | -742.91 | ±1.0 | | 78.074 | | 287.652 | | 15.298 | | # |
| CF3CH2OH | | 100.03983 | -885.686 | -872.188 | ±8. | | 92.610 | | 317.911 | | 18.507 | | # |
| CF3CH2OH+ cation | | 100.03928 | 201.493 | 208.116 | ±8. | | 96.278 | | 328.453 | | 19.164 | | # |
| CF3CH2OH- anion | | 100.04037 | -727.267 | -709.539 | ±8. | | 103.298 | | 343.238 | | 20.420 | | # |
| C2H3I IodoEthylene <~> | | 153.94969 | 130.56 | 139.6 | ±1.12 | | 56.071 | | 299.640 | | 12.368 | | # |
| C2H3N CH3CN Methylcyanide | | 41.05196 | 74.04 | 81.09 | ±0.37 | | 52.249 | | 243.267 | | 12.094 | | # |
| C2H3N CH3NC Methylcyanate | | 41.05196 | 163.5 | 169.982 | ±7.2 | | 52.947 | | 246.658 | | 12.660 | | # |
| C2H3N cy(-CH=CH-NH-)1H aziridin | | 41.05196 | 377.677 | 385.257 | ±8. | | 52.533 | | 249.962 | | 11.564 | | # |
| C2H3N cy(-CH2CH=N-)2H aziridin | | 41.05196 | 293.906 | 282.278 | ±8. | | 45.962 | | 245.879 | | 10.779 | | # |
| C2H3NO NCCH2OH | | 57.05136 | -49.710 | -39.971 | ±8. | | 64.965 | | 280.796 | | 13.745 | | # |
| C2H3NO2 NCCH2-O-OH | | 73.05136 | 29.476 | 39.641 | ±8. | | 82.503 | | 323.081 | | 17.659 | | # |
| C2H3NO2 Nitroethylene | | 73.05076 | 29.518 | 42.235 | ±8.0 | | 73.68 | | 300.503 | | 15.107 | | # |
| C2H3NO4 CH3C(O)-O-NO2 | | 105.04956 | -303.65 | -287.915 | ±8.0 | | 101.794 | | 351.943 | | 20.765 | | # |
| C2H3NO5 CH3C(O)-OO-NO2 | | 121.04896 | -254.64 | -237.021 | ±8.0 | | 116.800 | | 373.968 | | 23.223 | | # |
| C2H3NS HS-CH2-CN | | 73.11796 | 130.461 | 138.941 | ±8. | | 72.659 | | 303.105 | | 15.076 | | # |
| C2H3ClN2 3 Me-3-ChloroDiazirinef | | 90.51140 | 218.f | 230.287 | ±40. | | 79.946 | | 303.405 | | 15.782 | | # |
| C2H3N3 Cy 1-H-1,2,4-Triazine | | 69.06544 | 806.25 | 822.226 | ±0.8 | | 58.488 | | 270.231 | | 11.845 | | # |
| 1,1,1-C2H3(NO2)3 cr CH3C(NO2)3 (s) | |  | -112.97 |  | ±0.8.4 | |  | |  | |  | | X |
| C2H3O (CH3CO) RADICAL<~> | | 43.04462 | -10.3 | -3.6 | ±0.41d | | 50.785 | | 267.448 | | 12.385 | | # |
| C2H3O+ (CH3CO+) cation | | 43.04471 | 665.789 | 666.3d | ±1.1 | | 52.589 | | 243.392 | | 11.977 | | # |
| C2H3O-c (CH3CO-) anion | | 43.04462 | -55.6 | -43.8d | ±1.9 | | 57.121 | | 258.942 | | 12.590 | | # |
| C2H3O (CH2=CHO\*) Radical | | 43.04462 | 12.753 | 20.189 | ±8. | | 52.398 | | 258.818 | | 11.713 | | # |
| OH3C2 (\*CH2CHO) RAD <!> | | 43.04462 | 12.753  15.79h | 19.833 | ±8  0.86h. | | 54.335 | | 264.204 | | 12.069 | | # |
| C2H3O (\*CH=CH-OH) | | 43.04462 | 141.505 | 147.660 | ±8. | | 58.496 | | 266.788 | | 12.994 | | # |
| C2H3O OXYRANE RAD <!> | | 43.04462 | 164.473 | 172.900 | ±8.0 | | 45.741 | | 252.528 | | 10.723 | | # |
| C2H3O2 HOCH2C\*=O | | 59.04402 | -145.42 | -136.978 | ±8. | | 66.163 | | 304.877 | | 15.044 | | # |
| C2H3O2 HOC\*HCHOH | | 59.04402 | -176.05 | -167.064 | ±8. | | 63.064 | | 325.723 | | 14.503 | | # |
| C2H3O2 \*COOCH3 RADICAL | | 59.04402 | -163.39 | -154.616 | ±8.0 | | 66.197 | | 288.777 | | 14.720 | | # |
| C2H3O2 CH3C(O)O\* Acetic Rad | | 59.04402 | -192.79 | -183.115 | ±8. | | 65.149 | | 284.722 | | 13.814 | | # |
| C2H3O2 H2C=CHOO Vinylperoxy | | 59.04402 | 105.772 | 115.350 | ±8. | | 65.002 | | 284.555 | | 13.910 | | # |
| C2H3O2 CH3O-\*C=O | | 59.04402 | -160.5 | -160.342 | ±1.2 | | 65.585 | | 293.197 | | 15.336 | | # |
| C2H3O3 CH3-C(O)-OO | | 75.04352 | -159.28 | -148.043 | ±8. | | 83.661 | | 304.462 | | 17.042 | | # |
| C2H4 ETHYLENE <^!> | | 28.0536 | 52.500 | 61.025 | ±.15d | | 42.887 | | 219.322 | | 10.519 | | † |
| C2H4+ | | 28.05261 | 1074.46 | 1074.912 | ±0.15d | | 48.804 | | 246.866 | | 12.395 | | # |
| C2H4-d | | 28.0537 | 219.4d | 232.1 | ±2.0 | | 48.945 | | 222.983 | | 11.281 | | # |
| CH3CH singlet c | | 28.05316 | 366.85 | 374.724 | ±1.12 | | 47.351 | | 226.164 | | 11.169 | | # |
| CH3CH triplet c | | 28.05316 | 354.46 | 361.5d | ±1.11 | | 48.988 | | 240.764 | | 11.909 | | # |
| CH3CH+ c 1-Ethylium-1-yl | | 28.0526 | 1184.77 | 1185.7d | ±2.52 | |  | |  | |  | | X |
| CH3CH- Ethylidene anion | | 28.05370 | 314.68 | 328.54 | ±2.04 | | 48.254 | | 234.158 | | 11.380 | | # |
| C2H4Br CH3CHBr Br-ethylidene | | 107.95716 | 130.332 | 146.440 | ±8. | | 71.288 | | 301.875 | | 15.175 | | # |
| C2H4Br2 liq. CH2Br-CH2Br liquid | | 187.8611 | -79.31d |  | ±1.24 | |  | |  | |  | | X |
| C2H4Br2 CH2Br-CH2Br | | 187.8611 | -37.5 | -10.491 | ±1.3d | | 75.948 | | 329.088 | | 16.422 | | # |
| C2H4Br2 CHBr2-CH3 liquid | | 187.8611 | -66.3d |  | ±1.34 | |  | |  | |  | | X |
| C2H4Br2 CH3-CHBr2 | | 187.8611 | -36.3d | -9.3d | ±7.8d | | 79.452 | | 327.355 | | 16.288 | | # |
| C2H4CL CH3CHCl\* RADICAL | | 63.50586 | 80.718 | 90.154 | ±8. | | 63.575 | | 286.929 | | 14.198 | | # |
| C2H4CL CH2ClCH2\* RADICAL | | 63.50586 | 97.998 | 108.416 | ±8. | | 58.631 | | 284.827 | | 13.216 | | # |
| C2H4ClF ClFHC-CH3 | | 82.50426 | -310.70 | -296.966 | ±8. | | 70.860 | | 291.429 | | 14.313 | | # |
| C2H4CL2 liq. CH2CL-CH2CLliq.a | | 98.95856 | -165.24d |  | ±0.59 | |  | |  | |  | | X |
| C2H4CL2 CH2CL-CH2CL FR150 | | 98.95856 | -130.07 | -117.37 | ±0.6 | | 72.544 | | 303.542 | | 15.531 | | # |
| C2H4CL2 liq. CH3-CHCL2 liq.a | | 98.95856 | -158.11d |  | ±1.03 | |  | |  | |  | | X |
| C2H4CL2 CH3-CHCL2 | | 98.95856 | -127.48 | -114.438 | ±1.1d | | 75.454 | | 304.249 | | 15.283 | | # |
| C2H4O2CL2 Cl2-Peroxyethane | | 130.95796 | -231.38 | -215.17 |  | | 109.993 | | 362.046 | | 20.697 | | # |
| C2H4F CH3CHF α Radical <~> | | 47.05216 | -75.659 | -65.6 | ±8. | | 58.671 | | 273.994 | | 13.397 | | # |
| C2H4F CH2FCH2\* β Radical <~> | | 47.05156 | -61.091 | -51.271 | ±8. | | 60.737 | | 278.832 | | 13.636 | | # |
| C2H4F2 CH2F-CH2F HFC152<~> | | 66.04997 | -450.36 | -436.747 | ±4.92 | | 66.868 | | 286.321 | | 14.255 | | # |
| C2H4F2 CH3-CHF2 HFC-152a | | 66.04997 | -500.45 | -486.52 | ±5.6 | | 67.266 | | 282.502 | | 13.939 | | # |
| (CIH2)2 cr | | 281.86210 | 9.26d |  | ±0.6d | |  | |  | |  | | X |
| (CIH2)2 | | 281.86210 | 73.123 | 88.350 | ±0.9 | | 77.887 | | 340.936 | | 17.012 | | # |
| C2H4ON \*C(O)CH2NH2 Rad. | | 58.05930 | 29.3 | 41.35 | ±3.3 | | 74.484 | | 304.116 | | 15.667 | | # |
| 1,1-C2H4(NO2)2 liq | | 120.06424 | -149.37 |  | ±0.42 | |  | |  | |  | | X |
| 1,2-C2H4(NO2)2 liq | | 120.06424 | -178.24 |  | ±0.42 | |  | |  | |  | | X |
| 1,2-C2H4(NO2)2 1,2-DinitroEthane | | 120.06424 | -96.65 | -72.50 | ±1.26 | | 105.233 | | 401.082 | | 20.926 | | # |
| 1,2-C2H4(NO2)2+1,2DinitroEthane+ | | 120.06369 | 1002.717 | 1016.909 | ±8. | | 110.808 | | 416.045 | | 23.080 | | # |
| 1,2-C2H4(NO2)2- 1,2-DinitroEthane- | | 120.06479 | -205.276 | 177.665 | ±8. | | 106.148 | | 413.155 | | 22.280 | | # |
| C2H4O VINYL-ALCOHOL | | 44.05256 | -124.683 | -114.308 |  | | 62.518 | | 260.949 | | 13.009 | | # |
| C2H4O OXYRANE  <!> | | 44.05316 | -52.635 | -40.082 | ±0.44d | | 47.624 | | 242.870 | | 10.831 | | † |
| CH3CHO (liq) Acetaldehyde (l) c | | 44.05316 | -191.68d | -186.97d | ±0.35 | | 89.05 | | 117.3 | |  | | X |
| CH3CHO ACETALDEHYDE <~> | | 44.05316 | -166.19 | -155.70 | ±0.32d | | 55.319 | | 263.952 | | 12.897 | | † |
| CH3CHO | | 44.05316 |  | -75.95 | ±2.36 | |  | |  | |  | | X |
| CH3CHO+d | | 44.05201 | 828.2d | 832.01d | ±0.29g | | 58.506 | | 269.216 | | 13.206 | | # |
| CH3CHO- | | 44.05311 | -76.0d | -59.3d | ±2.5d | | 57.011 | | 267.304 | | 13.285 | | # |
| HOCH2CHO Acetaldehyde-1-ol | | 60.05196 | -306.55 | -294.036 | ±8. | | 66.391 | | 309.242 | | 15.206 | | # |
| CH3COOH liquid Acetic Acid c | | 60.05196 | -484.21d |  | ±0.17d | | 123.386 | | 159.829 | |  | |  |
| CH3COOH ACETIC ACID | | 60.05196 | -432.253 | -418.12 | ±0.49d | | 63.439 | | 283.473 | | 13.597 | | † |
| CH3COOH+ cation | | 60.05141 | 600.250 | 607.450 | ±8. | | 76.617 | | 306.654 | | 16.445 | | # |
| CH3COOH- anion | | 60.05251 | -322.170 | -303.813 | ±8. | | 82.210 | | 312.209 | | 17.352 | | # |
| (HCOOH)2 Formic Acid dimmer | | 92.05076 | -820.943 | -804.171 |  | | 96.142 | | 332.785 | | 19.632 | | † |
| HCOOCH3 (liq) Methyl Formatec | | 60.05196 | -386.146 |  | ±0.578 | |  | |  | |  | | X |
| HCOOCH3 MethylFormate | | 60.05196 | -357.796 | -344.396 | ±0.6 | | 62.436 | | 286.254 | | 14.323 | | # |
| C2H4O3 HOCH2COOH | | 76.05136 | -583.0 | -567.9 | ±10. | | 87.074 | | 318.610 | |  | | # |
| C2H4S CH2=CHSH | | 60.11916 | 80.475 | 90.314 | ±8. | | 63.260 | | 275.636 | | 13.616 | | # |
| C2H4S-cyclo -CH2-CH2-S- | | 60.11916 | 78.847 | 90.976 | ±8. | | 52.391 | | 255.070 | | 11.326 | | # |
| cy-C2H4S+ (-CH2-CH2-S-)+ | | 60.11861 | 959.600 | 965.002 | ±8. | | 54.800 | | 262.601 | | 11.637 | | # |
| cy-C2H4S- (-CH2-CH2-S-)- | | 60.11971 | 89.282 | 105.512 | ±8. | | 62.545 | | 273.620 | | 13.189 | | # |
| C2H4S2 CH3-S-CH=S | | 92.18516 | 78.185 | 89.762 | ±8. | | 77.657 | | 299.960 | | 16.271 | | # |
| C2H4S2 HS-CH2-CH=S | | 92.18516 | 108.751 | 120.668 | ±8. | | 78.840 | | 316.034 | | 15.950 | | # |
| C2H4S2+ HS-CH2-CH=S+ | | 92.18461 | 983.244 | 988.741 | ±8. | | 80.389 | | 323.048 | | 16.173 | | # |
| C2H4S2- HS-CH2-CH=S- | | 92.18570 | 45.714 | 60.949 | ±8. | | 90.773 | | 345.885 | | 18.829 | | # |
| C2H4S4 2(HS)C=C(SH)2 | | 156.31716 | 159.373 | 170.530 | ±8. | | 137.717 | | 406.563 | | 25.534 | | # |
| C2H4S4 1,2,4,5-HexaCyC2H4S4 C2H4S4 | | 156.31716 | 105.060 | 120.373 | ±8. | | 112.256 | | 348.918 | | 21.379 | | # |
| C2H4Si CH2=CH-SiH | | 56.13866 | 307.432 | 315.538 | ±8. | | 65.371 | | 278.892 | | 14.155 | | # |
| C2H4Si+ CH2=CH-SiH cation | | 56.13111 | 1122.630 | 1124.454 | ±8. | | 65.910 | | 276.057 | | 13.997 | | # |
| C2H4Si- CH2=CH-SiH anion | | 56.13921 | 200.882 | 214.961 | ±8. | | 67.638 | | 276.355 | | 14.121 | | # |
| C2H5 ETHYL RADICAL <!> | | 29.06110 | 119.7 | 130.773 | ±0.36d | | 50.679 | | 242.984 | | 12.204 | | #† |
| C2H5+ | | 29.06055 | 909.095 | 914.835 | ±0.41d | | 48.713 | | 237.490 | | 11.340 | | # |
| C2H5- Ethanided | | 29.61649 | 138.43 | 156.402 | ±2.4 | | 50.513 | | 239.988 | | 11.502 | | # |
| C2H5Br (liq)c | | 108.9651 | -91.46d | -55.93d | ±0.28d | |  | |  | |  | | X |
| C2H5Br Bromoethane <~> | | 108.9651 | -63.54d | -41.55d | ±0.27 | | 64.206 | | 287.668 | | 13.584 | | #† |
| BrCH2CH2OH (liq) | | 124.9645 | -275.17d |  | ±0.47d | |  | |  | |  | | X |
| BrCH2CH2OH | | 124.9645 | -220.75 | -196.523 | ±0.53 | | 77.931 | | 325.767 | | 15.651 | | # |
| C2H5CL (liq) | | 64.5138 | -135.75d | -134.13d | ±0.22d | |  | |  | |  | | X |
| C2H5CL CHLOROETHANE | | 64.5138 | -111.235 | -96.65 | ±0.22 | | 62.654 | | 276.218 | | 13.283 | | # |
| ClCH2CH2OH (liq) | | 80.5132 | -315.09d |  | ±0.54d | |  | |  | |  | | X |
| ClCH2CH2OH | | 80.5132 | -266.76 | -249.809 | ±0.6 | | 76.044 | | 314.467 | | 15.256 | | # |
| C2H5CLO2 Chloroperoxyethane | | 96.5132 | -212.966 | -194.27 |  | | 92.223 | | 336.239 | | 17.853 | | # |
| C2H5F FLUOROETHANE<~> | | 48.0595 | -272.54 | -257.74 | ±0.94 | | 59.575 | | 270.630 | | 12.888 | | # |
| FCH2CH2OH | | 64.05890 | -424.32 | -407.063 | ±1.05 | | 72.550 | | 304.856 | | 14.773 | | # |
| C2H5I liq | | 155.96557 | -39.08d | -9.21d | ±0.38d | |  | |  | |  | | X |
| C2H5I IODOETHANE <~> | | 155.96557 | -7.047 | +8.253 | ±0.38d | | 71.670 | | 298.362 | | 14.575 | | # |
| ICH2CH2OH liq Iodoethanol liq | | 171.96497 | -207.2 |  | ±2.4d | |  | |  | |  | | X |
| ICH2CH2OH Iodoethanol | | 171.96497 | -150.20 | -131.872 | ±2.36 | | 77.483 | | 318.285 | | 15.888 | | # |
| C2H5N C2H3NH2 VinylAmine | | 43.06784 | 56.819 | 71.511 | ±8. | | 62.936 | | 264.299 | | 12.920 | | # |
| C2H5N azeridine cy(-CH2CH2NH-) | | 43.06784 | 129.819 | 146.255 | ±8 | | 51.223 | | 250.221 | | 11.076 | | # |
| NH2CH2C(O)OH (cr) Glycine solid | | 75.06664 | -333.5 |  |  | | 409.6 | |  | |  | | X |
| C2H5NO2 Glycine NH2CH2C(O)OH | | 75.06664 | -391.706 | -372.393 | ±8 | | 87.389 | | 359.646 | | 16.979 | | # |
| C2H5NO2 (liq) NITROETHANE | | 75.06664 | -143.93 |  | ±0.42 | |  | |  | |  | | X |
| C2H5NO2 NITROETHANE | | 75.06664 | -107.972 | -88.531 | ±8 | | 80.584 | | 320.078 | | 16.851 | | # |
| C2H5NO2+ Nitroethane cation | | 75.06609 | 947.706 | 959.538 | ±8 | | 85.546 | | 332.304 | | 17.661 | | # |
| C2H5NO2- NITROETHANE anion | | 75.06719 | -128.177 | -102.989 | ±8 | | 84.369 | | 327.119 | | 17.468 | | # |
| C2H5ONO2 ETHYLNITRATE | | 91.06604 | -154.984 | -132.642 | ±8. | | 94.998 | | 325.634 | | 18.291 | | # |
| CH3OC(O)NH2 MethylCarbamate | | 75.06664 | -412. | -392.6 | ±3. | | 88.782 | | 307.374 | | 16.905 | | # |
| C2H5N3 Ethyl Azide | | 71.08132 | 266.872 | 287.394 | ±8. | | 80.026 | | 303.042 | | 15.761 | | # |
| C2H5N3O5 NENA HN(NO2)CH2 CH2ONO2 | | 151.07832 | -75.07 | -44.758 | ±3. | | 138.102 | | 433.078 | | 27.670 | | # |
| C2H5O\* ETHOXY RADICAL | | 45.06050 | -11.47 | -1.52 | ±0.5 | | 63.473 | | 272.575 | | 17.666 | | # |
| C2H5O+ d Ethyloxyoxoniumylidene | | 45.0600 | 981.63 | 989.1d | ±1.75 | |  | |  | |  | | X |
| C2H5O- c | | 45.06105 | -184.37 | -163.672 | ±0.51d | | 58.967 | | 266.118 | | 13.117 | | # |
| C\*H2CH2OH RADICAL | | 45.06050 | -25.82 | -13.3 | ±0.6 | | 68.358 | | 297.629 | | 15.095 | | # |
| CH2CH2OH+ | |  | 1013.79 |  | ±1.57 | |  | |  | |  | | X |
| CH3C\*HOH RADICAL | | 45.06050 | -55.29 | -41.93 | ±0.6 | | 64.038 | | 288.991 | | 14.263 | | # |
| CH3C\*HOH+ Hydroxyethylium | | 45.95995 | 601.016 | 609.389 | ±0.4d | | 59.266 | | 264.216 | | 13.047 | | # |
| CH3C\*HOH- | | 45.0610 | -39.32 | -19.95 | ±2.4 | | 68.077 | | 282.703 | | 14.446 | | # |
| (CH2-CH2)OH+ Ethylene oxide- oxonium (Protonatedoxirane) | | 45.05995 | 715.07d | 725.04d | ±0.62d | | 52.329 | | 246.649 | | 11.266 | | # |
| C2H5O Dimethylether Radical | | 45.06050 | -1.887 | 11.191 | ±8.0 | | 66.484 | | 281.716 | | 14.539 | | # |
| C2H5O+ CH3-O-CH2+ | | 45.05995 | 676.909 | 678.982 | ±8. | | 59.088 | | 264.746 | | 13.149 | | # |
| C2H5O2 HOCH2CH2O\* | | 61.05990 | -159.636 | -143.869 | ±8 | | 71.493 | | 329.555 | | 16.190 | | # |
| C2H5O2 HOCH2C\*HOH | | 61.05990 | -207.443 | -192.194 | ±8. | | 75.813 | | 336.908 | | 16.709 | | # |
| C2H5O2 EthylPeroxy Radical | | 61.05990 | -28.70 | -12.642 | ±8.4 | | 76.155 | | 308.996 | | 15.897 | | # |
| C2H5O2 \*C2H4OOH Radical | | 61.05990 | 40.543 | 63.548 | ±8. | | 85.355 | | 302.325 | | 17.952 | | # |
| C2H5S\* EthylThio Radical | | 61.12710 | 97.6 | 111.4 | ±8. | | 64.353 | | 284.751 | | 13.877 | | # |
| C2H6 ETHANE <^!> | | 30.06904 | -83.852 | -68.232 | ±0.2 | | 52.501 | | 229.221 | | 11.892 | | † |
| C2H6+ | | 30.06849 | 1036.13 | 1044.68 | ±0.6 | | 60.532 | | 239.247 | | 12.760 | | # |
| C2H6- | | 30.06959 | -13.22 | +8.327 | ±3.1 | | 55.704 | | 236.279 | | 12.117 | | # |
| C2H6Bi Bi(CH3)2 Radical | | 239.04942 | 265.000 |  | ±22. | | 87.130 | | 330.692 | | 17.416 | | # |
| C2H6N (CH3)2N\* Dimethylazide | | 44.07578 | 159.854 | 177.58 | ±8. | | 66.912 | | 308.930 | | 14.120 | | # |
| C2H6N \*CH2-NH-CH3 | | 44.07578 | 156.58 | 174.07 | ±8. | | 70.233 | | 279.671 | | 14.498 | | # |
| C2H6N CH3CH2NH\* Ethylamine | | 44.07578 | 150.2 | 168.1 | ±8. | | 67.198 | | 269.796 | | 13.937 | | # |
| C2H6N2 AZOMETHANE | | 58.08252 | 193.866 | 213.543 | ±8. | | 77.639 | | 289.748 | | 16.504 | | # |
| C2H6N2O (CH3)2N-N=O | | 74.08192 | 58.622 | 80.785 | ±8. | | 91.732 | | 309.776 | | 18.358 | | # |
| C2H6N2O+ (CH3)2N-N=O cation | | 74.08137 | 914.958 | 930.103 | ±8. | | 92.558 | | 316.072 | | 18.457 | | # |
| C2H6N2O- (CH3)2N-N=O anion | | 74.08247 | 82.269 | 109.374 | ±8. | | 98.178 | | 318.380 | | 19.047 | | # |
| C2H6N2O2 (CH3)2N-NO2 | | 90.08192 | -4.8 | 20.279 |  | | 103.204 | | 328.138 | | 19.783 | | # |
| C2H5OH(L) ETHANOL LIQUID | | 46.06904 | -277.51 | -269.74 | ±0.22d | | 112.250 | | 160.100 | | 24.082 | | † |
| C2H5OH ETHANOL <^> | | 46.06904 | -234.95 | -217.641 | ±0.22d | | 65.309 | | 280.593 | | 14.542 | | † |
| C2H5OH+ | | 46.06789 | 784.495 | 796.087 | ±0.74 | | 70.662 | | 285.132 | | 14.062 | | # |
| CH3OCH3 DIMETHYLETHER | | 46.06904 | -183.935 | -166.438 | ±0.45 | | 65.823 | | 267.381 | | 14.354 | | # |
| CH3OH-CH2+ oxonium cation | | 46.06789 | 797.630 | 808.080 | ±8. | | 72.130 | | 282.717 | | 15.204 | | # |
| C2H6OS CH3CHOHSH | | 78.13444 | -218.112 | -198.611 | ±8. | | 87.856 | | 304.223 | | 16.782 | | # |
| C2H6O2 liq HO-CH2-CH2-OH liq c | | 62.06784 | -455.169 |  | ±0.375 | |  | |  | |  | | X |
| C2H6O2 1,2-Ethane DiOl | | 62.06784 | -389.362 | -369.547 | ±0.49d | | 74.572 | | 323.647 | | 16.376 | | # |
| C2H6O2 PEROXYETHANE | | 62.06784 | -162.080 | -142.228 | ±8. | | 80.747 | | 315.739 | | 16.340 | | # |
| CH3OOCH3 Dimethylperoxyde | | 62.06784 | -125.5 | -106.773 | ±5.0 | | 84.582 | | 304.378 | | 17.464 | | # |
| C2H6S C2H5SH Ethanethiol | | 62.13504 | -43.514 | -27.099 | ±8. | | 71.312 | | 300.135 | | 15.509 | | # |
| C2H6S (CH3SCH3)Methylsulfide | | 62.13504 | -35.376 | -19.028 | ±8. | | 71.824 | | 285.936 | | 15.576 | | # |
| C2H6S2 CH3-SS-CH3 | | 94.20164 | -17.732 | -1.486 | ±8. | | 90.588 | | 359.431 | | 20.089 | | # |
| C2H6S2 CH3CH(SH)2 | | 94.20104 | -8.841 | +9.474 | ±8. | | 94.614 | | 336.961 | | 18.021 | | # |
| C2H6Sb Sb(CH3)2 | | 151.82904 | 143.93 |  | ±4.5 | | 78.064 | | 326.197 | | 17.351 | | # |
| C2H6Si CH2=CH-SiH3 | | 58.15454 | 90.174 | 106.267 | ±8. | | 75.903 | | 280.937 | | 14.636 | | # |
| C2H6Si+ CH2=CH-SiH3 cation | | 58.15399 | 1062.586 | 1070.361 | ±8. | | 80.135 | | 300.154 | | 16.145 | | # |
| C2H6Si- CH2=CH-SiH3 anion | | 58.15509 | 165.192 | 183.899 | ±8. | | 89.718 | | 303.118 | | 17.357 | | # |
| C2H6Si CH2=SiH-CH3 | | 58.15454 | 125.817 | 140.865 | ±8. | | 82.212 | | 287.045 | | 15.681 | | # |
| C2H6Si+ CH2=SiH-CH3 cation | | 58.15399 | 938.099 | 945.379 | ±8. | | 81.677 | | 302.032 | | 16.633 | | # |
| C2H6Si- CH2=SiH-CH3 anion | | 58.15509 | 131.628 | 151.072 | ±8. | | 87.328 | | 299.695 | | 16.631 | | # |
| C2H6Zn DiMethylZinc Zn(CH3)2 | | 95.45904 | 55.400 | 70.493 | ±5.9 | | 83.376 | | 305.332 | | 18.076 | | # |
| C2H7+ Ethane Protonated cation  CH3-H+-CH3 | | 31.07643 | 865.155 | 876.184 | ±8. | | 64.400 | | 257.199 | | 14.305 | | # |
| C2H7N (liq) CH3-NH-CH3 c | | 45.08372 | -41.104 |  | ±0.7 | |  | |  | |  | | X |
| C2H7N CH3-NH-CH3 | | 45.08372 | -15.259 | +6.501 | ±0.69d | | 68.541 | | 267.185 | | 14.320 | | # |
| C2H7N CH3CH2NH2 | | 45.08372 | -47.946 | -26.072 | ±8. | | 69.963 | | 270.795 | | 14.321 | | # |
| C2H7N2 (CH3)2N-NH\* | | 59.09046 | 207.685 | 232.276 | ±8. | | 81.384 | | 294.772 | | 15.824 | | # |
| C2H7N2 \*CH2(CH3)N-NH2 | | 59.09046 | 258.655 | 281.792 | ±8. | | 90.949 | | 322.581 | | 17.279 | | # |
| C2H7O+ (CH3)2OH+ | | 47.07583 | 562.238 | 570.996 | ±8. | | 69.946 | | 273.423 | | 14.933 | | # |
| C2H7O+ C2H5-OH2+ | | 47.07583 | 527.762 | 536.286 | ±8. | | 72.680 | | 280.690 | | 15.171 | | # |
| C2H7PO3 (CH3O)2PH=O | | 110.04894 | -719.769 | -695.215 | ±8. | | 124.610 | | 395.893 | | 25.571 | | # |
| C2H7PO3+ (CH3O)2PH=O+ | | 110.04839 | 102.220 | 119.654 | ±8. | | 126.740 | | 404.779 | | 26.494 | | # |
| C2H7P C2H5PH2 | | 62.05074 | -30.861 | -8.733 | ±8. | | 75.523 | | 286.070 | | 14.977 | | # |
| C2H7P+ C2H5PH2+ | | 62.05019 | 834.725 | 849.147 | ±8. | | 80.003 | | 295.471 | | 15.680 | | # |
| C2H7P- C2H5PH2- | | 62.05129 | 114.687 | 141.770 | ±8. | | 81.127 | | 294.352 | | 15.463 | | # |
| C2H7P (CH3)2PH | | 62.05074 | -50.459 | -28.456 | ±8. | | 78.433 | | 280.375 | | 15.102 | | # |
| C2H7P+ (CH3)2PH+ cation | | 62.05019 | 765.566 | 780.603 | ±8. | | 81.922 | | 290.444 | | 15.871 | | # |
| C2H8N2 SYM Dimethylhydrazine | | 60.09840 | 106.173 | 133.504 | ±8. | | 86.934 | | 310.941 | | 17.319 | | # |
| C2H8N2 UDMH | | 60.09840 | 93.487 | 121.271 | ±8. | | 90.405 | | 305.644 | | 16.866 | | # |
| C2H8P C2H5PH3 protonated | | 63.05868 | 155.021 | 180.275 | ±8. | | 81.719 | | 285.437 | | 16.086 | | # |
| C2H8P+ C2H5PH3+ cation | | 63.05813 | 645.136 | 663.877 | ±8. | | 81.210 | | 292.300 | | 16.271 | | # |
| C2H8P- C2H5PH3- anion | | 63.05923 | 79.500 | 109.453 | ±8. | | 86.166 | | 288.875 | | 16.737 | | # |
| C2H8Si CH3SiH2CH3 | | 60.17042 | -88.190 | -65.677 | ±8. | | 90.149 | | 289.540 | | 16.683 | | # |
| C2H8Si+ CH3SiH2CH3+ cation | | 60.16987 | 893.340 | 906.884 | ±8. | | 104.302 | | 313.942 | | 19.455 | | # |
| C2H8Si- CH3SiH2CH3- anion | | 60.17097 | 68.684 | 96.104 | ±8. | | 98.317 | | 303.243 | | 17.974 | | # |
| C2H8Si C2H5SiH3 | | 60.17042 | -36.116 | -12.942 | ±8. | | 85.192 | | 291.590 | | 16.023 | | # |
| C2H8Si+ C2H5SiH3+ cation | | 60.16987 | 929.961 | 943.743 | ±8. | | 96.348 | | 307.231 | | 17.853 | | # |
| C2H8SiO SiH3CH2CH2OH | | 76.16982 | -190.556 | -166.875 | ±8. | | 99.748 | | 316.856 | | 19.414 | | # |
| CCN Cyanomethylidyne <~> | | 38.02814 | 679.07 | 674.474 | ±4.4d | | 44.231 | | 237.159 | | 11.089 | | #† |
| CCN+ | | 38.02759 | 1721.81 | 1710.21 | ±6.08 | | 45.805 | | 234.357 | | 11.847 | | # |
| CCN- | | 38.02869 | 403.05 | 405.662 | ±5.83 | | 40.937 | | 221.099 | | 10.027 | | # |
| CNC <~> | | 38.02814 | 675.85 | 670.935 | ±4.0d | | 45.042 | | 233.804 | | 11.357 | | #† |
| CNC+c | | 38.02759 | 1623.85 | 1612.15 | ±6.2d | | 45.473 | | 228.587 | | 11.946 | | # |
| CNC-c | | 38.0287 | 475.63 | 478.1d | ±5.76 | |  | |  | |  | | X |
| N(CC) c cyclo | | 38.02814 | 725.46 | 721.491 | ±4.95 | | 39.399 | | 238.890 | | 10.411 | | # |
| C2NO O=C\*-CN | | 54.02754 | 210.00 | 207.188 | ±10. | | 56.145 | | 278.187 | | 13.594 | | #† |
| C2N2 NCCN DiCyanogen <^> | | 52.03488 | 309.28 | 307.342 | ±0.43 | | 57.085 | | 242.204 | | 12.715 | | † |
| NCCN+ | | 52.03433 | 1606.684 | 1598.26d | ±0.43 | | 56.884 | | 249.252 | | 12.828 | | # |
| NCCN-c | | 52.0354 | 278.3d | 281.4d | ±2.7d | |  | |  | |  | | X |
| CNNC Diisocyanogen | | 52.0349 | 613.0 | 610.1 | ±1.7 | |  | |  | |  | | X |
| CNNC+d *trans-cis-*equil | | 52.03433 | 1832.17 | 1823.0d | ±3.40 | | 56.010 | | 280.826 | | 13.478 | | # |
| CNNC+c *cis* | | 52.03433 | 1843.92 | 1835.0d | ±3.5d | |  | |  | |  | | X |
| CNNC-c | | 52.0354 | 457.36 | 456.7d | ±5.50 | |  | |  | |  | | X |
| CC(NN) cyclo | | 52.0349 | 836.03 | 833.6d | ±3.52 | |  | |  | |  | | X |
| NNCC Diazoethylenylidene | | 52.0349 | 659.5 | 656.9 | ±3.0 | |  | |  | |  | | X |
| NNCC+ Diazoethylenylidene+ | | 52.03433 | 1785.3d | 1777.0d | ±6.1d | |  | |  | |  | | X |
| NNCC- Diazoethylenylidene- | | 52.03543 | 532.3d | 536.0d | ±5.8d | | 57.934 | | 284.378 | | 13.726 | | # |
| CNCN Isocyanogen C=N-CN | | 52.03488 | 413.04 | 410.376 | ±1.54 | | 54.451 | | 290.381 | | 13.441 | | # |
| CNCN + | | 52.03433 | 1660.3d | 1652.8d | ±1.7d | | 54.908 | | 282.958 | | 13.154 | | # |
| CNCN- *trans*-equil | | 52.03543 | 381.4d | 383.9d | ±2.9d | | 55.757 | | 275.641 | | 13.523 | | # |
| CNCN- cis | | 52.03543 | 383.3d | 386.6d | ±2.9d | |  | |  | |  | | X |
| (CN)2Hg Hg(CN)2(solid) | | 252.62488 | 263.6 |  | ±8.4 | |  | |  | |  | | X |
| (CN)2Hg Hg(CN)2(gas) | | 252.62488 | -372.4 | -370.741 | ±9.4 | | 83.042 | | 341.379 | | 18.461 | | # |
| C2N2O2Hg Hg-Fulminate | | 284.62368 | 396.894 | 404.358 | ±20. | | 104.559 | | 354.029 | | 21.336 | |  |
| C2(NO2)2 Dinitroacetylene | | 116.03248 | 349.046 | 356.251 | ±8 | | 102.603 | | 353.895 | | 20.933 | | # |
| C2N3 (CN)2N\* radical | | 66.04162 | 512.749 | 513.522 | ±8 | | 65.553 | | 286.422 | | 14.334 | | # |
| C2N3+ CN)2N\*+ radical cation | | 66.04107 | 1670.67 | 1664.29 | ±8 | | 68.048 | | 204.232 | | 15.080 | | # |
| C2N3- CN)2N\*- radical anion | | 66.04217 | 104.250 | 111.704 | ±8 | | 62.329 | | 276.973 | | 13.643 | | # |
| C2(NO2)4 Tetranitroethylene | | 208.04356 | ? 324.3 | N/A |  | | 184.031 | | 468.771 | | 35.016 | | # |
| C2N6O3 FTDO explosive | | 156.06004 | 661.7 | 680.8 | ±16.7 | | 121.751 | | 358.564 | | 21.409 | | # |
| C2(NO2)6 cr Hexanitroethane | | 300.05464 | 80.33 |  | ±0.42 | |  | |  | |  | | X |
| C2(NO2)6 Hexanitroethane | | 300.05464 | 142.256 | 168.321 | ±0.84 | | 286.780 | | 624.839 | | 54.133 | | # |
| C2O <!> | | 40.02080 | 385.68 | 381.641 | ±1.9 | | 43.134 | | 233.624 | | 10.486 | | # |
| C=O=C triplet | | 40.02080 | 656.9d | 652.6d | ±3.3d | |  | |  | |  | | X |
| C=O=C singlet | | 40.02080 | 725.2d | 720.8d | ±1.7d | | 37.395 | | 233.411 | | 10.175 | | # |
| COC+d C=O-C doublet | | 40.02025 | 1589.1d | 1575.8d | ±2.3d | | 45.231 | | 245.747 | | 11.418 | | # |
| COC+d  C=O-C quartet | | 40.0203 | 1822.4d | 1812.2d | ±2.3d | |  | |  | |  | | X |
| COC- c C=O-C | | 40.02135 | 547.95 | 550.592 | ±2.02 | | 40.940 | | 221.850 | | 10.003 | | # |
| CCO Dicarbon monoxide | | 40.02080 | 378.9d | 374.8d | ±1.3d | |  | |  | |  | | X |
| CCO singlet | | 40.02080 | 457.9d | 453.5d | ±1.3d | | 42.991 | | 225.193 | | 10.550 | | # |
| CCO+c | | 40.02025 | 1442.8d | 1431.5d | ±2.2d | | 47.324 | | 237.047 | | 11.435 | | # |
| CCO-a | | 40.02135 | 150.08d | 152.6d | ±1.35 | | 40.940 | | 227.613 | | 10.003 | | # |
| C2S2 | | 88.15340 | 376.660 | 373.831 |  | | 62.030 | | 274.120 | | 13.760 | | † |
| C2Si see SiC2 | |  |  |  |  | |  | |  | |  | |  |
| C2.231H3.006O3.721N0.751 Nitrocellulose | | 99.87 | -291.462 |  | ±1. | |  | |  | |  | | X |
| C3 singlet 1Σ+g 1,2-Propadiene-1,3-diylidene | | 36.03210 | 822.025 | 813.770 | ±1.1d | | 42.203 | | 237.613 | | 12.109 | | #† |
| C3 Cyclo c singlet | | 36.03210 | 1005.9d | 999.1d | ±2.7d | |  | |  | |  | | X |
| C3 Cyclo c also triplet | | 36.03210 | 911.90d | 905.0d | ±2.0d | |  | |  | |  | | X |
| C3+ c Cyclo Propynylidyne | | 36.0316 | 1967.d | 1953.7d | ±2.2d | |  | |  | |  | | X |
| C3- Cyclo | | 36.0326 | 663.5 | 662.577 | ±8 | | 38.428 | | 228.532 | | 10.281 | | # |
| C3+ d linear | | 36.03155 | 1988.9d | 1973.9d | ±3.d | | 45.509 | | 223.300 | | 11.844 | | # |
| C3+ c g CAS # 118090-85-0 | | 36.0316 | 1967.1d | 1953.8d | ±2.4d | |  | |  | |  | | X |
| C3- c | | 36.0326 | 623.41d | 622.2d | ±1.7d | |  | |  | |  | | X |
| C3Br2 BrC\*=C=C\*Br | | 195.84010 | 611.533 | 622.068 | ±8 | | 77.501 | | 335.224 | | 17.146 | | # |
| C3Br3 Br2C=C=C\*Br | | 275.74410 | 449.906 | 468.756 | ±8 | | 96.993 | | 393.290 | | 21.090 | | # |
| C3Br3 1,2,3-triBrCyPropene-1-yl | | 275.74410 | 529.192 | 548.69 | ±8 | | 94.196 | | 423.079 | | 20.443 | | # |
| C3Br4 Br2C=C=CBr2 | | 355.64810 | 316.394 | 343.175 | ±8 | | 117.375 | | 420.589 | | 25.420 | | # |
| C3Cl2 ClC\*=C=C\*Cl biradical | | 106.93750 | 519.876 | 514.996 | ±8. | | 77.130 | | 319.091 | | 17.220 | | # |
| C3Cl2 Cy (-ClC=C=CCl-) | | 106.93750 | 441.194 | 426.215 | ±8. | | 69.740 | | 302.556 | | 14.979 | | # |
| C3Cl3 1,2,3-triClCyPropene-1-yl | | 142.3902 | 398.434 | 396.717 | ±8 | | 88.840 | | 347.538 | | 18.649 | | # |
| C3Cl3 Cl2C=C=CCl\* radical | | 142.3902 | 311.296 | 307.497 | ±8 | | 95.298 | | 372.338 | | 20.731 | | # |
| C3Cl3O\* Cl2C=C=CCl(O\*) rad. | | 158.38960 | 95.571 | 94.555 | ±8 | | 105.684 | | 397.707 | | 22.288 | | # |
| C3Cl4 Cl2C=C=CCl2 | | 177.8429 | 135.1 | 134.08 | ±8 | | 109.297 | | 371.955 | | 22.545 | | # |
| C3D4 Propyne-d4 CD3C≡CD | | 44.08851 | 173.408 | 179.640 |  | | 68.774 | | 259.569 | | 14.066 | | # |
| C3D4 Cyclopropene-D4 | | 44.08851 | 263.592 | 271.241 |  | | 63.845 | | 254.235 | | 12.650 | | # |
| C3D6 Cyclopropane-D6 | | 48.11671 | 32.850 | 48.523 |  | | 72.723 | | 251.483 | | 13.195 | | # |
| C3D6O Acetone-D6 | | 64.11611 | -264.663 | -249.067 | ±8 | | 86.865 | | 306.821 | | 17.612 | | # |
| C3F Radical | | 55.030503 | 564.957 | 559.052 | ±8 | | 55.612 | | 277.062 | | 13.479 | | # |
| C3F3 FCC-CF2\* | | 93.02731 | -134.419 | -135.23 | ±8 | | 81.990 | | 326.463 | | 17.210 | | # |
| C3F3 \*CC-CF3 | | 93.02731 | -79.078 | -79.609 | ±8 | | 80.749 | | 313.306 | | 16.929 | | # |
| C3F4 PerFluoroAllene | | 112.02571 | -553.685 | -551.89 | ±8 | | 92.135 | | 336.733 | | 19.021 | | # |
| C3F5N C2F5-C≡N | | 145.03085 | -929.490 | -923.418 |  | | 122.514 | | 372.496 | | 23.487 | | # |
| C3F5N- C2F5-C≡N- anion | | 145.03140 | -965.922 | -956.307 | ±8 | | 131.732 | | 393.329 | | 25.620 | | # |
| C3F6 Hexafluoropropene | | 150.02252 | -1157.253 | -1150.95 | ±8 | | 121.759 | | 373.675 | | 23.337 | | # |
| C3F7 RADICAL | | 169.02182 | -1347.122 | -1339.5 | ±8 | | 135.964 | | 416.386 | | 26.401 | | # |
| C3F8 FC-218 | | 188.01933 | -1784.70 | -1773.9 | ±8. | | 149.409 | | 399.506 | | 27.628 | | # |
| C3H HC≡C-C | | 37.04004 | 719.393 | 714.091 | ±8 | | 53.430 | | 247.795 | | 12.696 | | # |
| C3HBr2 1,3-DiBromoAllene Rd | | 196.84804 | 420.032 | 434.370 | ±8 | | 82.624 | | 349.563 | | 17.576 | | # |
| C3HBr2 1,1-DiBromoAllene Rd | | 196.84804 | 406.015 | 419.337 | ±8 | | 88.647 | | 353.450 | | 18.593 | | # |
| C3HBr2O BrHC=C=CBr(O\*) | | 212.84744 | 195.142 | 210.448 | ±8 | | 97.345 | | 394.220 | | 20.949 | | # |
| C3HBr2O Br2C=C=CH(O\*) | | 212.84744 | 239.032 | 254.141 | ±8 | | 97.059 | | 384.601 | | 21.145 | | # |
| C3HBr3 TriBromoAllene | | 276.75204 | 234.185 | 306.937 | ±8 | | 100.773 | | 389.538 | | 21.373 | | # |
| C3HCl2 DiChloroAllenyl Radical | | 107.94544 | 328.356 | 326.877 | ±8 | | 82.314 | | 340.860 | | 18.055 | | # |
| C3HCl2 1,1-DiChloroAllenyl Rd | | 107.94544 | 311.633 | 310.755 | ±8 | | 85.060 | | 329.338 | | 17.453 | | # |
| C3HCl2O\* H(Cl)C=C=CCl(O\*) | | 123.94484 | 104.792 | 105.885 | ±8. | | 93.127 | | 365.659 | | 19.823 | | # |
| C3HCl2O\* Cl2C=C=CH(O\*) | | 123.94484 | 151.578 | 152.696 | ±8 | | 92.814 | | 359.360 | | 19.797 | | # |
| C3HCl3 TriChloroAllene | | 143.39814 | 148.871 | 150.575 | ±8 | | 94.649 | | 353.019 | | 19.463 | | # |
| C3HF7 FC-227EA | | 169.02092 | -1564.82 | -1552.4 | ±8 | | 136.690 | | 399.058 | | 25.901 | | # |
| C3HN HC≡CCN CyanoAcetylene | | 51.04678 | 368.414 | 367.225 | ±8 | | 62.633 | | 247.991 | | 12.918 | | # |
| C3H2(1) CyPropenylidene f <!> | | 38.04798 | 496.140 | 477.960 | ±0.47 | | 44.220 | | 236.803 | | 10.644 | | # |
| C3H2+ CyPropenylidene f cation | | 38.0474 | 1387.2 | 1382.0 | ±1.2 | |  | |  | |  | | X |
| C3H2- CyPropenylidene f anion | | 38.04853 | 537.60f | 544.3 | ±2.2 | | 48.334 | | 245.575 | | 11.152 | | # |
| C3H2 CyPropyne (CC)CH2 f | | 38.0480 | 790.6f | 791.1 | ±1.4 | |  | |  | |  | | X |
| C3H2 H2C\*-C≡C\*f Propadienyliden <!> | | 38.04888 | 555.64f | 554.970 | ±0.43f | | 54.719 | | 249.679 | | 12.298 | | # |
| C3H2(3) \*HC=C=CH\* <!> | | 38.04888 | 755.254 | 751.668 | ±62.7 | | 67.953 | | 260.782 | | 15.215 | |  |
| C3H2(1) HC-C≡CH\* <!> | | 38.04888 | 817.972 | 816.374 | ±62.7 | | 58.770 | | 251.691 | | 13.227 | |  |
| HCCCH+ Propynylidene cationf | | 38.04743 | 1419.597 | 1410.8 | ±1.2 | | 61.546 | | 265.394 | | 13.780 | | # |
| HCCCH- Propargylenidene anionf | | 38.04853 | 432.36f | 436.54f | ±0.98 | | 58.922 | | 250.889 | | 12.875 | | # |
| HCCCH cis Propynylidene f | | 38.04798 | 599.60f | 598.192 | ±1.5f | | 57.789 | | 245.850 | | 13.037 | | # |
| HCCCH triplet f | | 38.04798 | 546.08f | 543.08f | ±0.67 | |  | |  | |  | | X |
| C3H2Br2 HBrC=C=CHBr | | 197.85598 | 250.120 | 268.615 | ±8 | | 84.110 | | 340.818 | | 17.653 | | # |
| C3H2Cl HClC=C=H\* | | 73.50068 | 328.164 | 329.399 | ±8 | | 72.438 | | 296.950 | | 14.984 | | # |
| C3H2Cl2 HClC=C=CClH | | 108.95338 | 161.440 | 165.569 | ±8 | | 80.178 | | 316.701 | | 16.680 | | # |
| C3H2Cl2O ClHC=C=CCl-OH | | 124.95278 | -4.954 | +0.493 | ±8 | | 96.536 | | 355.053 | | 19.703 | | # |
| C3H2F3 CF3-CH=CH\* | | 95.04319 | -376.895 | -369.47 | ±8 | | 90.727 | | 323.105 | | 17.442 | | # |
| C3H2F3 CF3-C\*=CH2 | | 95.04319 | -374.941 | -367.82 | ±8 | | 91.100 | | 125.439 | | 17.741 | | # |
| C3H2F4 CF3-CF=CH2 | | 114.04159 | -813.261 | -803.168 | ±8. | | 101.255 | | 327.768 | | 19.186 | | # |
| C3H2F4 CF3-CH=CHF trans | | 114.04159 | -817.989 | -808.361 | ±8. | | 98.883 | | 329.426 | | 19.220 | | # |
| C2H2F6 CF3-CHF-CHF2 | | 152.03840 | -1322.600 | -1308.617 | ±9 | | 124.365 | | 369.443 | | 24.121 | | # |
| C3H2N HC\*=CH-CN | | 52.05472 | 442.855 | 445.486 | ±8 | | 59.531 | | 272.030 | | 13.333 | | # |
| C3H2N4O4 DiNitro-1,3-Imidazole | | 158.07254 | 120.918 | 141.714 | ±12.5 | | 137.176 | | 403.986 | | 25.533 | | # |
| C3H2S2 S=CH-S-C≡CH | | 102.17998 | 376.552 | 379.219 | ±8 | | 88.144 | | 325.354 | | 17.785 | | # |
| C3H2S2+ S=CH-S-C≡CH cation | | 102.17943 | 1241.358 | 1237.735 | ±8 | | 86.995 | | 335.200 | | 17.909 | | # |
| C3H3 PROPARGYL RADICA<!> | | 39.05592 | 351.506 | 353.7493 | ±0.5 | | 64.891 | | 256.659 | | 13.620 | | #† |
| C3H3 Propynyl Rad.H3CC≡C\*<!> | | 39.05592 | 528.35 | 531.813 | ±1.1d | | 53. | | 250.9 | | 12.400 | | #† |
| C3H3+ H3C-C≡C\*+ | | 39.0554 | 1542.2d | 1537.d | ±16.d | |  | |  | |  | | X |
| C3H3- H3C-C≡C\*- | | 39.05647 | 251.585 | 261.405 | ±0.71 | | 52.301 | | 252.945 | | 12.240 | | # |
| C3H3 Allenyl RadicalCH2=C=CH\* | | 39.05592 | 348.427 | 352.384 | ±8 | | 55.262 | | 253.192 | | 11.905 | | # |
| C3H3+ [CH2=C=CH]+ cation | | 39.05537 | 1201.645 | 1198.416 | ±8 | | 59.173 | | 239.329 | | 12.894 | | # |
| [CH2CCH]+ CAS# 21540-27-2 | | 39.05537 | 1194.25 | 1190.86d | ±0.47 | | 61.433 | | 249.712 | | 13.241 | | # |
| C3H3- [CH2=C=CH]- anion | | 39.05647 | 255.995 | 265.575 | ±0.79d | | 57.768 | | 252.063 | | 12.480 | | # |
| C3H3 CycloPropenyl Radical<!> | | 39.05592 | 488.064 | 492.719 | ±0.92d | | 50.459 | | 232.865 | | 11.207 | | # |
| C3H3 CH2(CH=C\*) CyPrRad | | 39.05592 | 523.964 | 528.592 | ±0.85 | | 50.378 | | 253.102 | | 11.235 | | # |
| CLC3H3 1-Chloro-1-propyne | | 74.50862 | 184.711 | 189.553 | ±8 | | 71.364 | | 283.822 | | 15.611 | | # |
| C3H3Cl CH2Cl-CCH | | 74.50862 | 181.042 | 186.923 | ±8 | | 70.579 | | 291.229 | | 14.572 | | # |
| 3-C3H3Cl CY | | 74.50862 | 240.216 | 247.474 | ±8 | | 64.699 | | 274.948 | | 13.195 | | # |
| C3H3Cl CHCl=C=CH2 | | 74.50862 | 175.310 | 181.577 | ±8 | | 68.274 | | 288.295 | | 14.186 | | # |
| C3H3F2 \*CF2-CH=CH2 | | 77.05273 | -224.440 | -216.932 | ±8 | | 89.452 | | 322.532 | | 17.180 | | # |
| C3H3F3 CF3-CH=CH2 | | 96.05113 | -631.131 | -619.51 | ±6. | | 90.704 | | 319.468 | | 17.481 | | # |
| C3H3I CH2ICCH Propargyl Iod. | | 165.96039 | 269.072 | 276.353 | ±12.5 | | 74.028 | | 310.672 | | 15.180 | | # |
| C3H3I CH2=C=CHI Allenyl Iod. | | 165.96039 | 264.117 | 272.127 | ±12.5 | | 70.463 | | 305.857 | | 14.451 | | # |
| C3H3N CH2=CHCN | | 53.06266 | 184.037 | 190.874 | ±8 | | 59.387 | | 263.290 | | 13.361 | | # |
| C3H3N cy(-CH=CHCH=N-) azete | | 53.06266 | 460.866 | 469.119 | ±8 | | 57.755 | | 261.980 | | 11.945 | | # |
| C3H3ON (Cyclo) Oxazole | | 69.06206 | -15.468 | -2.726 | ±8 | | 58.893 | | 270.124 | | 11.795 | | # |
| C3H3ON (Cyclo) Isoxazole | | 69.06206 | 81.199 | 93.865 | ±8 | | 59.736 | | 270.690 | | 11.872 | | # |
| C3H3NS (Cyclo) Thiazole | | 85.12866 | 151.494 | 163.370 | ±8 | | 66.727 | | 281.916 | | 12.734 | | # |
| C3H3NS (Cyclo) Isothiazole | | 85.12866 | 159.733 | 171.655 | ±8 | | 66.453 | | 281.503 | | 12.687 | | # |
| C3H3N3 1,3.5 Triazine cy | | 81.07614 | 224.593 | 240.191 | ±8. | | 67.767 | | 270.403 | | 13.269 | | # |
| C3H3(NO2)5 liq.  11122-Pentanitropropane | |  | -57.32 |  | ±0.42 | |  | |  | |  | | X |
| C3H3O CH2=CHC\*=O acryl rad<!> | | 55.05532 | 88.530 | 94.536 | ±8 | | 62.578 | | 300.914 | | 14.197 | | # |
| C3H3O+ CH2=CHC\*=O+ cation | | 55.05477 | 776.781 | 767.212 | ±8 | | 62.421 | | 273.836 | | 13.347 | | # |
| C3H3O- CH2=CHC\*=O- anion | | 55.05587 | 36.756 | 47.769 | ±8 | | 70.405 | | 286.558 | | 15.137 | | # |
| C3H3O \*CH2-CH=C=O | | 55.05532 | 93.560 | 98.786 | ±8 | | 70.422 | | 294.130 | | 14.977 | | # |
| H4C3 PROPYNE <!> | | 40.06386 | 184.9 | 191.966 | ±0.38d | | 60.731 | | 248.429 | | 13.031 | | † |
| C3H4 ALLENE <!> | | 40.06386 | 190.92 | 198.412 | ±0.37d | | 58.88 | | 243.630 | | 12.605 | | † |
| C3H4 CYCLOPROPENE <!> | | 40.06386 | 283.93 | 292.653 | ±0.59d | | 52.883 | | 243.605 | | 11.374 | | #† |
| C3H4CL \*CH=CH-CH2CL | | 75.51656 | 250.253 | 259.680 | ±8. | | 73.850 | | 303.749 | | 15.261 | | # |
| CLC3H4 \*CH2-CH=CHCL | | 75.51656 | 137.444 | 147.12 | ±8. | | 71.705 | | 303.390 | | 15.012 | | # |
| C3H4N CH3-CH\*-CN | | 54.07060 | 222.706 | 232.213 | ±8. | | 72.044 | | 298.672 | | 14.925 | | # |
| C3H4N2 Cy 1,3-DIAZOLE C3H4N2 | | 68.07734 | 134.014 | 150.376 | ±8 | | 64.620 | | 273.159 | | 12.404 | | # |
| C3H4N2 Cy 1,2-Pyrazole C3H4N2 | | 68.07734 | 180.481 | 196.898 | ±8 | | 64.116 | | 272.969 | | 12.350 | | # |
| 1,3,3 TRI-NITRO-AZETIDINE | | 192.08812 | 128.449 | 171.220 | ±8. | | 134.987 | | 357.315 | | 20.706 | |  |
| C3H4O ACROLEIN (2-Propenal)  CH2=CHCH=O <!> | | 56.06326 | -68.065 | -59.554 | **±**8 | | 72.005 | | 307.778 | | 15.925 | | # |
| C3H4O CH3CH=C=O MeKetene | | 56.06326 | -66.241 | -56.663 | **±**8 | | 69.592 | | 276.650 | | 14.858 | | # |
| C3H4O2 CH2=CH-C(O)-OH | | 72.06266 | -326.051 | -312.52 | **±**8 | | 79.301 | | 313.570 | | 15.243 | | # |
| C3H4S HC≡CCH2SH | | 72.12986 | 238.66 | 245.901 | ±8. | | 80.628 | | 297.840 | | 16.267 | | # |
| C3H4S+ HC≡CCH2SH+ cation | | 72.12931 | 1164.83 | 1166.57 | ±8. | | 81.796 | | 311.267 | | 15.835 | | # |
| C3H4S- HC≡CCH2SH- anion | | 72.13041 | 243.495 | 251.02 | ±8. | | 102.570 | | 364.665 | | 21.703 | | # |
| C3H4S HC≡CH-S-CH3 | | 72.12986 | 237.689 | 245.843 | ±8. | | 82.246 | | 300.699 | | 16.355 | | # |
| C3H4S+ HC≡CH-S-CH3+ | | 72.12931 | 1101.066 | 1102.697 | ±8. | | 81.908 | | 318.891 | | 16.680 | | # |
| C3H4S2 S=CH-S-CH=CH2 | | 104.19586 | 196.506 | 205.931 | ±8. | | 93.298 | | 362.033 | | 19.495 | | # |
| C3H4S2- S=CH-S-CH=CH2- | | 104.19641 | 110.126 | 124.788 | ±8. | | 99.957 | | 362.971 | | 20.245 | | # |
| C3H5 Symmetric Allyl Radical | | 41.0727 | 168.600 | 180.398 | **±**1.5 | | 61.825 | | 257.876 | | 12.533 | | #† |
| C3H5+ CH2=CH-CH2\*+ symetric | | 41.07125 | 959.22h | 940.482 | ±0.45 | | 58.605 | | 258.621 | | 12.638 | | # |
| C3H5- CH2=CH-CH2\* allyl anion | | 41.0723 | 116.91h | 134.12 | ±0.24 | |  | |  | |  | | X |
| T-C3H5 CH3C\*=CH2 “ " <~> | | 41.0727 | 252.58h |  | ±0.77h | | 61.663 | | 266.064 | |  | |  |
| CH3C\*=CH2+ 1-Methylethenylium | | 41.07125 | 992.283h | 995.2 | ±2.0h | | 68.533 | | 270.433 | | 14.604 | | # |
| CH3C\*=CH2- [1-Methylethenyl anion](https://atct.anl.gov/Thermochemical%20Data/version%201.122p/species/?species_number=1386) | | 41.07234 | 182.0 | 199.4  ±2.0 | | | 60.663 | | 261.693 | |  | | # |
| S-C3H5 CH3CH=CH\* “ “ <~> | | 41.07180 | 265.533  269.44h | 276.287  280.86 | ±8.  0,8h | | 63.362 | | 271.305 | | 13.577 | | # |
| C3H5 Cyclo | | 41.07180 | 279.9  290.7h | 292.716 | ±10.5  1.4h | | 55.701 | | 251.486 | |  | | # |
| C3H5Br3O CBr3CH2CH2OH | | 296.78320 | -167.820 | -130.039 | **±**12. | | 133.73 | | 413.693 | | 27.144 | | # |
| C3H5Cl 1-Chloro-1-propene | | 76.5245 | -8.100 | +4.937 | **±**8. | | 76.450 | | 299.193 | | 15.884 | | # |
| C3H5CL 3-Chloro-1-propene | | 76.5245 | 0.369 | 14.052 | ±8. | | 74.210 | | 307.919 | | 15.239 | | # |
| C3H5N PROPIONITRILE | | 55.07944 | 53.191 | 66.974 | ±8. | | 72.039 | | 285.205 | | 14.883 | | # |
| C3H5NO Acrylamide solid | | 71.07794 | -212.08 |  | ±0.3 | | 110.58 | |  | |  | | X |
| C3H5NO Acrylamide liquid | | 71.07794 | -224. |  |  | |  | |  | |  | | X |
| CH2=CHC(O)-NH2 Acrylamide | | 71.07794 | -130.378 | -115.713 | ±8. | | 82.703 | | 334.240 | | 17.440 | | # |
| CH2=CHC(O)-NH2+ cation | | 71.07739 | 806.466 | 816.056 | ±8. | | 82.035 | | 337.906 | | 17.141 | | # |
| CH2=CHC(O)-NH2- anion | | 71.07849 | -108.278 | -87.713 | ±8. | | 90.848 | | 348.493 | | 18.857 | | # |
| CH3CH=CHNO2 Nitropropylene | | 87.07824 | 9.987 | 29.046 | ±8.9 | | 93.59 | | 330.004 | | 18.288 | |  |
| C3H5NO2 NitroCycloPropane | | 87.07824 | 21.033 | 41.466 | ±8. | | 90.786 | | 311.278 | | 16.913 | | # |
| C3H5NO4 Glycidyl-Nitrate | | 119.07614 | -157.072 | -134.345 | ±8. | | 116.586 | | 405.524 | | 23.300 | | # |
| C3H5N3O6 liq 1,1,1-Trinitropropane | |  | -120.92 |  | ±0.42 | |  | |  | |  | | X |
| C3H5N3O9 (liq) Nitroglycerine | | 227.08752 | -369.86 |  | ±2. | |  | |  | |  | | X |
| C3H5N3O9 Nitroglycerine | | 227.08752 | -279.073 | -246.14 | ±2.7 | | 234.24 | | 545.865 | | 43.458 | |  |
| C2H5CO Propanal Radical | | 57.0712 | -32.83 | -19.862 | **±**8. | | 67.859 | | 308.527 | | 15.703 | | # |
| CH2COCH3 Acetone Radical | | 57.0712 | -33.34  -31.76h | -20.617 | ±8.  ±0.98 | | 72.843 | | 307.518 | | 15.948 | | # |
| C3H5O Propylene Oxide Rad | | 57.0712 | 104.069 | 118.072 | **±**8. | | 71.197 | | 293.196 | | 14.667 | | # |
| C3H5O2 Propanoic acid Radical | | 73.07060 | -213.175 | -197.658 | **±**8. | | 79.370 | | 337.845 | | 17.494 | | # |
| C3H5O2 CH3-C(O)-OCH2\* | | 73.07060 | -221.639 | -205.562 | **±**8. | | 85.269 | | 316.985 | | 16.934 | | # |
| C3H6 PROPYLENE <~> | | 42.07974 | 20.000 | 35.014 | ±0.33d | | 64.433 | | 266.668 | | 13.551 | | † |
| C3H6 CYCLOPROPANE <&> | | 42.07974 | 53.30 | 70.455 | ±0.53d | | 55.572 | | 237.488 | | 11.410 | | † |
| C3H6N2O2 N-NITRO-AZETIDIN | | 102.09292 | 114.123 | 141.198 |  | | 100.656 | | 328.954 | | 18.840 | |  |
| C3H6N2O4 O2N-(CH2)3NO2 | | 134.09082 | -141.0 | -112.1 |  | | 127.545 | | 411.883 | | 25.692 | | # |
| C3H6N2O4 C2H5CH(NO2)2 | | 134.09082 | -104.6 | -76.4 |  | | 137.553 | | 404.492 | | 26.398 | | # |
| C3H6N2O4 (CH3)2C(NO2)2 | | 134.09082 | -72.496 | -51.933 | ±21.3 | | 139.720 | | 401.341 | | 27.032 | | # |
| C3H6N5O4 RDX radical | | 176.11104 | 239.6 | 275.3 | ±50. | | 172.633 | | 464.000 | | 32.415 | | # |
| C3H6N5O4 RDX radical linear \*CH-N(NO2)-CH2-N(NO2)-CH2-NH\* | | 176.11104 | 288.11 | 320.4 | ±50. | | 182.541 | | 496.296 | | 35.334 | | # |
| C3H6N6O6 RDX Solid | | 222.11748 | 79.078 |  |  | | 248.95 | | 259.8 | |  | |  |
| C3H6N6O6 RDX 135 Triazine | | 222.11748 | 192.000 | 233.285 |  | | 230.174 | | 482.441 | | 39.331 | |  |
| C3H5OH 2-Propen-1-ol CH2=CHCH2OH | | 58.07914 | -123.645 | -105.820 | ±8 | | 76.848 | | 304.783 | | 15.080 | | # |
| C3H5OH 1-Propen 1-ol  CH3CH=CHOH | | 58.07914 | -145.963 | -129.493 | ±8 | | 80.079 | | 295.360 | | 16.434 | | # |
| C3H5OH 1-Propen-2-ol  CH3C(OH)=CH2 | | 58.07914 | -163.176 | -146.178 | ±8 | | 80.493 | | 292.412 | | 15.907 | | # |
| C3H5OH CycloPropanol | | 58.07914 | -101.504 | -82.242 | ±8. | | 71.826 | | 279.262 | | 13.643 | | # |
| C2H5CHO Propionaldehyde <!> | | 58.07914 | -185.155 | -167.543 | ±8. | | 75.275 | | 288.844 | | 15.293 | | # |
| CH3COCH3 (L) Acetone liq.c | | 58.08004 | -247.46d | -244.34d | ±0.37d | | 125.018 | | 200.414 | |  | |  |
| CH3COCH3 ACETONE <~> | | 58.08004 | -214.814 | -199.39d | ±0.37d | | 74.207 | | 295.660 | | 16.193 | | †# |
| C3H6O PROPYLENE OXIDE   <!> | | 58.07914 | -92.760 | -74.271 | ±8. | | 72.671 | | 281.487 | | 14.415 | | # |
| C3H6O CY OXETANE CycloTrimethylene Oxide | | 58.07914 | -81.086 | -61.49 | ±8. | | 61.826 | | 274.672 | | 13.499 | | # |
| C3H6O Vinylmethylether | | 58.07914 | -100.378 | -83.824 | ±8. | | 76.313 | | 308.229 | | 16.351 | | # |
| C3H6O2 Propionic acid | | 74.07854 | -450.868 | -431.289 | ±8. | | 82.546 | | 333.431 | | 17.666 | | # |
| C3H6O2(liq) Methylacetate liq. | | 74.07854 | -445.89 |  |  | |  | |  | |  | | X |
| C3H6O2 Methylacetate ester. | | 74.07854 | -415.170 | -396.272 | **±**8. | | 85.346 | | 321.527 | | 18.347 | | # |
| C3H6O2(liq.) Ethylformate ester | | 74.07854 | -394.2 |  | **±**0.8 | |  | |  | |  | | X |
| C3H6O2 Ethylformate ester | | 74.07854 | -377.188 | -357.631 | **±**8. | | 84.642 | | 329.799 | | 17.688 | | # |
| C3H6O2 Glycidol OxyraneMethanol | | 74.07854 | -239.572 | -218.285 | **±**8. | | 84.003 | | 317.884 | | 15.959 | | # |
| C3H6O2 Hydroxyacetone | | 74.07854 | -358.079 | -339.727 | **±**8. | | 97.070 | | 339.595 | | 18.892 | | # |
| C3H6O3 Lactic Acid CH3CH(OH)COOH | | 90.07794 | -610.278 | -587.408 | **±**8. | | 101.214 | | 354.204 | | 18.715 | | # |
| (CH2O)3 Cy 1,3,5-Trioxane | | 90.07794 | -476.05 | -449.479 | ±8. | | 81.394 | | 288.603 | | 15.013 | | # |
| C3H6O3 DiMeCarbonat (CH3)2CO3 | | 90.07794 | -578.534 | -556.574 | ±8. | | 100.963 | | 323.847 | | 19.625 | | # |
| C3H6S HS-CH2-CH=CH2 | | 74.14574 | 62.614 | 79.166 | ±8. | | 84.015 | | 311.148 | | 16.424 | | # |
| C3H6S+ HS-CH2-CH=CH2+ | | 74.14519 | 935.141 | 945.249 | ±8. | | 83.482 | | 312.229 | | 15.824 | | # |
| C3H6S CH3-S-CH=CH2 | | 74.14574 | 64.492 | 79.786 | ±8. | | 82.046 | | 327.046 | | 17.683 | | # |
| C3H6S+ CH3-S-CH=CH2+ | | 74.14519 | 874.770 | 883.677 | ±8. | | 82.876 | | 332.834 | | 17.819 | | # |
| C3H6S THIETHANE | | 74.14574 | 65.220 | 84.226 | ±8. | | 70.419 | | 282.055 | | 13.971 | | # |
| 1,3-C3H6S2 cy Dithiolane | | 106.21174 | 139.172 | 159.557 | ±8. | | 88.195 | | 324.318 | | 17.004 | | # |
| N-C3H7 PROPYL RADICALg <~> | | 43.08768 | 100.81g | 118.639 | ±0.61 | | 71.304 | | 290.457 | | 14.970 | | †# |
| N-C3H7+ PROPYL cation g | | 43.08713 | 844.847 | 856.87g | ±0.83 | | 67.153 | | 268.895 | | 13.388 | | # |
| N-C3H7- PROPYL anion | | 43.08823 | 98.821 | 123.369 | ±8. | | 70.080 | | 272.498 | | 13.785 | | # |
| I-C3H7 Isopropyl RADICALg <~> | | 43.08768 | 88.68g | 105.280 | ±0.67 | | 107.116 | | 435.879 | | 27.147 | | †# |
| i-C3H7+ Isopropyl cationg | | 43.08713 | 811.817 | 822.88 | ±0.26 | | 71.863 | | 264.792 | | 14.236 | | # |
| i-C3H7- Isopropyl anion | | 43.08823 | 104.516 | 128.767 | ±8. | | 68.184 | | 261.021 | | 13.582 | | # |
| n-C3H7Cl Propyl Chloride | | 78.54038 | -131.892 | -110.470 | ±8. | | 81.117 | | 300.995 | | 15.968 | | # |
| i-C3H7Cl iso-Propyl Chloride | | 78.54038 | -145.227 | -123.532 | ±8. | | 82.505 | | 298.435 | | 15.694 | | # |
| i-C3H7Cl+ i-PropylChloride cation | | 78.53983 | 899.531 | 913.716 | ±8. | | 92.430 | | 305.371 | | 17.007 | | # |
| i-C3H7Cl- i-PropylChloride anion | | 78.54093 | -189.870 | -165.584 | ±8. | | 95.461 | | 330.864 | | 19.300 | | # |
| 1-C3H7I Iodopropane | | 169.99215 | -30.177 | -10.2 | ±2 | | 94.506 | | 353.401 | | 19.420 | | # |
| 2-C3H7I 2-Iodopropane | | 169.99215 | -40.79 | -20.1 | ±2 | | 91.324 | | 335.155 | | 18.707 | | # |
| C3H5NH2 CY-PROPYLAMINE | | 57.09442 | 79.4 | 102.718 | ±8. | | 74.006 | | 274.444 | | 13.816 | | # |
| C3H7N AZETIDINE | | 57.09442 | 98.198 | 122.224 |  | | 67.14 | | 267.274 | | 13.087 | | # |
| 1-C3H7NO2 liq 1-Nitropropane liq | | 89.09322 | -167.78 |  | ±0.84 | |  | |  | |  | | X |
| 1-C3H7NO2 1-Nitropropane | | 89.09322 | -128.46 | -102.277 | ±8. | | 104.549 | | 358.359 | | 19.633 | | # |
| 1-C3H7NO2+ 1-Nitropropane+ | | 89.09267 | 901.121 | 915.727 | ±8. | | 117.510 | | 395.848 | | 24.329 | | # |
| 1-C3H7NO2- 1-Nitropropane anion | | 89.09377 | -153.210 | -122.118 | ±8. | | 108.565 | | 361.413 | | 20.744 | | # |
| 2-C3H7NO2 liq 2-Nitropropane liq | | 89.09322 | -180.33 |  | ±0.42 | |  | |  | |  | | X |
| C3H7NO3 NPN Propylnitrate | | 105.09262 | -183.18 | -154.215 | ±8. | | 111.467 | | 375.141 | | 21.194 | | # |
| C3H7NO3- Propylnitrate anion | | 105.09317 | -251.885 | -232.551 | ±8. | | 125.788 | | 416.330 | | 26.330 | | # |
| C3H7NO3 IPN Isoproppylnitrate | | 105.09262 | -200.55 | -172.796 | ±8. | | 120.928 | | 356.816 | | 22.399 | | # |
| C3H7NO3+ IPN Isoproppylnitrate | | 105.09207 | 826.735 | 844.783 | ±8. | | 133.134 | | 380.419 | | 25.340 | | # |
| C3H7NO3- IPN Isoproppylnitrate | | 105.09317 | -278.977 | -250.576 | ±8. | | 130.000 | | 388.811 | | 25.647 | | # |
| C3H7NO3 L-Serine (gas) | | 105.09262 | -579.11 | -551.829 | ±8. | | 118.076 | | 404.228 | | 22.876 | | # |
| C3H7NO3 L-Serine (solid) | | 105.09262 | -732.73 |  | ±0.28 | |  | | 149.16 | |  | | X |
| C3H7N3O5 Methyl-NENA CH3-N(NO2)CH2CH2ONO2 | | 165.10490 | -106.5 | -69.281 |  | | 149.349 | | 464.325 | | 30.285 | | # |
| C3H7O N-PROPOXY RAD. | | 59.08708 | -35.468 | -14.540 | ±8. | | 81.695 | | 302.058 | | 16.211 | | # |
| C3H7O iso-propoxy rad | | 59.08708 | -47.614 | -26.097 | ±8. | | 82.265 | | 289.902 | | 15.622 | | # |
| C3H7O (CH3)2C\*-OH isopropanol | | 59.08708 | -98.487 | -78.352 | ±8. | | 85.989 | | 308.740 | | 17.004 | | # |
| C3H7O+ Me Oxyrane protonate | | 59.08653 | 648.00 | 663.775 | ±8. | | 76.735 | | 284.409 | | 14.821 | | # |
| C3H7O+ CyTrimethyleneoxide  Protonated | | 59.08653 | 640.85 | 657.96 | ±8. | | 68.609 | | 271.860 | | 13.527 | | # |
| C3H7O2 PropylPeroxy Radical | | 75.08648 | -42.468 | -19.712 | ±8. | | 90.029 | | 324.857 | | 18.723 | | # |
| C3H7O2 iso-PropylPeroxy RAD | | 75.08648 | -65.061 | -42.161 | ±8. | | 97.746 | | 333.498 | | 18.579 | | # |
| C3J7O2 CH3OCH\*OCH3 Methylal | | 75.08648 | -163.055 | -140.221 | ±8. | | 94.613 | | 316.664 | | 18.645 | | # |
| CH3OCH\*OCH3- Methylal RAD an | | 75.08703 | -188.088 | -161.000 | ±8. | | 97.007 | | 312.573 | | 18.623 | | # |
| CH3OCH2OCH2\* radical C1 methylal | | 75.08648 | -156.381 | -133.540 | ±8. | | 98.588 | | 324.326 | | 18.637 | | # |
| CH3OCH2OCH2\*+ cation C1 methylal | | 75.08593 | 485.780 | 500.420 | ±8. | | 97.861 | | 318.579 | | 18.459 | | # |
| CH3OCH2OCH2\*- anion C1 methylal | | 75.08703 | -176.975 | -149.552 | ±8. | | 97.336 | | 316.531 | | 18.220 | | # |
| C3H7S C3H7S\* ThiopropylRad. | | 75.15368 | 75.513 | 95.137 | ±8. | | 87.069 | | 324.010 | | 17.687 | | # |
| C3H7S CH3CHS\*CH3h | | 75.15368 | 70.131 | 89.714 | ±8. | | 87.941 | | 313.855 | | 17.688 | | # |
| C3H8 PROPANE HC 290 <~> | | 44.09562 | -104.68 | -82.388 | ±0.29d | | 73.589 | | 270.315 | | 14.741 | | † |
| C3H8N (CH3)2NCH2\* | | 58.10236 | 142.4 | 166.687 | ±1.4 | | 91.103 | | 301.392 | | 17.161 | | # |
| C3H7OH PROPANOL | | 60.09592 | -255.2 | -231.35 |  | | 84.978 | | 323.367 | | 17.519 | | † |
| (CH3)2CHOH (l) iso-Propanol liqc | | 60.09592 | -318.17d | -305.36d | ±0.37d | |  | |  | |  | | X |
| (CH3)2CHOH 2-Propanol <&> | | 60.09592 | -272.7 | -248.59 | ±0.37d | | 89.594 | | 309.226 | | 17.265 | | † |
| C3H8O CH3OC2H5 Me-Et-Ether | | 60.09502 | -220.643 | -196.204 | ±8. | | 82.490 | | 301.277 | | 16.934 | | # |
| C3H8O+ (CH3)2O-CH2+ | | 60.09447 | 772.823 | 783.086 | ±8. | | 93.481 | | 312.207 | | 18.716 | | # |
| C3H8O2 n-Peroxypropane | | 76.09442 | -181.786 | -156.330 | ±8. | | 97.346 | | 367.594 | | 20.391 | | # |
| C3H8O2 iso-Peroxypropane | | 76.09442 | -201.752 | -174.540 | ±8. | | 102.975 | | 323.392 | | 18.501 | | # |
| C3H8O2 CH3-O-CH2-O-CH3 | | 76.09530 | -345.967 | -321.13 | ±8. | | 100.842 | | 347.098 | | 20.938 | | # |
| C3H8O2 1,3-Propanediol | | 76.09442 | -407.484 | -380.396 | ±8. | | 96.450 | | 330.228 | | 18.625 | | # |
| C3H8O3 (L) Glycerol (liq) | | 92.09382 | -669.6 |  | ±0.6 | | 218.9 | | 37.87(s) | |  | | X |
| C3H8O3 Glycerol/Glycerin  HOCH2CHOHCH2OH | | 92.09382 | -577.9 | -552.153 | ±1.1 | | 131.648 | | 400.000 | | 24.306 | | # |
| C3H7SH 1-PropaneThiol | | 76.16162 | -64.890 | -42.311 | ±8. | | 89.535 | | 343.373 | | 18.866 | | # |
| (CH3)2CH(SH) 2-Propanethiol | | 76.16162 | -77.237 | -52.610 | ±8. | | 91.469 | | 298.300 | | 16.818 | | # |
| CH3)2CH(SH)+ 2-Propanethiol+ | | 76.16107 | 810.00 | 829.03 | ±8. | | 95.810 | | 308.691 | | 17.599 | | # |
| C3H9Bi TriMethylBismutine | | 254.08394 | 194. |  | ±14. | | 125.791 | | 360.814 | | 23.738 | | # |
| C3H9N (liq) c | | 59.11030 | -45.739 |  | ±0.6 | |  | |  | |  | | X |
| C3H9N (CH3)3N | | 59.11030 | -24.023 | +4.062 | ±0.62 | | 91.106 | | 292.444 | | 17.517 | | # |
| C3H9O+ (CH3)3O+ cation | | 61.10241 | 541.716 | 556.731 | ±8. | | 90.997 | | 299.987 | | 18.197 | | # |
| C3H9O+ n-C3H7OH2+ cation | | 61.10241 | 501.846 | 495.649 | ±8. | | 92.343 | | 316.534 | | 17.760 | | # |
| i-C3H9O+ (CH3)2CHOH2+ cation | | 61.10241 | 471.809 | 465.612 | ±8. | | 97.788 | | 315.417 | | 18.657 | | # |
| C3H9PO3 (CH3O)3P | | 124.07552 | -692.829 | -663.441 | ±8. | | 144.598 | | 445.586 | | 30.259 | | # |
| C3H9PO3+ (CH3O)3P+ | | 124.07497 | 107.755 | 130.156 | ±8. | | 146.712 | | 411.477 | | 29.738 | | # |
| C3H9PO3- (CH3O)3P- | | 124.67606 | -554.940 | -533.226 | ±8. | | 155.927 | | 459.012 | | 31.983 | | # |
| C3H9PO4 (CH3O)3P=O | | 140.07492 | -1050.598 | -1081.86 | ±8. | | 158.601 | | 417.959 | | 31.261 | | # |
| C3H9P C3H7PH2 | | 76.07732 | -54.087 | -26.023 | ±8. | | 97.639 | | 327.112 | | 18.563 | | # |
| C3H9P+ C3H7PH2+ cation | | 76.07677 | 805.470 | 825.800 | ±8. | | 102.483 | | 331.662 | | 19.362 | | # |
| C3H9P- C3H7PH2- anion | | 76.07787 | 104.284 | 131.101 | ±8. | | 121.350 | | 388.893 | | 25.510 | | # |
| C3H9P (CH3)3P | | 76.07732 | -96.826 | -70.268 | ±8. | | 105.108 | | 316.612 | | 20.069 | | # |
| C3H9P+ (CH3)3P+ | | 76.07677 | 671.430 | 690.172 | ±8. | | 108.082 | | 332.011 | | 21.337 | | # |
| C3H9P- (CH3)3P- | | 76.07787 | 106.980 | 133.172 | ±8. | | 127.777 | | 362.244 | | 25.597 | | # |
| C3H9Sb Sb(CH3)3 | | 166.86356 | 38.5 | 62.9 | ±4.2 | | 113.001 | | 361.073 | | 23.510 | | # |
| C3H9Si Si(CH3)3 radical | | 73.18906 | 24.175 | 48.091 | ±8. | | 112.449 | | 324.106 | | 20.568 | | # |
| C3H9Si+ Si(CH3)3 + cation | |  | 630.2 |  | ±6. | |  | |  | |  | | X |
| C3H10Si (CH3)3SiH | | 74.1970 | -153.193 | -125.366 | ±8. | | 117.339 | | 319.711 | | 20.891 | | # |
| C3N2O NC-CO-CN | | 80.0449 | 247.5 | 246.523 | ±6.4 | | 80.854 | | 310.032 | | 17.148 | | # |
| C3N3P P(CN)3 | | 109.02608 | 473.721 | 473.433 | ±8. | | 106.879 | | 348.565 | | 21.813 | | # |
| C3N3P+ P(CN)3+ cation | | 109.02553 | 1599.627 | 1591.966 | ±8. | | 108.249 | | 361.103 | | 22.589 | | # |
| C3N3P- P(CN)3 anion | | 109.02663 | 315.715 | 319.084 | ±8. | | 114.134 | | 365.421 | | 23.940 | | # |
| C3O2 OCCCO cr | | 68.0309 | -119.4d | -134.5d | ±1.4d | |  | |  | |  | | X |
| C3O2 | | 68.0309 | -95.59 | -98.834 | ±1.4 | | 67.370 | | 276.816 | | 15.085 | | #† |
| OCCCO+ | | 68.03035 | 935.95 | 925.4d | ±1.41 | | 68.855 | | 273.531 | | 14.816 | | # |
| OCCCO- c | | 68.0314 | -135.61 | -133.1d | ±3.d | |  | |  | |  | | X |
| C4 singlet 1Ag  Bicyclo | | 48.04280 | 1055.713 | 1046.544 | ±8 | | 58.639 | | 245.962 | | 13.383 | | # |
| C4 triplet 3Σ-g | | 48.04280 | 1059.720 | 1050.435 | ±8 | | 59.078 | | 255.801 | | 13.499 | | #† |
| C4+ linear C≡C-C≡C+ | | 48.04225 | 2126.6g | 2109.8g | ±2.9 | | 62.873 | | 265.030 | | 15.012 | | # |
| C4- linear C≡C-C≡C- anion | | 48.04335 | 680.5 | 677.6 | ±1.2 | | 55.079 | | 243.863 | | 12.274 | | # |
| C4Cl2 Cl-CC-CCCl | | 118.94820 | 453.592 | 447.208 | ±8. | | 93.858 | | 319.209 | | 19.779 | | # |
| C4CL6 Perchloro-1,3-Butadiene | | 260.7590 | -7.209 | -7.411 | ±8. | | 158.984 | | 460.208 | | 31.959 | | # |
| C4D6 1,3-Butadiene d-6 | | 60.12741 | 64.94 | 77.47 | ±10.5 | | 91.494 | | 308.599 | | 17.386 | | # |
| C4F2 FCC-CCF | | 86.03961 | 215.309 | 210.191 | ±8. | | 88.863 | | 294.682 | | 18.157 | | # |
| C4F6 Perfluoro 1,3-Butadiene | | 162.03322 | -1004.160 | -997.710 |  | | 132.219 | | 394.728 | | 24.239 | | # |
| F6C4 Perfluorocyclobutene | | 162.03322 | -1210.887 | -1205.3 |  | | 131.312 | | 379.211 | | 25.135 | | # |
| C4F8 Perfluorocyclobutane | | 200.03002 | -1558.1 | -1510.6 |  | | 148.532 | | 401.246 | |  | |  |
| C4F10 FC-3110 Perfluorobutane | | 238.02803 | -2137.4 |  |  | | 189.038 | | 480.624 | |  | |  |
| C4H <I> | | 49.05074 | 780. | 775.015 | ±50. | | 64.851 | | 256.088 | | 13.433 | | # |
| C4H2 1,3-Butadiyne <!> | | 50.05868 | 460.365 | 458.744 | ±0.87d | | 73.733 | | 249.502 | | 14.303 | | #† |
| C4H2+ HCCCCH+ | | 50.05813 | 1447.72 | 1440.94 | ±0.9 | | 67.073 | | 244.003 | | 13.262 | | # |
| C4H2N2 Fumaronitrile  N≡C-CH=CH-C≡N | | 78.07216 | 330.996 | 334.8 | ±8. | | 85.445 | | 308.998 | | 17.549 | | # |
| C4H2S HCC-S-CCH | | 82.12468 | 531.936 | 532.048 | ±8. | | 91.840 | | 311.943 | | 18.025 | | # |
| C4H3 E,1-butene-3-yne-1-yl <~> | | 51.06662 | 543.104 | 545.65 | ±8 | | 71.773 | | 281.767 | | 14.371 | | # |
| C4H3 i,1-butene-3-yne-2-yl <~> | | 51.06662 | 501.829 | 502.00 | ±8. | | 77.383 | | 305.368 | | 16.739 | | # |
| C4H3 1,2,3-butatriene-4-yl | | 51.06662 | 501.829 | Resonant | With | | former | | species | |  | | X |
| 2-C4H3SNO2 2-Nitrothiophene | | 129.13816 | 104.324 | 119.291 | ±8. | | 103.268 | | 355.338 | | 19.376 | | # |
| 2-C4H3SNO2+ 2Nitrothiophene+ | | 129.13761 | 1043.048 | 1049.673 | ±8. | | 108.183 | | 370.940 | | 20.552 | | X |
| 2-C4H3SNO2- 2Nitrothiophene- | | 129.13871 | -7.189 | +12.313 | ±8. | | 110.964 | | 367.626 | | 20.415 | | X |
| 3-C4H3SNO2 3-Nitrothiophene | | 129.13816 | 513.762 | 526.845 | ±8. | | 112.605 | | 368.704 | | 21.260 | | # |
| C4H4 1-Butene 3-yne <~> | | 52.07456 | 287.859 | 294.717 | ±8. | | 71.612 | | 277.319 | | 14.292 | | # |
| C4H4 Cyclobutadiene | | 52.07456 | 431.722 | 440.911 | ±8. | | 58.200 | | 251.074 | | 11.961 | | #† |
| C4H4N Pyrrole Radical | | 66.08130 | 291.704 | 304.440 | ±8. | | 67.915 | | 274.651 | | 12.750 | | # |
| C4H4N- Pyrrole Radical anion | | 66.08185 | 81.433 | 100.675 | ±8. | | 65.970 | | 273.007 | | 12.441 | | # |
| C4H4N2 PYRAZINE | | 80.08804 | 195.811 | 212.069 | ±1.3 | | 73.945 | | 280.378 | | 13.562 | | # |
| C4H4N2 PYRIMIDINE | | 80.08804 | 196.648 | 212.864 | ±1. | | 73.69 | | 280.677 | | 13.645 | | # |
| C4H4N2 SUCCINONITRILE  N≡C-CH2-CH2-C≡N | | 80.08804 | 209.7 | 221.172 | ±0.9 | | 92.458 | | 325.114 | | 18.349 | | # |
| C4H4N2O2 N-NitroPyrole | | 112.00684 | 171.590 | 190.985 | ±8. | | 105.072 | | 335.719 | | 19.105 | | # |
| C4H4N2O2+ N-NitroPyrole cation | | 112.00629 | 1045.925 | 1057.912 | ±8. | | 109.696 | | 349.040 | | 20.209 | | # |
| C4H4N2O2- N-NitroPyrole anion | | 112.00739 | 71.834 | 92.793 | ±8. | | 112.944 | | 391.021 | | 23.042 | | # |
| C4H4N2O2 (cr) Uracil | | 112.08684 | -429.6 |  | ±0.6 | |  | |  | |  | | X |
| C4H4N2O2 Uracil | | 112.08684 | -301.5 | -281.85 | ±2.5 | | 107.172 | | 335.085 | | 18.847 | | # |
| C4H4O FURAN | | 68.07516 | -34.158 | -21.015 | ±8. | | 65.407 | | 267.239 | | 12.347 | | # |
| C4H4O+ FURAN cation | | 68.07341 | 832.265 | 838.666 | ±8. | | 65.938 | | 274.433 | | 12.578 | | # |
| C4H4O- FURAN anion | | 68.07451 | 118.871 | 136.423 | ±8. | | 74.820 | | 280.769 | | 13.766 | | # |
| C4H4O VINYL-KETENE | | 68.07516 | 22.719 | 31.98 | ±8. | | 81.797 | | 309.171 | | 16.229 | | # |
| C4H4O2 1,4-DIOXIN | | 84.07336 | -86.542 | -72.051 | ±8. | | 81.320 | | 284.595 | | 15.339 | | # |
| C4H4O4 Fumaric acid *trans* | | 116.07216 | -696.469 | -679.388 | ±8. | | 117.504 | | 376.826 | | 21.430 | | # |
| C4H4S Thiophene | | 84.14056 | 115.96 | 128.240 | ±8. | | 72.818 | | 278.908 | | 13.282 | | # |
| C4H4S+ Thiophene cation | | 84.14001 | 982.115 | 987.302 | ±8. | | 74.859 | | 287.882 | | 13.808 | | # |
| E-C4H5 1,3-butadiene 1-yl <~> | | 53.08250 | 363.339 | 373.360 | ±8. | | 74.144 | | 303.589 | | 15.362 | | # |
| I-C4H5 1,3-butadiene-2-yl | | 53.08250 | 315.223 | 325.419 | ±8. | | 77.138 | | 290.119 | | 15.188 | | # |
| T-C4H5 1,2,butadiene-4-yl <~> | | 53.08250 | 315.223 | Resonant |  | | with the | | former | | species | | X |
| C4H5 1-butyne-3-yl <~> | | 53.08250 | 318.432 | 327.890 | ±8. | | 81.537 | | 293.840 | | 15.926 | | # |
| C4H5 1-butyne-4-yl \*CH2CH2C≡CH | | 53.08250 | 376.18 | 385.19 | ±8. | | 84.712 | | 305.957 | | 16.373 | | # |
| C4H5 2-butyne-1-yl | | 53.08250 | 306.085 | 314.862 | ±8. | | 77.774 | | 300.775 | | 16.607 | | # |
| C4H5+ CH3-CC-CH2\*+ | | 53.08195 | 1083.0 | 1085.3 | ±8. | | 77.900 | | 295.958 | | 16.909 | | # |
| C4H5+ CH3-C\*=C=CH2+ | | 53.08195 | 1083.0 | Resonant | with | | the | | former | | species | | X |
| C4H5F5 CF3-CH2-CF2-CH3 | | 148.07451 | -1242.7 |  | ±8. | | 139.375 | | 372.408 | | 25.504 | | # |
| C4H5N PYRROLE | | 67.09044 | 108.18 | 124.857 | ±0.81 | | 71.6 | | 276.875 | | 13.042 | | # |
| C4H5N+ PYRROLE cation | | 67.08869 | 912.393 | 922.589 | ±8. | | 70.541 | | 276.348 | | 12.971 | | # |
| C4H5N- PYRROLE anion | | 67.08979 | 494.762 | 513.975 | ±8. | | 87.834 | | 297.806 | | 16.276 | | # |
| C4H5N Cyclopropanecarbonitrile  C4H5N | | 67.08924 | 184.096 | 198.729 | ±0.84 | | 78.733 | | 292.673 | | 15.086 | | # |
| C4H5N3O (cr) Cytosine Cy | | 111.10212 | -221.3 |  | ±2.3 | |  | |  | |  | | X |
| C4H5N3O Cytosine Cy | | 111.10212 | -69.5 | -45.433 | ±3.5 | | 114.046 | | 338.024 | | 18.663 | | # |
| C4H5O \*CH2CH2CH=C=O | | 69.08190 | 119.072 | 129.592 | ±8. | | 94.588 | | 343.805 | | 19.205 | | # |
| C4H5O CH3CH\*CH=C=O | | 69.08190 | 67.500 | 77.848 | ±8. | | 90.390 | | 342.574 | | 19.377 | | # |
| C4H5O2 CH3CH=CHC(O)O\* | | 85.08130 | -123.399 | -109.182 | ±8. | | 93.927 | | 358.064 | | 19.848 | | # |
| C4H5O2 \*CH=CHC(O)-OCH3 | | 85.08130 | -56.053 | -42.208 | ±8. | | 100.313 | | 351.572 | | 20.219 | | # |
| C4H5O2 CH2=C\*C(O)-OCH3 | | 85.08130 | -57.300 | -44.908 | ±8. | | 105.344 | | 372.811 | | 21.672 | | # |
| C4H6 1-Butayn Ethyl-acetylen <~> | | 67.09044 | 165.2 | 178.798 | ±0.85d | | 81.820 | | 291.210 | | 16.020 | | † |
| C4H6 2-ButaynDimethylacetylen | | 54.09044 | 146.314 | 159.388 | ±0.8d | | 77.886 | | 291.909 | | 16.544 | | †# |
| 1,3-C4H6 Butadiene <~> | | 54.09044 | 110.834 | 125.118 | ±8. | | 74.219 | | 293.330 | | 15.335 | | †# |
| 1,2-C4H6 Butadiene <~> | | 54.09044 | 161.314 | 175.436 | ±2. | | 78.663 | | 290.993 | | 15.496 | | # |
| C4H6 Cyclobutene | | 54.09164 | 156.7 | 173.761 | ±1.6d | | 64.414 | | 262.076 | | 12.558 | | † |
| C4H6 MethyleneCyclopropan C4H6 | | 54.09044 | 201. | 216.764 | ±2. | | 73.003 | | 270.423 | | 13.854 | | # |
| C4H6CL2 1,4-Dichlorobutene | | 124.99584 | -51.882 | -34.587 | ±8. | | 108.341 | | 386.083 | | 21.505 | | # |
| CL2C4H6 3,4-Dichlorobutene | | 124.99584 | -53.572 | -36.121 | ±8. | | 109.803 | | 379.398 | | 21.349 | | # |
| C4H6N4O12 Erythritol Tetra Nitrate | | 302.11020 | -447.69 | -399.66 |  | | 264.947 | | 680.976 | | 51.012 | | # |
| C4H6N8O8 BiCycloHMX solid | | 294.13956 | 172.3 |  |  | |  | |  | |  | | X |
| C4H6N8O8 BiCycloHMX gas BCHMX | | 294.13956 | 231.835 | 286.903 |  | | 240.868 | | 572.745 | | 43.952 | | # |
| C4H6O CH3CH2CH=C=O | | 70.08984 | -88.303 | -72.169 | ±8. | | 91.448 | | 343.487 | | 17.824 | | # |
| C4H6O (CH3)2C=C=O | | 70.08984 | -90.981 | -75.393 | ±8. | | 93.628 | | 301.334 | | 18.370 | | # |
| C4H6O 2,5 Di-Hydro FURAN | | 70.08984 | -63.911 | -44.234 | ±8. | | 72.849 | | 283.465 | | 14.282 | | # |
| C4H6O *trans*-Croton Aldehyde | | 70.08984 | -101.940 | -85.385 | ±0.49 | | 88.502 | | 307.987 | | 17.404 | | # |
| C4H6O *cis*-Methyl Vinyl Keton  CH3CO2CH=CH2 | | 70.08984 | -114.349 | -97.333 | ±8. | | 89.733 | | 314.569 | | 16.943 | | # |
| C4H6O *trans*-Methyl Vinyl Keton | | 70.08984 | -112.550 | -95.543 | ±8. | | 89.556 | | 314.470 | | 16.952 | | # |
| C4H6O *trans*-1,3-Butadiene-2-ol  CH2=C(OH)CH=CH2l | | 70.08984 | -66.931 | -49.053 | ±8. | | 89.870 | | 316.787 | | 16.080 | | # |
| C4H6O2 Crotonic acid E | | 86.08924 | -363.184 | -344.680 | ±8. | | 103.507 | | 343.679 | | 19.795 | | # |
| C4H6O2 CH2=CHC(O)-OCH3 | | 86.08924 | -309.386 | -291.690 | ±8. | | 101.460 | | 360.043 | | 20.603 | | # |
| C4H6O2 liq Diacetyl liquid c | | 86.08924 | -365.53d |  | ±0.57d | |  | |  | |  | | X |
| C4H6O2 CH3-C(O)-C(O)-CH3 | | 86.08924 | -325.482 | -310.25d | ±0.987 | | 102.375 | | 351.425 | | 21.089 | | # |
| C4H6O4 liq. Succinic acid c | | 118.08804 | -940.237d | -918.54d | ±0.132 | |  | |  | |  | | X |
| C4H6O4 HOOC-CH2CH2-COOHd | | 118.08804 | -817.729 | -794.955 | ±0.59 | | 124.337 | | 424.442 | | 24.204 | | # |
| C4H6O4 CH3-CO-OO-CO-CH3 | | 118.08804 | -500. | -477.02 | ±10 | | 122.291 | | 390.682 | | 23.944 | | # |
| C4H6S C2H3-S-C2H3 | | 86.15644 | 166.580 | 180.989 | ±8. | | 96.832 | | 348.299 | | 19.706 | | # |
| 2,5 C4H6S Dihydrothiophene | | 86.15644 | 85.872 | 104.666 | ±8. | | 80.794 | | 295.466 | | 15.237 | | # |
| C4H7 tt-1-Butene-1-yl <~> | | 55.09838 | 245.871 | 262.755 | ±8. | | 83.705 | | 311.281 | | 16.968 | | # |
| C4H7 cc-1-Butene-1-yl <~> | | 55.09838 |  | 264.85 | ±8. | |  | |  | |  | | X |
| C4H7 trans 1-Butene-2-yl | | 55.09838 | 231.162 | 248.45 | ±8. | | 83.973 | | 300.371 | | 16.425 | | # |
| C4H7 cis 1-Butne-2-yl | | 55.09838 |  | 248.11 | ±8. | |  | |  | |  | | X |
| C4H7 *trans*-2-Butene-2-yl | | 55.09838 | 223.853 | 239.743 | ±8. | | 83.237 | | 313.256 | | 17.962 | | # |
| C4H7 *cis*-2-Butene-2-yl | | 55.09838 |  | 243.09 | ±8. | |  | |  | |  | | X |
| C4H7 *trans* 3-Butene 1-yl Rad. | | 55.09838 | 204.595 | 220.915 | ±8. | | 84.719 | | 317.348\* | | 17.533 | | # |
| C4H7 cis 3-Butene-1-yl Radical | | 55.09838 |  | 223.01 | ±8. | | - | | - | |  | | X |
| C4H7 *trans* (CH2=CH\*CHCH3) | | 55.09838 | 136.111 | 153.553 | ±8 | | 80.787 | | 306.087\* | | 16.411 | | # |
| C4H7 *cis* –1-Methylallyl Radical | | 55.09838 |  | 156.48 | ±8. | |  | |  | |  | | X |
| C4H7 2-Methyl-Allyl Radical | | 55.09838 | 137.603 | 155.226 | ±5. | | 82.196 | | 300.803 | | 16.229 | | # |
| C4H7 Cyclobutyl Radical | | 55.09838 | 230.306 | 249.366 | ±8. | | 73.070 | | 286.490 | | 14.792 | | # |
| C4H7N C3H7CN Propylcyanide | | 69.10512 | 31.200 | 51.765 | ±8. | | 91.422 | | 310.996 | | 17.622 | | # |
| C4H7N3O9 liq NO3CH2CH(NO3)CH2CH2NO3 | | 241.11320 | -414. |  |  | |  | |  | |  | | X |
| C4H7N3O9 gas NO3CH2CH(NO3)CH2CH2NO3 | | 241.11320 | -361.7 | -318.32 |  | | 218.793 | | 580.703 | | 42.538 | | # |
| C4H7O \*CH2CH2CH2CH=O | | 71.09778 | 2.494 | 21.652 | ±8. | | 96.363 | | 368.530 | | 19.034 | | # |
| C4H7O CH3\*CHCH2CH=O | | 71.09778 | -12.510 | 5.510 | ±8. | | 101.188 | | 356.878 | | 20.172 | | # |
| C4H7O CH3CH2CH2\*C=O | | 71.09778 | -51.313 | -32.787 | ±8. | | 97.923 | | 352.974 | | 19.666 | | # |
| C4H7O C2H5C(O)CH2\*  2-Butanone | | 71.09778 | -56.233 | -36.974 | ±8 | | 100.468 | | 344.546 | | 18.934 | | # |
| C4H7O 2-Butanone Radical | | 71.09778 | -75.994 | -57.670 | ±8. | | 97.420 | | 344.655 | | 19.868 | | # |
| C4H7O CH2=C(CH3)CH2O\* | | 71.09778 | 55.748 | 75.378 | ±8. | | 96.143 | | 334.259 | | 18.562 | | # |
| C4H7O2 CH3CH2CH2C(O)O\* | | 87.09718 | -234.007 | -212.646 | ±8. | | 103.763 | | 378.873 | | 21.172 | | # |
| C4H7O2 \*CH2CH2C(O)OCH3 | | 87.09718 | -229.166 | -208.651 | ±8. | | 111.373 | | 376.723 | | 22.018 | | # |
| C4H7O2 CH3C(O)OCH2CH2\* | | 87.09718 | -236.773 | -216.138 | ±8. | | 108.389 | | 381.911 | | 21.898 | | # |
| C4H7O2 CH2=CHCH2CH2OO\* | | 87.09718 | 60.66 | 82.05 |  | | 106.957 | | 372.450 | | 21.145 | | # |
| C4H8 CH2=CH-CH2-CH3  <~> | | 56.10632 | -0.031 | 20.819 | ±0.47 | | 85.601 | | 305.372 | | 17.236 | | #† |
| H8C4 CH2=C(CH3)2 Isobutene<~> | | 56.10632 | -17.574 | 3.46d | ±0.52 | | 86.018 | | 287.454 | | 16.220 | | #† |
| C4H8 2-Butene trans | | 56.10632 | -11.185 | 9.391 | ±0.5 | | 87.670 | | 296.330 | | 17.510 | | † |
| C4H8 2-Butene cis | | 56.10632 | -7.340 | 13.946 | ±0.52 | | 80.150 | | 301.310 | | 16.800 | | † |
| C4H8 CYCLOBUTANE <~> | | 56.10632 | 28.4 | 52.889 |  | | 72.096 | | 259.083 | | 13.597 | | #† |
| C4H8CL2S Mustard | | 159.07772 | -124.77 | -100.66 |  | | 136.283 | | 420.586 | | 27.569 | | # |
| Beta HMX solid | | 296.15664 | 74.894 |  |  | | 307.302 | | 320.0 | |  | |  |
| C4H8N8O8 HMX  HMX Structure<http://www.chemicalbook.com/ProductChemicalPropertiesCB1453029_EN.htm> | | 296.15664 | 187.862 | 245.304 | ±25.1 | | 275.455 | | 568.833 | | 50.045 | |  |
| C4H8O Cyclobutanol cyC4H7OH | | 72.10572 | -145.126 | -119.188 | ±8. | | 91.517 | | 295.917 | | 16.489 | | # |
| C4H8O 2-Methyl-Allyl Alcohol | | 72.10572 | -161.143 | -137.34 | ±8 | | 100.007 | | 316.183 | | 18.622 | | # |
| C4H8O n-Butanal | | 72.10572 | -206.137 | -182.183 | ±8. | | 95.543 | | 327.343 | | 18.473 | | # |
| C4H8O 2-BUTANONE | | 72.10572 | -239.973 | -218.121 | ±8. | | 101.003 | | 340.043 | | 20.754 | | # |
| H8C4O 2,3-Dimethyloxyrane | | 72.10572 | -137.658 | -113.00 | ±8. | | 95.471 | | 303.780 | | 17.777 | | # |
| OC4H8 ETHYL-OXYRANE | | 72.10572 | -115.960 | -91.115 | ±8 | | 91.134 | | 316.499 | | 17.582 | | # |
| C4H8O Tetrahydrofuran, Oxolan | | 72.10572 | -182.498 | -155.522 | ±8 | | 78.225 | | 302.550 | | 15.450 | | # |
| C4H8O2 (liq) Butyric acid | | 88.10512 | -533.92 |  | ±0.59 | |  | |  | |  | | X |
| C4H8O2 Butyric acid | | 88.10512 | -455.780 | -429.750 | ±8. | | 102.582 | | 367.660 | | 20.736 | | # |
| C4H8O2 Methyl Propionate | | 88.10512 | -437.291 | -412.905 | ±8. | | 107.873 | | 375.707 | | 22.381 | | # |
| C4H8O2 Ethyl Acetate | | 88.10512 | -448.550 | -424.136 | ±8. | | 107.786 | | 377.409 | | 22.352 | | # |
| C4H8O2 1,4 DIOXANE | | 88.10512 | -295.068 | -265.482 | ±8. | | 91.821 | | 304.207 | | 17.180 | | # |
| C4H8O2 1-Peroxy-3-Butene | | 88.10512 | -76.237 | -50.932 | ±8. | | 11.779 | | 363.541 | | 21.461 | | # |
| (CH3COOH)2 Acetic Acid dimer | | 120.1048 | -929.015 | -901.62 |  | | 137.254 | | 414.396 | | 28.053 | | † |
| C4H8O4 Tetraoxocan | | 120.10392 | -635.474 | -600.627 | ±8 | | 115.259 | | 326.918 | | 20.599 | | # |
| C4H8S Tetrahydrothiophen | | 88.17232 | -30.702 | -4.196 | ±8. | | 87.38 | | 300.156 | | 15.993 | | # |
| 1,4-C4H8S2 Dithiane | | 120.23832 | 20.635 | 48.493 | ±8. | | 109.655 | | 326.500 | | 19.053 | | # |
| 1,3-C4H8S2 Dithiane | | 120.23832 | 4.945 | 32.593 | ±8. | | 110.433 | | 333.844 | | 19.263 | | # |
| C4H9,n-Butyl Radical <~> | | 57.11426 | 81.80 | 105.91 | ±8. | | 94.555 | | 307.628 | | 19.797 | | #† |
| C4H9+ n-Butyl Radical cation | | 57.11371 | 807.763 | 832.436 | ±8. | | 89.402 | | 296.441 | | 16.787 | | # |
| C4H9- n-Butyl Radical anion | | 57.11481 | 77.780 | 108.353 | ±8. | | 91.774 | | 300.077 | | 17.223 | | # |
| *i*-C4H9 iso-Butyl Radical <~> | | 57.11426 | 73.785 | 97.92 | ±8. | | 98.111 | | 304.662 | | 18.063 | | # |
| *i*-C4H9+ iso-Butyl cation | | 57.11371 | 722.653 | 739.024 | ±8. | | 86.589 | | 310.974 | | 17.866 | | # |
| *i*-C4H9- iso-Butyl anion | | 57.11481 | 56.722 | 87.538 | ±8. | | 91.986 | | 288.992 | | 16.638 | | # |
| *s-*C4H9 *sec-*Butyl Radical <~> | | 57.11426 | 70.224  66.07h | 94.945 | ±8.  ±0.95h | | 86.395 | | 327.417 | | 17.538 | | # |
| *2-*C4H9+ *sec-*Butyl Radical cation | | 57.11371 | 782.282 | 799.648 | ±8. | | 94.357 | | 311.952 | | 17.737 | | # |
| *2-*C4H9- *sec-*Butyl Radical anion | | 57.11481 | 73.077 | 103.750 | ±8. | | 90.423 | | 307.179 | | 16.969 | | # |
| C4H9,t-Butyl Radical <~> | | 57.11426 | 55.070  50.30h | 79.719 | ±8.  0.66h | | 82.410 | | 323.393 | | 17.010 | | # |
| C4H9-, t-Butyl Radical anion | | 57.11481 | 46.982 | 78.132 | ±8. | | 89.172 | | 283.793 | | 16.312 | | # |
| C4H9N PYROLIDINE | | 71.12100 | -3.59 | 26.889 | ±0.8 | | 82.112 | | 309.206 | | 16.177 | | # |
| C4H9NO2 Nitrobutan | | 103.11980 | -152.452 | -120.911 | ±8. | | 124.993 | | 393.110 | | 23.794 | | # |
| C4H9NO2+ Nitrobutan cation | | 103.11925 | 868.097 | 888.551 | ±8. | | 138.481 | | 443.727 | | 28.337 | | # |
| C4H9NO2- Nitrobutan anion | | 103.12035 | -175.552 | -132.325 | ±8. | | 126.480 | | 420.284 | | 25.228 | | # |
| C4H9NO2 (CH3)3CNO2 | | 103.11980 | -182.004 | -149.238 | ±8. | | 125.357 | | 351.943 | | 22.569 | | # |
| C4H9NO2+ (CH3)3CNO2  cation | | 103.11925 | 836.600 | 859.553 | ±8. | | 135.823 | | 368.573 | | 24.431 | | # |
| C4H9NO2- (CH3)3CNO2 anion | | 103.12035 | -205.303 | -168.640 | ±8. | | 133.940 | | 356.742 | | 23.304 | | # |
| C4H9N3O5 Ethyl NENA C2H5N(NO2)CH2CH2ONO2 | | 179.13148 | -133.9 | -92.7 |  | | 183.712 | | 511.444 | | 35.769 | | # |
| C4H9O n-BUTOXY RAD | | 73.11366 | -56.350 | -29.003 | ±8. | | 101.794 | | 349.126 | | 19.314 | | # |
| C4H9O I-BUTOXY RAD | | 73.11366 | -65.070 | -36.703 | ±8. | | 101.777 | | 319.038 | | 18.294 | | # |
| C4H9O S-BUTOXY RAD | | 73.11366 | -69.84 | -41.88 | ±8. | | 102.025 | | 327.058 | | 18.700 | | # |
| C4H9O T-BUTOXY RAD | | 73.11366 | -86.923 | -58.899 | ±8. | | 106.062 | | 309.188 | | 18.637 | | # |
| C4H9O C2H5-O-CH2CH2\* | | 73.11366 | -44.095 | -18.932 | ±8. | | 109.732 | | 366.749 | | 21.498 | | # |
| C4H9O C2H5-O-CH\*CH3 | | 73.11366 | -74.697 | -49.959 | ±8. | | 109.080 | | 370.674 | | 21.922 | | # |
| C4H8OH+ cy Tetrahydrofuran  Oxonium (CH2CH2CH2CH2)OH+ | | 73.11311 | 529.067 | 553.199 | ±8. | | 86.994 | | 293.796 | | 15.892 | | # |
| C4H9O2 Peroxy n-Butane RAD | | 89.11306 | -63.530 | -34.746 | ±8. | | 111.895 | | 381.549 | | 22.217 | | # |
| C4H9O2 Peroxy s-Butane RAD | | 89.11306 | -84.557 | -55.898 | ±8. | | 116.539 | | 380.506 | | 22.482 | | # |
| C4H9O2 Peroxy T-Butane RAD | | 89.11306 | -106.412 | -78.159 | ±8. | | 122.218 | | 367.903 | | 22.748 | | # |
| C4H10 n-Butane HC 600 <~> | | 58.1222 | -125.790 | -98.46 | ±0.38d | | 98.651 | | 309.884 | | 19.227 | | † |
| C4H10+ n-Butane cation | | 58.12165 | 886.163 | 906.253 | ±8. | | 102.474 | | 315.735 | | 19.151 | | # |
| C4H10- n-Butane anion | | 58.12275 | -69.187 | -35.454 | ±8. | | 95.482 | | 306.469 | | 17.950 | | # |
| I-C4H10 ISOBUTANE <&> | | 58.1222 | -134.990 | -106.37 | ±0.40d | | 96.643 | | 295.493 | | 17.936 | | † |
| I-C4H10+ ISOBUTANE cation | | 58.12165 | 887.444 | 907.204 | ±8. | | 105.894 | | 309.257 | | 19.194 | | # |
| I-C4H10- ISOBUTANE anion | | 58.12274 | -75.593 | -40.284 | ±8. | | 93.282 | | 292.598 | | 16.703 | | # |
| C4H10FO2P SARIN | | 140.09316 | -1005.834 | -971.27 | ±20 | | 159.442 | | 411.754 | | 30.443 | | # |
| C4H10N2 1,4-Piperazine | | 86.13568 | 32.058 | 70.65 | ±8. | | 96.860 | | 301.189 | | 16.633 | | # |
| C4H10O-N 1-BUTANOL | | 74.1216 | -275.981 | -245.721 | ±8. | | 108.033 | | 361.703 | | 20.634 | | # |
| C4H10O-S 2-BUTANOL | | 74.1216 | -295.332 | -265.572 | ±8. | | 111.128 | | 354.836 | | 21.134 | | # |
| C4H10O Isobutanol CH3CH(CH3)CH2OH | | 74.1216 | -283.8 | -253.94 | ±0.9 | | 112.354 | | 351.556 | | 21.035 | | # |
| C4H10O-T 2-Methyl-2-propanol | | 74.1216 | -315.415 | -285.128 | ±8. | | 113.481 | | 335.551 | | 20.607 | | # |
| C4H10O DiEthylEther | | 74.1216 | -254.948 | -224.468 | ±8. | | 105.009 | | 345.73 | | 20.415 | | # |
| C4H10O2 nButyl Hydroperoxide | | 90.1210 | -202.602 | -171.262 | ±8. | | 122.721 | | 373.151 | | 23.895 | | # |
| C4H10O2 t Butyl Hydropeoxide | | 90.1210 | -241.090 | -210.203 | ±8. | | 136.548 | | 354.252 | | 24.347 | | # |
| C4H10O2 1,4-butanediol | | 90.1210 | -432.048 | -398.417 | ±8. | | 115.030 | | 355.844 | | 21.604 | | # |
| C4H10O3 DiEthyleneGlycol  (HOCH2CH2)2O | | 106.1204 | -551.380 | -520.119 | ±0.79 | | 145.521 | | 430.402 | | 28.314 | | # |
| C4H10O4 C4(OH)4 1,2,3,4-Erythritol | | 122.1198 | -762.3 | -720.7 | ±15. | | 137.197 | | 394.501 | | 22.346 | | # |
| C4H10S 1-Butanethiol C4H9SH | | 90.1882 | -85.923 | -57.029 | ±8. | | 110.052 | | 372.824 | | 22.073 | | # |
| C4H10S DiEthylSulfide (C2H5)2S | | 90.1882 | -81.659 | -52.591 | ±8. | | 107.788 | | 357.377 | | 21.899 | | # |
| C4H11O+ (CH3)2O-C2H5+ | | 75.12899 | 497.984 | 519.411 | ±8. | | 110.480 | | 331.076 | | 21.307 | | # |
| C4H11O+ (C2H5)2OH+ | | 75.12899 | 468.077 | 489.895 | ±8. | | 112.598 | | 326.792 | | 20.917 | | # |
| C4H11P (C2H5)2PH | | 90.10390 | -85.521 | -51.804 | ±8. | | 120.258 | | 342.245 | | 22.432 | | # |
| C4H11P+ (C2H5)2PH+ | | 90.10335 | 711.000 | 736.585 | ±8. | | 123.744 | | 353.035 | | 23.168 | | # |
| C4H11P- (C2H5)2PH- | | 90.10445 | 95.064 | 127.587 | ±8. | | 133.245 | | 431.934 | | 28.307 | | # |
| C4H12Si Si(CH3)4 | | 88.22358 | -219.338 | -186.489 | ±8. | | 145.448 | | 344.106 | | 25.391 | | # |
| C4H12Si+ Si(CH3)4+ cation | | 88.22303 | 706.536 | 728.016 | ±8. | | 156.214 | | 361.645 | | 27.654 | | # |
| C4H12Si (C2H5)2SiH2 | | 88.22358 | -106.002 | -72.329 | ±8. | | 129.567 | | 372.008 | | 24.567 | | # |
| C4H12Si+ (C2H5)2SiH2+ cation | | 88.22303 | 821.349 | 845.565 | ±8. | | 140.733 | | 386.178 | | 26.787 | | # |
| C4H12Sn Sn(CH3)4 | | 178.84808 | -20.502 | +11.004 | ±4.2 | | 145.919 | | 410.093 | | 29.840 | | # |
| C4H12Sn H2Sn(C2H5)2 | | 178.84808 | 56.484 | 90.910 | ±4.2 | | 143.567 | | 410.046 | | 26.920 | | # |
| C4N2 Carbon Subnitrid | | 76.0574 | 529.2 | 524.285 | ±0.8 | | 86.326 | | 290.524 | | 17.799 | | † |
| C4N8O6 DDFP | | 256.09312 | 724.250 | 753.182 | ±12.5 | | 201.048 | | 493.698 | | 36.003 | | # |
| C5 1Σ+g singlet | | 60.05350 | 1072.112 | 1061.180 | ±8. | | 75.507 | | 271.677 | | 16.192 | | †# |
| C5Cl6 PerChloroCycloPentadiene | | 272.76970 | -11.7 | -11.066 | ±4.4 | | 165.769 | | 449.904 | | 32.177 | | # |
| C5F6 PerFluoroCycloPentadiene | | 174.04392 | -932.986 | -928.15 | ±8. | | 144.089 | | 393.515 | | 26.906 | | # |
| C5F12 FC 4-1-12 | | 288.03584 | -2543.311 |  |  | | 229.036 | | 555.108 | |  | |  |
| C5H | | 61.06144 | 860.0 | 853.43 | ±75. | | 80.114 | | 281.338 | | 16.071 | | # |
| C5H2 \*HC=C=C=C=CH\* <~> | | 62.06938 | 691.299 | 690.360 |  | | 82.497 | | 266.537 | | 14.674 | | # |
| C5H2CL2O CY | | 148.97418 | -12.17 | -5.59 | ±8. | | 111.295 | | 349.650 | | 20.679 | | # |
| C5H2CL3 CY | | 168.42748 | 152.68 | 158.05 | ±8. | | 118.207 | | 369.252 | | 22.140 | | # |
| C5H2Cl3 ClHC=C=CCl-CCl=CH\* | | 168.42748 | 460.064 | 462.152 | ±8. | | 131.611 | | 413.831 | | 25.420 | | # |
| C5H2N3O6\* 1,3,4-triNitroCPD-1-yl | | 200.08600 | 155.034 | 173.336 | ±8. | | 182.182 | | 424.849 | | 34.479 | | # |
| C5H3 1,3-Pentadiyne-5-yl Rad. | | 63.07882 | 602.58 |  |  | | 87.499 | | 295.196 | |  | |  |
| C5H3 HC≡C-CH\*C≡CH <~> | | 63.07882 | 564.61 |  | ±43 | | 93.241 | | 306.147 | |  | |  |
| C5H3 Cyclopentatriene-yl | | 63.07732 | 718.836 | 722.751 | ±8. | | 73.211 | | 286.057 | | 14.055 | | # |
| C5H3+ Cyclopentatriene-yl Cation | | 63.07677 | 1523.7 | 1521.6 | ±8. | | 71.775 | | 278.711 | | 13.832 | | # |
| C5H3Cl3 1,2,4-triCl-2,4-CYdiene | | 169.43542 | 61.513 | 71.033 | ±8. | | 118.468 | | 372.260 | | 22.221 | | # |
| C5H3Cl3O CY | | 185.43482 | -104.72 | -93.65 | ±8. | | 139.671 | | 397.902 | | 25.014 | | # |
| C5H3N HC≡C-CH=CH-CN | | 77.08406 | 422.613 | 426.538 | ±8. | | 93.766 | | 318.598 | | 18.380 | | # |
| C5H4 1,3-Pentadiyne | | 64.08526 | 411.835 | 416.818 | ±8. | | 86.669 | | 291.342 | | 17.221 | | # |
| C5H4 1,4-Pentadiyne | | 64.08526 | 451.964 | 434.773 | ±8. | | 89.940 | | 305.243 | | 17.191 | | # |
| C5H4 Pentane-Tetraene | | 64.08526 | 444.466 | 449.702 | ±8. | | 86.132 | | 287.480 | | 16.968 | | # |
| H4C5 1,2-Pentadiene-4-yne | | 64.08526 | 433.354 | 438.929 | ±8. | | 86.751 | | 301.509 | | 16.628 | | # |
| C5H4 1,2,4-Cyclo-Pentatriene. | | 64.08526 | 548.644 | 557.214 | ±8. | | 72.062 | | 279.037 | | 13.633 | | # |
| C5H4N \*CH=CH-CH=CH-CN | | 78.09200 | 502.942 | 510.320 | ±8. | | 97.601 | | 341.652 | | 19.160 | | # |
| C5H4N meta-Pyridyl Radical | | 78.09200 | 405.241 | 418.146 | ±8. | | 74.123 | | 292.227 | | 13.634 | | # |
| C5H4N4 Purine C5H4N4 | | 120.11222 | 272.270 | 294.347 | ±8. | | 103.224 | | 322.840 | | 17.466 | | # |
| C5H4O Cyclopentadiene-1-one<!> | | 80.08466 | 55.229 | 66.855 |  | | 80.941 | | 289.952 | | 14.958 | | # |
| C5H4O2 3 Ketene | | 96.08556 | -105.834 | -95.030 | ±8 | | 101.982 | | 361.789 | | 20.080 | | # |
| C5H4O2 Furfural | | 96.08406 | -159.046 | -145.549 | ±8 | | 92.927 | | 328.843 | | 17.386 | | # |
| C5H4O2 Pyran-2(α)-one | | 96.08406 | -205.589 | -190.847 | ±8. | | 90.574 | | 308.935 | | 16.142 | | # |
| C5H4O2 Pyran-4/()-one | | 96.08406 | -167.737 | -153.021 | ±8. | | 90.121 | | 303.825 | | 16.168 | | # |
| C5H5 1-Pentyne-3-ene-5-yl | | 65.09320 | 384.93 | 394.23 | ±8. | | 92.828 | | 310.776 | | 17.130 | | # |
| C5H5+ 1-Pentyne-3-ene-5-yl cation | | 65.09265 | 1149.0 | 1152.2 | ±8. | | 86.823 | | 303.652 | | 16.970 | | # |
| C5H5 CY Cyclopentadienyl Rad. <!> | | 65.09320 | 263.269  261.39h | 275.251 | ±8  0.93h. | | 77.582 | | 300.406 | | 15.155 | | # |
| C5H5+ CY Cyclopentadienyl Cation | | 65.09265 | 1110.8  1074.75h | 1116.8 | ±8.  0.93h | | 75.683 | | 278.266 | | 14.260 | | # |
| C5H5- Cyclopentadienyl anion | | 65.09375 | 82.279  87.1h | 101.750  100.1h | ±8.  1.1h | | 73.238 | | 270.985 | | 13.164 | | # |
| C5H5N CH2=CH-CH=CH-CN | | 79.09994 | 238.944 | 250.471 | ±8. | | 99.632 | | 336.825 | | 19.246 | | # |
| C5H5N PYRIDINE | | 79.09994 | 140.080 | 156.922 | ±8. | | 77.746 | | 282.762 | | 13.931 | | # |
| C5H5NO2 NitroCycloPentadiene | | 111.09874 | 126.696 | 146.916 | ±8. | | 104.237 | | 345.720 | | 19.233 | | # |
| C4H2O2N-CH3 Me-Maleinimide C5H5NO2 | | 111.09874 | -256.0 | -237.615 | ±1.5 | | 112.143 | | 342.156 | | 21.068 | | # |
| C4H4NCOOH Pyrrole-2-carboxylic acid C5H5NO2 | | 111.09874 | -288.106 | -268.607 | ±8. | | 112.219 | | 350.843 | | 19.954 | | # |
| C5H4N2O4 Orotic acid  C5H4N2O4 | | 156.09634 | -538.9 | -516.29 |  | | 145.213 | | 403.337 | | 25.627 | | # |
| C5H5N5 (cr) Adenine Cy | | 135.12690 | 96.9 |  | ±1.3 | |  | |  | |  | | X |
| C5H5N5 Adenine Cy | | 135.12690 | 225.7 | 252.165 | ±3.5 | | 129.836 | | 351.909 | | 21.648 | | # |
| C5H5N5O (cr) Guanine solid | | 151.1263 | -183.8 |  | ±0.9 | |  | |  | |  | | X |
| C5H5N5O Guanine Cy | | 151.1263 | 16.0 | 44.29 | ±5. | | 145.812 | | 371.844 | | 24.160 | | # |
| C5H4OH CYCLO RAD <!> | | 81.0926 | 67.036 | 81.734 | ±8. | | 94.197 | | 309.874 | | 16.080 | | # |
| 1,3C5H5O CY RADICAL <!> | | 81.0926 | 38.689 | 53.951 | ±8. | | 85.879 | | 305.606 | | 15.515 | | # |
| 1,4C5H5O CY RADICAL <!> | | 81.0926 | 72.73 | 87.983 | ±8. | | 90.479 | | 307.805 | | 15.525 | | # |
| 2,4-c-C5H5O CY RADICAL <!> | | 81.0926 | 217.045 | 232.282 | ±8. | | 86.614 | | 305.729 | | 15.541 | | # |
| C5H5O2 2-pentenedialdehyde R | | 97.0920 | -31.45 | -18.540 | ±8. | | 108.258 | | 388.719 | | 22.613 | | # |
| C5H5O2 2-pentenedialdehyde R | | 97.0935 | -84.144 | -70.281 | ±8. | | 105.719 | | 371.864 | | 21.255 | | # |
| C5H6 1,2,4-Pentatriene | | 66.10114 | 252.617 | 265.126 | ±8. | | 93.762 | | 316.977 | | 18.163 | | # |
| C5H6 1-ene-3-yne | | 66.10114 | 253.927 | 267.143 | ±8. | | 92.856 | | 305.417 | | 17.456 | | # |
| C5H6 3-enE-1-yne | | 66.10114 | 252.638 | 266.263 | ±8. | | 91.771 | | 305.044 | | 17.047 | | # |
| C5H6 liq Cyclopentadiene liq h | | 66.10114 | 109.87h |  | ±0.58h | |  | |  | |  | | X |
| C5H6 CYCLOPENTADIENE<!> | | 66.10114 | 132.76g | 150.079 | ±0.76g | | 74.140 | | 273.241 | | 13.353 | | #† |
| C5H6+ 2,4-Cyclopentadiene cation | | 66.10059 | 1560.30 | 983.47 | ±8. | | 74.399 | | 275.991 | | 13.751 | | # |
| C5H6N2 2-AMINOPYRIDINE | | 94.11462 | 118.085 | 140.843 | ±8. | | 99.446 | | 312.178 | | 16.584 | | # |
| C5H6N2O2 (cr) Thymine CY | | 126.11342 | -462.8 |  | ±1.1 | |  | |  | |  | | X |
| C5H6N2O2 Thymine CY | | 126.11342 | -338.0 | -312.889 | ±2.5 | | 132.918 | | 359.633 | | 22.921 | | # |
| 2,4-C5H5OH <!> | | 82.10054 | -1.233 | +17.008 | ±8. | | 90.122 | | 313.406 | | 16.771 | | # |
| 1,3-C5H5OH | | 82.10204 | -37.851 | -18.509 | ±8. | | 91.400 | | 308.264 | | 15.671 | | # |
| 1,4 C5H5OH | | 82.10204 | -41.40 | -22.023 | ±8. | | 91.363 | | 308.113 | | 15.633 | | # |
| C5H6O Pyran 2,5-Hexadiene 1oxo | | 82.10204 | -10.399 | +9.191 | ±8. | | 84.819 | | 294.627 | | 15.422 | | # |
| 2-C5H6O 2-Methyl-Furan | | 82.10054 | -78.316 | -59.522 | ±8. | | 89.800 | | 303.662 | | 16.217 | | # |
| 3-C5H6O 3-Methyl-Furan | | 82.10054 | -67.132 | -48.348 | ±8. | | 89.932 | | 303.871 | | 16.228 | | # |
| 2-C5H6O2 Furfuryl Alcohol Structural formula of furfuryl alcohol | | 98.09994 | -216.99 | -196.899 | ±8. | | 101.795 | | 353.865 | | 19.260 | | # |
| C5H7 1,3-Pentadien-5-yl | | 67.10908 | 205.455 | 222.877 | ±8. | | 92.672 | | 325.606 | | 17.484 | | # |
| C5H7 1,4-Pentadien-3-yl | | 67.10908 | 205.455 | 223.086 | ±8. | | 93.92 | | 323.195 | | 17.275 | | # |
| C5H7+ 1,4-Pentadien-3-yl cation | | 67.10853 | 928.070 | 938.960 | ±8. | | 90.439 | | 302.224 | | 17.396 | | # |
| C5H7- 1,4-Pentadien-3-yl anion | | 67.10963 | 112.783 | 135.208 | ±8. | | 99.075 | | 304.785 | | 18.189 | | # |
| C5H7 Cy 1-penten-3-yl | | 67.10908 | 172.623 | 192.745 | ±8. | | 79.939 | | 296.325 | | 14.785 | | # |
| C5H7 Cy 1-penten-4-yl | | 67.10908 | 223.94 | 243.815 | ±8. | | 80.499 | | 290.579 | | 15.031 | | # |
| C5H7CL | | 102.56178 | 58.091 | 76.235 | ±8 | | 110.072 | | 374.067 | | 21.352 | | # |
| C5H7CL2 | | 138.01448 | 110.926 | 128.756 | ±8 | | 132.403 | | 444.862 | | 26.257 | | # |
| C5H7NO | | 97.11522 | -96.843 | -78.691 | ±8 | | 127.323 | | 391.075 | | 25.429 | | # |
| C5H7O 1-Cypenten-4-oxy Rad. | | 83.10848 | 95.04 | 117.53 | ±8. | | 92.705 | | 317.690 | | 16.752 | | # |
| C5H8 1-Pentyne HCCC3H7 | | 68.11702 | 143.930 | 164.061 | ±3.5 | | 101.499 | | 327.860 | | 19.009 | | # |
| C5H8 2-Pentyne CH3-CC-C2H5 | | 68.11702 | 128.449 |  | ±3.5 | | 99.590 | | 332.600 | |  | | # |
| C5H8 1,3-Pentadiene | | 68.11702 | 84.157 | 105.770 | ±8. | | 94.718 | | 318.284 | | 17.527 | | # |
| C5H8+ 1,4 Pentadiene cation | | 68.11647 | 995.219 | 1009.749 | ±8. | | 97.446 | | 310.935 | | 17.931 | | # |
| C5H8 ISOPRENE | | 68.11702 | 76.161 | 97.942 | ±8. | | 95.762 | | 316.277 | | 17.359 | | # |
| C5H8 Cyclopentene | | 68.11702 | 37.317  33.85h | 681.61 | ±8.  0.45h | | 79.055 | | 284.799 | | 14.659 | | #† |
| C5H8- Cyclopentene anion | | 68.11756 | 198.346 | 227.354 | ±8. | | 87.171 | | 291.323 | | 15.885 | | # |
| C5H8CL CH2ClCH=CHCH2CH2 | | 103.56972 | 158.197 | 179.288 | ±8. | | 119.551 | | 399.520 | | 22.640 | | # |
| PETN Solid | | 316.13828 | -538.481 |  | ±0.84 | | 353.757 | |  | |  | |  |
| C5H8N4O12 PETN | | 316.13828 | -387.02 | -332.00 |  | | 294.758 | | 614.706 | | 53.542 | |  |
| C5H8O Cyclopentanone | | 84.11642 | -197.401 | -171.29 | ±5.4 | | 97.436 | | 309.296 | | 17.366 | | # |
| C5H8O 1,5-Cyclopenten-2-ol | | 84.11642 | -126.579 | -99.582 | ±8. | | 96.604 | | 315.064 | | 16.583 | | # |
| C5H8O2 *trans* Pentenoic acid | | 100.11582 | -381.836 | -357.745 | ±8. | | 119.232 | | 401.920 | | 23.709 | | # |
| C5H8O2 Methyl Butenoate | | 100.11582 | -345.967 | -322.161 | ±8. | | 123.680 | | 382.548 | | 24.015 | | # |
| C5H8O2 MethylMetacrylate | | 100.11582 | -336.1 | -311.185 | ±0.6 | | 121.552 | | 357.622 | | 22.905 | | # |
| C5H8O3 Levulinic acid  CH3-C(O)-CH2CH2COOH | | 116.11522 | -611.923 | -584.969 | ±8. | | 133.653 | | 391.127 | | 25.206 | | # |
| C5H8O4 Glutaric acid  HOOC(CH2)3COOH | | 132.11462 | -837. | -808.663 | ±8. | | 144.164 | | 461.348 | | 28.163 | | # |
| C5H8O4 DiMethyl Malonate  CH3OOCCH2COOCH3 | | 132.11462 | -739. | -711.462 | ±0.45 | | 148.617 | | 441.618 | | 28.962 | | # |
| C5H9 CY | | 69.12496 | 111.131 | 138.404 | ±8. | | 88.092 | | 298.784 | | 16.101 | | # |
| C5H9 2-PENTEN-5-YL | | 69.12496 | 174.615 | 196.937 | ±8. | | 110.968 | | 357.785 | | 21.052 | | # |
| H9C5 2-PENTEN-1-YL | | 69.12496 | 116.700 | 140.617 | ±8. | | 106.281 | | 347.013 | | 19.457 | | # |
| C5H9 3M-1-BUTEN3YL | | 69.12496 | 102.479 | 126.521 | ±8. | | 106.535 | | 329.883 | | 19.332 | | # |
| C5H9 3M-1-BUTEN1YL | | 69.12496 | 219.091 | 243.190 | ±8. | | 105.817 | | 335.407 | | 19.275 | | # |
| C5H9 3M-1-BUTEN4YL | | 69.12496 | 180.356 | 204.114 | ±8. | | 108.450 | | 348.534 | | 19.616 | | # |
| C5H9N 1,2,3,6-TetraHydroPyridine | | 83.13170 | 273.454 | 305.013 | ±8. | | 96.132 | | 302.073 | | 16.150 | | # |
| C5H9NO2 cy CycloNitroPentan | | 115.13050 | 1051.778 | 1086.536 | ±8. | | 117.325 | | 362.006 | | 21.632 | | # |
| C5H9NO4 Glutamic acid (amino)  HO-C(O)CH2CH2CH(NH2)COOH | | 147.12930 | -817.972 | -781.560 | ±4.2 | | 163.203 | | 445.395 | | 28.658 | | # |
| C5H9O2 C4H9C(O)O\* Valeryl | | 101.12376 | -255.550 | -226.845 | ±8. | | 125.431 | | 377.951 | | 23.349 | | # |
| C5H9O2 C3H7C(O)OCH2\* C0 | | 101.12376 | -258.818 | -232.358 | ±8. | | 131.482 | | 414.869 | | 25.594 | | # |
| C5H9O2 C2H5CH\*C(O)OCH3C2 | | 101.12376 | -281.328 | -255.386 | ±8. | | 129.041 | | 424.815 | | 26.112 | | # |
| C5H9O2 CH3CH\*CH2C(O)OCH3 | | 101.12376 | -260.388 | -235.465 | ±8. | | 132.918 | | 426.760 | | 26.931 | | # |
| C5H9O2 CH2\*C2H4C(O)OCH3 | | 101.12376 | -251.668 | -225.677 | ±8. | | 131.262 | | 419.488 | | 26.064 | | # |
| C5H9P (CH3)3C-C≡P | | 100.09872 | 82.693 | 110.233 | ±8. | | 121.359 | | 330.936 | | 21.194 | | # |
| C5H9P- (CH3)3C-C≡P- anion | | 100.09927 | 117.394 | 148.540 | ±8. | | 124.387 | | 338.416 | | 22.262 | | # |
| C5H10 1-PENTENE <!> | | 70.13290 | -21.28 | +4.648 |  | | 108.200 | | 347.110 | | 21.680 | | † |
| C5H10 2-PENTENE | | 70.13290 | -30.334 | -4.166 | ±8. | | 100.615 | | 370.097 | | 21.440 | | # |
| C5H10 2MB-1ene | | 70.1329 | -33.924 | -6.613 | ±8. | | 102.803 | | 342.019 | | 20.297 | | # |
| C5H10 2MB-2ene | | 70.1329 | -39.794 | -13.205 | ±8. | | 103.667 | | 337.685 | | 21.019 | | # |
| C5H10 2MB-3ene | | 70.1329 | -28.142 | -1.589 | ±8. | | 105.189 | | 349.980 | | 21.056 | | # |
| C5H10 Cyclopentane | | 70.1344 | -77.1 | -44.515 | ±0.44g | | 82.760 | | 293.007 | | 15.023 | | † |
| C5H10N2O3 Glutamine (amino )  NH2-C(O)CH2CH2CH(NH2)COOH | | 146.14458 | -631.784 | -591.312 | ±4.2 | | 166.908 | | 428.267 | | 28.826 | | # |
| C5H10O Cyclopentanol C5H9OH | | 86.1323 | -240.065 | -206.835 | ±8. | | 103.848 | | 334.704 | | 18.718 | | # |
| C5H10O PentaHydroPYRAN | | 86.1338 | -224.283 | -189.04 | ±0.84 | | 96.359 | | 301.959 | | 16.710 | | # |
| C5H10O 2-MethylTetraHydroFuran | | 86.1323 | -225.062 | -191.55 | ±8. | | 99.564 | | 323.289 | | 18.437 | | # |
| C5H10O2 Pentanoic (Valeric) acid | | 102.13170 | -477.018 | -444.615 | ±8. | | 122.513 | | 393.642 | | 23.886 | | # |
| C5H10O2 (CH3)3CCOOH (Pivalic) | | 102.13170 | -507.1 | -474.456 | ±0.8 | | 132.901 | | 363.332 | | 23.644 | | # |
| C5H10O2(liq) MethylButyrate | | 102.13170 | -497.1 |  |  | |  | |  | |  | | X |
| C5H10O2 MethylButyrate | | 102.13170 | -457.884 | -426.201 | ±8. | | 125.394 | | 373.612 | | 24.605 | | # |
| C5H10O2(liq) Ethyl Propionate | | 102.13170 | -505.59 |  | ±0.5 | |  | |  | |  | | X |
| C5H10O2 Ethyl Propionate | | 102.13170 | -470.696 | -439.503 | ±8. | | 124.994 | | 402.675 | | 25.096 | | # |
| C5H10O2 CH2=CH(CH2)3OOH | | 102.13170 | -98.738 | -67.50 | ±8. | | 132.168 | | 394.552 | | 25.058 | | # |
| C5H10O3 (C2H5)2CO3 EtCarbonate | | 118.13110 | -633.022 | -599.375 | ±8. | | 145.838 | | 406.386 | | 26.980 | | # |
| N-C5H11 n-pentyl <!> | | 71.14084 | 60.98 | 90.91 | ±8. | | 114.642 | | 367.172 | | 21.905 | | #† |
| S-C5H11 2-pentyl | | 71.14084 | 49.275 | 78.74 | ±8. | | 111.887 | | 363.372 | | 22.373 | | # |
| T-C5H11 1,1-dimethyl-1-propyl | | 71.14084 | 43.72 | 74.74 | ±8. | | 110.092 | | 359.010 | | 20.817 | | #† |
| C5H11 1,1-dimethyl-3-propyl | | 71.14084 | 55.7 | 85.76 | ±8. | | 121.015 | | 344.879 | | 21.796 | | # |
| C5H11 neopentyl | | 71.14234 | 34.392 |  |  | | 118.84 | | 333.423 | |  | |  |
| C5H11N cyclo Piperidine | | 85.14758 | -19.405 | 18.945 | ±8. | | 100.922 | | 311.365 | | 17.827 | | # |
| C5H11NO2 Nitropentane | | 117.14788 | -164.431 | -123.37 | ±2.1 | | 137.100 | | 390.905 | | 23.792 | |  |
| C5H11N2O2P Tabun | | 162.12688 | -484.800 | -446.291 |  | | 190.337 | | 467.656 | | 36.043 | | # |
| C5H11N3O5 Propyl-NENA | | 193.15806 | -154.808 | -107.012 |  | | 199.630 | | 538.994 | | 38.751 | | # |
| C5H11O+ PentahydroPyran protonate | | 87.13969 | 510.967 | 541.740 | ±8 | | 106.110 | | 317.820 | | 18.644 | | # |
| C5H12(l) PENTANE liq g | | 72.14878 | -173.12 | -156.15 |  | |  | |  | |  | | X |
| C5H12 PENTANE <!> | | 72.14878 | -152.310 | -116.659 | ±8 | | 112.146 | | 348.294 | | 20.426 | | #† |
| I-C5H12(l) Isopentane liqg | | 72.14878 | -178.53 |  |  | |  | |  | |  | | X |
| I-C5H12 Isopentane | | 72.14878 | -153.70 | -119.63 |  | | 118.870 | | 343.740 | | 22.008 | | † |
| (CH3)4C(l) Neopentane liqg | | 72.14878 | -189.96 |  |  | |  | |  | |  | | X |
| CH3C(CH3)2CH3 Neopentane | | 72.14878 | -168.255 | -133.6 | ±8. | | 121.911 | | 309.573 | | 21.421 | | † |
| C5H12O 1-Pentanol C5H11OH | | 88.14818 | -297.286 | -260.514 | ±8. | | 117.224 | | 403.533 | | 23.645 | | # |
| C5H12O 2-Pentanol C3H7CH(OH)CH3 | | 88.14818 | -316.687 | -280.593 | ±8. | | 129.850 | | 385.251 | | 24.322 | | # |
| C5H12O 3-Pentanol C2H5CH(OH)C2H5 | | 88.14818 | -316.478 | -280.395 | ±8. | | 129.872 | | 380.443 | | 24.334 | | # |
| C5H12O 3Methyl-Butane-1ol | | 88.14818 | -298.424 | -261.452 | ±8. | | 124.316 | | 381.340 | | 23.444 | | # |
| C5H12O liquid MTBE | | 88.14818 | -313.6 | -293.85 |  | | 187.510 | | 265.650 | |  | |  |
| C5H12O Me-Tertiary Butyl Ether C5H12O | | 88.14818 | -288.273 | -252.38 | ±8. | | 136.565 | | 358.566 | | 24.522 | | # |
| C5H12O2 Pentyl-Hydroperoxide | | 104.14758 | -223.948 | -185.53 | ±8. | | 133.051 | | 413.969 | | 26.358 | | # |
| C5H13O+ (C2H5)2OCH3+ | | 89.15557 | 455.722 | 484.205 | ±8. | | 132.290 | | 349.675 | | 23.773 | | # |
| C5N4 C(CN)4 TetraCyanoMethane | | 116.08046 | 672.80 | 670.647 | ±9.20 | | 125.161 | | 358.507 | | 24.761 | | # |
| C5O5Fe Fe(CO)5 | | See | Fe(CO)5 |  |  | |  | |  | |  | |  |
| C6 linear singlet 1A'1 | | 72.0642 | 1227.3 | 1216.08 | ±8. | | 83.768 | | 288.457 | | 17.550 | | # |
| C6 linear triplet 3Σ-g | | 72.0642 | 1283.971 | 1272.522 | ±8. | | 84.585 | | 300.600 | | 17.770 | | # |
| C6CL6 Hexachlorobenzene | | 284.78040 | -42.526 | -41.486 | ±8. | | 174.696 | | 438.879 | | 32.824 | | # |
| C6CL6- Hexachlorobenzene anion | | 284.78095 | -133. | -129.291 | ±9.6 | | 187.884 | | 485.910 | | 36.352 | | # |
| C6D5 Deuterated phenyl radical | | 82.13651 | 315.700 | 327.525 |  | | 94.997 | | 300.504 | | 15.919 | | † |
| C6D6 Deuterated Benzene | | 84.14881 | 58.157 | 73.86 |  | | 100.398 | | 282.629 | | 16.325 | | † |
| C6F6 Hexafluorobenzene | | 186.05462 | -968.621 | -964.118 | ±8. | | 157.939 | | 384.462 | | 28.293 | | # |
| C6F6- Hexafluorobenzene anion | | 186.05517 | -997.0 | -988.407 | ±9.6 | | 164.950 | | 411.681 | | 30.401 | | # |
| C6F14 FC 51-14 Perfluorohexane | | 338.04364 | -2949.201 |  |  | | 269.551 | | 629.592 | |  | |  |
| C6F15N (L) (C2F5)3N (liq) | | 371.0469 | -3172 |  |  | | 527.100 | | 379.490 | |  | | X |
| C6F15N (C2F5)3N | | 371.0469 | -3138. |  |  | |  | |  | |  | | X |
| C6H <!> | | 73.07394 | 1000. | 991.8 | ±75. | | 95.617 | | 305.418 | | 18.757 | | # |
| C6HCL5 Pentachlorobenzen | | 250.33564 | -36.3 | -32.42 | ±3.7 | | 159.291 | | 427.213 | | 29.625 | | # |
| C6H2 <!> | | 74.08008 | 700.82 | 696.0 |  | | 103.919 | | 298.911 | | 19.608 | | † |
| C6H2CL4 1,2,3,4-Chlorobenzen | | 215.89088 | -13.071 | -6.239 | ±8. | | 143.507 | | 398.859 | | 26.320 | | # |
| C6H2CL4 1,2,3,5-Chlorobenzen | | 215.89088 | -18.464 | -11.75 | ±8. | | 143.922 | | 400.437 | | 26.439 | | # |
| C6H2CL3O Trichlorophenoxy ra | | 196.43758 | -27.48 | -20.29 | ±8.4 | | 140.508 | | 398.583 | | 25.714 | | # |
| C6H2CL3O Trichlorophenol Rad | | 196.43758 | 101.51 | 107.37 | ±8.4 | | 144.581 | | 410.077 | | 25.386 | | # |
| C6H2CL3O3 Peroxybiciclo Rad. | | 228.43638 | 131.42 | 142.99 |  | | 174.462 | | 429.942 | |  | | # |
| C6H2CL3O3 Peroxybicyclo Rad | | 228.43638 | 28.95 | 40.414 |  | | 171.330 | | 433.035 | |  | | # |
| C6H2(NO2)3 TriNitroPhenyl Rad. | | 212.0967 | 286.6 | 306.15 |  | | 179.914 | | 494.073 | | 34.280 | | # |
| C6H2(NO2)3O\* TriNitroPhenol Rad | | 228.09610 | 1.25 | 22.234 | ±8. | | 195.625 | | 517.227 | | 37.195 | | # |
| C6H3 H2C=C=C=C=C=CH\* <I> | | 75.08802 | 725.07 | 724.08 | ±8. | | 102.068 | | 328.116 | | 20.012 | | # |
| C6H3 H2C=C\*-C≡C-C≡CH <!> | | 75.08802 | 725.087 | 724.100 | ±8. | | 102.051 | | 328.107 | | 20.011 | | # |
| C6H3 Cy o-Benzyne-o-yl Rad. | | 75.08802 | 728.911 | 733.879 | ±8. | | 75.851 | | 293.013 | | 14.055 | | # |
| C6H3Cl3 1,2,3-trichlorobenzen | | 181.44612 | 6.711 | 14.425 | ±8. | | 127.690 | | 370.460 | | 23.081 | | # |
| C6H3Cl3 1,3,5-trichlorobenzen | | 181.44612 | -4.314 | 5.25 | ±8. | | 128.171 | | 364.132 | | 23.231 | | # |
| C6H3CL3O Trichlorophenol | | 197.44552 | -189.07 | -176.92 | ±8.4 | | 142.427 | | 397.903 | | 24.984 | | # |
| C6H3CL3O linear | | 197.44552 | -19.83 | +17.3 |  | | 39.200 | | 109.923 | |  | |  |
| C6H3CL3O2 CY | | 213.44492 | -277.25 | -263.99 |  | | 162.216 | | 420.242 | | 28.219 | | # |
| C6H3I o-Iodo-Benzyne | | 201.99249 | 534.715 | 542.244 | ±12. | | 96.910 | | 340.309 | | 18.093 | | # |
| C6H3(NO2)2 DiNitroBenzene rad | | 167.09910 | 302.08 | 320.25 |  | | 145.001 | | 435.239 | | 26.890 | | # |
| C6H3(NO2)3 (sol) Trinitrobenzene | | 213.10464 | -37.24 |  | ±1.25 | |  | |  | |  | | X |
| C6H3(NO2)3 Trinitrobenzene | | 213.10464 | 62.342 | 82.617 |  | | 205.633 | | 485.335 | | 37.794 | |  |
| C6H2(NO2)3OH (sol) Trinitrophenol | | 229.10404 | -217.9 |  | ±2. | |  | |  | |  | | X |
| C6H2(NO2)3OH Trinitrophenol | | 229.10404 | -139.5 | -111.75 |  | | 192.811 | | 495.618 | | 34.611 | | # |
| 1,2-C6H4 o-BENZYNE <!> | | 76.09596 | 461.135 | 470.128 | ±1.4d | | 78.406 | | 283.240 | | 14.265 | | # |
| 1,2-C6H4+ o-BENZYNE cation | | 76.0954 | 1397.5d | 1398.8d | ±3.0d | |  | |  | |  | | X |
| 1,2-C6H4- c o-BENZYNE anion | | 76.09651 | 400.5d | 409.3d | ±1.4 | | 106.701 | | 337.133 | | 20.795 | | # |
| 1,3-C6H4 m-BENZYNE | | 76.09596 | 523.690 | 532.497 | ±8. | | 80.202 | | 283.810 | | 14.451 | | # |
| 1,4-C6H4 p-BENZYNE | | 76.09596 | 574.254 | 582.364 | ±8. | | 85.476 | | 282.239 | | 15.147 | | # |
| 1  C u0 p0 c0 {3,S} {6,S} {7,S} {8,S} 2  C u0 p0 c0 {4,S} {5,S} {9,S} {10,S} 3  C u0 p0 c0 {1,S} {4,T} 4  C u0 p0 c0 {2,S} {3,T} 5  C u0 p0 c0 {2,S} {6,T} 6  C u0 p0 c0 {1,S} {5,T} 7  H u0 p0 c0 {1,S} 8  H u0 p0 c0 {1,S} 9  H u0 p0 c0 {2,S} 10 H u0 p0 c0 {2,S} C6H4 Cyclohexa-1,4-diyne | | 76.09596 | 454.215 |  |  | | 83.68 | | 178.782 | |  | | # |
| C6H4 TRANS | | 76.09596 | 523.105 | 527.104 | ±8. | | 102.894 | | 317.187 | | 19.328 | | # |
| C6H4 CIS | | 76.09596 | 524.218 | 528.632 | ±8. | | 101.969 | | 317.563 | | 18.843 | | # |
| C6H4 HEXAPENTAENE | | 76.09596 | 568.263 | 572.160 | ±8. | | 99.977 | | 309.859 | | 19.359 | | # |
| C6H4 TRIENE-5YNE | | 76.09596 | 559.706 | 563.792 | ±8. | | 101.909 | | 325.109 | | 19.172 | | # |
| C6H4CL –ortho Radical | | 111.55046 | 303.173 | ? | ±28.9 | | 100.842 | | 329.678 | | ?? | | # |
| C6H4CL –metha Radical | | 111.55046 | 297.02 |  | ±28.0 | | 101.165 | | 329.135 | |  | | # |
| C6H4CL –para Radical | | 111.55046 | 298.86 |  | ±28.0 | | 101.264 | | 329.476 | |  | | # |
| C6H4CLO o-Chlorophenoxy Rad | | 127.54806 | 32.895 | 45.773 | ±8. | | 109.172 | | 338.965 | | 19.310 | | # |
| C6H4CLO CyHexadiene Rad | | 127.54806 | 225.91 | 237.50 |  | | 112.226 | | 359.349 | | 20.599 | | # |
| C6H4CL2 o-Dichlorobenzen | | 147.00136 | 28.464 | 40.970 | ±8. | | 111.879 | | 347.871 | | 19.933 | | # |
| C6H4CL2 m-Dichlorobenzen | | 147.00136 | 22.656 | 35.089 | ±8. | | 112.361 | | 343.476 | | 20.005 | |  |
| C6H4CL2 p-Dichlorobenzen | | 147.00136 | 23.104 | 35.493 | ±8. | | 112.303 | | 337.735 | | 20.049 | | # |
| C6H4CL2O Z 2,4Dichlorophenol | | 163.00076 | -158.009 | -143.023 | ±8. | | 128.644 | | 364.031 | | 21.793 | | # |
| C6H4CL2O E 2,4Dichlorophenol | | 163.00076 | -145.398 | -131.202 | ±8. | | 130.914 | | 368.913 | | 22.582 | | # |
| o-C6H4I Radical | | 203.00043 | 427.186 | 439.032 |  | | 97.752 | | 346.415 | | 18.010 | | # |
| o-C6H4I2 | | 329.90490 | 248.95 | 263.625 | ±5.9 | | 113.052 | | 386.892 | | 21.778 | | # |
| m-C6H4I2 | | 329.90490 | 243.509 | 257.766 |  | | 118.125 | | 384.828 | | 22.196 | | # |
| p-C6H4I2 | | 329.90490 | 242.700 | 257.177 |  | | 114.640 | | 365.746 | | 21.976 | | # |
| C6H4NO2 m-NitroBenzene Radic | | 122.10150 | 317.566 | 333.558 |  | | 111.539 | | 362.811 | | 20.280 | | # |
| C6H4N2O4 1,3 DiNitroBenzene | | 168.10704 | 51.88 | 74.25 |  | | 146.438 | | 418.208 | | 26.915 | | # |
| C6H4N4O2 4-Nitro-PhenylAzide | | 164.12172 | 389.7 | 410.723 | ±5.2 | | 157.694 | | 420.170 | | 28.254 | | # |
| C6H4O2 O=C6H4=O | | 108.09476 | -121.478 | -108.376 | ±8 | | 105.614 | | 320.469 | | 18.835 | | # |
| C6H5 CHAIN | | 77.10390 | 587.852 | 595.974 |  | | 104.083 | | 332.937 | | 19.369 | | # |
| C6H5 PHENYL RAD <!> | | 77.10390 | 337.3 | 351.2 | ±0.6 | | 77.04 | | 286.135 | | 13.591 | | # |
| C6H5+ singlet c | | 77.10335 | 1143.03d | 1148.98 | ±0.93 | | 87.110 | | 289.117 | | 15.313 | | # |
| C6H5+ triplet c Phenylium | | 77.10335 | 1245.87 | 1257.9d | ±3.18 | | 87.110 | | 298.252 | | 15.313 | | # |
| C6H5- Phenided | | 77.10445 | 225.8  231.79g | 244.89d | ±0.44d | | 79.653 | | 283.88 | | 14.172 | | # |
| C6H5 FULVENYL RAD-6-yl | | 77.10390 | 467.315 | 479.324 | ±8. | | 87.147 | | 297.813 | | 15.482 | | # |
| C6H5 FULVENYL RAD-2-yl | | 77.10390 | 490.365 |  | ±51.5 | | 93.077 | | 307.123 | |  | | # |
| C6H5Br (liq) Bromobenzenb | | 157.0079 | 60.2 |  | ±1.3 | |  | |  | |  | | X |
| C6H5Br Bromobenzen | | 157.0079 | 104.9 | 127.219 | ±1.3. | | 97.507 | | 324.774 | | 17.433 | | # |
| C6H5Br+ " cation | | 157.00735 | 979.957 | 995.518 | ±1.22 | | 99.933 | | 334.250 | | 17.993 | | # |
| C6H5BrO 2-Bromophenol (Z) cis | | 173.00730 | -63.72 | -39.09 | ±8. | | 113.188 | | 350.929 | | 19.051 | | # |
| C6H5BrO 2-Bromophenol-(E) *trans* | | 173.00730 | -70.208 | -46.085 | ±8. | | 115.810 | | 356.656 | | 19.968 | | # |
| C6H5Cl (liq) Chlorobenzenb | | 112.55660 | 11.3 |  | ±0.6 | |  | |  | |  | | X |
| C6H5CL Chlorobenzen | | 112.55660 | 52.287 | 67.461 | ±0.61d | | 96.152 | | 313.366 | | 16.908 | | # |
| C6H5CL+ | | 112.55605 | 934.796 | 943.089 | ±0.6 | | 98.934 | | 323.710 | | 17.591 | | # |
| C6H5CLO o-Chlorophenol (Z) | | 128.55600 | -130.942 | -113.250 | ±8. | | 112.581 | | 341.454 | | 18.729 | | # |
| C6H5CLO o-Chlorophenol (E) | | 128.55600 | -117.834 | -100.912 | ±8. | | 114.787 | | 346.205 | | 19.500 | | # |
| C6H5CLO 2,4-Cy-hexadiene.. | | 128.55600 | -35.75 | -19.81 |  | | 113.199 | | 352.445 | | 20.480 | | # |
| C6H5CLO 2,5 Cy-hexadiene… | | 128.55600 | -55.87 | -39.79 |  | | 113.969 | | 346.868 | | 20.347 | | # |
| C6H5F (liq) Fluorobenzenb | | 96.10230 | -150.02d | -152.44d | ±1.0 | |  | |  | |  | | X |
| C6H5F Fluorobenzen | | 96.10230 | -115.4 | -99.459 | ±1.0 | | 92.385 | | 301.688 | | 15.963 | | # |
| C6H5F+ | | 96.10175 | 779.76 | 788.600 | ±1.0 | | 96.139 | | 313.190 | | 16.866 | | # |
| C6H5I (liq) Iodobenzenb | | 204.00837 | 113.1 | 113.0d | ±1.1 | |  | |  | |  | | X |
| C6H5I Iodobenzen | | 204.00837 | 161.9 | 177.906 | ±1.1 | | 99.983 | | 335.00 | | 18.083 | | # |
| C6H5I+ | | 204.00782 | 1013.62 | 1023.108 | ±1. | | 101.121 | | 343.093 | | 18.404 | | # |
| C6H5NO NITROSOBENZENE | | 107.11004 | 198.075 | 215.586 | ±1.5d | | 106.354 | | 332.852 | | 18.655 | | # |
| C6H5NO2 NITRO-BENZENE | | 123.11124 | 56.823 | 76.774 | ±8. | | 116.112 | | 348.687 | | 20.555 | | # |
| C6H5NO2 Picolinic acid C6H5NO2 | | 123.10944 | -233.522 | -213.579 | ±8. | | 116.419 | | 361.590 | | 20.564 | | # |
| C6H5O PHENOXY RAD <!> | | 93.10330 | 61.56  55.80h | 76.511  71.08h | ±8.  0.88h | | 98.411 | | 312.038 | | 16.880 | | # |
| C6H5O Cy-hexadiene-1one-2yl | | 93.10330 | 246.58 | 260.42 |  | | 98.386 | | 332.759 | |  | | # |
| C6H5OO PEROXYPHENYL rad | | 109.10270 | 141.612 | 158.975 | ±8. | | 108.706 | | 339.197 | | 18.808 | | # |
| C6H6(L) <~> | | 78.11184 | 49.08 | 50.695 | ±0.26d | | 135.95 | | 173.44 | | 30.110 | | † |
| C6H6 BENZENE 1 C 0 {2,B} {6,B} 2 C 0 {1,B} {3,B} 3 C 0 {2,B} {4,B} 4 C 0 {3,B} {5,B} 5 C 0 {4,B} {6,B} 6 C 0 {1,B} {5,B}  <!> | | 78.11184 | 82.88 | 100.41 | ±0.26d | | 81.934 | | 269.158 | | 14.195 | | † |
| C6H6+ Benzene Cation | | 78.11129 | 982.3 | 991.762 | ±0.3 | | 89.226 | | 286.476 | | 16.065 | | # |
| C6H6- c | |  | 193.12 | 211.6d | ±3.7d | |  | |  | |  | | X |
| C6H6 FULVENE | | 78.11184 | 216.296 | 232.556 | ±8. | | 87.862 | | 292.468 | | 15.465 | | # |
| C6H6 BENZVALENE | | 78.11364 | 384.9 | 403 | ±8.3 | | 80.825 | | 284.701 | |  | | # |
| C6H6 1,5-Hexadiyine | | 78.11364 | 417.166 | 428.062 | ±8. | | 111.036 | | 336.936 | | 20.829 | | # |
| C6H6 2,4-Hexadiyne | | 78.11364 | 369.100 | 379.830 | ±8. | | 103.026 | | 335.627 | | 20.995 | | # |
| C6H6 1,3-Hexadiyne | | 78.11364 | 392.363 | 404.299 | ±8. | | 107.021 | | 328.174 | | 19.790 | | # |
| C6H6 1,2,4,5 Hexatetraene | | 78.11364 | 396.229 | 407.942 | ±8. | | 102.421 | | 343.852 | | 20.012 | | # |
| C6H6 1,2-Hexadiene-5-yne | | 78.11184 | 416.397 | 427.901 | ±8. | | 107.981 | | 336.97 | | 20.274 | | # |
| C6H6 3,4-Dimethylene1Cyclobutene | | 78.11184 | 339.937 | 354.726 | ±8. | | 94.844 | | 302.603 | | 16.936 | | # |
| C6H6 1,3-Hexadiene-5-yne | | 78.11184 | 343.49 | 355.494 | ±8. | | 105.878 | | 328.006 | | 19.721 | | # |
| C6H6 1,3-Butadiene-2-Ethynyl | | 78.11184 | 346.469 | 358.998 | ±8. | | 105.579 | | 325.120 | | 19.196 | | # |
| C6H6N C6H5NH\* | | 92.11858 | 251.7 | 271.7 | ±3.3 | | 96.841 | | 314.851 | | 16.026 | | # |
| C6H6N2 N(-CH=CH-)3N triCy | | 106.12532 | 530.573 | 554.646 | ±8. | | 104.941 | | 299.475 | | 16.423 | | # |
| C6H6N2 NC-CH2CH=CHCH2CN | | 106.12532 | 290.068 | 306.184 | ±8. | | 125.794 | | 380.718 | | 24.279 | | # |
| C6H6N2O2 o-NitroAminoBenzen C6H6N2O2 | | 138.12412 | 65.7 | 90.5 | ±12.5 | | 139.679 | | 384.205 | | 24.329 | | # |
| C6H6N2O2 m-NitroAminoBenzen | | 138.12412 | 62.5 |  | ±1.8 | |  | |  | |  | | X |
| C6H6N2O2 p-NitroAminoBenzen | | 138.12412 | 55.2 | 80.276 | ±1.8 | | 141.058 | | 372.585 | | 24.000 | | # |
| C6H6N6O6 TATB | | (see | Burcat.thr) |  |  | |  | |  | |  | | X |
| C6H5OH PHENOL   <!> | | 94.11124 | -92.864 | -73.896 | ±8. | | 101.895 | | 316.067 | | 17.097 | | #† |
| C6H5OH+ Phenol cation | | 94.11069 | 739.409 | 751.664 | ±8. | | 98.850 | | 317.174 | | 16.376 | | # |
| C6H6O 2,4-Cyclohexadiene1one | | 94.11124 | -21.63 | -3.31 |  | | 99.188 | | 322.935 | |  | | # |
| C6H6O Oxepin (cy) | | 94.11124 | 89.697 | 108.34 | ±8. | | 99.660 | | 309.917 | | 17.422 | | # |
| 1,2-C6H4(OH)2 Catechol **:** C6H6O2 | | 110.11064 | -279.190 | -256.039 | ±8. | | 119.511 | | 331.200 | | 20.254 | | # |
| C6H5OOH Hydroperoxyphenyl | | 110.11064 | -2.678 | 18.039 | ±8. | | 114.440 | | 350.539 | | 19.688 | | # |
| C6H6O6 HexaHydroxyBenzene | | 174.10824 | -974.035 | -946.597 |  | | 196.099 | | 437.156 | | 30.327 | | # |
| C6H5SH BenzeneThiol | | 110.17784 | 107.654 | 125.116 | ±8. | | 107.254 | | 332.426 | | 18.676 | | # |
| C6H5SH- BenzeneThiol anion | | 110.17839 | 150.955 | 172.992 | ±8. | | 115.667 | | 339.646 | | 19.303 | | # |
| C6H7 1,4 CYCLO Radical <~> | | 79.11978 | 210.823 | 231.054 | ±8 | | 90.246 | | 300.298 | | 15.729 | | # |
| C6H7 1,3 Cy 5-Radical 1 C 0 {2,D} {6,S} 2 C 0 {1,D} {3,S} 3 C 0 {2,S} {4,D} 4 C 0 {3,D} {5,S} 5 C 1 {4,S} {6,S} 6 C 0 {1,S} {5,S} | | 79.11978 | 210.815 | 231.047 | ±8 | | 90.235 | | 306.054 | | 15.727 | | # |
| C6H7+ 1,4 Cy Radical cation | | 79.11923 | 878.1 | 892.2 | ±8 | | 88.167 | | 293.690 | | 15.618 | | # |
| C6H7 1,3,5-Hexatriene-6-yl | | 79.11798 | 431.387 | 446.410 | ±8. | | 110.758 | | 363.629 | | 20.937 | | # |
| C6H7-1 CY C5H5-1-CH2\* | | 79.11798 | 334.092 | 351.954 | ±6.3 | | 100.095 | | 326.062 | | 18.098 | | # |
| C6H7-3 CY C5H5-3-CH2\* | | 79.11798 | 247.316 | 265.583 | ±19.2 | | 101.756 | | 321.686 | | 17.693 | | # |
| C6H7-1 CY C5H4-1-\*-CH3 | | 79.11978 | 221.007 | 238.873 | ±8 | | 103.103 | | 314.389 | | 18.094 | | # |
| C6H7-1+ CY C5H4-1-\*-CH3+ | | 79.11923 | 1004.62 | 1016.33 | ±8. | | 96.768 | | 313.124 | | 18.055 | | # |
| C6H5NH2(L) aniline | | 93.12652 | 31.50 | 37.774 |  | | 191.92 | | 191.060 | | 34.020 | | † |
| C6H7N ANILINE | | 93.12652 | 87.04 | 109.957 | ±0.88 | | 104.537 | | 311.678 | | 17.377 | | # |
| C6H7N+ C6H5-NH2 Aniline cation | | 93.12597 | 845.704 | 861.719 | ±8. | | 103.355 | | 313.420 | | 16.834 | | # |
| C6H7N 1H-Azepine Strukturformel von 1H-Azepin | | 93.12652 | 264.625 | 287.673 | ±8. | | 101.258 | | 313.415 | | 17.246 | | # |
| C6H7O11N3 Cellulose Trinitrate 14.13% N | | 297.1334 | -653.541 | -600.965 | ±35. | | 267.384 | | 449.830 | | 44.129 | |  |
| C6H7.45O10.1N2.55  NitroStarch | | 276.59 | -710.025 |  |  | |  | |  | |  | | X |
| C6H7.55O5(NO2)2.45 | | 272.25 | -703.44 |  |  | |  | |  | |  | | X |
| C6H7P C6H5-PH2 | | 110.09354 | 126.771 | 149.063 | ±8. | | 106.996 | | 335.241 | | 19.028 | | # |
| C6H7P+ C6H5-PH2+ cation | | 110.09299 | 953.638 | 968.512 | ±8. | | 113.768 | | 335.167 | | 19.633 | | # |
| C6H7P- C6H5-PH2- anion | | 110.09408 | 162.364 | 188.397 | ±8. | | 121.274 | | 340.826 | | 20.321 | | # |
| C6H8 DIHYDROBENZVALENE | | 80.12772 | 230.12 | 255.3 | ±8.3 | | 89.425 | | 293.780 | |  | | # |
| C6H8 CY 1,3-C5H5-5-CH3 | | 80.12772 | 112.257 | 135.267 | ±8. | | 95.574 | | 310.854 | | 17.183 | | # |
| C6H8 CY 1,3-C5H5-3-CH3 | | 80.12772 | 99.303 | 121.918 | ±8. | | 97.546 | | 312.884 | | 17.579 | | # |
| C6H8 1,3,5-HEXATRIENE | | 80.12772 | 152.214 |  |  | | 107.911 | | 330.388 | |  | |  |
| H8C6 (1,3-CYCLO) | | 80.12772 | 109.2 | 133.14 | ±8. | | 94.168 | | 240.221 | | 16.256 | | # |
| C6H8 (1,4-CYCLO) | | 80.12772 | 109.45 | 133.08 | ±8. | | 94.057 | | 238.906 | | 16.559 | | # |
| C6H8O 2,5-DiMethylFuran (Cy) | | 96.12712 | -121.821 | -97.623 | ±8. | | 115.388 | | 334.641 | | 20.335 | | # |
| C6H8O 3,4-DiMethylFuran (Cy) | | 96.12712 | -101.383 | -77.163 | ±8. | | 115.635 | | 328.674 | | 20.313 | | # |
| C6H8O3 2,5-DiHydroxyMetylFuran | | 128.12592 | -401.664 | -374.536 | ±12.5 | | 141.880 | | 420.474 | | 26.086 | | # |
| C6H8O7 (S) Citric acid solid  C6H8O7 | | 192.12352 | -1544.0 |  | ±4.6 | |  | |  | |  | | X |
| C6H8O7 Citric acid gas anhydrous | | 192.12352 | -1399.13 | -1363.9 |  | | 188.936 | | 528.690 | | 35.351 | | # |
| C6H8O9N2CelluloseDinitrate11.11%N | | 252.1358 | -753.58 | -705.189 | ±25. | | 241.715 | | 412.465 | | 39.533 | |  |
| C6H8Si C6H5-SiH3 | | 108.21322 | 123.056 | 146.625 | ±8. | | 114.369 | | 337.995 | | 19.842 | | # |
| C6H8Si- C6H5-SiH3 anion | | 108.21377 | 164.700 | 191.615 | ±8. | | 128.950 | | 349.744 | | 22.002 | | # |
| C6H9 1,3 hexadiene 5-yl Rad. | | 81.13566 | 173.49 | 195.692 | ±8. | | 119.775 | | 370.613 | | 22.225 | | # |
| 1,3-C6H9 hexadiene 6-yl Rad. | | 81.13566 | 265.533 | 286.651 | ±8. | | 120.582 | | 389.084 | | 22.990 | | # |
| C6H9 Cyclohexenyl-3 | | 81.13566 | 131.47 | 159.011 | ±8. | | 97.860 | | 313.685 | | 16.886 | | # |
| C6H9 CY 1- C5H6-4-CH3-4-yl | | 81.13566 | 188.468 | 214.322 | ±8. | | 103.489 | | 321.009 | | 18.574 | | # |
| C6H9 CY 1- C5H7-4-CH2\* | | 81.13566 | 215.731 | 241.534 | ±8. | | 106.551 | | 323.588 | | 18.625 | | # |
| C6H9 CY 1-C5H7-3-CH2\* | | 81.13566 | 212.464 | 237.965 | ±8. | | 104.037 | | 333.573 | | 18.926 | | # |
| C6H9 CY 1-C5H7-1-CH2\* | | 81.13566 | 124.89 |  |  | | 94.663 | | 323.377 | |  | |  |
| C6H9I CY 1-C6H9-3-I | | 208.04013 | 69.0 | 99.331 | ±21. | | 116.001 | | 360.644 | | 20.731 | | # |
| C6H9N3 1,3,5-TriAminoBenzen | | (see | Burcat.thr) |  |  | |  | |  | |  | | X |
| C6H10 1-Hexyne | | 82.14360 | 122.3 | 147.990 | ±1.2 | | 123.932 | | 374.180 | | 22.971 | | # |
| C6H10 2-Hexyne | | 82.14360 | 107.7 |  | ±2.4 | |  | |  | |  | | X |
| C6H10 1,3-HEXADIENE | | 82.14360 | 58.513 | 84.568 | ±8. | | 120.575 | | 372.675 | | 22.606 | | # |
| C6H10 (L) Cyclohexene liq | | 82.14360 | -103.284 |  |  | | 140.206 | | 216.187 | |  | |  |
| C6H10 Cyclohexene | | 82.14360 | -4.6 | +26.79 |  | | 101.464 | | 310.632 | | 17.271 | | † |
| C6H10 C5H7-CH3 Cypentene-4 | | 82.14360 | 8.46 | 38.49 | ±8. | | 101.249 | | 309.518 | | 17.208 | | # |
| C6H10O5 Cellulose crystalline | | 162.14060 | -2812.40 |  | ±1.7 | |  | |  | |  | | X |
| C6H10O5 Starch crysraline | | 162.14060 | -974.1 | -903.837 | ±2.1 | | 205.700 | | 182.200 | |  | | # |
| (C6H10O5)n Cellulose n=500-5000 | | 162.14060 | -960.45 | -933.944 | ±20. | | 171.565 | | 293.791 | | 43.856 | |  |
| C6H10O5 (S) Levoglucosan solid | | 162.14060 | -959.1 |  | ±2.1 | |  | |  | |  | | X |
| C6H10O5 Levoglucosan | | 162.14060 | -824.5 | -779.7 | ±2.7 | | 161.350 | | 401.922 | | 25.542 | | # |
| C6H11 CH2=CHC3H6CH2\* <!> | | 86.15334 | 162.502 | 190.886 | ±8. | | 127.963 | | 417.768 | | 24.512 | | # |
| C6H11 CH3CH=CHC2H4CH2\* | | 86.15334 | 153.862 | 181.880 | ±8. | | 129.760 | | 404.206 | | 24.878 | | # |
| C6H11 trans 3-hexene-6-yl Rad | | 83.15334 | 154.540 | 183.164 | ±8 | | 128.546 | | 401.219 | | 24.272 | | # |
| C6H11 CH2=C(CH2\*)C3H7 | | 83.15334 | 95.340 | 125.298 | ±8 | | 125.511 | | 391.885 | | 22.942 | | # |
| C6H11 CH2=C(CH3)C3H6\* | | 83.15334 | 149.787 |  |  | | 130.797 | | 390.786 | |  | |  |
| C6H11 CH3C(CH2\*)=CHC2H5 | | 83.15154 | 90.847 | 121.134 | ±8. | | 122.131 | | 383.848 | | 22.609 | | # |
| C6H11 CH3C(CH3)=CHC2H4\* | | 83.15334 | 141.838 |  |  | | 124.520 | | 387.438 | |  | |  |
| C6H11 (CH3)2C=CHCH\*CH3 | | 83.15154 | 72.91 | 101.569 | ±8. | | 128.105 | | 375.530 | | 24.237 | | # |
| C6H11 (CH3)2CHCH\*CH=CH2 | | 83.15154 | 91.232 | 119.916 | ±8. | | 135.913 | | 384.042 | | 24.212 | | # |
| C6H11 2-Methyl-1-pentene-4-yl | | 83.15154 | 136.913 | 165.834 | ±8. | | 127.708 | | 386.671 | | 23.975 | | # |
| C6H11 Cyclohexyl Radical | | 83.15154 | 75.839 | 110.421 | ±8. | | 106.108 | | 317.527 | | 18.513 | | # |
| C6H11+ Cyclohexyl Rad. cation | | 83.15099 | 768.333 | 796.300 | ±8. | | 107.709 | | 315.207 | | 18.731 | | # |
| C6H11- Cyclohexyl Rad. anion | | 83.15209 | 101.370 | 83.063 | ±8. | | 104.494 | | 315.794 | | 18.307 | | # |
| C6H11I Iodo-CycloHexane | | 210.05601 | -50.0 | -11.926 | ±4.7 | | 121.960 | | 363.668 | | 21.420 | | # |
| C6H11O2 Caproyl Radical | | 115.15034 | -278.4 | -243.938 | ±12.5 | | 145.374 | | 434.509 | | 27.114 | | # |
| C6H12 TRANS-3-HEXENE | | 84.15948 | -50.417 | -17.218 | ±8. | | 128.815 | | 365.867 | | 23.931 | | # |
| C6H12 1-HEXENE <!> | | 84.15948 | -39.4 | -6.4 | ±8 | | 125.177 | | 398.579 | | 24.110 | | #† |
| C6H12 2MP-1ene | | 84.15948 | -55.484 | -22.617 | ±8 | | 124.379 | | 390.430 | | 24.263 | | # |
| C6H12 2MP-2ene | | 84.15948 | -60.007 | -27.366 | ±8 | | 123.322 | | 381.027 | | 24.489 | | # |
| C6H12 4MP-2ene CIS | | 84.15948 | -53.53 | -20.82 | ±8 | | 123.126 | | 380.119 | | 24.421 | | # |
| C6H12 4MP-2ene TRANS | | 84.15948 | -56.89 | -24.26 | ±8 | | 123.325 | | 380.623 | | 24.504 | | # |
| C6H12(L) Cyclohexane liq | | 84.15948 | -156.231 |  |  | | 156.482 | | 204.347 | |  | |  |
| C6H12 CYCLOHEXANE | | 84.15948 | -123.3 | -83.715 | ±0.68 | | 105.343 | | 297.389 | | 17.545 | | † |
| C6H12(L) MethylCyclopentane liq | | 84.15948 | -137.7 |  | ±0.71 | | 158.699 | | 247.944 | |  | |  |
| C6H12 MethylCyclopentane | | 84.15948 | -105.855 | -125.053 | ±8. | | 106.784 | | 322.836 | | 19.198 | | # |
| C6H12 Ethyl-Cyclobutane | | 84.15948 | -27.7 | +8.837 | ±0.7 | | 111.475 | | 344.506 | | 20.593 | | # |
| C6H12N2 TriEthyleneDiAmine  drawing of Triethylenediamine | | 112.17296 | 95.650 | 142.613 | ±8. | | 117.370 | | 319.188 | | 18.837 | | # |
| C6H12O Cyclohexanol chair | | 100.15888 | -293.098 | -251.287 | ±8. | | 120.753 | | 332.710 | | 19.659 | | # |
| C6H12O Oxepane | | 100.15888 | -224.53 | -183.24 | ±8. | | 116.490 | | 331.752 | | 20.187 | | # |
| C6H12O 2,5DiMethylTetraHydroFuran**:** C6H12O | | 100.15888 | -262.429 | -222.572 | ±8. | | 123.843 | | 345.507 | | 21.612 | | # |
| C6H12O2 liq. Caproic acid (liq.) | | 116.15828 | -581.8 |  | ±1.1 | | 225.1 | |  | |  | | X |
| C6H12O2 C5H11COOH Caproic | | 116.15828 | -498.206 | -459.568 | ±8. | | 142.527 | | 421.649 | | 27.172 | | # |
| C6H12O2 liq. Methyl Valereate | | 116.15828 | -514.2 |  | ±7.1 | |  | |  | |  | | X |
| C6H12O2 C4H9COOCH3 Methyl Valereate | | 116.15828 | -448.847 | -411.914 | ±8. | | 148.507 | | 441.134 | | 28.876 | | # |
| C6H12O2 liq. Ethyl Butyrate (liq) | | 116.15828 | -528.4 |  | ±0.79 | |  | |  | |  | | X |
| C6H12O2 C3H7COOC2H5 Ethyl Butyrate | | 116.15828 | -462.863 | -425.524 | ±8. | | 144.783 | | 443.565 | | 28.471 | | # |
| C6H12O6 α D Glucose (cr) | | 180.15588 | -1273.700 | -1190.641 | ±1.2 | | 201.300 | | 209.500 | |  | | # |
| C6H12O6 Cy α/β Glucopyranose  beta-D-Glucose | | 180.15588 | -1040.142 | -990.924 | ±12.5 | | 205.153 | | 482.620 | | 33.952 | | # |
| C6H12O6 Cy α/β Fructopyranose | | 180.15588 | -1039.3 |  | ±12.5 | |  | |  | |  | | X |
| C6H12O6 Cy α/β Glucofuranose  β-D-Ribose | | 180.15588 | -1025.08 |  | ±12.5 | |  | |  | |  | | X |
| C6H12O6 Glucose chain C6H12O6 | | 180.15588 | -1016.24 | -966.61 | ±12.5 | | 205.551 | | 472.415 | | 33.543 | | # |
| C6H12O6 D-Mannose **:** C6H12O6 | | 180.15588 | -1035.02 | -982.36 |  | | 206.012 | | 483.873 | | 33.507 | | # |
| C6H12O7 Gluconic acid **:** C6H12O7 | | 196.15528 | -1329.26 | -1278.13 | ±12.5 | | 216.499 | | 490.528 | | 36.380 | | # |
| N-C6H13 n - HEXYL RAD. <!> | | 85.16742 | 38.5 | 70.881 |  | | 141.790 | | 408.339 | | 28.983 | | #† |
| 2-C6H13 2-HEXYL RAD. <!> | | 85.16922 | 28.158 | 61.309 | ±8. | | 147.533 | | 428.452 | | 28.213 | | # |
| C6H13 2MP-1YL | | 85.16922 | 35.635 | 70.799 | ±8 | | 140.892 | | 399.411 | | 26.200 | | # |
| C6H13 2MP-5YL | | 85.16922 | 32.367 | 67.427 | ±8. | | 139.391 | | 414.154 | | 26.304 | | # |
| C6H13-S 2ME - 4PENTYL | | 85.16922 | 20.079 | 55.023 | ±8. | | 141.737 | | 402.960 | | 26.420 | | # |
| C6H13-T 2ME 2PENTYL | | 85.16922 | 17.209 | 52.180 | ±8. | | 139.289 | | 404.566 | | 26.392 | | # |
| C6H13N3O5 Butyl-NENA | | 207.18464 | -175.310 | -121.079 |  | | 219.381 | | 553.272 | | 41.839 | | # |
| C6H14(L) n-Hexane | | 86.17536 | -198.660 | -179.98 | ±0.48 | | 195.480 | | 296.090 | | 46.920 | | † |
| C6H14 n-Hexane <!> | | 86.17536 | -166.92 | -130.02 | ±0.48d | | 142.59 | | 388.85 | | 28.702 | | † |
| H14C6 2-METHYLPENTANE | | 86.17536 | -171.678 | -133.185 | ±8. | | 146.626 | | 395.895 | | 27.105 | | # |
| C6H14 3MethylPentane | | 86.17536 | -170.025 | -130.403 | ±8. | | 139.531 | | 395.888 | | 25.976 | | # |
| C6H14 2,2-DMBUTANE | | 86.17536 | -184.125 | -144.475 | ±8. | | 143.153 | | 373.705 | | 25.947 | | # |
| C6H14 2,3-DMBUTANE | | 86.17536 | -175.941 | -136.096 | ±8. | | 141.413 | | 373.502 | | 25.753 | | # |
| C6H14O (L) 1-Hexanol (liq) | | 102.17476 | -377.5 |  | ±0.44 | | 243.2 | | 287.4 | |  | | X |
| C6H14O 1-Hexanol | | 102.17476 | -314.7 | -269.230 | ±1.4 | | 139.043 | | 376.040 | | 24.468 | | # |
| C6H14O 2-Hexanol | | 102.17476 | -337.963 | -293.886 | ±8. | | 145.466 | | 384.291 | | 25.861 | | # |
| C6H14O 3-Hexanol | | 102.17476 | -332.8 | -290.429 |  | | 154.62 | | 381.688 | | 27.567 | | # |
| C6H14O DiPropyl ether | | 102.17476 | -292.5 | -248.97 | ±8. | | 142.775 | | 390.698 | | 26.355 | | # |
| C6H14O2 1,6-n-Hexadiol | | 118.17416 | -467.436 | -421.704 |  | | 155.199 | | 414.829 | | 28.545 | | # |
| C6H14O3 DimethyleneGlycolDimethylEtherC6H14O3 | | 134.17356 | -521.3 | -475.8 |  | | 173.361 | | 450.613 | | 33.107 | | # |
| C6H14O6 Sorbitol (gas) HOCH2(CHOH)4CH2OH | | 182.17176 | -1162.315 | -1104.640 |  | | 213.152 | | 480.064 | | 33.963 | | # |
| C6H15Bi Bi(C2H5)3 | | 296.1636 | 216.0 |  | ±17. | | 166.237 | | 507.172 | | 33.637 | | # |
| C6H15N N(C2H5)3 | | 101.19004 | -96.7 | -52.3 | ±8. | | 153.104 | | 436.303 | | 29.817 | | # |
| C6H15O+ (C2H5)3O+ | | 103.18215 | 414.698 | 449.283 | ±8. | | 155.400 | | 370.702 | | 27.192 | | # |
| C6H15PO3 (C2H5O)3P | | 166.15526 | -808.0 | -758.238 | ±4. | | 201.070 | | 509.025 | | 38.450 | | # |
| C6H15P P(C2H5)3 | | 118.15706 | -146.465 | -102.687 | ±8. | | 161.983 | | 451.179 | | 31.413 | | # |
| C6H15P+ P(C2H5)3+ cation | | 118.15651 | 577.8 | 614.7 | ±4. | | 171.363 | | 439.254 | | 32.096 | | # |
| C6H15Sb Sb(C2H5)3 | |  | 48.7 | +41. | ±11. | |  | |  | |  | | X |
| C6N4 TetraCyanoEthylene | | 128.09116 | 683.331 | 680.464 | ±8. | | 135.244 | | 386.043 | | 26.528 | | # |
| C6N6O6 BENZOTRIFUROXAN | | 252.10284 | N/A | N/A |  | | 200.972 | | 416.395 | |  | |  |
| C6O6W W(CO)6 | | 351.90060 | WC6O6 | See under |  | |  | | W(CO)6 | |  | | # |
| C6N6O12 HexaNitroBenzene | | 348.09744 | 17.489 | 44.587 |  | | 293.817 | | 664.089 | | 57.314 | | # |
| C6T6 Benzene Hexatritium | | 90.1632 | 29.173 | 44.113 | ±8. | | 104.950 | | 287.907 | | 17.088 | | # |
| C7 linear singlette 1Σg+ | | 84.0749 | 1322.34 | 1309.34 | ±8. | | 98.927 | | 314.106 | | 20.372 | | # |
| C7F16 Perfluoroheptane | | 124.9 | -3383.97 |  |  | | 300.804 | | 704.075 | |  | |  |
| C7H | | 85.08284 | 1090. | 1080.1 | ±100. | | 110.882 | | 330.513 | | 21.504 | | # |
| C7H4 CH(C≡CH)3 | | 88.10666 | 725.786 | 727.696 | ±8. | | 122.862 | | 342.282 | | 22.401 | | # |
| C7H4(NO2)3 TNBenzyl radical | | 226.12328 | 158.574 | 184.984 |  | | 214.316 | | 491.241 | | 36.982 | | # |
| C7H5N C6H5-CN Benzonitrile | | 103.12134 | 213.066 | 227.443 | ±8. | | 105.310 | | 328.810 | | 18.503 | | # |
| C7H5NO Benzoxazole | | 119.12024 | 28.61 | 48.207 | ±0.5 | | 106.837 | | 323.591 | | 17.623 | | # |
| C7H5NO Anthranil | | 119.12024 | 183.2 | 202.491 | ±8. | | 108.914 | | 325.602 | | 17.934 | | # |
| C7H5NS 1,3-Benzothioazole | | 135.18734 | 204.17 | 222.44 | ±0.37 | | 115.156 | | 336.221 | | 19.922 | | # |
| 1,2-C7H5NS 1,2-Benzothioazole | | 135.18734 | 218.237 | 236.417 | ±8. | | 115.283 | | 336.894 | | 19.113 | | # |
| C7H5N2O4 2,4-DiNitroToluene-6-yl | | 181.12568 | 268.613 | 292.273 |  | | 177.746 | | 443.328 | | 30.915 | | # |
| C7H5N2O5 2-Me-3,5-NitroPhenoxy | | 197.12508 | -16.736 | +8.522 |  | | 192.961 | | 464.658 | | 33.657 | | # |
| TNT Solid | | 227.13122 | -63.178 |  | ±5.0 | | 244.680 | | 284.9 | |  | |  |
| C7H5N3O6 TNT | | 227.13122 | 24.1 | 53.992 | ±3.5 | | 215.417 | | 481.936 | | 37.698 | | # |
| C7H5(NO2)2-ONO | | 227.13122 | -42.012 | -14.260 |  | | 218.764 | | 515.965 | | 39.838 | | # |
| C7H5N5O8 Tetryl Solid | | 287.1435 | 41.003 |  | ±4.6 | | 302.08 | | 330.1 | |  | |  |
| C7H5N5O8 Tetryl (g)  C7H5N5O8 | | 287.1435 | 152.3 | 186.99 | ±12.5 | | 262.381 | | 632.445 | | 50.253 | | # |
| C7H5O C6H5-C\*=O | | 105.11400 | 116.8 | 130.49 | ±8. | | 108.240 | | 342.800 | | 19.194 | | # |
| C7H6N2O4(s) 2,4-DiNitroToluene | | 182.13362 | -66.4 |  | ±3. | |  | |  | |  | | X |
| C7H6N2O4 2,4-DiNitroToluene | | 182.13362 | 33.2 | 61.24 | ±3.3 | | 172.330 | | 446.473 | | 30.767 | | # |
| C7H6O BENZALDEHYDE | | 106.12404 | -39.179 | -21.320 | ±8. | | 111.428 | | 336.148 | | 19.260 | | # |
| C7H6O2 (cr) Benzoic Acid solid | | 122.12134 | -385.2 |  |  | |  | | 167.7 | |  | | X |
| C7H6O2 C6H5-C(O)OH | | 122.12134 | -299.344 | -279.062 | ±8. | | 119.577 | | 362.037 | | 21.177 | | # |
| C7H6O3 HO-C6H4-COOH p-Ben | | 138.12074 | -492.6 | -469.685 | ±2.2 | | 138.074 | | 396.157 | | 22.884 | | # |
| C7H6S BenzThioAldehyde | | 122.18854 | 190.330 | 170.588 | ±8. | | 111.730 | | 338.291 | | 19.742 | | # |
| C7H6S+ BenzThioAldehyde+ | | 122.18799 | 1017.0 | 1027.3 | ±8. | | 113.705 | | 346.279 | | 20.121 | | # |
| C7H6S- BenzThioAldehyde- | | 122.18909 | 76.740 | 99.39 | ±8. | | 116.329 | | 344.556 | | 20.112 | | # |
| C7H7 2,4,6-Cycloheptatriene-1-yl | | 91.13048 | 280.696 | 298.308 | ±8. | | 109.167 | | 332.619 | | 19.401 | | # |
| C7H7 BENZYL RADICAL <!> | | 91.13048 | 208.0 | 226.8 | ±1.9 | | 109.700 | | 318.229 | | 18.178 | | # |
| C7H7+ C6H5CH2\*+ | | 91.12993 | 918.76 | 933.06 | ±8. | | 99.312 | | 306.083 | | 16.513 | | # |
| C7H7 o-Toluene radical | | 91.13048 | 311.708 | 329.95 | ±8.8 | | 103.671 | | 338.718 | | 18.770 | | # |
| C7H7 p-Toluene radical | | 91.13048 | 311.708 |  | ±8.8 | | 99.035 | | 318.863 | |  | |  |
| C7H7 Quadricyclene Appex Rad. | | 91.13048 | 534.519 | 556.275 | ±2.2 | | 95.877 | | 297.781 | |  | | # |
| C7H7 Quadricyclene Basis Rad. | | 91.13048 | 581.346 | 603.316 | ±2.2 | | 90.683 | | 299.778 | |  | | # |
| C7H7 Quadricyclene Shoulder R | | 91.13048 | 588.94 | 611.424 | ±2.2 | | 90.774 | | 299.687 | |  | | # |
| C7H7+ C5H4\*CH=CH2 | | 91.12993 | 1065.60 | 1077.11 | ±8. | | 109.06 | | 324.049 | | 19.303 | | # |
| C7H7NO 2-AcetylPyridine | | 121.13662 | -41.3 | -18.394 | ±2.9 | | 127.181 | | 374.262 | | 22.782 | | # |
| *p*-C7H7NO2 *p*-NitroToluene | | 137.13620 | 30.96 | 63.000 | ±3.9 | | 99.574 | | 343.083 | | 17.928 | | # |
| *o*-C7H7NO2 2-NitroToluene | | 137.13620 | 33.89 | 59.919 |  | | 138.079 | | 381.637 | | 23.999 | | # |
| C7H7O C6H5-CH2O\* | | 107.12988 | 125.909 | 146.9 | ±8. | | 117.167 | | 351.816 | | 20.362 | | # |
| C7H7O2 p-Guiacyl rad | | 123.12928 | 0.6 | 23.64 |  | | 131.568 | | 369.211 | | 22.654 | | # |
| TOLUENE(L) | | 92.13842 | 12.18 | 19.957 | ±0.36d | | 157.29 | | 221.030 | | 33.470 | | † |
| C7H8 TOLUENE <!> | | 92.13842 | 50.17 | 73.476 | ±0.37d | | 103.279 | | 320.187 | | 17.940 | | † |
| C7H8 (liq) Norbornadienec | | 92.13842 | 179.14d |  | ±1.d | |  | |  | |  | | X |
| C7H8 Norbornadiene | | 92.13842 | 212.5d | 238.345 | ±1.2d | | 98.054 | | 293.803 | | 15.402 | | # |
| C7H8 (liq) Quadricyclene | | 92.13842 | 302.1 |  | ±2.2 | |  | |  | |  | | X |
| C7H8 Quadricyclene | | 92.13842 | 337.23 | 363.987 | ±2.2 | | 91.551 | | 228.420 | |  | | # |
| C7H8 1,3,5-Cycloheptatriene | | 92.13842 | 371.138 | 394.044 | ±8. | | 107.362 | | 315.427 | | 18.340 | | # |
| C7H8 1,6-Heptadiyne | | 92.13842 | 395.739 | 413.020 | ±8. | | 130.046 | | 361.047 | | 23.966 | | # |
| C7H8O CRESOL | | 108.13782 | -132.298 | -108.55 |  | | 128.026 | | 360.116 | | 21.838 | | † |
| C7H8O BENZYL-ALCOHOL | | 108.13782 | -94.6 | -70.081 | ±3.0 | | 119.290 | | 360.634 | | 21.068 | | # |
| C7H8O C6H5OCH3 Anisole | | 108.13782 | -73.505 | -48.750. | ±8. | | 119.860 | | 349.135 | | 20.832 | | # |
| C7H8O+ C6H5OCH3  cation | | 108.13727 | 733.590 | 751.103 | ±8. | | 123.266 | | 360.289 | | 21.668 | | # |
| C7H8OS Benzyl Alcohol Mercaptan | | 140.20382 | -85.939 | -59.533 |  | | 141.244 | | 384.301 | | 23.593 | | # |
| C7H8O2 m-Guaiacol | | 124.1372 | -249.6 | -222.82 |  | | 135.6 | | 382.066 | | 23.219 | | # |
| C7H9 2-CH3-4=CH2-1CyPenten | | 93.14636 | 190.862 | 216.044 | ±8. | | 118.751 | | 344.962 | | 20.298 | | # |
| C7H10 Cyclopentyl-Acetylene | | 94.15430 | 166.096 | 194.511 | ±8. | | 118.125 | | 349.171 | | 21.300 | | # |
| C7H10 5,5 dimethyl-1,3-CPD | | 94.15430 | 81.211 | 109.705 | ±8. | | 122.658 | | 333.143 | | 21.221 | | # |
| C7H10 2,5 dimethyl-1,3-CPD | | 94.15430 | 74.659 | 103.023 | ±8. | | 120.843 | | 341.862 | | 21.352 | | # |
| C7H10 2,4 dimethyl-1,3-CPD | | 94.15430 | 63.513 | 91.186 | ±8. | | 121.800 | | 347.404 | | 22.042 | | # |
| C7H10 2,3 dimethyl-1,3-CPD | | 94.15430 | 61.894 | 89.955 | ±8. | | 117.103 | | 344.813 | | 21.654 | | # |
| C7H10 NORBORNENE | | 94.15430 | 79.806 | 113.391 | ±8. | | 100.827 | | 305.343 | | 16.129 | | # |
| C7H10N2O2 Cyclo(Pro-Gly) | | 154.16658 | -341.012 | -301.25 | ±12.5 | | 158.210 | | 401.299 | | 27.301 | | # |
| C7H11 CH2=CHCH\*CH2CH2CH=CH2 | | 95.16224 | 199.12 | 228.538 | ±8. | | 128.837 | | 413.554 | | 24.524 | | # |
|  | |  |  |  |  | |  | |  | |  | |  |
| C7H12 NORBORNANE | | 96.17018 | -53.572 | -12.727 | ±4.2 | | 109.112 | | 308.182 | | 17.338 | | # |
| C7H12 1-Heptyne | | 96.17018 | 103.800 | 135.768 | ±2.6 | | 143.815 | | 400.484 | | 26.215 | | # |
| C7H12 CY-HEPTENE | | 96.17018 | -7.866 | 30.578 | ±8. | | 120.515 | | 324.394 | | 19.739 | | # |
| C7H12 CH2=CHCH2CH2CH2CH=CH2 | | 96.17018 | 65.07 | 98.56 | ±8. | | 128.189 | | 403.896 | | 24.692 | | # |
| C7H13 Cycloheptanyl Radical | | 97.17812 | 77.739 | 118.315 | ±8. | | 126.683 | | 353.102 | | 21.841 | | # |
| C7H13 1-Heptyl-4/5 ene | | 97.17812 | 132.2 | 194.632 |  | | 148.532 | | 435.136 | |  | |  |
| C7H13 1-Heptene-4-yl | | 97.17812 | 129.7 | 192.117 |  | | 149.900 | | 505.000 | |  | |  |
| C7H14 n-HEPTENE <!> | | 98.18816 | -62.76 | -26.9 |  | | 153.500 | | 425.600 | | 30.790 | | † |
| C7H14(L) Cycloheptane liq | | 98.18606 | -230.387 |  |  | | 180.707 | | 242.547 | |  | |  |
| C7H14 CY-HEPTANE | | 98.18606 | -115.6 | -69.83 | ±8. | | 123.552 | | 340.393 | | 20.882 | | # |
| C7H14O Methyl Isoamyl Ketone (CH3)2CHCH2CH2C(=O)CH3 | | 114.18546 | -307.56 | -266.18 |  | | 160.711 | | 429.073 | | 29.614 | | # |
| C7H14O2 (liq) Enanthic acid | | 130.18486 | -608.5 |  | ±0.9 | |  | |  | |  | | X |
| C7H14O2 n-Heptanoic acid | | 130.18486 | -534.3 | -489.48 | ±12.5 | | 162.604 | | 448.539 | | 30.514 | | # |
| C7H14O2 Me-Hexanoate | | 130.18486 | -505.43 | -461.8 | ±12.5 | | 169.320 | | 451.890 | | 31.739 | | # |
| C7H14O2 Ethyl Pentanoate | | 130.18486 | -512.65 |  | ±12.5 | |  | |  | |  | | X |
| C7H15 n-HEPTYL RAD. <!> | | 99.19400 | 17.9 | 55.242 |  | | 164.430 | | 448.029 | | 33.543 | | #† |
| C7H15 NEOHEPTYL-1 | | 99.1961 | 3.000 | 44.181 | ±8. | | 164.117 | | 426.783 | | 29.704 | | # |
| C7H15 NEOHEPTYL-2 | | 99.19400 | -2.926 | 37.433 | ±8. | | 168.595 | | 430.562 | | 30.526 | | # |
| C7H15N3O5 Pentyl-NENA | | 221.21122 | -195.811 | -135.708 |  | | 239.882 | | 591.344 | | 45.487 | | # |
| C7H15O 3,3dimethyl1-pentanoxy | | 115.1955 | -142.256 |  |  | | 171.86 | | 328.026 | |  | |  |
| C7H16(L) n-Heptan | | 100.20194 | -224.35 | -201.87 | ±0.74d | | 224.980 | | 328.560 | | 52.640 | | † |
| C7H16 n-HEPTAN <!> | | 100.20194 | -187.78 | -145.88 | ±0.74d | | 165.180 | | 428.095 | | 33.221 | | † |
| C7H16 iso-Heptan | | 100.20194 | -194.600 | -150.40 |  | | 164.500 | | 420.500 | | 30.920 | | † |
| C7H16 NEOHEPTAN | | 100.20194 | -199.284 | -150.56 | ±8. | | 157.434 | | 359.044 | | 26.395 | | # |
| C7H16FO2P Soman  CH3C(CH3)2CH(CH3)OP(=O)F(CH3) | | 182.17290 | -1076.543 | -982.971 |  | | 229.702 | | 518.230 | |  | | # |
| C7H15OH n-Heptanol | | 116.20134 | -339.741 | -296.292 | ±1.6 | | 185.339 | | 486.155 | | 36.010 | | # |
| C7H15OH Neoheptanol | | 116.20134 | -359.657 | -319.671 |  | | 179.907 | | 493.957 | | 39.474 | | # |
| C8 (1Ag) linear singlette | | 96.08560 | 1458.866 | 1445.44 |  | | 107.988 | | 330.429 | | 21.848 | | # |
| C8 (3Σ-g) linear triplet | | 96.08560 | 1513.8 | 1500.3 | ±8. | | 100.651 | | 301.647 | | 21.932 | | # |
| C8H CH≡C-C≡C-C≡C-C≡C\* | | 97.09354 | 1230.0 | 1218.5 | ±100. | | 125.662 | | 354.191 | | 24.131 | | # |
| C8H2 CH≡C-C≡C-C≡C-C≡CH | | 98.10388 | 900.0 | 891.8 | ±60. | | 134.364 | | 348.303 | | 25.093 | | # |
| C8H4O3 Phthalic anhidride | | 148.11560 | -371.0 | -355.152 | ±5.0 | | 133.189 | | 364.261 | | 22.537 | | # |
| C8H4O4(S) 3-hydroxyphthalic anhydride | | 164.11496 | -680.8 |  | ±7.2 | | 186.60 | |  | |  | | X |
| C8H4O4 | | 164.11496 | -576.4 | -558.763 | ±8. | | 149.653 | | 382.695 | | 25.087 | | # |
| C8H5 CH≡C-CH=CH-CH=C\*C≡CH | | 101.12530 | 808.453 | 812.494 | ±8. | | 141.494 | | 402.387 | | 26.558 | | # |
| C8H5 C6H5C≡C\* | | 101.12530 | 654.934 | 665.190 | ±8. | | 108.279 | | 334.534 | | 19.342 | | # |
| C8H5 o-C6H4\*C≡CH | | 101.12530 | 559.0 | 569.1 |  | | 113.041 | | 339.080 | | 19.471 | | # |
| C8H6 C6H5C≡CH <!> | | 102.13324 | 317.683 | 330.632 | ±8. | | 125.784 | | 334.300 | | 20.883 | | # |
| C8H6 Pentalene BiCycloOctaTetraene | | 102.13324 | 374.857 | 391.355 | ±8. | | 104.650 | | 312.047 | | 17.335 | | # |
| C8H6 Benzocyclobutene | | 102.13324 | 410.015 | 426.377 | ±8. | | 105.597 | | 312.114 | | 17.471 | | # |
| C8H6O BENZOFURANE | | 118.13264 | 17.0 | 37.048 | ±1.5 | | 111.964 | | 326.193 | | 18.124 | | # |
| C8H6O2 Benzodioxin | | 134.13204 | -71.2 | -49.95 | ±6. | | 128.967 | | 347.408 | | 21.265 | | # |
| C8H6S BENZOTHIOPHENE | | 134.19924 | 165.703 | 184.431 | ±8. | | 119.919 | | 338.823 | | 19.517 | | # |
| C8H7 *n*-STYRYL RADICAL | | 103.14358 | 393.5 | 411.737 | ±8. | | 117.820 | | 349.841 | | 19.830 | | # |
| C8H7 *i*-STYRYL RADICAL | | 103.14118 | 367.686 | 385.134 | ±8. | | 120.881 | | 355.861 | | 20.618 | | # |
| C8H7 o-C6H4CH=CH2 | | 103.14118 | 401.827 | 420.034 | ±8. | | 116.318 | | 350.846 | | 19.860 | | # |
| C8H7 1,3,5,7Cy-octateraene-1-yl | | 103.14118 | 503.921 | 522.020 | ±8. | | 118.407 | | 340.591 | | 19.948 | | # |
| C8H7 2,3,5,7Cy-octateraene-1-yl | | 103.14118 | 503.795 | 521.914 | ±8. | | 118.425 | | 340.577 | | 19.948 | | # |
| C8H7N INDOLE | | 117.14792 | 156.5 | 179.576 | ±1.25 | | 121.626 | | 332.432 | | 19.325 | | # |
| C8H7N o-C6H4(CH3)CN | | 117.14792 | 187.8 | 207.9 |  | | 126.286 | | 364.066 | | 22.306 | | # |
| C8H8 CUBANE | | 104.14912 | 611.253 | 639.285 | ±8. | | 93.988 | | 269.749 | | 14.269 | | # |
| C8H8 STYRENE   <!> | | 104.14912 | 149.13 | 171.65 | ±8. | | 117.80 | | 338.530 | | 19.781 | | #† |
| C8H8 1,3,5,7 Cyclooctateraene | | 104.14912 | 297.6 | 319.294 | ±1.3 | | 122.616 | | 327.102 | | 20.607 | | # |
| C8H8 2,3,5,7 Cyclooctateraene | | 104.14912 | 389.434 | 411.499 | ±8. | | 118.990 | | 338.828 | | 20.235 | | # |
| C8H8 Benzocyclobutane | | 104.14912 | 200.476 | 224.662 | ±8. | | 109.342 | | 317.617 | | 18.115 | | # |
| C8H8O Acetophenone  C8H8O | | 120.14852 | -86.7 | -63.26 | ±1.7 | | 132.600 | | 374.437 | | 23.205 | | # |
| C8H8O2 MethylBenzoate solid | | 136.14792 | -328.94 |  | ±0.74 | |  | |  | |  | | X |
| C8H8O2 MethylBenzoate | | 136.14792 | -273.187 | -247.825 | ±0.77 | | 141.791 | | 395.350 | | 25.355 | | # |
| C8H8O3 Methyl Paraben | | 152.149 | -463.587 |  |  | | 170.750 | | 454.508 | |  | | X |
| C8H8O3 Methyl Salicylate Skeletal formula | | 152.149 | -458.817 |  |  | | 179.950 | | 441.035 | |  | | X |
| C8H9 C6H5CH2CH2\* | | 105.15706 | 237.714 | 262.114 | ±8. | | 130.543 | | 359.343 | | 22.135 | | # |
| C8H9 C6H5CH\*CH3 | | 105.15706 | 185.841 | 210.129 | ±8. | | 127.246 | | 365.597 | | 22.246 | | # |
| C8H9 1,3-BiMeBenzen-5-yl | | 105.15706 | 266.3 | 290.285 |  | | 123.521 | | 365.106 | | 22.550 | | # |
| C8H9 1,2-CH3C6H4CH2\* | | 105.15706 | 181.799 | 207.049 | ±8. | | 128.223 | | 348.836 | | 21.285 | | # |
| C8H9+ meta CH3C6H4CH2\*+ | | 105.15651 | 871.6 | 890.46 | ±8. | | 125.468 | | 349.393 | | 21.480 | | # |
| C8H10(L) C6H5C2H5 liq | | 106.16500 | -12.468 |  |  | | 185.895 | | 255.182 | |  | |  |
| C8H10 C6H5C2H5  <!> | | 106.16500 | 29.790 | 58.81 | ±8. | | 129.799 | | 337.688 | | 22.280 | | #† |
| C8H10 o-Di Methyl Benzene  C8H10 | | 106.16500 | 18.464 | 47.858 | ±8. | | 121.692 | | 353.784 | | 21.374 | | # |
| C8H10 p-Di METHYLBENZENE | | 106.16500 | 19.652 | 50.476 | ±8. | | 118.286 | | 352.115 | | 19.944 | | # |
| C8H12 3,6-di-CH3-1,4-hexadiene | | 108.18088 | 52.622 | 88.364 | ±8. | | 139.021 | | 352.015 | | 23.495 | | # |
| C8H14 1-Octayne HC≡CC6H13 | | 110.19676 | 80.700 | 119.446 | ±3.4 | | 161.622 | | 423.116 | | 28.959 | | # |
| C8H14 2-Octayne CH3C≡CC5H11 | | 110.19676 | 68.300 |  | ±1.5 | |  | |  | |  | | X |
| C8H14 CH(-CH2-CH2-)3CH | | 110.19676 | -99.035 | -51.705 | ±1. | | 125.174 | | 327.572 | | 20.374 | | # |
| C8H14 1,5-Hexadiene-3,4-dimethyl | | 110.19676 | 26.8 | 65.76 | ±26. | | 163.802 | | 406.037 | | 28.720 | | # |
| C8H14 trans- Bicyclo[3.3.0]octane | | 110.19676 | -67. |  | ±3. | |  | |  | |  | | X |
| C8H14 liq *cis*-Bicyclo[3.3.0]octane | | 110.19676 | -136. |  | ±1. | |  | |  | |  | | X |
| C8H14 *cis*-Bicyclo[3.3.0]octane | | 110.19676 | -93. | -46.183 | ±2. | | 127.575 | | 340.935 | | 20.887 | | # |
| C8H15 1-Octen-4-yl | | 111.20710 | 109.1 | 181.039 |  | | 172.717 | | 481.400 | |  | |  |
| 1-C8H16 1-OCTENE <!> | | 112.21264 | -83.59 | -42.768 |  | | 176.100 | | 464.840 | | 35.350 | | † |
| C8H16 CycloOctane | | 112.21264 | -114.386 | -62.136 | ±8. | | 143.577 | | 341.566 | | 23.923 | | # |
| C8H16O2 (liq) Caprylic acid | | 144.21144 | -634.8 |  | ±0.8 | |  | |  | |  | | X |
| C8H16O2 n-Octanoic acid | | 144.21144 | -553.96 | -502.584 | ±12.5 | | 185.105 | | 476.251 | | 33.476 | | # |
| N-C8H17 N-OCTYL RAD | | 113.22058 | -2.51 | +39.794 |  | | 187.070 | | 487.729 | | 38.103 | | #† |
| C8H17 2,3,3-TriMethylPentan | | 113.22058 | -20.083 | +29.026 |  | | 187.522 | | 412.106 | | 31.298 | | # |
| C8H18(L) n-Octane <!> | | 114.22852 | -250.260 | -227.11 | ±0.79d | | 254.150 | | 361.071 | | 61.490 | | † |
| C8H18 OCTANE <!> | | 114.22852 | -208.75 | -161.89 | ±0.79d | | 187.780 | | 467.352 | | 37.780 | | † |
| C8H18(L) isooctane 2,2,4 t.m.penta | | 114.22852 | -259.160 | -224.71 | ±1.5d | | 239.000 | | 328.110 | | 50.190 | | † |
| C8H18 ISO-OCTANE | | 114.22852 | -224.01 | -171.54 | ±1.5d | | 188.410 | | 423.090 | | 32.170 | | † |
| C8H18(L) 2,3,3-triMethylPentane | | 114.22852 | -253.7 |  | ±1.4 | |  | |  | |  | | X |
| C8H18 2,3,3-TriMethylPentane | | 114.22852 | -216.4 | -162.415 | ±1.4 | | 186.214 | | 399.026 | | 30.656 | | # |
| C8H18O Octanol C8H17OH | | 130.22792 | -356.00 | -300.63 | ±5. | | 182.727 | | 471.669 | | 33.612 | | # |
| (CH3)3C-OO-C(CH3)3 Liquid | | 146.22732 | -380.8 |  | ±2.0 | |  | |  | |  | | X |
| C8H18O2 (CH3)3C-OO-C(CH3)3 | | 146.22732 | -343. |  |  | | 219.150 | | 482.400 | |  | |  |
| C8H20Pb (C2H5)4Pb Liquid | | 323.4444 | 53.0 |  | ±5. | |  | |  | |  | | X |
| C8H20Pb (C2H5)4Pb Gas | | 323.4444 | 109.6 | 169.315 | ±5.1 | | 233.217 | | 477.890 | |  | | # |
| C9 (1Σ+g) | | 108.0963 | 1563.57 | 1553.48 | ±8. | | 122.991 | | 356.062 | | 24.670 | | # |
| C9H | | 109.10424 | 1310. | 1296.8 | ±125. | | 140.858 | | 379.086 | | 26.889 | | # |
| C9H4 C(CCH)4 | | 112.12806 | 913.78 | 918.435 |  | | 126.858 | | 330.747 | |  | | # |
| C9H6N 2 Quinolyl | | 128.15068 | 414.216 | 433.474 | ±8. | | 123.575 | | 340.796 | | 19.963 | | # |
| C9H6O2 Coumarin | | 146.14274 | -176.8 | -155.891 | ±1.8 | | 138.750 | | 363.779 | | 22.657 | | # |
| C9H7 1-INDENYL | | 115.15188 | 285.6 | 304.521 | ±22 | | 128.21 | | 342.843 | | 20.199 | | # |
| C9H7 3-INDENYL Rad | | 115.15188 | 430.726 | 450.705 |  | | 117.958 | | 337.956 | | 19.141 | | # |
| C9H7 7-Indenyl Rad | | 115.15188 | 420.492 | 440.471 | ±12. | | 117.958 | | 337.956 | | 19.141 | | # |
| C9H7+ C6H5CH=C=CH\*+ | | 115.15133 | 1128.8 | 1139.4 | ±8. | | 130.197 | | 358.376 | | 22.341 | | # |
| C9H7 o-C6H4-C≡CH(CH2\*) | | 115.15188 | 433.462 | 450.39 |  | | 138.220 | | 359.573 | | 22.192 | | # |
| C9H7 p-C6H4-C≡CH(CH2\*) | | 115.15188 | 430.952 | 448.536 |  | | 135.173 | | 349.701 | | 21.536 | | # |
| C9H7N QUINOLINE  C9H7N | | 129.15862 | 200.52 | 223.454 |  | | 129.153 | | 344.075 | | 20.521 | | # |
| C9H7N ISOQUINOLINE  C9H7N | | 129.15862 | 204.61 | 227.487 |  | | 128.983 | | 344.568 | | 20.578 | | # |
| C9H8 INDENE | | 116.15982 | 164.138 | 187.693 | ±1 | | 124.226 | | 335.846 | | 19.799 | | # |
| C9H8 o-EthynylToluene | | 116.15982 | 280.07 | 299.6 | ±17. | | 140.119 | | 364.777 | | 23.836 | | # |
| C9H8 m-EthynylToluene | | 116.15982 | 275.31 | 295.09 | ±17. | | 136.183 | | 363.845 | | 23.568 | | # |
| C9H8 p-EthynylToluene p-HC≡C-C6H4-CH3 | | 116.15982 | 275.89 | 297.88 |  | | 127.979 | | 348.429 | | 21.376 | | # |
| C9H8 C6H5-CH2C≡CH | | 116.15982 | 299.6 |  |  | | 136.398 | | 372.794 | |  | | # |
| C9H8 C6H5-C≡C-CH3 | | 116.15982 | 268.2 | 288.2 | ±2.2 | | 131.273 | | 368.649 | | 23.388 | | # |
| C9H9 Indanyl Radical any location | | 117.16776 | 249.166 | 275.607 | ±8. | | 128.908 | | 346.062 | | 21.146 | | # |
| C9H10 INDANE | | 118.1757 | 60.9 | 92.3 | ±2.1 | | 125.732 | | 336.366 | | 20.412 | | # |
| C9H10 METHYLSTYRENE | | 118.17570 | 112.968 | 141.060 |  | | 138.712 | | 373.528 | | 23.730 | | # |
| C9H10 C6H5-CH2CH=CH2 | | 118.17570 | 136.4 | 163.95 |  | | 137.938 | | 386.823 | | 24.269 | | # |
| C9H10 1,2-C6H4-CH=CH2(CH3) | | 118.17570 | 277.82 | 305.8 |  | | 142.317 | | 366.065 | | 24.019 | | # |
| C9H10 CycloPropylbenzene  C9H10 | | 118.17570 | 150.7 | 180.334 | ±1. | | 133.441 | | 356.283 | | 22.188 | | # |
| C9H11NO2 PhenylAlanine C9H11NO2 | | 165.18918 | -321.750 | -282.290 | ±4.2 | | 179.967 | | 442.003 | | 29.612 | | # |
| C9H10O2 Ethyl Benzoate solid | | 150.17450 | -365.230 |  | ±0.94 | |  | |  | |  | | X |
| C9H10O2 Ethyl Benzoate | | 150.17450 | -306.570 | -275.309 | ±0.97 | | 163.940 | | 433.694 | | 29.241 | | # |
| C9H11 C6H5-CH2CH2CH2\* Rad | | 119.18364 | 214.639 | 244.241 |  | | 150.956 | | 413.439 | | 26.454 | | # |
| C9H12 C(CH=CH2)4 | | 120.19158 | 250.6 | 279.18 |  | | 174.032 | | 417.887 | | 31.734 | | # |
| C9H12 1,3,5-Trimethylbenzene | | 120.19158 | -16.067 | 44.22 |  | | 147.800 | | 385.300 | |  | |  |
| C9H12 1,2,4-Trimethylbenzene | | 120.19158 | -13.933 | 46.36 |  | | 154.508 | | 395.765 | |  | |  |
| C9H12 Propylbenzene  C9H12 | | 120.19158 | 7.82 | 42.33 | ±0.84 | | 145.803 | | 403.398 | | 25.779 | | # |
| C9H12 Isopropyl Benzene (liq.) | | 120.19158 | -41.2 |  | ±1.1 | |  | |  | |  | | X |
| C9H12 Isopropyl Benzene C9H12Cumene | | 120.19158 | 3.9 | 38.5 | ±1.1 | | 150.426 | | 376.905 | | 25.647 | | # |
| C9H16 1-Nonenyl CH3(CH2)6C≡CH | | 124.22334 | 63.000 | 106.800 | ±1. | | 181.172 | | 477.050 | | 33.427 | | # |
| C9H17 1-Nonenyl Radical <!> | | 125.23398 | 88.400 | 169.860 |  | | 195.709 | | 520.900 | |  | |  |
| C9H18 1-Nonene <!> | | 126.24192 | -432.207 |  |  | | 200.269 | | 505.000 | |  | |  |
| C9H18 1,3,5-triMeCyclohexane cis | | 126.23922 | -887.426 | -830.260 |  | | 177.075 | | 380.828 | | 28.528 | | # |
| C9H18O2 (liq) Pelargic acid | | 158.23802 | -658.0 |  | ±0.9 | |  | |  | |  | | X |
| C9H18O2 n-Nonanoic acid | | 158.23802 | -573.6 | -516.938 | ±12.5 | | 206.200 | | 515.713 | | 37.686 | | # |
| C9H18O6 cyTriAcetoneTriPeroxy | | 222.23562 | -395.472 | -331.52 | ±22 | | 302.788 | | 499.584 | | 47.780 | | # |
| N-C9H19 n-NONYL RAD <!> | | 127.24716 | -23.2 | +24.064 |  | | 209.710 | | 527.419 | | 42.664 | | #† |
| N-C9H20 liq. NONANE | | 128.2578 | -275.475 |  |  | | 284.386 | | 393.673 | |  | |  |
| N-C9H20 NONANE <!> | | 128.2551 | -228.300 | -169.307 | ±1. | | 186.962 | | 482.757 | | 35.169 | | # |
| 1-C9H20O 1-Nonanol | | 144.25450 | -377.0 | -315.495 | ±9. | | 199.781 | | 502.547 | | 36.997 | | # |
| C10 (1A'l) cyclic Singlet | | 120.10700 | 1459.363 | 1443.5 |  | | 132.726 | | 373.758 | | 26.376 | | # |
| C10 estimated linear singlet | | 120.10700 | 1665.0 |  | ±12.5 | |  | |  | |  | | X |
| C10 (3Σ-g) linear triplet | | 120.10700 | 1741.11 | 1725.189 |  | | 133.694 | | 382.818 | | 26.460 | | # |
| C10D8 NAPHTHALENE-D8 | | 136.21982 | 118.050 | 139.214 |  | | 156.120 | | 350.531 | | 23.647 | | # |
| C10H | | 121.11494 | 1450. | 1435.2 | ±125. | | 155.644 | | 402.686 | | 29.534 | | # |
| C10H2 | | 122.12288 | 1120. | 1108.5 | ±80. | | 164.350 | | 396.743 | | 30.501 | | # |
| C10H4Cl4 2,3,6,7-Cl-Naphthalen | | 265.94956 | 50.21 | 62.584 |  | | 192.982 | | 449.224 | | 32.457 | | # |
| C10H6 Naphtyne | | 126.15764 | 500.825 | 515.5 |  | | 132.178 | | 347.542 | | 21.264 | |  |
| C10H6 1,3-EthynylBenzene | | 126.15464 | 552.121 | 562.954 | ±8. | | 149.360 | | 372.020 | | 25.106 | | # |
| C10H7 Naphtyl Radical | | 127.16558 | 396.225 | 415.418 |  | | 132.216 | | 352.133 | | 20.980 | |  |
| C10H7 C6H5CH=CH-C≡C\* | | 127.16558 | 687.515 | 701.677 | ±20 | | 144.738 | | 406.909 | | 26.011 | | # |
| C10H7 C6H4\*CH=CH-C≡CH | | 127.16558 | 630.612 | 645.066 | ±20 | | 148.770 | | 402.203 | | 25.719 | | # |
| C10H7 C6H4(C2H)CH=CH\* | | 127.16558 | 617.140 | 631.762 |  | | 152.555 | | 393.607 | | 25.551 | | # |
| C10H7I (L) 1-Iodonaphthalene Liq. | | 254.06705 | 162. |  | ±6.3 | |  | |  | |  | | X |
| C10H7I 1-Iodonaphthalene | | 254.06705 | 234. |  | ±8.8 | | 158.574 | | 394.133 | |  | |  |
| C10H7O\* Naphthol Radical | | 143.15498 | 115.478 | 136.47 |  | | 146.882 | | 373.015 | | 23.522 | |  |
| H8C10 AZULENE | | 128.17052 | 308.00 | 331.306 |  | | 132.175 | | 348.306 | | 21.101 | | # |
| C10H8 NAPHTHALENE  <!> | | 128.17052 | 150.582 | 174.276 | ±1.5 | | 131.920 | | 333.267 | | 20.713 | | † |
| C10H8 | | 128.17052 | 377.732 | 396.805 | ±17. | | 149.806 | | 386.765 | | 25.334 | | # |
| C10H8 Penta Fulvalene Skeletal formula | | 128.17052 | 374.422 | 396.023 | ±8. | | 137.780 | | 352.832 | | 22.806 | | # |
| C10H8O Naphtol | | 144.17292 | -30.794 | -6.37 |  | | 154.318 | | 368.709 | | 24.318 | | # |
| C10H9+ Protonated Azulene+ | | 129.17791 | 889. | 909.5 |  | | 135.256 | | 354.804 | | 21.951 | | # |
| C10H9 2-HydroNaphthalen Rad | | 129.17846 | 229.534 | 255.533 |  | | 143.289 | | 363.659 | | 22.643 | |  |
| C10H9 C6H5CH=CHCH=CH\* | | 129.17846 | 444.508 | 466.692 | ±20 | | 152.314 | | 419.069 | | 26.458 | | # |
| C10H9 1-Methyl-1-Indenyl Rad | | 129.17846 | 262.337 | 287.549 | ±20 | | 144.004 | | 369.098 | | 23.429 | | # |
| C10H9 7-Methyl-1-Indenyl Rad | | 129.17846 | 262.086 | 287.435 |  | | 140.773 | | 370.873 | | 23.292 | | # |
| C10H9 1-Methylene-Indene Rad | | 129.17846 | 337.649 | 363.520 | ±20 | | 144.045 | | 364.065 | | 22.771 | | # |
| C10H9 2-Methylene Indene Rad | | 129.17846 | 266.5 |  | ±20 | |  | |  | |  | | X |
| C10H10 1,2-DihydroNapthalene | | 130.1864 | 117.152 | 147.213 |  | | 143.955 | | 359.383 | | 22.797 | |  |
| C10H10 1,1’-BiCycloPentadiene | | 130.1864 | 291.625 | 320.336 |  | | 143.016 | | 385.011 | | 24.164 | | # |
| C10H10 2,2’’-BiCycloPentadiene | | 130.1864 | 291.056 | 318.773 |  | | 150.301 | | 386.504 | | 25.159 | | # |
| C10H10 1-Methyl Indene  C10H10 | | 130.1864 | 184.933 | 214.695 | ±20 | | 144.346 | | 360.391 | | 23.113 | | # |
| C10H10 2-Methyl Indene | | 130.1864 | 173.636 | 202.811 | ±20 | | 146.240 | | 364.509 | | 23.701 | | # |
| C10H10 3-Methyl Indene | | 130.1864 | 173.218 | 202.400 | ±20 | | 146.056 | | 364.755 | | 23.694 | | # |
| C10H10 7-Methyl Indene | | 130.1864 | 130.96 | 160.15 | ±17. | | 145.505 | | 364.732 | | 23.686 | | # |
| C10H10 o-Ethyl-Ethyny Benzene | | 130.1864 | 259.74 | 285.47 | ±17. | | 158.091 | | 404.167 | | 27.151 | | # |
| C10H10 p-Ethyl-EthynylBenzene | | 130.1864 | 254.973 | 281.140 | ±17. | | 155.663 | | 406.408 | | 26.709 | | # |
| C10H12O3 Coniferyl alcohol | | 180.20048 | -367.77 | -327.93 |  | | 200.139 | | 476.25 | | 34.521 | | # |
| C10H13 C5H7-C5H6\* | | 133.21322 | 197.15 |  | ±20 | | 149.452 | | 395.356 | |  | |  |
| C10H14 3,3-C5H7-C5H7 bicyclo | | 134.21816 | 108.784 | 152.131 | ±20 | | 155.753 | | 401.109 | | 26.465 | | # |
| 11-C10H15 JP-10 apex Radical | | 135.22910 | 105.650 | 157.726 |  | | 142.526 | | 359.233 | | 21.970 | | # |
| 6-C10H15 JP-10 Tert side Rad. | | 135.22910 | 96.32 | 149.14 |  | | 138.190 | | 355.345 | | 21.225 | | # |
| C10H15 C5H8\*-C5H7 | | 135.22910 | 171.54 | 217.32 | ±125.5 | | 166.487 | | 419.405 | | 28.268 | | # |
| C10H15O3PS2 Fenthion | | 278.33006 | -688.77 | -638.62 | ±20. | | 288.227 | | 575.876 | | 51.104 | | # |
| C10H16 exo THDCPD(liq) | | 136.23404 | -126.4 |  |  | |  | |  | |  | | X |
| C10H16 endo THDCPD (liq) | | 136.23404 | -114.7 |  |  | |  | |  | |  | | X |
| C10H16 exo THDCPD (g) | | 136.23404 | -76.6 | -21.09 | ±8. | | 149.304 | | 358.467 | | 22.767 | | # |
| C10H16 endo THDCPD (g) | | 136.23404 | -63.4 | -7.498 | ±8. | | 149.986 | | 353.758 | | 22.378 | | # |
| C10H16 adamantane (g) | | 136.23404 | -135.6 | -77.656 | ±8. | | 142.684 | | 317.860 | | 20.336 | | # |
| C10H16 JP-10 (g) fuel Equil mix | | 136.23404 | -76.555 |  | ±8. | | 149.306 | | 358.457 | |  | | X |
| C10H16 +Limonene C10H16 | | 136.23404 | 3.090 | 50.937 | ±1.02 | | 182.526 | | 420.085 | | 30.433 | | # |
| C10H16 -Terpinene | | 136.23404 | 5.439 | 51.989 | ±13.5 | | 182.998 | | 426.208 | | 31.730 | | # |
| C10H16 -Terpinene | | 136.23404 | 11.715 | 58.258 | ±13.5 | | 183.097 | | 420.527 | | 31.737 | | # |
| C10H16 Terpinolene C10H16 | | 136.23404 | 20.083 | 67.436 | ±13.5 | | 186.603 | | 410.990 | | 30.927 | | # |
| C19H16O (Solid) Camphor | | 152.23344 | -319. |  | ±3. | | 271.2 | |  | |  | | X |
| C10H16O g Camphor **:** C10H16O | | 152.23344 | -263.174 |  | ±3. | | 194.138 | | 499,697 | |  | | # |
| C10H18 (liq) 1,1'-Bicyclopentyl | | 138.24992 | -179.3 |  | ±1.0 | | 238.9 | |  | |  | | X |
| C10H18 1,1'-Bicyclopentyl  C10H18 | | 138.24992 | -127.8 | -70.05 |  | | 167.750 | | 427.551 | | 29.001 | | # |
| C10H18 1-Decyne HC≡C-C8H17 | | 138.24992 | 41.900 | 92.217 | ±3.4 | | 198.190 | | 505.767 | | 36.431 | | # |
| C10H19 1-Decenyl 4/5 Radical | | 139.26086 | 67.900 | 158.882 |  | | 218.653 | | 560.300 | |  | |  |
| C10H19 1-Decenyl 3 Radical | | 139.26086 | 2.600 | 93.582 |  | | 221.077 | | 567.300 | |  | |  |
| C10H20 1-Decene <!> | | 140.26580 | -123.900 | -66.221 |  | | 202.582 | | 511.975 | | 37.537 | | # |
| C10H20 2-Decene-trans | | 140.26580 | -136.200 | -78.629 |  | | 199.059 | | 516.993 | | 37.645 | | # |
| C10H20 3-Decene-trans | | 140.26580 | -135.500 | -77.332 |  | | 197.988 | | 515.334 | | 37.048 | | # |
| C10H20 cyclo CycloDecane | | 140.26580 | -154.4 | -89.5 | ±1.7 | | 184.236 | | 388.931 | | 30.321 | | # |
| C10H20O2 (liq) Capric acid | | 172.26460 | -713.7 |  | ±0.9 | |  | |  | |  | | X |
| C10H20O2 n-Decanoic acid | | 172.26460 | -593.7 | -529.69 | ±12.5 | | 225.282 | | 524.779 | | 39.879 | | # |
| N-C10H21 n-Decyl 1-Radical<!> | | 141.27374 | -43.8 | +8.426 |  | | 232.350 | | 567.109 | | 47.224 | | #† |
| C10H21 n-Decyl – 2-Radical <!> | | 141.27374 | -58.100 | +2.060 |  | | 215.469 | | 524.944 | | 39.290 | | # |
| C10H21 n-Decyl-3/4 Radical<!> | | 141.27674 | -58.200 |  |  | | 230.534 | | 567.300 | |  | |  |
| N-C10H22 liq DECANE | | 142.28468 | -301.039 |  |  | | 314.511 | | 425.889 | |  | |  |
| N-C10H22 gas-DECANE <!> | | 142.28468 | -249.534 | -192.75 |  | | 233.049 | | 545.677 | | 46.903 | | # |
| C10H22 2,2,3,3,4 PentaMethyl-Pentane | | 142.28168 | -244.597 | -178.597 | ±2.5 | | 226.655 | | 449.077 | | 37.685 | | # |
| 1-C10H22O 1-Decanol | | 158.28111 | -395. | 462.743 | ±10. | | 218.651 | | 534.304 | | 40.281 | | # |
| C10H22O4 TPGME C10H22O4 | | 206.27928 | -812.1 | -738.945 |  | | 273.234 | | 557.023 | | 47.874 | | # |
| C11 singlet | | 132.11770 | 1792.06 | 1775.137 | ±8. | | 144.086 | | 394.396 | | 28.517 | | # |
| C11H radical | | 133.12564 | 1530. | 1513.5 | ±150. | | 170.848 | | 427.700 | | 32.321 | | # |
| HC11N HC10CN | | 147.13238 | 1270. | 1253.8 | ±100. | | 190.022 | | 458.112 | | 36.314 | | # |
| 1-C10H7C\*O Naphtaldehyde Rad. | | 155.17598 | 174.891 | 193.741 |  | | 161.693 | | 399.949 | | 26.717 | |  |
| 1-C10H7CHO Naphtaldehyde C11H8O | | 156.18392 | 30.543 | 54.59 |  | | 162.397 | | 383.881 | | 25.754 | |  |
| C11H8 1-Ethynyl-Indene | | 140.18122 | 415.764 | 436.369 |  | | 153.101 | | 378.856 | | 24.856 | | # |
| C11H8 7-Ethynyl-Indene | | 140.18122 | 390.284 | 410.764 |  | | 154.528 | | 377.364 | | 24.951 | | # |
| 1-C10H7-CH2\* Methyl-Naphthyl | | 141.19246 | 272.797 | 297.846 |  | | 158.090 | | 378.770 | | 24.645 | |  |
| C11H9 1-C10H6\*-3-CH3 Rad. | | 141.18916 | 367.35 | 393.3 |  | | 152.892 | | 371.356 | | 23.744 | | # |
| C11H9 1-CH3-3-C10H6\* Rad | | 141.18916 | 367.355 | 392.737 |  | | 152.859 | | 375.537 | | 24.313 | | # |
| C11H10 1-C10H7-CH3 MethylNaphthalen | | 142.20040 | 116.106 | 145.0 |  | | 157.922 | | 381.348 | | 25.026 | |  |
| C11H10 C6H5-1-C5H5 | | 142.19710 | 238.07 | 266.9 |  | | 151.509 | | 390.667 | | 25.112 | | # |
| C11H11 1,2-H-Naphthalene-1-Me-2yl | | 143.20504 | 208.974 | 241.733 |  | | 161.429 | | 382.675 | | 25.404 | | # |
| C11H11 1,7-DiMethyl-1-Indenyl | | 143.20504 | 214.304 | 245.35 |  | | 169.212 | | 392.335 | | 27.112 | | # |
| C11H12 1-Methyl-1,2 Dihydro-Naphthalene | | 144.21298 | 104.47 | 141.39 | ±17. | | 162.316 | | 377.375 | | 25.486 | | # |
| C11H12 1,1 DiMethyl Indene  C11H12 | | 144.21298 | 107.110 | 142.882 |  | | 170.066 | | 381.707 | | 26.625 | | # |
| C11H12 1,7 DiMethyl Indene | | 144.21298 | 99.579 | 134.861 |  | | 169.807 | | 386.907 | | 27.115 | | # |
| C11H20O2 Methyl-9-Decenoate | | 184.27530 | -448.32 | -388.31 |  | | 241.627 | | 579.043 | | 44.940 | | # |
| C11H22O2 n-Undecanoic acid | | 186.29118 | -612.96 | -543.14 | ±12.5 | | 245.847 | | 577.079 | | 43.603 | | # |
| C11H22O2 MethylDecanoate | | 186.29118 | -584.1 | -516.58 | ±12.5 | | 254.904 | | 567.095 | | 45.899 | | # |
| C11H23 -1 n-Undecyl-1 | | 155.30032 | -64.4 |  |  | | 254.4 | | 602.9 | |  | |  |
| C11H24 N-UNDECANE <!> | | 156.31156 | -270.286 | -208.54 |  | | 255.684 | | 584.923 | | 51.463 | | # |
| C11H24O 1-Undecanol | | 172.30766 | -420.0 | -302.5 |  | | 270.286 | | 635.55 | |  | |  |
| C11N \*C10-CN Radical | | 146.12444 | 1500. | 1479.45 | ±150. | | 185.004 | | 462.108 | | 36.477 | | # |
| C12 Σ+g linear singlet | | 144.12840 | 1913.7 | 1895.3 | ±12.5 | | 158.347 | | 416.774 | | 31.035 | | # |
| C12 linear triplet | | 144.12840 | 1964.1 | 1945.56 | ±12.5 | | 159.729 | | 427.047 | | 31.198 | | # |
| O-C12D9 O-BIPHENYL Radical | | 162.25532 | 386.5 | 407.176 |  | | 194.573 | | 428.719 | | 30.527 | | # |
| C12D10 BIPHENYL – D | | 164.26942 | 138.410 | 163.029 |  | | 199.244 | | 413.432 | | 30.868 | | # |
| C12H | | 145.13634 | 1670. | 1651.89 | ±150. | | 185.671 | | 451.233 | | 34.985 | | # |
| C12H2 | | 146.14428 | 1340. | 1325.2 | ±100. | | 194.154 | | 445.249 | | 35.889 | | # |
| C12H4CL4O 2,3,6,7 | | 305.97036 | -50. | -35.924 | ±10 | | 225.108 | | 496.028 | | 38.205 | |  |
| C12H4CL4O 2,4,6,8 | | 305.97036 | -58. | -44.108 | ±10 | | 225.552 | | 493.238 | | 38.388 | |  |
| C12H4CL4O2 2,3,7,8 | | 321.96976 | -136.1 | -120.71 | ±10 | | 241.524 | | 513.049 | | 41.226 | | # |
| C12H4CL4O2 1,3,6,8 | | 321.96976 | -174.10 | -158.934 | ±10 | | 241.685 | | 520.954 | | 41.454 | | # |
| C12H4CL4O2 1,3,7,9 | | 321.96976 | -174.130 | -158.961 | ±10 | | 241.657 | | 520.551 | | 41.452 | |  |
| C12H4CL4O3 1,3,6,8 | | 337.97276 | -295.37 | -278.36 |  | | 256.811 | | 533.525 | | 43.948 | |  |
| C12H4CL5O2 spiro radical | | 357.42246 | -95.550 | -80.345 | ±10 | | 264.387 | | 571.035 | | 46.006 | | # |
| C12H4CL5O2 6-2’ ether radical | | 357.42246 | -125.900 | -112.30 | ±10 | | 266.495 | | 600.066 | | 47.612 | | # |
| C12H4CL6O2 2-6’ ether | | 392.87516 | -201.95 | -187.778 | ±10 | | 287.872 | | 625.238 | | 51.630 | | # |
| C12H4CL6O2 Biphenyl-diol | | 392.87876 | -321.92 | -305.6 | ±33.5 | | 286.707 | | 573.925 | | 49.483 | |  |
| C12H5CL3O3 2,4,7 trichloro | | 303.52800 | -348.99 | -329.03 |  | | 241.279 | | 505.020 | | 40.642 | |  |
| C12H5CL4O2 6-6’ ether radical | | 322.98130 | -85.52 | -69.659 | ±25.1 | | 250.467 | | 582.730 | | 44.993 | |  |
| C12H5CL4O3 radical | | 338.97710 | -432.42 | -412.55 | ±62.8 | | 265.578 | | 551.043 | | 45.331 | |  |
| C12H5CL4O3 radical | | 338.97710 | -321.79 | -301.82 | ±62.8 | | 263.787 | | 550.127 | | 45.226 | |  |
| C12H5CL5O2 6-6’ ether | | 358.43040 | -265.590 | -247.196 | ±10. | | 272.572 | | 577.900 | | 47.051 | | # |
| C12H6CL2O DCDF | | 237.08084 | 5.2 | 25.245 | ±24.7 | | 192.255 | | 439.242 | |  | | # |
| C12H6CL2O2 DCDD | | 253.08024 | -89.3 | -67.92 | ±26.6 | | 209.088 | | 461.386 | |  | | # |
| C12H6CL4O2 6-2’ ether | | 323.98564 | -207.57 | -187.21 |  | | 256.821 | | 561.466 | | 44.729 | |  |
| 1-C10H7-C≡C\* EthynylNaphthyl | | 151.18758 | 694.962 | 710.644 |  | | 162.077 | | 397.847 | | 26.598 | |  |
| C12H7 5-Acenaphtylenyl Rad. | | 151.18398 | 525.300 | 544.948 | ±8. | | 146.923 | | 338.218 | | 22.633 | | # |
| C12H8 Acenaphthylene | | 152.19552 | 259.7 | 283.489 | ±5.9 | | 148.772 | | 338.676 | | 22.726 | | # |
| C12H8 Biphenylene C12H8 | | 152.19192 | 417.20 | 440.025 | ±1.9 | | 150.492 | | 359.810 | | 23.689 | | # |
| C10H7-C≡CH EthynylNaphthalen | | 152.19552 | 379.070 | 398.592 |  | | 169.895 | | 391.974 | | 26.992 | |  |
| C12H8Cl2O2 | | 255.09612 | -231.794 | -167.418 |  | | 238.488 | | 528.021 | |  | |  |
| C12H8O Di-Benzo-Furan | | 168.19132 | 55.3 | 80.812 | ±0.3 | | 163.566 | | 375.274 | | 25.229 | | # |
| C12H8O2 Di-Benzo-p-Dioxin | | 184.19432 | -50.1 | -23.24 | ±2.2 | | 180.004 | | 396.647 | | 28.336 | | # |
| C12H8S Di-Benzo-Thiophene | | 184.25792 | 211.3 | 235.78 | ±4.5 | | 168.265 | | 387.659 | | 26.450 | | # |
| 1-C10H7-CH=CH\* Vinyl-Naphthyl | | 153.20346 | 469.863 | 492.963 |  | | 172.891 | | 404.234 | | 27.649 | |  |
| 1-C10H7-C\*=CH2 | | 153.20346 | 412.208 | 434.879 |  | | 175.034 | | 407.260 | | 28.077 | |  |
| C12H9 8-C10H6\*-CH=CH2 | | 153.19986 | 465.262 | 489.2 |  | | 163.749 | | 410.373 | | 26.810 | | # |
| O-C12H9 O-BIPHENYL RAD | | 153.2031 | 427.73 | 451.889 |  | | 163.048 | | 405.110 | | 26.589 | | † |
| p-C12H9CL ChloroBiphenyl | | 188.65256 | 149.79 | 175.72 |  | | 177.275 | | 423.758 | | 29.406 | | # |
| C12H9N CARBAZOLE | | 167.2102 | 200.7 |  |  | | 176.877 | | 388.305 | |  | |  |
| 1-C10H7-CH=CH2 | | 154.21140 | 215.058 | 242.302 |  | | 173.671 | | 400.851 | | 27.738 | |  |
| C12H10 Heptalene | | 154.20780 | 411.4 | 439.727 |  | | 166.517 | | 381.190 | | 26.655 | | # |
| C12H10 BIPHENYL   <!> | | 154.21140 | 182.13 | 210.329 | ±0.7 | | 166.179 | | 388.941 | | 26.783 | | † |
| (C6H5)2N\* Biphenylamin Rad. | | 168.21454 | 354.5 | 384.78 | ±3.3 | | 175.395 | | 429.789 | | 29.036 | | # |
| C12H11 1-C10H7-CH2CH2\* | | 155.21934 | 292.88 | 322.861 |  | | 185.266 | | 418.370 | | 29.235 | |  |
| C12H11 1-C10H7-CH\*-CH3 | | 155.21934 | 220.497 | 250.340 |  | | 184.272 | | 426.717 | | 29.373 | |  |
| C12H12 1,3-DimethylNaphthalen | | 156.22368 | 83.68 | 118.14 |  | | 178.694 | | 404.153 | | 29.075 | | # |
| 1-C10H7-C2H5 EthylNaphthalen | | 156.22728 | 96.901 | 131.723 |  | | 181.943 | | 406.323 | | 28.829 | |  |
| C12H12O 1-C10H7CH2CH2OH | | 172.22668 | -52.718 | -16.807 |  | | 195.002 | | 447.806 | | 31.880 | |  |
| C12H12Si (C6H5)2SiH2 | | 184.30918 | N/A | N/A |  | | 188.570 | | 461.454 | | 31.414 | |  |
| C12H18 HexaMethyl Benzene | | 162.27132 | -77.4 |  | ±2.5 | | 241.500 | | 454.8 | |  | | # |
| C12H20O10 Cellobiose biradical | | 324.2812 | -1392.7 |  | ±150. | | 343.12 | | 587.58 | |  | |  |
| C12H22O11 Cellobiose/Maltose | | 342.29648 | -2162.7 |  | ±30. | | 376.72 | | 776.41 | |  | |  |
| C12H22O11 solid Sucrose  C12H22O11 | | 342.2965 | -2228.9 |  |  | | 424.3 | | 392.4 | |  | | X |
| C12H23 liquid JET-A(L) | | 167.31102 | -303.469 |  |  | | 350.336 | | 448.112 | |  | | † |
| C12H23 JET-A (Kerosine) gas | | 167.31102 | -211.46 |  |  | | 293.494 | | 612.539 | |  | | † |
| C12H23O2 O=CH(CH2)10CH2O\* | | 199.30982 | -303.2 |  |  | | 294.1 | | 691.2 | |  | |  |
| C12H23O2 C6H13C(O)CH2CHO\*C3H7 | | 199.30982 | -351.0 |  |  | | 295.8 | | 676.97 | |  | |  |
| C12H24 CycloDodecane | | 168.31896 | -228.446 | -150.694 |  | | 224.464 | | 459.344 | | 36.507 | | # |
| C12H24O2 n-Dodecanoic acid liq | | 200.31776 | -775.1 |  |  | |  | |  | |  | | X |
| C12H24O2 n-Dodecanoic acid | | 200.31776 | -633.0 | -557.9 | ±15. | | 267.397 | | 588.617 | | 47.848 | | # |
| C12H25-1 n-Dodecyl-1 | | 169.32690 | -84.93 | -12.102 |  | | 252.414 | | 569.132 | | 45.666 | | # |
| C12H26 N-DODECANE <!> | | 170.33844 | -290.872 | -224.17 |  | | 278.32 | | 624.253 | | 56.024 | |  |
| C12H26O (liq.) 1-Dodecanol | | 186.33424 | -528.5 |  | ±0.8 | | 438.42 | |  | |  | | X |
| C12H26O 1-Dodecanol | | 186.33424 | -440.99 | -313.926 |  | | 294.554 | | 674.879 | |  | |  |
| C13H9 1-Phenalenyl Radical | | 165.21056 | 264.3 | 291.327 | ±8. | | 164.097 | | 376.488 | | 24.775 | | # |
| C13H9N ACRIDINE | | 179.2212 | 273.9 |  |  | | 177.643 | | 394.998 | |  | |  |
| C13H9N PHENANTHRIDINE | | 179.2212 | 240.5 |  |  | | 184.131 | | 391.6 | |  | |  |
| C13H10 Fluorene | | 166.21850 | 175. | 205.189 |  | | 166.651 | | 381.181 | | 25.847 | | # |
| C13H10 Phenalene | | 166.21850 | 189.4 | 219.636 | ±8. | | 167.435 | | 385.909 | | 25.800 | | # |
| C13H10O Benzophenone | | 182.21790 | 63.6 | 92.5 | ±12.5 | | 189.484 | | 443.111 | | 31.486 | | # |
| C13H12 BiPhenylMethane | | 168.23438 | 164.7 | 200.4 | ±0.7 | | 173.300 | | 430.772 | | 28.786 | | # |
| C13H12 p-BiPhenylMethane p-C6h5-C6H4-CH3 | | 168.23438 | 146.02 | 180.4 |  | | 181.845 | | 423.14 | | 30.113 | | # |
| C13H12 1-Me-2-Ethynyl Naphthalene | | 168.23438 | 181.75 | 216.42 | ±17. | | 186.907 | | 412.125 | | 29.835 | | # |
| C13H12  1-Me-1,2-H-Acenaphthylene | | 168.23438 | 102.00 | 139. | ±17. | | 175.629 | | 385.712 | | 27.522 | | # |
| C13H14 PropylNaphthalene | | 170.25026 | 76.567 | 117.516 |  | | 193.938 | | 456.288 | | 32.024 | | # |
| C13H26O2 liq n-Tridecanoic acid | | 214.34434 | -807.2 |  |  | |  | |  | |  | | X |
| C13H26O2 n-Tridecanoic acid | | 214.34434 | -660.235 | -580.2 | ±8. | | 286.957 | | 637.985 | | 52.424 | | # |
| C13H26O2 Methyl-Dodecanoate | | 214.34434 | -623.4 | -490.9 | ±15. | | 313.382 | | 666.511 | |  | |  |
| C13H28 n-TriDecane (liquid) | | 184.36142 | -377.7 |  | ±1.6 | |  | |  | |  | | X |
| C13H28 n-TriDecane | | 184.36142 | -311.5 | -179.251 | ±1.6 | | 303.340 | | 661.449 | |  | |  |
| C14H6(NO2)6 solid HNS | | 450.23068 | 58.07 |  | ±10. | |  | |  | |  | | X |
| C14H6(NO2)6 HexaNitroStilbene | | 450.23068 | 238.4 | 285.396 |  | | 411.150 | | 773.618 | | 71.248 | | # |
| C14H8 5-EthynylAcenaphthenyl | | 176.21332 | 453.25 | 473.58 | ±20. | | 181.900 | | 403.852 | | 28.294 | | # |
| C14H9 1-Antryl | | 177.22126 | 480.2 | 504.75 | ±8. | | 184.7 | | 408.7 | | 28.300 | |  |
| C14H9 2-Antryl | | 177.22126 | 478.5 | 503.06 | ±8. | | 184.9 | | 408.5 | | 28.300 | |  |
| C14H9 10-Antryl | | 177.22126 | 488.0 | 512.66 | ±8. | | 184.2 | | 409.1 | | 28.300 | | X |
| C14H9 1-Phenantryl | | 177.22126 | 458.0 | 482.65 | ±8. | | 184.1 | | 409.5 | | 28.200 | |  |
| C14H9 2-Phenantryl | | 177.22126 | 457.0 | 481.56 | ±8. | | 184.4 | | 409.5 | | 28.300 | |  |
| C14H9 3-Phenantryl | | 177.22126 | 456.4 | 480.96 | ±8. | | 184.4 | | 409.3 | | 28.300 | |  |
| C14H9 4-Phenantryl | | 177.22126 | 450.8 | 475.45 | ±8. | | 183.8 | | 408.3 | | 28.200 | |  |
| C14H9 9-Phenantryl | | 177.22126 | 456.2 | 480.75 | ±8. | | 184.3 | | 409.8 | | 28.300 | |  |
| C14H10 ANTHRACENE | | 178.2292 | 223. | 251.67 | ±10. | | 184.876 | | 392.664 | | 28.423 | | # |
| C14H10 PHENANTHRENE | | 178.2292 | 202.2 | 231.15 | ±2.3 | | 186.788 | | 394.304 | | 28.137 | | # |
| C14H10 5-VinylAcenaphthenyl | | 178.2292 | 291.9 | 320. | ±20. | | 185.949 | | 418.396 | | 29.014 | | # |
| C14H10O Phenanthrenol (any loc) | | 194.22860 | 33. |  |  | | 217.3 | | 429.78 | |  | |  |
| C14H12 solid t-Stilbene | | 180.24508 | 136.73 |  | ±10. | |  | |  | |  | | X |
| C14H12 trans-Stilbene | | 180.24508 | 223.3 | 255.957 | ±4. | | 203.066 | | 447.878 | | 32.901 | | # |
| C14H13 s-BiBenzyl Radical | | 181.25302 | 255.6 |  |  | | 208.8 | | 463.62 | |  | |  |
| C14H14 BIBENZYL <!> | | 182.26096 | 135.6 | 175.94 | ±1.3 | | 202.411 | | 477.207 | | 33.684 | | # |
| C14H28 1-Tetradecene | | 196.37212 | -206.522 | -128.536 |  | | 315.306 | | 696.218 | | 55.316 | |  |
| C14H28 CycloTetraDecane | | 196.37212 | -239.2 | -149.55 | ±2.3 | | 264.975 | | 551.862 | | 43.654 | | # |
| C14H28O2(liq) Myristic acid | | 228.37092 | -834.1 |  |  | |  | |  | |  | | X |
| C14H28O2 Myristic acid | | 228.37092 | -672.369 | -584.956 | ±15.ee300 | | 307.636 | | 647.184 | | 54.570 | | # |
| C14H28O2 (liq) Ethyl Dodecanoate | | 228.37092 | -732.6 |  |  | |  | |  | |  | | X |
| C14H28O2 Ethyl Dodecanoate | | 228.37092 | -657.7 | -515.7 | ±15. | | 333.465 | | 702.915 | |  | |  |
| C14H30 (liq) n-Tetradecane | | 198.3880 | -403.3 |  | ±1.8 | |  | |  | |  | | X |
| C14H30 n-Tetradecane | | 198.3880 | -332.1 | -255.47 | ±1.8 | | 323.591 | | 702.494 | | 65.145 | | # |
| C15H12 1-Me-Anthracene | | 192.25578 | 184.93 | 220.43 |  | | 203.843 | | 421.630 | | 31.112 | | # |
| C15H12 4 Me-Phenantrene | | 192.25578 | 195.8 | 232.5 | ±1.1 | | 196.471 | | 420.683 | | 29.917 | | # |
| C15H14 9,9-DiMethyl Fluorene | | 194.27166 | 105.3 | 147.061 |  | | 217.560 | | 426.500 | | 33.318 | | # |
| C15H16O2 BisPhenol | | 228.28634 | -251.040 | -197.048 |  | | 256.429 | | 489.212 | | 38.236 | | # |
| C15H30 1-Pentadecene | | 210.39870 | -227.233 | -147.982 |  | | 338.151 | | 735.171 | | 63.573 | |  |
| C15H30O2(liq) Pentadecanoic acid | | 242.3975 | -862.4 |  |  | |  | |  | |  | | X |
| C15H30O2 Pentadecanoic acid | | 242.3975 | -701.238 | -608.971 | ±8. | | 327.780 | | 696.299 | | 59.237 | | # |
| C15H30O2(liq) MethylMyristate | | 242.3975 | -759.4 |  |  | |  | |  | |  | | X |
| C15H30O2 MethylMyristate | | 242.3975 | -662.746 |  | ±15. | | 360.242 | | 731.782 | |  | |  |
| C15H32 (liq) n-Pentadecane | | 212.41458 | -428.8 |  | ±2.0 | |  | |  | |  | | X |
| C15H32 n-Pentadecane | | 212.41458 | -354.8 | -273.213 | ±2.0 | | 346.226 | | 741.823 | | 69.705 | | # |
| C15H32O n-Pentadecanol | | 228.41398 | -504.574 |  |  | | 361.581 | | 790.734 | |  | | # |
| C16H9 1-Pyrenyl Radical | | 201.24266 | 476.9 | 501.96 | ±8. | | 201.5 | | 418.9 | | 29.9 | |  |
| C16H9 2-Pyrenyl Radical | | 201.24266 | 473.8 | 498.76 | ±8. | | 202.0 | | 419.0 | | 30.00 | |  |
| C16H9 4-Pyrenyl Radical | | 201.24266 | 479.2 | 504.26 | ±8. | | 201.7 | | 419.2 | | 29.9 | |  |
| C16H10 PYRENE | | 202.2506 | 225.5 | 254.82 | ±2.5 | | 202.501 | | 407.507 | | 29.878 | | # |
| C16H10 1-EthynylAnthracene <http://luceneservice.lookchem.com/UploadMol/111/11198842.jpg> | | 202.25060 | 444.3 | 470.5 |  | | 212.460 | | 440.143 | | 32.937 | | # |
| C16H29O2 Palmitoleate Rad. O\* | | 253.40026 | -348.5 | -260.537 | ±25. | | 336.544 | | 708.254 | | 60.334 | | # |
| C16H30O2 cis-Palmitoleic acid | | 254.40820 | -585.342 | -493.4 | ±25. | | 341.122 | | 698.610 | | 60.651 | | # |
| C16H31O2 Palmitate Radical O\* | | 255.41614 | -475.3 | -380.46 | ±12.5 | | 343.345 | | 714.875 | | 61.951 | | # |
| C16H32O2 (liq) Palmitic acid | | 256.42408 | -848.8 |  | ±2.2 | |  | |  | |  | | X |
| C16H32O2 Palmitic acid | | 256.42408 | -711.698 | -612.164 | ±25. | | 346.926 | | 703.076 | | 61.491 | | # |
| C16H32O2(liq) EthylMyristate | | 256.42408 | -802.9 |  |  | |  | |  | |  | | X |
| C16H32O2 EthylMyristate | | 256.42408 | -697.054 |  | ±15. | | 379.070 | | 769.019 | |  | |  |
| C16H33 2-HEXADECYL Rad. | | 225.43802 | -181.67 | -25.09 |  | | 366.100 | | 818.976 | |  | | # |
| C16H34 n-HEXADECANE | | 226.44596 | -374.51 | -213.7 |  | | 370.284 | | 780.943 | |  | | # |
| C16H34O n-Hexadecanol | | 242.44056 | -517.5 | -413.665 | ±3.2 | | 337.303 | | 705.377 | | 61.319 | | # |
| C17H12 1-Methyl Pyrane | | 216.27718 | 192.9 | 228.6 | ±35. | | 217.515 | | 435.778 | | 32.985 | | # |
| C17H31O2 Margaroleate RadO\* | |  | -368.2 |  | ±25. | |  | |  | |  | |  |
| C17H31O2 MePalmitolea te-C0-yl | | 267.42684 | -378.6 | -285.249 | ±15. | | 366.327 | | 740.672 | | 64.495 | | # |
| C17H32O2 MargarOleic acid | | 268.43478 | -605.425 | -507.259 | ±25. | | 356.161 | | 724.299 | | 63.913 | | # |
| C17H32O2(liq) MethylPalmitoleate | | 268.43478 | -674.29 |  |  | |  | |  | |  | | X |
| C17H32O2 cis-MethylPalmitoleate | | 268.43478 | -576.14 |  | ±15. | | 386.183 | | 835.545 | |  | |  |
| C17H33O2 Margareate Rad O\* | | 269.44272 | -494.967 | -394.08 | ±15. | | 363.591 | | 741.763 | | 65.427 | | # |
| C17H33O2 MePalmitate-C16-yl | | 269.44272 | -492.04 |  | ±8. | | 409.39 | | 897.8 | |  | |  |
| C17H34O2 Margaric acid | | 270.45066 | -731.363 | -625.83 | ±8. | | 366.798 | | 729.877 | | 65.014 | | # |
| C17H34O2(liq) MethylPalmitate | | 270.45066 | -1441.8 |  | ±3.8 | |  | |  | |  | | X |
| C17H34O2 MethylPalmitate | | 270.45066 | -702.075 |  | ±25. | | 404.174 | | 796.634 | |  | |  |
| C17H36 (liq) n-Heptadecane | | 240.46774 | -479.5 |  | ±2.4 | |  | |  | |  | | X |
| C17H36 n-Heptadecane | | 240.46774 | -393.9 | -302.349 | ±2.4 | | 391.497 | | 820.482 | | 78.785 | | # |
| C18H10 1-Ethynyl Pyrene  1-ETHYNYLPYRENE Structure | | 226.27200 | 456.5 | 483.1 | ±30. | | 229.166 | | 450.792 | | 34.667 | | # |
| C18H12 Naphthacene | | 228.28788 | 302. | 337.48 | ±15. | | 227.829 | | 440.252 | | 34.291 | | # |
| C18H12 (s) Triphenylene solid | | 228.28788 | 146.5 |  | ±1.5 | |  | |  | |  | | X |
| C18H12 Triphenylene | | 228.28788 | 278.0 | 312.98 | ±10. | | 227.580 | | 446.288 | | 34.792 | | # |
| C18H14 1-EthylPyrene | | 230.30376 | 176.9 |  |  | | 249.366 | | 490.574 | |  | |  |
| C18H15Bi(sol) (C6H5)3Bi s | |  | 469.2  489.7 |  | ±20. | |  | |  | |  | | X |
| C18H15Bi (C6H5)3Bi | | 440.29208 | 590 | 542.8 | ±20. | | 122.860 | | 409.202 | | 47.165 | | # |
| C18H15N (s) TriPhenylAmine | | 245.31844 | 235. |  | ±3. | |  | |  | |  | | X |
| C18H15N (C6H5)3N | | 245.31844 | 327 | 371.585 | ±4.2 | | 260.410 | | 523.427 | | 42.224 | | # |
| C18H15P TriPhenylPhosphine  (C6H5)3P | | 262.28546 | 336.0 | 379.821 |  | | 262.883 | | 557.371 | | 44.013 | | # |
| C18H16Si (C6H5)3SiH | | 260.40514 | N/A | N/A |  | | 266.088 | | 571.093 | | 44.360 | |  |
| C18H29O2 Linolenate Rad. O\* | | 277.42166 | -132.63 |  | ±25. | | 363.702 | | 754.722 | | 64.877 | | # |
| C18H30O2 (liq) α Linolenic acid | | 278.42960 | -508.8 |  |  | |  | |  | |  | | X |
| C18H30O2 αLinolenic acid | | 278.42960 | -369.45 | -279.48 | ±25. | | 360.644 | | 756.212 | | 64.700 | | # |
| C18H31O2 Linoleate Radical O\* | | 279.43754 | -258.153 | -165.4 | ±25. | | 367.963 | | 769.453 | | 66.170 | | # |
| C18H32O2 (liq) Linoleic acid | | 280.44548 | -634.7 |  |  | |  | |  | |  | | X |
| C18H32O2 Linoleic acid | | 280.44548 | -494.97 | -397.1 | ±25. | | 370.428 | | 744.563 | | 65.259 | | # |
| C18H33O2 Oleate Radical O\* | | 281.45342 | -388.275 | -288.418 | ±12.5 | | 374.717 | | 776.117 | | 67.510 | | # |
| C18H34 1-Octadecyne | | 250.46256 | -123.579 | -35.485 |  | | 402.668 | | 836.131 | | 74.726 | | # |
| C18H34O2 (liq) Oleic acid | | 282.46136 | -764.8 |  |  | |  | |  | |  | | X |
| C18H34O2 Oleic acid | | 282.46136 | -624.67 | -520.81 | ±25. | | 379.761 | | 765.174 | | 67.739 | | # |
| C18H34O2 EthylPalmitOleate | | 282.46136 | -610.03 |  |  | | 409.614 | | 863.996 | |  | |  |
| C18H34O3 Ricinoleic acid | | 298.46076 | -816.717 | -809.985 | ±25. | | 389.473 | | 778.111 | | 69.209 | | # |
| C18H35O2 Stearate Radical O\* | | 283.46930 | -514.63 | -413.734 | ±25. | | 402.870 | | 833.512 | | 74.937 | | # |
| C18H36 1-Octadecene | | 252.47844 | -289.03 | -193.548 |  | | 406.768 | | 852.030 | | 75.906 | | # |
| C18H36O2 Stearic acid | | 284.47724 | -751.028 | -639.66 | ±31. | | 388.310 | | 765.562 | | 68.705 | | # |
| C18H36O2 (liq) Ethyl Palmitate | | 284.47724 | -860.2 |  |  | |  | |  | |  | | X |
| C18H36O2 Ethyl Palmitate | | 284.47724 | -736.384 | -556.31 | ±25. | | 423.421 | | 834.29 | |  | |  |
| C18H38 (l) n-Octadecane liquid | | 254.49432 | -505.4 |  | ±2.7 | |  | | 696.6 | |  | | X |
| C18H38 n-Octadecane | | 254.49432 | -414.55 | -318.039 | ±2.7 | | 414.132 | | 859.812 | | 83.345 | | # |
| C18H38O n-Octadecanol | | 270.49372 | -566.472 |  |  | | 430.199 | | 907.503 | |  | | # |
| C19H16 TriPhenylMethane | | 244.33034 | 276.1 | 324.05 | ±5. | | 247.611 | | 539.601 | | 39.810 | | # |
| C19H32O2(liq) MethylLinolenate | | 292.45618 | -472.75 |  |  | |  | |  | |  | | X |
| C19H32O2 MethylLinolenate | | 292.45618 | -358.15 | -193.96 | ±20. | | 406.266 | | 868.6 | |  | |  |
| C19H34O2(liq) MethylLinoleate | | 294.47206 | -604.88 |  |  | |  | |  | |  | | X |
| C19H34O2 MethylLinoleate | | 294.47206 | -485.762 | -313.11 | ±15. | | 418.400 | | 887.01 | |  | |  |
| C19H36O2(liq) Methyl Oleate | | 296.48794 | -727.64 |  |  | |  | |  | |  | | X |
| C19H36O2 Methyl Oleate | | 296.48794 | -615.885 | -434.76 | ±15. | | 430.115 | | 932.195 | |  | |  |
| C19H38O2(S) Methyl Stearate | | 298.50382 | -945.6 |  |  | |  | |  | |  | | X |
| C19H38O2 Methyl Stearate | | 298.50382 | -741.82 | -552.23 | ±35. | | 450.617 | | 861.9 | |  | |  |
| C19H40 (liq) n-Nanodecane | | 268.52090 | -530.9 |  | ±2.9 | |  | |  | |  | | X |
| C19H40 n-Nanodecane | | 268.52090 | -435.1 | -333.627 | ±2.9 | | 436.810 | | 898.723 | | 87.906 | | # |
| C20H10 Corannulene | | 250.29340 | 463.712 | 495.843 | ±7.3 | | 216.018 | | 412.967 | | 31.264 | | # |
| C20H12 Perylene | | 252.30928 | 306.0 | 340.0 | ±0.8 | | 254.201 | | 475.499 | | 37.878 | | # |
| C20H12 Benzo[a]Pyrene | | 252.30928 | 289.5 |  |  | | 254.800 | | 468.700 | |  | |  |
| C20H14 Alpha BiNaphtyl C20H14 | | 254.32516 | 315.055 | 395.402 |  | | 278.654 | | 513.795 | |  | |  |
| C20H14N4 Porphyrin/Porphyn (solid) | | 310.35200 | 1106.9 |  | ±3.6 | |  | |  | |  | | X |
| C20H32O2 Arachidonic acid | | 304.46688 | -342.5 | -248. | ±60. | | 403.402 | | 776.744 | | 70.717 | | # |
| C20H34O2 Ethyl Linolenate | | 306.48276 | -392.04 | -218.33 |  | | 428.44 | | 889.1 | |  | |  |
| C20H36O2 Ethyl Linoleate | | 308.49864 | -522.58 | -340.4 |  | | 445.18 | | 918.39 | |  | |  |
| C20H38O2 Gondoic acid | | 310.51452 | -689.7 | -573.2 |  | | 419.352 | | 815.869 | | 74.108 | | # |
| C20H38O2(liq) Ethyl Oleate | | 310.51452 | -773.25 |  |  | |  | |  | |  | | X |
| C20H38O2 Ethyl Oleate | | 310.51452 | -649.775 | -459.13 |  | | 452.29 | | 981.86 | |  | |  |
| C20H39O2 Archidate Rad. O\* | | 311.52246 | -554. | -440.4 | ±25. | | 442.784 | | 890.297 | | 82.276 | | # |
| C20H40O2(liq) Arachidic acid | | 312.53040 | -1012.6 |  |  | |  | |  | |  | | X |
| C20H40O2 Arachidic acid | | 312.53040 | -790.36 | -667.28 | ±22.6 | | 425.56 | | 820.830 | | 76.037 | | # |
| C20H40O2 MeNanodecanoate | | 312.53040 | -763.5 |  |  | | 477.8 | | 1000.7 | |  | |  |
| C20H40O2 (S) Ethyl Stearate | | 312.53040 | -984.6 |  |  | |  | |  | |  | | X |
| C20H40O2 Ethyl Stearate | | 312.53040 | -775.7 | -576.6 | ±50. | | 467.35 | | 905. | |  | |  |
| C20H42 (l) n-Eicosane liquid | | 282.54748 | -556.5 |  | ±3.1 | |  | |  | |  | | X |
| C20H42 n-Eicosane | | 282.54748 | -455.8 | -349.366 | ±3.1 | | 459.403 | | 938.053 | | 92.466 | | # |
| C20H42O n-Eicosanol | | 298.54688 | -607.726 |  |  | | 475.972 | | 985.499 | |  | | # |
| C21H12 Sumanene | | 264.31998 | 535.3 | 573.110 | ±9. | | 246.805 | | 443.280 | | 35.122 | | # |
| C21H42O2 Methyl Eicosanate | | 326.55698 | -781.153 | -572.5 | ±35. | | 495.804 | | 924.246 | |  | |  |
| C21H44 n-Uneicosane | | 296.57406 | -476.588 | -365.16 | ±10. | | 482.039 | | 977.299 | | 97.023 | | # |
| C22H14 Pentacene | | 278.34656 | 389.000 | 428.03 | ±15. | | 277.388 | | 494.673 | | 41.423 | | # |
| C22H14 Pentafene | | 278.35315 | 345.000 |  |  | | 282.920 | | 501.187 | |  | |  |
| C22H18 (C10H7-CH2-)2 | | 282.37832 | 279.073 | 378.46 |  | | 320.9 | | 597.89 | |  | |  |
| C22H44O2 n-Behenic acid | | 340.58356 | -845.3 | -709.5 | ±35. | | 468.476 | | 873.849 | | 82.404 | | # |
| C22H44O2 EthylEicosanate | | 340.58356 | -815.043 |  | ±35. | | 512.958 | | 962.32 | |  | |  |
| C22H46 n-Docosane | | 310.60064 | -497.059 |  |  | | 509.193 | | 1013.281 | |  | |  |
| C23H46 1-Tricosene | | 322.61134 | -391.622 |  |  | | 520.490 | | 1053.531 | |  | |  |
| C23H47 1-Ticosenyl radical | | 323.61928 | -311.290 |  |  | | 528.858 | | 1075.706 | |  | |  |
| C23H48 n-Tricosane | | 324.62722 | -517.561 |  |  | | 532.205 | | 1052.443 | |  | |  |
| C24CL12 Perchloro-coronene | | 713.68920 | 146.6 | 146.7 | ±35. | | 458.824 | | 803.678 | | 80.264 | | # |
| C24H12 Coronene | | 300.35208 | 307.5 | 345.262 | ±10. | | 262.602 | | 458.935 | | 38.331 | | # |
| C24H17 Triphenylbenzene Rad. | | 305.39898 | 623.2 |  |  | | 323.134 | | 652.000 | |  | |  |
| C24H18 Triphenylbenzene | | 306.39972 | 373.38 | 432.36 | ±15. | | 320.200 | | 604.870 | | 51.514 | | # |
| C24H20Pb(S) TetraPhenyl Lead | | 515.6156 | 515. |  | ±15. | |  | |  | |  | | X |
| C24H20Pb Pb(C6H5)4 | | 515.6156 | 674. | 727.7 | ±15. | | 371.099 | | 722.859 | | 63.103 | | # |
| C24H46O2 15-Nervonic acid | | 366.62084 | -771.95 | -633.69 | ±40. | | 503.772 | | 958.23 | | 90.477 | | # |
| C24H48O2 n-Lignoceric acid | | 368.63672 | -886.6 | -740.6 | ±40. | | 507.208 | | 944.963 | | 91.171 | | # |
| C25H20 C(C6H5)4 | | 320.42630 | 393. | 449.2 | ±6.3 | | 334.652 | | 654.026 | | 54.783 | | # |
| C25H52 n-Pentacosane | | 352.68038 | -558.56 |  | ±10. | | 574.540 | | 1130.84 | |  | | # |
| C28H58 n-Octacosane | | 394.76012 | -620.487 |  | ±25. | | 644.336 | | 1255.20 | |  | | # |
| C30H10 Half-BuckminsterFullerene | | 370.40040 | 1139.303 | 1168.575 | ±12. | | 323.869 | | 494.466 | | 44.674 | | # |
| C30H62 n-Triacotane | | 422.81320 | -662.05 |  | ±10. | | 688.34 | | 1326.55 | |  | | # |
| C31H64 n-HenTriacotane | | 436.83986 | -682.2 |  | ±10. | | 718.500 | | 1373.40 | |  | | # |
| C32H13 Ovalenyl Radical | | 397.44562 | 663.541 | 701.746 | ±20. | | 359.727 | | 558.246 | | 50.510 | | # |
| C32H14 Ovalene | | 398.45356 | 418.4 | 460.8 | ±12. | | 361.353 | | 546.813 | | 50.580 | | # |
| C44H30N4 5,10,15,20-Tetra-Phenyl-Porphyrin/Porphyne (sol) | | 614.73580 | 784. |  | ±15. | |  | | 679.0 | |  | | X |
| C44H30N4 5,10,15,20-Tetra-Phenyl-Porphyrin/Porphyne gas | | 614.73580 | 1004. |  | ±10 | |  | | 946.8 | |  | | X |
| C57H104O9 GlycerinTriRicinoleate | |  | -2199.5 |  |  | |  | |  | |  | | X |
| C60 (cr) BuckminsterFullerene | | 720.64200 | 2346. | 2337. | ±12. | | 525.6 | | 427.1 | | 72.520 | | # |
| C60 gas Buckminster Fullerene | | 720.64200 | 2511.7 | 2516.484 | ±30. | | 498.510 | | 534.818 | | 58.426 | | # |
| C62H111O9 (L) Castor oil natural | | 1000.54 | -2620.6 |  | ±100. | |  | |  | |  | | X |
| C70(cr) Footballene crystal | | 840.74900 | 2555. | 2551.625 | ±22 | | 625.6 | | 452.7 | | 77.120 | | # |
| C70 Footballene | | 840.74900 | 2652. | 2660.33 | ±34. | | 558.171 | | 589.537 | |  | | # |
| JET-A(L) | | 167.31102 | -303.469 |  |  | | 350.336 | | 448.112 | |  | | † |
| JET-A(G) (C12H23) | | 167.31102 | -211.46 |  |  | | 293.494 | | 612.539 | |  | | † |
| Ca (S) REFERENCE ELEMENT | | 40.07800 | 0. | 0. |  | | 25.75 | | 42.536 | | 5.783 | | † |
| Ca (gas) | | 40.07800 | 177.8 | 177.386 | ±0.8 | | 20.786 | | 154.887 | | 6.197 | | † |
| Ca+ | | 40.07740 | 773.2 |  | ±0.2 | | 20.786 | | 160.650 | | 6.197 | | † |
| CaCO3 (S) Calcium Carbonate | | 100.08690 | -1206.600 | -1201.223 |  | | 83.472 | | 91.710 | | 14.480 | | # |
| CaO (S) | | 56.07740 | -634.920 | -631.548 | ±0.9 | | 42.050 | | 38.100 | | 6.750 | | † |
| CaO gas | | 56.07740 | 38.005 | 39.175 | ±10. | | 32.454 | | 219.715 | | 8.953 | | † |
| CaO+ | | 56.07885 | 710.238 | 705. | ±10. | | 34.537 | | 233.606 | | 9.163 | | † |
| Cd (S,L) REFERENCE ELEMENT | | 112.41100 | 0. | 0. |  | | 26.020 | | 51.800 | | 6.247 | | † |
| Cd gas | | 112.41100 | 111.800 | 111.850 |  | | 20.786 | | 167.750 | | 6.197 | | † |
| Cd+ | | 112.41045 | 985.754 | 979.606 |  | | 20.786 | | 173.513 | | 6.197 | | † |
| CL <~> | | 35.4527 | 121.302 | 119.620 | ±0.002 | | 21.838 | | 165.192 | | 6.272 | | † |
| CL+ | | 35.45215 | 1378.80 | 1370.807 | ±0.002 | | 22.959 | | 167.558 | | 6.388 | | † |
| CL - <~> | | 35.45325 | -233.543 | -228.952 | ±0.003 | | 20.786 | | 253.358 | | 6.197 | | † |
| CuCl (see under Cu) | |  |  |  |  | |  | |  | |  | |  |
| DCL | | 37.4668 | -93.547 | -93.333 | ±0.21 | | 29.170 | | 192.773 | | 8.661 | | † |
| DOCL | | 53.4662 | -79.539 | -76.648 | ±2.1 | | 38.585 | | 240.321 | | 10.325 | | † |
| CLF <&> | | 54.4511 | -55.701d | -55.706 | ±0.063 | | 32.085 | | 217.943 | | 8.908 | | † |
| CLF+ g | | 54.45055 | 1171.967g | 1165.59g | ±0.59 | | 31.389 | | 222.729 | | 16.372 | | # |
| CLF- g | | 54.45165 | -261.587g | -258.2d | ±0.8g | | 36.487 | | 235.643 | | 9.922 | | # |
| CLO3F | | 102.4493 | -23.799 | -15.076 |  | | 64.927 | | 278.989 | | 13.299 | | † |
| CLF3 <&> | | 92.44791 | -164.6 | -160.5 | ±5. | | 64.061 | | 282.152 | | 13.728 | | † |
| ClF5 | | 130.44472 | -238. | -229.277 | ±7. | | 97.167 | | 310.257 | | 17.930 | | † |
| HCL <^~> | | 36.46094 | -92.31 | -92.125 | ±0.006 | | 29.136 | | 186.901 | | 8.640 | | † |
| HCL+ | | 36.46009 | 1143.81 | 1137.794 | ±0.005 | | 29.146 | | 193.202 | | 8.643 | | # |
| HCL- c | | 36.46118 | -30.7g | -25.5d | ±3.d | | 34.749 | | 205.189 | | 9.316 | | # |
| HCLO\*g Chlorosyl hydride | | 52.46004 | 139.100 | 141.960 | ±2.3g | | 38.339 | | 238.443 | | 10.304 | | # |
| HOCLd Hypochlorous acid <~> | | 52.46004 | -76.149 | -73.205 | ±0.028 | | 37.264 | | 236.971 | | 10.221 | | # |
| HOCL+ c | | 52.45949 | 996.91 | 993.784 | ±3.13 | | 36.042 | | 240.932 | | 10.093 | | # |
| HOCL- g Hypochlorous acid | | 52.46059 | 196.4 | 196.7 | ±2.2.g | |  | |  | |  | | X |
| HCLO2 | | 68.45944 | 20.92 | 25.94 | ±1.67 | | 50.512 | | 281.726 | | 12.531 | | # |
| HCLO3 HO-ClO2 | | 84.45884 | -10.878 | -3.200 | ±1.25 | | 63.375 | | 299.446 | | 14.166 | | # |
| HCLO4 HO-ClO3 | | 100.45824 | -0.418 | +11.234 | ±1. | | 69.774 | | 300.191 | | 14.532 | | # |
| HCLH+ Chloroniumd | | 37.46803 | 884.6d | 881.5d | ±1.2d | | 33.938 | | 206.343 | | 9.949 | | # |
| CLNH2 (see NCLH2) | | 51.47532 |  |  |  | |  | |  | |  | | # |
| ICl cr | | 162.35717 | -65.537d | -36.511d | ±0.063 | |  | |  | |  | | X |
| ICL | | 162.35717 | 17.39 | 19.029 | ±0.01 | | 35.532 | | 247.451 | | 9.549 | | # |
| ClNO c  (see NOCl) | | 65.45884 | 52.517 | 54.419 | ±0.065 | |  | |  | |  | | † |
| ClNO2 | | See NO2Cl |  |  |  | |  | |  | |  | |  |
| ClONO2 Chloronitrate | | 97.45764 | 22.389 | 29.466 | ±8. | | 68.705 | | 302.565 | | 14.869 | | # |
| CLO <~> | | 51.4521 | 101.7 | 101.385 | ±0.03 | | 33.804 | | 233.421 | | 9.246 | | #† |
| CLO+g | | 51.45155 | 1156.53 | 1150.58d | ±0.66 | | 30.381 | | 206.006 | | 8.741 | | # |
| CLO- c | | 51.45265 | -124.53 | -118.62d | ±0.13 | | 34.184 | | 198.763 | | 9.193 | | # |
| CLO2 (O=ClO\*) | | 67.4515 | 99.035 | 101.518 | ±6.3 | | 41.921 | | 257.555 | | 10.788 | | #† |
| CLOO\* <~> | | 67.4518 | 101.671 | 102.712 | ±4.0 | | 47.463 | | 276.894 | | 12.230 | | # |
| CLO3 | | 83.45090 | 185.351 | 190.574 | ±1.67 | | 56.096 | | 282.289 | | 12.388 | | # |
| CLO4 radical | | 99.4503 | 272.671 | 279.875 | ±8. | | 72.691 | | 289.473 | | 14.427 | | # |
| CLS | | See SCL |  |  |  | |  | |  | |  | |  |
| TCl Tritium Chloride | | 38.469 | -97.424 | -88.803 | ±8. | | 29.273 | | 196.081 | | 8.672 | | # |
| CL2 REFERENCE ELEMEN<^> | | 70.9054 | 0 | 0 |  | | 33.949 | | 223.082 | | 9.181 | | † |
| CL2+c | | 70.9049 | 1114.07 | 1107.90 | ±0.2 | | 36.417 | | 228.704 | | 9.376 | | # |
| CL2-d | | 70.90595 | -235.88 | -230.7d | ±1.8d | | 37.706 | | 222.426 | | 10.283 | | # |
| Cl2Cu (see under Cu) | |  |  |  |  | |  | |  | |  | |  |
| CL2NH DicloroAmine | | (see under NCL2H) | |  |  | |  | |  | |  | | # |
| CL2O Cl-O-CL <~> | | 86.90480 | 78.743 | 80.569 | ±0.67 | | 47.811 | | 267.951 | | 11.695 | | #† |
| CL2O ClClO | | 86.90480 | 140.683 | 141.981 | ±8. | | 48.845 | | 278.463 | | 12.223 | | # |
| CL2O2 | | 102.9042 | 131.754 | 135.345 | ±1.25 | | 65.034 | | 295.883 | | 14.273 | | # |
| CL2O7 ClO3-O-ClO3 | | 182.90120 | 275.726 | 293.029 | ±8.4 | | 118.323 | | 400.922 | | 22.258 | | # |
| CL3Cu3 (See under Cu) | |  |  |  |  | |  | |  | |  | |  |
| CL3N (See under NCL3) | | 120.36484 |  |  |  | |  | |  | |  | | # |
| Co (cr,l) Reference Element | | 58.93320 | 0. | 0. |  | | 24.802 | | 30.067 | | 4.771 | | † |
| Co Cobalt gas | | 58.93320 | 428.432 | 426.853 | ±4.2 | | 23.024 | | 179.520 | | 6.360 | | † |
| Co+ | | 58.93265 | 1193.003 | 1185.285 |  | | 22.271 | | 178.340 | | 6.292 | | † |
| Co- anion | | 58.3375 | 358.414 | 363.076 | ±2.1 | | 22.439 | | 178.414 | | 6.307 | | † |
| Cr(cr) REFERENCE ELEMENT | | 51.9961 | 0 | 0 |  | | 23.434 | | 23.618 | | 4.057 | | † |
| Cr | | 51.9961 | 397.48 | 395.34 | ±4.2 | | 20.786 | | 174.313 | | 6.197 | | † |
| Cr+ cation | | 51.99555 | 1056.209 | 1047.872 |  | | 20.786 | | 173.029 | | 6.197 | | # |
| CrCl | | 87.4488 | 129.9 | 129.159 | ±2.7 | | 34.684 | | 249.790 | | 9.389 | | # |
| CrClO | |  | -117.9 |  | ±9.6 | |  | | 301.01 | | 13.574 | | X |
| CrClO2 | |  | -310.3 |  | ±21.6 | |  | | 309.81 | | 14.449 | | X |
| CrCl2 | | 122.90150 | -117.6 | -117.85 | ±1.7 | | 53.795 | | 275.620 | | 13.490 | | # |
| CrCl2O | |  | -336.5 |  | ±22.5 | |  | | 333.03 | | 16.784 | | X |
| CrCl2O2 | | 154.90030 | -519.2 | -515.35 | ±4.2 | | 84.052 | | 329.53 | | 18.066 | | # |
| CrCl3(cr) | | 158.35420 | -556.472 |  |  | | 91.799 | | 123.010 | |  | | # |
| CrCl3 | | 158.35420 | -283.0 | -282.707 | ±6.1 | | 74.546 | | 325.46 | | 17.536 | | # |
| CrCl3O | |  | -507.8 |  | ±3.0 | |  | | 357.32 | | 20.049 | | X |
| CrCl4 | | 193.80690 | -396.5 | -395.831 | ±13.8 | | 96.120 | | 317.625 | | 21.751 | | # |
| CrCl5 | | 229.25696 | -389.6 | -389.026 |  | | 120.170 | | 394.161 | | 26.436 | | # |
| CrCl6 | | 264.71230 | -345.3 | -344.58 | +50. | | 143.573 | | 414.95 | | 30.878 | | # |
| Cr(OH)6 | | 154.04014 | -1016.17 | -988.022 | ±33.5 | | 161.489 | | 368.630 | | 26.812 | | # |
| CrN(s) | | 66.00284 | -117.152 | -116.465 | ±8.4 | | 52.677 | | 37.711 | | 7.705 | | † |
| CrN | | 66.00284 | 505.009 | 504.523 | ±20.9 | | 30.754 | | 230.556 | | 8.778 | | † |
| CrO | | 67.99550 | 188.280 | 187.849 | ±41.8 | | 31.321 | | 239.271 | | 8.828 | | # |
| CrO2 | | 83.9949 | -108.043 | -106 | ±15. | | 41.971 | | 265.575 | | 10.694 | | † |
| CrO3 | | 99.9943 | -322.037 | -318.00 | ±15. | | 58.658 | | 269.408 | | 13.040 | | † |
| CrO3- | | 99.9949 | -738.9 | -729.049 | ±34. | | 60.322 | | 277.590 | | 13.423 | | # |
| Cr2 (g) | | 103.99220 | 611.287 | 610.014 |  | | 35.006 | | 229.381 | | 9.387 | | # |
| Cr2N(s) | | 117.99894 | -125.520 |  | ±12.6 | | 66.065 | | 64.921 | |  | | † |
| Cr2O3(s) | | 151.9904 | -1140.6 | -1134.766 | ±8.4 | | 120.08 | | 81.100 | | 15.300 | | † |
| Cr2FeO4 | | 223.8348 | -1458.12 |  |  | | 133.69 | | 141.963 | |  | |  |
| Cr3C2(S) | | 180.0103 | -85.354 |  |  | | 99.326 | | 85.437 | |  | |  |
| Cr7C3(S) | | 400.0057 | -160.666 |  |  | | 209.764 | | 200.999 | |  | |  |
| C6Cr23(S) | | 1267.9763 | -328.444 |  |  | | 628.117 | | 612.119 | |  | |  |
| Cu (cr) REFERENCE ELEMRNT | | 63.546 | 0. | 0. |  | | 24.440 | | 33.150 | | 5.004 | | † |
| Cu | | 63.546 | 337.4 | 336.207 |  | | 20.786 | | 166.399 | | 6.197 | | † |
| Cu+ | | 63.54545 | 1089.080 | 1081.689 |  | | 20.786 | | 160.636 | | 6.197 | | † |
| Cu- | | 63.54654 | 212.719 | 217.723 |  | | 20.786 | | 160.636 | | 6.197 | | † |
| CuCl | | 98.99870 | 91.090 | 91.213 | ±1.67 | | 35.262 | | 237.210 | | 9.471 | | † |
| CuCl2(S) | | 134.4520 | -217.986 | -218.798 |  | | 71.873 | | 108.516 | | 14.983 | | † |
| CuF | | 82.54440 | -12.550 | -12.217 | ±16.7 | | 33.380 | | 226.498 | | 9.083 | | † |
| CuF2 | | 101.54281 | -266.940 | -265.167 | ±12.55 | | 47.988 | | 267.090 | | 12.056 | | † |
| CuO | | 79.54540 | 306.270 | 305.863 | ±41.8 | | 35.693 | | 234.621 | | 9.751 | | † |
| Cu2 | | 127.0920 | 485.340 | 485.418 | ±12.6 | | 36.585 | | 241.724 | | 9.934 | | † |
| Cu3Cl3 | | 296.9961 | -258.270 | -258.510 | ±2.09 | | 124.572 | | 429.553 | | 28.724 | | † |
| D | | 2.0141 | 221.717 | 219.804 | ±0.001 | | 20.786 | | 123.352 | | 6.197 | | † |
| D+ | | 2.01355 | 1540.320 | 1532.210 | ±0.000 | | 20.786 | | 117.585 | | 6.197 | | † |
| D- | | 2.01465 | 142.75d | 146.99d | ±0.002 | | 20.786 | | 117.592 | | 6.197 | | † |
| DF | | 21.01251 | -276.228 | -276.169 | ±0.8 | | 29.137 | | 179.705 | | 8.638 | | † |
| DI | | 128.91857 | 26.26 | 28.46 | ±0.5 | | 29.321 | | 212.423 | | 8.685 | | # |
| HD | | 3.02204 | 0.319 | 0.328 | ±8.3E-5 | | 29.200 | | 143.801 | | 8.509 | | † |
| HD+ | | 3.02149 | 1496.793 | 1490.60 | ±2.6E-5 | | 29.334 | | 155.552 | | 8.614 | | † |
| NHD Radical | | 17.02878 | 67.66 | 76.778 | ±8. | | 35.521 | | 232.424 | | 10.521 | | # |
| HDO | | 19.02144 | -245.280 | -242.35 |  | | 33.798 | | 199.517 | | 9.926 | | † |
| HDO2 | | 35.02084 | -140.242 | -134.38 |  | | 43.779 | | 243.581 | | 11.335 | | † |
| DN | | 16.0208 | (see ND) |  |  | |  | |  | |  | |  |
| DOT Deuterium-Tritium Water | | 21.02955 | -258.588 | -255.647 | ±8. | | 34.255 | | 206.587 | | 9.968 | | # |
| DO2 | | 34.0129 | 6.487 | 9.387 |  | | 35.845 | | 232.883 | | 10.065 | | † |
| DO2- | | 34.01345 | -104.796 | -95.713 |  | | 36.041 | | 227.860 | | 10.080 | | † |
| SD | | 34.0801 | 140.14 | 140.17 | ±0.52 | | 29.239 | | 198.212 | | 8.666 | | # |
| SiD | | 30.09960 | 361.749 | 367.565 | ±8. | | 29.555 | | 198.661 | | 8.686 | | # |
| SiD+ | | 30.09905 | 1145.161 | 1125.316 | ±8. | | 29.516 | | 193.017 | | 8.684 | | # |
| SiD- | | 30.10015 | 295.917 | 300.917 | ±8. | | 29.764 | | 193.429 | | 8.699 | | # |
| Si2D | | 58.18510 | 493.18 | 491.3 | ±8. | | 46.438 | | 284.446 | | 12.607 | | # |
| DT Deutherium Tritide D3H | | 5.03015 | 0.089 | 0.089 |  | | 29.196 | | 154.880 | | 8.589 | | # |
| D2 REFERENCE ELEMENT <^> | | 4.0282 | 0 | 0 |  | | 29.195 | | 144.96 | | 8.569 | | † |
| D2+ | | 4.02766 | 1498.586 | 1492.29 | ±0.00 | | 29.510 | | 156.735 | | 8.651 | | † |
| D2- | | 4.02875 | 235.161 | 241.213 |  | | 30.315 | | 158.261 | | 8.714 | | † |
| ND2 | | 18.0349 | 290.762 | 296.930 | ±0.6 | | 45.729 | | 243.380 | | 11.121 | | # |
|  | N2D2 *cis* (see under N2 species) | 32.0416 | 202.857 | 209.788 | |  | | 39.025 | | 224.095 | | 10.308 | | | #† | |
| D2N2O2 NitroAmine-D2 | | 64.04048 | -12.527 | +0.110 | ±8. | | 63.736 | | 275.964 | | 13.282 | | # |
| D2O <^> | | 20.0276 | -249.209 | 246.261 | ±0.067 | | 34.265 | | 198.342 | | 9.960 | | † |
| D2O2 | | 36.027 | -144.3 | -138.61 |  | | 45.252 | | 242.085 | | 11.563 | | † |
| D2S | | 36.0942 | -24.047 | -21.114 | ±0.8 | | 35.795 | | 215.316 | | 10.089 | | † |
| SiD2 D-Si-D | | 32.11370 | 262.824 | 264.418 | ±8. | | 37.031 | | 217.458 | | 10.193 | | # |
| SiD2+ cation | | 32.11315 | 1155.624 | 1150.938 | ±8. | | 37.518 | | 222.013 | | 10.276 | | # |
| SiD2*–* | | 32.11425 | 147.281 | 161.210 | ±8. | | 37.761 | | 224.001 | | 10.252 | | # |
| SiD2T2 Silane-D2-T2 | | 38.1458 | 4.824 | 13.255 | ±10. | | 55.247 | | 233.027 | | 11.719 | | # |
| Si2D2 D-SiSi-D | | 60.19920 | 451.340 | 451.964 | ±8. | | 59.768 | | 272.843 | | 14.380 | | # |
| Si2D2- anion | | 60.19975 | 262.738 | 270.136 | ±8. | | 58.791 | | 272.728 | | 13.535 | | # |
| ND3 Amonia-d3 | | 20.04901 | -145.378 | -139.2 |  | | 29.143 | | 178.409 | | 8.642 | | † |
| SiD3 | | 34.12781 | 191.761 | 196.765 | ±8. | | 45.928 | | 229.809 | | 11.067 | | # |
| SiD3+ cation | | 34.12726 | 996.129 | 988.839 | ±8. | | 45.179 | | 223.200 | | 10.967 | | # |
| SiD3- anion | | 34.12835 | 37.431 | 55.003 | ±8. | | 45.331 | | 224.113 | | 10.894 | | # |
| SiD4 | | 36.14191 | 22.792 | 31.610 | ±8. | | 52.240 | | 219.352 | | 11.537 | | # |
| D4Ge | | 80.66640 | 84.934 | 94.798 | ±5. | | 55.008 | | 232.029 | | 11.911 | | # |
| D4Sn TetrahydroStanum-d4 | | 126.76640 | 167.218. | 177.203 | ±6. | | 62.794 | | 248.508 | | 13.476 | | # |
| ELECTRON GAS e- <^~> | | 0.00055 | 0 | 0 |  | | 20.786 | | 20.979 | | 6.197 | | † |
| F <~> | | 18.9984 | 79.39 | 77.274 | ±0.058 | | 22.747 | | 158.752 | | 6.518 | | † |
| F+ | | 18.99785 | 1766.661 | 1758.165 | ±0.059 | | 23.497 | | 182.644 | | 6.197 | | † |
| F- c | | 18.99895 | -255.31 | -250.897 | ±0.06 | | 20.786 | | 145.578 | | 6.197 | | † |
| HF liquid | | 20.00634 | -302.45d |  | ±0.17d | |  | |  | |  | | X |
| HFa <^~> | | 20.00634 | -272.864 | -272.817 | ±0.06 | | 29.138 | | 173.783 | | 8.599 | | † |
| HF+a Fluoroniumyld | | 20.00579 | 1281.847 | 1275.62 | ±0.06d | | 29.102 | | 183.236 | | 8.676 | | # |
| HF- g | | 20.00689 | -81.1 | -75.4d | ±2.0g | | 32.281 | | 211.973 | | 8.935 | | # |
| HOF Hypofluorous acid <~> | | 36.00574 | -87.262 | -84.364 | ±0.18 | | 35.94 | | 226.757 | | 10.088 | | # |
| HOF+ | | 36.00519 | 1145.29 | 1142.103 | ±0.87 | | 34.509 | | 230.946 | | 9.977 | | # |
| HOF- Hypoflorous acid | | 36.00629 | 145.7g | 152.7d | ±3.8d | |  | |  | |  | | X |
| HFH+ Fluoronium | | 21.01373 | 778.39d | 775.1d | ±1.2d | | 33.610 | | 191.063 | | 9.931 | | # |
| IF Iodine Monofluoride | | 145.90287 | -94.76 | -92.85 |  | | 33.383 | | 236.138 | | 9.091 | | # |
| FNO see NOF | |  |  |  |  | |  | |  | |  | |  |
| FNO2 see NO2F | |  |  |  |  | |  | |  | |  | |  |
| FNO3 see NO3F | |  |  |  |  | |  | |  | |  | |  |
| FO Fluoroxyl radical <~> | | 34.9978 | 111.267 | 110.632 | ±0.15d | | 31.995 | | 216.396 | | 9.388 | | † |
| FO+ c | | 34.99725 | 1348.77g | 1342.39d | ±0.78 | | 29.537 | | 199.357 | | 8.690 | | # |
| FO- g Hypofluoriteg | | 34.99835 | -114.93g | -108.90g | ±0.48 | | 31.787 | | 196.769 | | 8.871 | | # |
| FO2 O-F-O <~> | | 50.9972 | 521.222 | 523.776 | ±0.88 | | 41.126 | | 251.289 | | 10.538 | | #† |
| OFO+ Dioxofluorine cation | | 50.99665 | 1671.0g | 1667.0 | ±2.8 | | 44.084 | | 244.071 | | 10.970 | | # |
| OFO- Dioxofluorine | | 50.99775 | 148.1g | 155.9 | ±2.5 | | 47.958 | | 257.173 | | 11.676 | | # |
| FO2 F-O-O Dioxygenyl Fluoride | | 50.9972 | 25.4 | 26.93d | ±0.26d | | 44.453 | | 259.511 | | 11.256 | | † |
| FO2+ F-O-O+ Fluorodioxidenium | | 50.99665 | 1225.7g | 1221.9 | ±2.0g | | 40.241 | | 247.719 | | 10.542 | | # |
| FO2- FOO- | | 50.99775 | -262.3 | -256.9 | ±1.9g | | 46.032 | | 257.921 | | 11.618 | | # |
| TF Tritium Fluoride | | 22.01445 | -291.964 | -273.501 |  | | 29.147 | | 183.110 | | 8.652 | | # |
| FW see WF | |  |  |  |  | |  | |  | |  | |  |
| F2 REFERENCE ELEMEN<^~> | | 37.99681 | 0 | 0 |  | | 31.304 | | 202.792 | | 8.825 | | † |
| F2+ | | 37.99626 | 1520.777 | 1513.989 | ±0.175 | | 33.528 | | 210.831 | | 9.415 | | # |
| F2- | | 37.99736 | -297.7d | -292.3d | ±1.6d | | 35.581 | | 218.211 | | 9.572 | | # |
| HF2 FHFc | | 39.00475 | -203.8d | -203.7d | ±2.5d | |  | |  | |  | | X |
| HF2+ FHF+a | |  | 1182.8 |  | ±10.9 | |  | |  | |  | | X |
| HF2- c FHF- | | 39.00529 | -720.37 | -711.53 | ±2.30 | | 38.935 | | 229.453 | | 10.418 | | # |
| HF2+ FFH+ d | | 39.0042 | 1178.76 | 1175.5d | ±2.0d | |  | |  | |  | | X |
| HF2- FFH- c | |  | -483.77 | -477.2d | ±3.2d | |  | |  | |  | | X |
| HF2+a | |  | 779.197 |  | ±10. | |  | |  | |  | | X |
| H2F2 | | 40.01269 | -569.924 | -566.5 | ±4. | | 58.132 | | 260.905 | | 13.869 | | † |
| F2O F-O-F <~> | | 53.99621 | 24.5 | 26.754 | ±0.25d | | 43.495 | | 247.508 | | 10.912 | | † |
| F2O+ F-O-F+ | | 53.99566 | 1296.48 | 1292.885 | ±0.67d | | 40.649 | | 250.062 | | 10.563 | | # |
| F2O- F-O-F- | | 53.99675 | -200.58 | -194.62 | ±3.65 | | 53.280 | | 270.801 | | 13.407 | | # |
| FFOFluorosyl fluoride | | 53.99621 | 189.53d | 189.2d | ±4.8d | |  | |  | |  | | X |
| FFO+ c | | 53.99566 | 1419.6g | 1413.0 | ±3.5g | |  | |  | |  | | X |
| FFO- c | |  | -59.17d | -53.6d | ±6.1d | |  | |  | |  | | X |
| F2O2 OOF2 | | 69.99561 | 71.25 | 75.5d | ±7.8d | |  | |  | |  | | X |
| F2O2 F-O-O-F <~> | | 69.99561 | 32.87 | 36.597 | ±0.38d | | 62.073 | | 277.214 | | 13.778 | | † |
| F2O2+ F-O-O-F+ | | 69.99506 | 1286.2g | 1283.6g | ±2.3 | | 57.726 | | 279.227 | | 13.453 | | # |
| F2O2+ F-O-O-F+ *cis* | | 69.99506 | 1289.0 | 1287.1 | ±2.3g | |  | |  | |  | | X |
| F2O2- F-O-O-F- c | | 69.99615 | -257.2. | -251.0g | ±28.g | |  | |  | |  | | X |
| F2O3 F-O-O-O-F | | 85.99500 | 111.32 | 116.82 | ±7.59 | | 75.661 | | 303.972 | | 16.347 | | # |
| F2S2 F-S-S-F See S2F2 | |  | -322.2 |  | ±2.1 | |  | |  | |  | | # |
| F2S2 SSF2 See S2F2 | |  | -331.8 |  | ±2.1 | |  | |  | |  | | # |
| F2W See WF2 | |  | -86.19 |  | ±13.5 | |  | |  | |  | | # |
| F3 c | | 56.99521 | 87.1d | 86.3d | ±3.7d | |  | |  | |  | | X |
| F3+ c | | 56.99466 | 1533.6g | 1529.5g | ±2.3g | |  | |  | |  | | X |
| F3- c | | 56.99576 | -370.48d | -363.3d | ±3.2d | | 50.819 | | 284.322 | | 12.254 | | # |
| H3F3 | | 60.01903 | -883.677 | -873. | ±8. | | 73.884 | | 280.947 | | 15.263 | | † |
| F3W See WF3 | |  |  |  |  | |  | |  | |  | | # |
| H4F4 | | 80.02537 | -1186.93 | -1174. | ±12. | | 104.022 | | 350.016 | | 21.654 | | † |
| F4W See WF4 | |  |  |  |  | |  | |  | |  | | # |
| H5F5 | | 100.03172 | -1490.19 | -1475. | ±20. | | 134.161 | | 417.286 | | 28.045 | | † |
| F5W See WF5 | |  |  |  |  | |  | |  | |  | | # |
| H6F6 <^> | | 120.03806 | -1805.54 | -1788. | ±8. | | 163.735 | | 486.619 | | 34.334 | | † |
| H7F7 | | 140.0444 | -2099.7 | -2080. | ±30. | | 194.438 | | 548.654 | | 40.827 | | † |
| Fe(a) REFERENCE ELEMENT | | 55.847 | 0 | 0 |  | | 25.094 | | 27.321 | | 4.507 | | † |
| Fe | | 55.847 | 415.5 | 413.128 | ±1.3 | | 25.675 | | 180.49 | | 6.850 | | † |
| Fe+ | | 55.84645 | 1181.144 | 1175.59 |  | | 26.068 | | 181.859 | | 6.936 | | † |
| Fe- | | 55.84755 | 393.338 | 397.4 |  | | 25.023 | | 180.2 | | 6.642 | | † |
| FeC5O5 (liq) Fe(CO)5 liquid | | 195.8955 | -766.09 | -787.55 | ±7.1 | | 233.785 | | 337.078 | | 52.934 | | † |
| FeC5O5 Fe(CO)5 | | 195.8955 | -727.850 | -729.521 | ±7.1 | | 170.705 | | 439.291 | | 33.145 | | † |
| FeCL | | 91.2997 | 251.036 | 249.76 | ±84. | | 38.223 | | 257.577 | | 10.377 | | † |
| FeClO(s) Iron Oxychloride | | 107.2971 | -410.994 | -410.497 | ±0.92 | | 70.5 | | 82.55 | | 12.940 | | † |
| FeCL2(s) | | 126.7524 | -341.833 | -344.418 | ±0.42 | | 76.664 | | 117.947 | | 16.273 | | † |
| FeCL2 | | 126.7504 | -141 | -141.59 | ±2.1 | | 57.571 | | 299.287 | | 14.277 | | † |
| FeCL3(s) | | 162.2051 | -399.237 | -400.399 | ±0.84 | | 96.943 | | 147.821 | | 19.441 | | † |
| FeCL3 | | 162.2031 | -253.13 | -253.07 | ±5 | | 77.703 | | 344.210 | | 18.214 | | † |
| Fe0.947O(s) Wustite | | 71.8444 | -272.037 |  |  | | 47.990 | | 57.488 | |  | | † |
| FO  FO X5Δ | | 71.84614 | 251.040 | 251.050 | ±20.9 | | 31.406 | | 241.926 | | 8.837 | | † |
| FeO2 (av OFeO, CyFe(O2),FeOO) | | 87.8438 | 75.55 | 77. | ±10. | | 45.581 | | 273.117 | | 11.741 | | # |
| Fe(OH)2(s) | | 89.85968 | 5 |  | ±2.9 | | 97.069 | | 87.864 | |  | | † |
| Fe(OH)2 | | 89.85968 | -330.536 | -323.09 | ±2.1 | | 71.505 | | 283.092 | | 14.209 | | † |
| Fe(OH)3(s) | | 106.86702 | -832.627 |  | ±12.6 | | 101.671 | | 104.600 | |  | | † |
| FeS(a) | | 87.911 | -101.818 | -100.116 | ±0.8 | | 50.543 | | 60.312 | | 9.414 | | † |
| FeS(G) | | 87.911 | 370.767 |  |  | | 34.002 | | 252.344 | |  | | † |
| FeSO4(s) | | 151.9086 | -928.848 | -919.338 | ±8.4 | | 100.583 | | 120.955 | | 16.769 | | † |
| FeS2(s) Pyrite | | 119.9770 | -171.544 | -167.854 | ±2.1 | | 62.124 | | 52.915 | | 9.641 | | † |
| Fe2CL4 | | 253.5008 | -431.370 | -433.843 | ±4.2 | | 125.876 | | 464.506 | | 29.849 | | † |
| Fe2CL6 | | 324.4062 | -654.378 | -658.268 | ±8.4 | | 173.665 | | 536.945 | | 40.448 | | † |
| Fe2O3(S) Solid-A Hematite | | 159.6882 | -817.088 |  |  | | 103.763 | | 87.404 | |  | | † |
| Fe2(SO4)3 Solid | | 399.8808 | -2582.99 |  | ±1.7 | | 264.722 | | 307.524 | |  | | † |
| Fe3C (S) Solid-A | | 179.546 | 25.104 |  |  | | 105.868 | | 104.6 | |  | |  |
| Fe3O4(S) Solid-A Magnetite | | 231.5326 | -1118.38 | -1112.264 |  | | 150.791 | | 146.147 | | 24.762 | | † |
| Ga(cr,l) REFERENCE ELEMENT | | 69.72300 | 0 | 0 |  | | 26.099 | | 41.220 | | 5.640 | | † |
| Ga(g) Galium | | 69.72300 | 272.000 | 271.089 |  | | 25.347 | | 169.045 | | 6.551 | | † |
| Ga+ | | 69.72245 | 856.688 | 849.934 |  | | 20.786 | | 161.793 | | 6.197 | | † |
| Ge(S) Reference Element | | 72.61 | 0. | 0. |  | | 23.222 | | 31.090 | | 4.636 | | † |
| Ge | | 72.61 | 367.8 | 365.038 | ±2. | | 30.733 | | 167.909 | | 7.399 | | † |
| Ge- | | 72.61055 | 245.4 | 249.25 | ±1. | | 21.985 | | 180.831 | | 6.981 | | † |
| GeBr | | 152.5140 | 137.438 | 144.470 | >±4.2 | | 37.250 | | 257.225 | | 9.864 | | † |
| GeBr2 | | 232.4180 | -60.963 | -46.00 | ±5. | | 55.757 | | 319.172 | | 14.193 | | † |
| GeBr3 | | 312.3220 | -119.031 | -96.164 | >±50. | | 78.139 | | 363.175 | | 18.549 | | † |
| GeBr4 | | 392.2260 | -291. | -261.29 | ±6. | | 101.687 | | 396.195 | | 23.963 | | † |
| GeCl | | 108.0627 | 69.030 | 68.66 | ±18. | | 36.990 | | 245.904 | | 9.599 | | † |
| GeCl2 singlet | | 143.5154 | -166.9 | -166.39 | ±5. | | 53.806 | | 296.332 | | 13.307 | | †# |
| GeCl2 triplet | | 143.5154 | 102.3 | 102.525 | ±5. | | 54.217 | | 307.835 | | 13.593 | | # |
| GeCl3 | | 178.9681 | -234.4 | -233.69 | ±5. | | 76.149 | | 338.232 | | 17.700 | | †# |
| GeCl4 | | 214.4208 | -500.9 | -498.55 | ±5. | | 95.975 | | 348.572 | | 21.150 | | †# |
| GeF4 | | 148.60361 | -1190.2 | -1185-5 | ±0.5 | | 81.674 | | 271.954 | | 17.589 | | # |
| GeH3Cl | | 111.08652 | 57.70 | 67.63 | ±5. | | 54.795 | | 273.113 | | 11.995 | | # |
| GeD4 see D4Ge | | 80.66640 |  |  | ±5. | |  | |  | |  | | # |
| GeH4 | | 76.64176 | 90.3 | 101.125 | ±5. | | 45.011 | | 217.303 | | 10.748 | | †# |
| GeS (solid) | | 104.676 | -61.2 | -61.738 | ±1.2 | | 47.767 | | 66.932 | | 8.281 | | # |
| GeS | | 104.676 | 106.9 | 106.809 | ±3. | | 33.701 | | 241.275 | | 9.14 | | # |
| GeS2 (solid) | | 136.742 | -127.8 | -127.09 | ±1. | | 65.700 | | 93.600 | | 12.750 | | † |
| GeS2 linear | | 136.742 | 112. | 112.18 | ±20. | | 54.622 | | 269.454 | | 13.286 | | #† |
| Ge2 Digermanium | | 145.22 | 471.5 | 470.08 | ± | | 41.681 | | 256.453 | | 10.696 | | † |
| Ge2S2 cyclo | | 209.352 | 107.9 | 108.37 | ±7. | | 76.053 | | 339.490 | | 17.627 | |  |
| H <^!> | | 1.00794 | 217.998 | 216.034 | ±0.001 | | 20.786 | | 114.718 | | 6.197 | | † |
| H+ | | 1.00739 | 1536.244 | 1528.084 | ±0.000 | | 20.786 | | 108.948 | | 6.197 | | † |
| H- | | 1.00849 | 139.031 | 143.246 | ±1.E-5 | | 20.786 | | 108.961 | | 6.197 | | † |
| HIa <^~> | | 127.91241 | 26.558 | 28.734 | ±0.047 | | 29.157 | | 206.592 | | 8.657 | | † |
| HOIg  Hypoiodous acid | | 143.91181 | -61.3g | -56.6g | ±2.0g | | 38.960 | | 245.972 | | 10.438 | | # |
| HNO <~> | | 31.01408 | 106.842 | 109.809 | ±0.125 | | 33.880 | | 220.920 | | 9.942 | | † |
| HNO+ Oxoammoniumyld | | 31.01353 | 1095.75 | 1092.48d | ±0.7d | | 34.456 | | 223.64 | | 9.982 | | # |
| HNO- | | 31.01463 | 70.91 | 80.038 | ±1.13 | | 34.539 | | 228.54 | | 9.979 | | # |
| HNO2 equil <~> | | 47.01348 | -78.70 | -73.05 | ±0.6 | | 46.320 | | 254.071 | | 11.597 | | #† |
| HNO2 HONO *trans* | | 47.01348 | -79.19 | -73.043d | ±0.077 | | 44.646 | | 248.087 | | 10.912 | | # |
| HNO2 HONO *cis* Nitrous acid | | 47.01348 | -77.61d | -71.25d | ±0.39d | |  | |  | |  | | X |
| HNO2+ *trans* and equil HONO+ Hydroxyoxoamoniumyl | | 47.01293 | 983.44 | 983.74 | ±1.58 | | 43.076 | | 251.006 | | 10.748 | | # |
| HNO2- *trans*  HONO- | | 47.01403 | -116.90 | -106.678 | ±1.88 | | 54.990 | | 271.559 | | 13.224 | | # |
| HNO2- *cis-trans* equil c | | 47.01403 | -117.39 | -107.7d | ±1.87 | |  | |  | |  | | X |
| HNO2+ *cis* HONO+ | | 47.01293 | 1014.71 | 1014.933 | ±1.76 | | 43.505 | | 251.770 | | 10.828 | | # |
| HNO2- *cis* HONO- | | 47.01403 | -118.54 | -107.587 | ±1.87 | | 52.770 | | 265.574 | | 12.494 | | # |
| HNO3 liq | | 63.01288 | -173.26d | -178.98d | ±0.19d | |  | |  | |  | | X |
| HNO3 Nitric acid <~> | | 63.01288 | -134.3 | -124.58 | ±0.2d | | 54.092 | | 266.816 | | 11.876 | | # |
| HNO3+ | | 63.01233 | 1026.247 | 1029.193 | ±0.692 | | 57.868 | | 284.430 | | 12.446 | | # |
| HNO3- c Hydroxydioxonitrated | | 63.01343 | -201.66 | -191.2d | ±2.85 | |  | |  | |  | | X |
| HNO3 HOON=O Peroxynitrousg | | 63.01288 | -12.760 | -5.472 | ±0.36 | | 64.323 | | 280.522 | | 14.302 | | # |
| HNO4 HOONO2 PeroxyNitric aci | | 79.01228 | -56.923 | -46.213 | ±8. | | 72.419 | | 296.754 | | 15.219 | | # |
| HNO4+ HOONO2+ cation | | 79.01173 | 919.648 | 921.672 | ±8. | | 79.431 | | 322.436 | | 17.462 | | # |
| HN2O2 HN\*NO2 | | See after | N2O |  |  | |  | |  | |  | |  |
| HN3O4 | | See after | N3H |  |  | |  | |  | |  | |  |
| OH <^!> | | 17.00734 | 37.3 | 37.1 | ±0.3 | | 29.886 | | 183.737 | | 8.813 | | # |
| OH A 2Σ+ (excited) | | 17.00734 | 430.5 | 425.189 |  | | 29.153 | | 179.131 | | 13.887 | | # |
| OH+ | | 17.00679 | 1299.213 | 1292.987 | ±0.042 | | 29.196 | | 182.746 | | 8.603 | | † |
| OH- | | 17.00789 | -145.256 | -139.091 | ±0.036 | | 29.141 | | 172.542 | | 8.606 | | † |
| S-OH | | 49.07334 | -6.694 | -3.857 | ±15. | | 36.704 | | 239.812 | | 10.149 | | # |
| S-OH+ | | 49.07279 | 969.3 | 959.8 | ±2. | | 35.532 | | 233.034 | | 10.044 | | # |
| HS=O | | 49.07334 | -21.757 | -18.825 | ±15. | | 35.699 | | 241.683 | | 10.055 | | # |
| HS=O+ | | 49.07291 | 943.589 | 934.161 | ±8. | | 35.192 | | 235.185 | | 10.019 | | # |
| HS=O- | | 49.07389 | -147.265 | -132.091 | ±8. | | 37.486 | | 237.488 | | 10.207 | | # |
| HOT (3HOH) MonoTritium Water | | 20.02339 | -251.161 | -248.237 | ±8. | | 33.682 | | 202.150 | | 9.934 | | # |
| HO2 <!> | | 33.00674 | 12.296 | 15.208 | ±0.25 | | 34.893 | | 229.106 | | 10.002 | | †# |
| HO2+ | | 33.00619 | 1113.774 | 1110.565 | ±0.11d | | 33.515 | | 225.293 | | 9.926 | | # |
| HO2- | | 33.00728 | -97.677 | -88.811 | ±0.39d | | 37.720 | | 226.610 | | 10.245 | | †# |
| HO2S <~> | | 65.07274 | -235.622 | -230.676 | ±8. | | 50.609 | | 282.497 | | 12.380 | | # |
| HO3 HOOO *trans/* equil | | 49.00614 | 27.82d | 32.67 | ±0.74d | | 51.174 | | 265.654 | | 12.408 | | # |
| HOOO *cis* | | 49.00614 | 29.1d | 34.2d | ±1.1 | | 50.155 | | 262.776 | | 12.036 | | # |
| OO(H)O | | 49.00614 | 294.2d | 300.1d | ±1.3d | |  | |  | |  | | X |
| HO3+ equil HOOO+ equil | | 49.00559 | 1067.61 | 1067.736 | ±1.85 | | 44.833 | | 248.879 | | 10.931 | | # |
| HO3+ *cis* HOOO+c | | 49.00559 | 1083.3d | 1083.4d | ±1.8d | | 44.295 | | 248.749 | | 10.862 | | # |
| HOOO- *cis*d | | 49.00669 | -131.8d | -122.0d | ±1.6d | | 55.815 | | 269.157 | | 13.471 | | # |
| OO(H)O+d | | 49.00559 | 1296.9d | 1297.5d | ±1.6d | |  | |  | |  | | X |
| OO(H)O-d | | 49.00669 | 16.1d | 27.7d | ±1.4d | |  | |  | |  | | X |
| HSO3 HO-SO2 | | 81.07214 | -353.87 | -346.055 | ±8. | | 62.090 | | 300.731 | | 13.851 | | # |
| HPO | | 47.9811 | -93.7 | -89.9 | ±4.2 | | 35.829 | | 235.683 | | 10.065 | | #† |
| HPO2 HOPO | | 63.98050 | -468.6 | -461.7 | ±6.3 | | 48.874 | | 270.179 | | 11.409 | | # |
| HPO3 HOPO2 | | 79.97990 | -713.79 | -704.02 | ±8.4 | | 60.383 | | 282.465 | | 12.841 | | # |
| HPO4-2 | | see | Next to | PH4-3 |  | |  | |  | |  | | # |
| HPb See PbH | |  |  |  |  | |  | |  | |  | | # |
| HPt See PtH | |  |  |  |  | |  | |  | |  | | # |
| SH <~> | | 33.07394 | 141.87 | 141.212 | ±0.52 | | 32.446 | | 195.751 | | 9.274 | | # |
| SH- | | 33.07449 | -86.574 | -80.377 | ±0.12 | | 29.146 | | 186.638 | | 8.646 | | † |
| HS2 Hydrothiosulpheno Radical | | 65.13994 | 104.60 | 107.145 | ±10.46 | | 39.703 | | 253.304 | | 10.484 | | # |
| HT | | 4.02395 | 0.724 | 0.733 |  | | 29.165 | | 148.327 | |  | | # |
| H2 REFERENCE ELEMEN<^!> | | 2.01588 | 0 | 0 |  | | 29.210 | | 130.635 | | 8.449 | | #† |
| H2+ | | 2.01533 | 1494.677 | 1488.365 | ±1.10-5 | | 29.289 | | 142.370 | | 8.583 | | † |
| H2- | | 2.01643 | 311.68 | 317.725 | ±2.94 | | 29.556 | | 143.747 | | 8.621 | | #† |
| H2O(cr) c \*Ice. Values at 273.15 K | | 18.01528 | -292.74\*\* | -286.3 | ±0.03 | | \*38.113 | | 41.327\* | |  | | † |
| H2O(L) | | 18.01528 | -285.83 | -286.922 | ±0.03 | | 75.351 | | 69.939 | | 13.278 | | † |
| H2O <^!> | | 18.01528 | -241.826 | -238.922 | ±0.03d | | 33.588 | | 188.829 | | 9.934 | | † |
| H2O+ | | 18.01473 | 981.806 | 978.491 | ±0.033 | | 33.683 | | 195.378 | | 9.934 | | † |
| H2PO HPOH | | 48.98904 | -102.1 | -94.6 | ±6.3 | | 53.345 | | 257.638 | | 10.711 | | # |
| H2O2(L) | | 34.01468 | -187.778 | -193.58 | ±0.08 | | 89.328 | | 109.604 | | 22.949 | | † |
| H2O2 <!> | | 34.01468 | -135.88 | -129.89 | ±0.64d | | 42.416 | | 234.542 | | 11.162 | | # |
| H2O2+ *trans* | | 34.01413 | 895.122 | 894.847 | ±0.621 | | 38.931 | | 243.420 | | 11.226 | | # |
| H2O2+ *cis* | | 34.01413 | 930.50 | 930.225 | ±1.03 | | 38.929 | | 243.416 | | 11.225 | | # |
| H2O3 HOOOH *trans* trioxidane | | 50.0140 | -90.49 | -81.39 | ±0.9 | | 55.668 | | 254.289 | | 12.388 | | # |
| H2O3 *cis* c HOOOH *cis* | | 50.0140 | -81.4d | -72.84d | ±0.92d | | 55.670 | | 254.286 | | 12.387 | | # |
| H2O3+ HOOOH+ | | 50.01353 | 926.42 | 929.544 | ±1.82 | | 53.370 | | 257.431 | | 12.167 | | # |
| H2O3+ HOOOH+ *trans* c,d | | 50.01353 | 925.6d | 928.6d | ±1.82 | |  | |  | |  | | X |
| H2PO4- | | see | PO4-3 |  |  | |  | |  | |  | | # |
| H2P2 | | 63.96340 | See | P2H2 |  | |  | |  | | 10.986 | | # |
| H2S <^~> | | 34.08188 | -20.6 | -17.67 | ±0.5 | | 34.255 | | 205.817 | | 9.958 | | † |
| H2S- anion | | 34.08243 | 114.588 | 122.469 | ±8. | | 44.045 | | 224.816 | | 11.196 | | # |
| H2SO4(L) | | 98.07948 | -813.989 | -811.975 | ±0.67 | | 138.584 | | 156.895 | | 28.226 | | † |
| H2SO4 | | 98.07948 | -732.7 | -720.85 | ±2.0 | | 90.235 | | 311.333 | | 18.391 | | # |
| H2S2 HS-SH | | 66.14788 | 15.500 | 21.243 | ±2.1 | | 48.745 | | 251.070 | | 11.549 | |  |
| H2S2 H2SS | | 66.14788 | 123.43 |  | ±4.2 | |  | |  | |  | | X |
| H3+ Trihydrogen Cation | | 3.02327 | 1112.89d | 1110.304d | ±0.013 | | 33.271 | | 147.528 | | 9.916 | | # |
| H3O+ Hydronium Cation | | 19.02267 | 603.417 | 604.215 | ±0.61d | | 35.485 | | 193.139 | | 10.046 | | † |
| H3O2- HOHOH-Trihydrogendioxide | | 35.02317 | -495.52.g | -487.26g | ±0.96g | |  | |  | |  | | X |
| H3O2+ H2OOH+ Hydroperoxonium | | 35.02207 | 734.6d | 738.7d | ±1.3d | | 44.091 | | 241.703 | | 10.943 | | # |
| H3PO HOPH2 | | 49.99698 | -210.0 | -198.9 | ±6.3 | | 48.348 | | 257.214 | | 11.230 | | # |
| H3PO | | 49.99698 | -215.5 | -203.5 | ±6.3 | | 41.660 | | 233.866 | | 10.441 | | # |
| H3PO3 gas (P(OH)3) | | 81.99578 | -771.02 | -755.56 | ±8. | | 84.344 | | 312.678 | | 15.622 | | # |
| H3PO3 O=PH(OH)2 | | 81.99578 | -820.754 | -804.3 | ±8. | | 75.978 | | 307.665 | | 14.635 | | # |
| H3PO4(S) Orthophosphoric acid | | 97.99518 | -1284.49 | -1266.046 |  | | 106.064 | | 110.544 | | 16.980 | | † |
| H3PO4(g) Orthophosphoric acid | | 97.99518 | -1118.71 | -1100.5 | ±8. | | 95.715 | | 327.316 | | 17.211 | | # |
| H4O2c (H2O)2  Water dimer | | 36.03056 | -499.63 | -492.22d | ±0.11 | |  | |  | |  | | X |
| H4P+ Phosphonium | | 35.00497 | See | PH4+ |  | |  | |  | |  | | # |
| H4P2 | | 65.97928 | See | P2H4 |  | |  | |  | | 13.621 | | # |
| He REFERENCE ELEMENT<^~> | | 4.00260 | 0 | 0 |  | | 20.786 | | 126.154 | | 6.197 | | † |
| He+ | | 4.00205 | 2378.519 | 2372.322 | ±0.001 | | 20.786 | | 131.915 | | 6.197 | | † |
| He++c | | 4.001505 | 7635.23 | 7622.839 | ±2.4E-5 | |  | |  | |  | | X |
| HeH+ | | 5.009993 | 1357.834 | 1353.391 | ±8. | | 29.101 | | 152.362 | | 8.676 | | # |
| Hg(cr,L) REFERENCE ELEMENT | | 200.5900 | 0 | 0 |  | | 27.978 | | 76.028 | | 9.343 | | † |
| Hg (gas) <&> | | 200.5900 | 61.38 | 64.53 | ±0.04 | | 20.786 | | 174.972 | | 6.197 | | † |
| Hg+ | | 200.58945 | 1074.643 | 1071.591 |  | | 20.786 | | 180.735 | | 6.197 | | † |
| HgBr2 (solid) | | 360.3980 | -175.31 |  |  | | 75.312 | | 170.314 | |  | | † |
| HgBr2 (gas) <&> | | 360.3980 | -91.312 | -73.107 |  | | 60.277 | | 320.227 | | 15.658 | | † |
| HgCl (gas) Calomel | | 236.0427 | 78.45 |  |  | | 36.34 | | 260.0 | |  | |  |
| HgCl2 (solid) | | 236.0427 | -230.12 |  |  | |  | |  | |  | | X |
| HgCl2 (liquid) | | 236.0427 | -213.22 |  |  | |  | |  | |  | | X |
| HgCl2 (gas) from 1500 K and up | | 271.4954 | -146.29 |  |  | |  | |  | |  | |  |
| HgO (solid) | | 216.5894 | -90.789 | -86.210 | ±0.1 | | 44.062 | | 70.270 | | 9.104 | | † |
| Hg(N3)2 | |  | 556.5 |  |  | |  | |  | |  | | X |
| Hg2N6 (solid) N3-Hg-Hg-N3 | | 485.22044 | 592.8 |  |  | |  | |  | |  | | X |
| Hg2N6 N3-Hg-Hg-N3 | | 485.22044 | 642.4 | 666.84 |  | | 129.253 | | 443.266 | | 28.607 | | # |
| I Iodine <~> | | 126.90447 | 106.76 | 107.161 | ±0.002 | | 20.786 | | 180.789 | | 6.197 | | † |
| I+ | | 126.90392 | 1121.345 | 1115.548 | ±0.006 | | 20.786 | | 182.644 | | 6.197 | | † |
| I- | | 126.90502 | -194.594 | -187.996 | ±0.039 | | 20.786 | | 169.262 | | 6.197 | | † |
| HI See under H | |  |  |  |  | |  | |  | |  | | † |
| INO2 NITRO-IODINE | | 172.91001 | 60.25 | 67.349 | ±4.2 | | 55.366 | | 289.237 | | 12.514 | | # |
| IO <~> | | 142.90387 | 125.0 | 127.0 | ±1.1 | | 32.863 | | 239.624 | | 9.008 | | # |
| IO+ g | | 142.90332 | 1064.1 | 1066.1 | ±2. | |  | |  | |  | | X |
| IO- g | | 142.90332 | -104.4 | -102.5 | ±1.2 | |  | |  | |  | | X |
| IO2 O-O-I | | 158.90327 | 116.5 | 118.973 | ±40 | | 48.727 | | 296.374 | | 12.806 | | # |
| IO2 O-I-O | | 158.90327 | 159.3 | 162.717 | ±25 | | 46.697 | | 281.231 | | 11.861 | | # |
| IO3 | | 174.90267 | 241.9 | 248.013 | ±50 | | 61.56 | | 292.975 | | 13.505 | | # |
| IT Tritium Iodide estimated | | 129.92052 | 17.369 | 27.968 | ±0.5 | | 29.738 | | 215.799 | | 8.701 | | # |
| I2 (cr) REFERENCE ELEMENT | | 253.80894 | 0. | 0. |  | | 54.440 | | 116.139 | | 13.196 | | † |
| I2 gas <^~> | | 253.80894 | 62.417 | 65.495 | ±0.004 | | 36.887 | | 260.687 | | 10.116 | | † |
| I2+ g | | 253.80839 | 966.605 | 963.523 | ±0.02g | | 36.507 | | 265.076 | | 9.963 | | # |
| I2- g | | 253.80949 | -186.92 | -178.13 | ±0.48 | |  | |  | |  | | X |
| I2O I-I-O | | 269.80834 | 106.7 | 110.545 | ±40 | | 52.359 | | 330.647 | | 13.691 | | # |
| I2O I-O-I | | 269.80834 | 119.5 | 123.899 | ±25 | | 51.874 | | 308.111 | | 13.137 | | # |
| Ir (solid) REFERENCE ELEMEN | | 192.217 | 0. | 0. |  | | 24.999 | | 35.480 | | 5.263 | | # |
| Ir (gas) Iridium | | 192.217 | 670.001 | 669.068 |  | | 20.786 | | 193.585 | | 6.197 | | # |
| K(S) REFERENCE ELEMENT | | 39.09830 | 0 | 0 |  | | 29.6 | | 64.680 | | 7.088 | | † |
| K (gas) <~> | | 39.09830 | 89.0 | 89.82 | ±0.4 | | 20.786 | | 160.342 | | 6.197 | | † |
| K+ <~> | | 39.09775 | 514.0 | 508.7 | ±0.4 | | 20.786 | | 154.578 | | 6.197 | | † |
| K- | | 39.09885 | 34.418 | 41.5 |  | | 20.786 | | 154.579 | | 6.197 | | X† |
| KNO3(S) | | 101.10320 | 494.0 | -488.31 | ±0.5 | | 95.060 | | 132.900 | |  | | † |
| KNO3 | | 101.10320 | -315.833 | -307.31 |  | | 68.358 | | 311.473 | | 15.917 | | † |
| KO <~> | | 55.09770 | 64.733 | 66.68 | ±20. | | 35.352 | | 241.198 | | 9.481 | | † |
| K2+ | | 78.19605 | 524.66 | 521.778 |  | | 38.133 | | 259.959 | | 10.861 | | X† |
| K2CO3 | | 138.2055 | -871.65 | -862.9 | ±20. | | 89.939 | | 345.508 | | 19.516 | | † |
| K2O | | 94.19600 | -74.09 | -69.429 |  | | 54.180 | | 286.548 | | 13.858 | | † |
| K2O2 | | 110.19540 | -191.566 | -185.0 |  | | 70.589 | | 306.461 | | 16.290 | | † |
| Kr REF ELEMENT <^> | | 83.8 | 0 | 0 |  | | 20.786 | | 164.086 | | 6.197 | | † |
| Kr+ | | 83.79945 | 1356.954 | 1350.76 | ±0.001 | | 20.786 | | 175.613 | | 6.197 | | † |
| KrF2 | | 121.79680 | 65.689 | 68.243 |  | | 54.139 | | 253.909 | | 12.468 | | # |
| KrH+ | | 84.8074 | 1110.91d | 1106.50d | ±0.70d | |  | |  | |  | | X |
| Li sol Reference Element | | 6,941 | 0. | 0. |  | | 24.881 | | 29.120 | |  | | † |
| Li gas | | 6.941 | 159.300 | 157.735 |  | | 20.786 | | 138.783 | | 6.197 | | † |
| Li+ cation | | 6.94045 | 685.719 | 677.017 |  | | 20.786 | | 133.018 | | 6.197 | | † |
| Li- anion | | 6.94155 | 93.475 | 98.107 |  | | 20.786 | | 133.020 | | 6.197 | | † |
| LiBr(S) cubic | | 86.84500 | -351.160 |  | ±0.27 | | 49.830 | | 74.010 | | 10.476 | | † |
| LiBr | | 86.84500 | -151.162 | -143.444 | ±4. | | 33.932 | | 224.225 | | 9.173 | | † |
| LiCl(S) | | 42.39370 | -408.540 |  | ±0.2 | | 47.990 | | 59.270 | | 9.300 | | † |
| LiCl | | 42.39370 | -193.780 | -193.617 | ±4. | | 33.254 | | 212.860 | | 9.060 | | † |
| LiF(S) | | 25.93940 | -618.300 |  | ±0.7 | | 41.800 | | 35.660 | | 6.473 | | † |
| LiF | | 25.93940 | -340.945 | -340.728 | ±3 | | 31.292 | | 200.300 | | 8.828 | | † |
| LiI(S) cubic | | 133.84547 | -273.200 |  | ±0.5 | | 51.040 | | 86.710 | | 11.360 | | † |
| LiI | | 133.84547 | -85.270 | -83.330 | ±8. | | 34.551 | | 232.220 | | 9.290 | | † |
| LiH(S) | | 7.94894 | -90.650 |  | ±20. | | 28.950 | | 20.600 | | 3.883 | | † |
| LiH | | 7.94894 | 139.264 | 139.444 |  | | 29.731 | | 170.907 | | 8.686 | | † |
| LiN | | 20.94774 | 334.720 | 139.444 | ±167. | | 32.839 | | 208.248 | | 8.999 | | † |
| LiNO2(s) | | 52.94654 | -368.300 |  | ±1. | | 63.000 | | 88.000 | | 12.100 | | † |
| LiNO2 | | 52.94654 | -202.031 | -197.753 | ±10. | | 56.959 | | 265.014 | | 13.369 | | † |
| LiNO3(s) hexagonal | | 68.94594 | -482.700 |  | ±0.5 | | 89.000 | | 104.000 | |  | | † |
| LiNO3 | | 68.94594 | -311.585 | -303.513 | ±10 | | 64.061 | | 278.287 | | 13.915 | | † |
| LiO | | 22.94040 | 72.914 | 72.524 | ±8 | | 32.317 | | 211.123 | | 9.362 | | † |
| LiOF | | 41.93880 | -92.048 | |  | |  | -89.4991 | | --- | --- | | | --- | --- | --- | --- | | ±41.8 | | 43.032 | | 246.026 | | 10.827 | | † |
| LiOH(s) | | 23.94834 | -487500 |  | ±0.4 | | 49.579 | | 42.810 | | 7.414 | | † |
| LiOH | | 23.94834 | -229.0 | -227.131 | ±5 | | 46.026 | | 214.377 | | 11.337 | | † |
| LiON | | 36.94714 | 179,912 | 181.918 | ±41.8 | | 44.424 | | 245.335 | | 11.301 | | † |
| Li2 | | 13.88200 | -215.9 | 215.489 | ±3 | | 36.103 | | 197.000 | | 9.675 | | † |
| Li2+ | | 13.88145 | 721.611 | 714.689 | ±5. | | 36.978 | | 207.572 | | 9.989 | | † |
| Li2Br2 | | 173.69000 | -495.834 | -479. | ±6 | | 75.105 | | 372.437 | | 16.950 | | . † |
| Li2CO3(S) monoclinic | | 73.89090 | -1214.1 |  | ±1. | | 98.320 | | 90.120 | | 15.180 | | † |
| Li2Cl2 | | 84.78740 | -597.539 | -595. | ±6 | | 72.625 | | 292.645 | | 15.906 | | † |
| Li2F2 | | 51.87881 | -935.323 | -931. | ±8 | | 64.770 | | 261.916 | | 13.766 | | † |
| Li2I2 | | 267.69094 | -362.801 | -358. | ±7. | | 76.762 | | 334.607 | | 17.659 | | † |
| Li2O (s) | | 29.88140 | -597.880 |  | ±30. | | 54.100 | | 37.610 | | 7.251 | | † |
| Li2O | | 29.88140 | |  | -165.840 | | --- | --- | | -166.525 | ±10. | | 50.286 | | 232.985 | | 12.485 | | † |
| Li2O+ | | 29.88085 | 439.095 | 433.473 | ±20. | | 51.385 | | 242.552 | | 13.029 | | † |
| Li2O2(s) | | 45.88080 | -632.5 |  | ±4. | | 75. | | 58. | |  | | † |
| Li2O2 | | 45.88080 | -279.398 | -275.002 | ±20. | | 59.412 | | 258.643 | | 13.548 | | † |
| Li2O2H2 | | 47.897 | -737. | -726.167 | ±10. | | 71.17 | | | 269.7 |  | | --- | --- | | | 15.854 | | † |
| Li2SO4(S) | | 109.94560 | -1436.0 |  | ±0.5 | | 117.570 | | 113.970 | | 18.631 | | † |
| Li2SO4 | | 109.94560 | -1041.816 | -1030.432 | ±117. | | 101.805 | | 322.826 | | 19.653 | | † |
| Li3+ | | 20.82245 | 756.591 | 751. | ±10. | | 54.285 | | 245.270 | | 13.289 | | † |
| Li3Br3 | | 260.53500 | -850.676 | -800. | ±10. | | 118.950 | | 401.354 | | 26.037 | | † |
| Li3Cl3 | | 127.18110 | -976.107 | -973. | ±10 | | 115.506 | | 367.816 | | -24.561 | | † |
| Li3F3 | | 77.81821 | -1524.597 | -1518. | ±10. | | 102.920 | | 316.818 | | 20.537 | | † |
| Li3I3 | | 401.53641 | -606.000 | -606. | ±10. | | 121.601 | | 425.290 | | 27.233 | | † |
| Mg (S) REFERENCE ELEMENT | | 24.30500 | 0 | 0 |  | | 24.775 | | 32.535 | | 4.979 | | † |
| Mg(L) | | 24.30500 | 4.79 |  |  | |  | |  | |  | | † |
| Mg (G) <&> | | 24.30500 | 147.10 | 145.90 | ±0.8 | | 20.786 | | 148.649 | | 6.197 | | † |
| Mg+ | | 24.30445 | 891.047 | 883.65 | ±1.3 | | 20.786 | | 154.412 | | 6.197 | | † |
| MgAl2O4 (S) | | 142.26568 | -2299.11 | -2332.17 | ±1.3 | | 116.198 | | 88.692 | | 64.480 | | † |
| MgAl2O4 (L) | | 142.26568 | -2106.53 |  |  | |  | |  | |  | | † |
| MgB2(s) | | 45.9270 | -92.0 | -91.392 | ±8.4 | | 47.823 | | 35.982 | | 6.799 | | # |
| MgB2 g | | 45.9270 | ??834.511 | 830.605 | ±8. | | 45.514 | | 250.119 | | 11.313 | | # |
| MgBr | | 104.2090 | 6.163 | 13.814 | ±20. | | 35.664 | | 244.976 | | 9.588 | | † |
| MgBr2(S) | | 184.1130 | -526.0 | -512.0 | ±2.5 | | 73.219 | | 117.0 | | 15.500 | | † |
| MgBr2(L) | | 184.1130 | -490.41 |  |  | |  | |  | |  | | † |
| MgBr2 | | 184.1130 | -306.743 | -292.0 | ±10. | | 58.550 | | 296.432 | | 14.757 | | † |
| MgCO3(S) Magnesium Carbonat | | 84.31390 | -1096. | -1088.58 | ±3. | | 76.108 | | 65.090 | | 11.630 | | † |
| MgCl <&> | | 59.75770 | -54.705 | -54.498 | ±6. | | 34.837 | | 233.423 | | 9.363 | | † |
| MgCl+ | | 59.75715 | 640.196 | 640.196 | ±84. | | 35.447 | | 228.559 | | 9.516 | | † |
| MgClF | | 78.75610 | -569.02 |  | ±21. | | 49.912 | | 265.994 | |  | |  |
| MgCl2 (S) | | 95.21040 | -644.3 | -643.910 | ±0.7 | | 71.384 | | 89.620 | | 13.770 | | † |
| MgCl2(L) | | 95.21040 | -601.58 |  |  | |  | |  | |  | | † |
| MgCl2 <&> | | 95.21040 | -399.170 | -398.91 | ±5. | | 56.548 | | 272.242 | | 13.901 | | † |
| MgF <&> | | 43.30340 | -232.267 | -231.844 | ±10. | | 32.580 | | 221.097 | | 8.969 | | † |
| MgF+ | | 43.30285 | 516.868 | 511.093 | ±38. | | 32.606 | | 215.334 | | 8.969 | | † |
| MgF2(S) | | 62.30181 | -1124.2 | -1120.3 | ±1.3 | | 61.587 | | 57.200 | | 9.920 | | † |
| MgF2(L) | | 62.30181 | -1072.35 |  |  | |  | |  | |  | | † |
| MgF2 <&> | | 62.30181 | -735.498 | -734.316 | ±16.7 | | 52.293 | | 247.556 | | 12.622 | | † |
| MgF2+ | | 62.30126 | 582.692 | 577.884 | ±20.9 | | 52.450 | | 258.148 | | 12.415 | | † |
| MgH | | 25.31294 | 229.786 | 230.317 | ±6. | | 29.587 | | 193.197 | | 8.682 | | † |
| MgOH | | 41.31234 | -132.429 | -130. | ±12. | | 46.497 | | 232.622 | | 11.124 | | † |
| MgOH+ | | 41.31179 | 615.769 | 612.937 | ± | | 43.216 | | 220.827 | | 10.188 | | † |
| MgH2 (S) | | 26.32088 | -75.7 | -67.563 | ±2. | | 35.35 | | 31.1 | | 5.31 | | † |
| Mg(OH)2(S) | | 58.31968 | -924.35 | -935.76 | ±2.1 | | 77.111 | | 63.180 | | 11.410 | | † |
| Mg(OH)2 gas | | 58.31968 | -551.996 | -547. | ±20 | | 80.668 | | 271.597 | | 17.132 | | † |
| MgI | | 151.20947 | 61.206 | 63.042 | ±20. | | 36.078 | | 252.815 | | 9.741 | | † |
| MgI2(S) | | 278.11394 | -370. | -368.825 | ±2.0 | | 74.475 | | 134.0 | | 17.000 | | † |
| MgI2(L) | | 278.11394 | -342.25 |  |  | |  | |  | |  | | † |
| MgI2 | | 278.11394 | -171.706 | -168.825 | ±15. | | 59.364 | | 313.820 | | 15.294 | | † |
| MgN | | 38.31174 | 288.7 | 289.02 | ±25.1 | | 32.733 | | 224.838 | | 8.989 | | † |
| MgO(S) | | 40.30440 | -601.6 | -597.441 | ±0.3 | | 37.237 | | 26.950 | | 5.160 | | † |
| MgO(L) | | 40.30440 | -532.61 |  |  | |  | |  | |  | | † |
| MgO | | 40.30440 | 32.261 | 32.671 | ±25.1 | | 32.111 | | 213.318 | | 8.909 | | † |
| MgS(S) | | 56.37100 | -348. | -346.939 | ±4.2 | | 45.560 | | 50.330 | | 8.330 | | † |
| MgS | | 56.37100 | 120.649 | 120.806 | ±30. | | 34.237 | | 225.448 | | 9.234 | | † |
| MgSO4(S) II | | 120.36860 | -1288.8 | -1277.45 | ±20.9 | | 96.399 | | 91.600 | | 15.400 | | † |
| MgSO4(L) | | 120.36860 | -1246.59 |  |  | |  | |  | |  | | † |
| MgSiO3 (S) | | 100.38870 | -1548.92 | -1539.813 | ±4.2 | | 81.927 | | 67.768 | | 12.113 | | † |
| MgSiO3 (L) | | 100.38870 | -1494.86 |  | ±20.9 | |  | |  | |  | | † |
| MgTiO3(S) | | 120.18320 | -1562.24 | -1552.74 | ±6.3 | | 91.881 | | 74.59 | | 3.240 | | † |
| MgTiO3(L) | | 120.18320 | -1497.63 |  | ±6.3 | |  | |  | |  | | † |
| MgTi2O5(S) | | 200.06200 | -2491.14 | -2477.25 | ±10.5 | | 146.858 | | 135.603 | | 5.363 | | † |
| MgTi2O5 (L) | | 200.06200 | -2382.31 |  | ±8.4 | |  | |  | |  | | † |
| Mg2 <&> | | 48.61000 | 276.555 | 276.971 | ±0.06 | | 24.199 | | 240.843 | | 9.542 | | † |
| Mg2F4 | | 124.60361 | -1718.37 | -1711.9 | ±37.7 | | 107.502 | | 337.018 | | 21.143 | | † |
| Mg2SiO4(S) | | 140.69310 | -2163.93 | -2150.67 | ±4.2 | | 118.688 | | 95.140 | | 4.130 | | † |
| Mg2SiO4(L) | | 140.69310 | -2113.88 |  | ±20.9 | |  | |  | |  | | † |
| Mg2TiO4(S) | | 160.48760 | -2164.35 | -2151.048 | ±6.3 | | 128.574 | | 115.102 | | 18.836 | | † |
| Mg2TiO4(L) | | 160.48760 | -2046.33 |  |  | |  | |  | |  | | † |
| Mg3N2 (S) cubic | | 100.92848 | -461.300 | -448.183 | ±2. | | 92.049 | | 85.00 | | 10.500 | | † |
| Mn (cr) Reference Element | | 54.93805 | 0. | 0. |  | | 26.280 | | 31.920 | | 4.980 | | X |
| Mn | | 54.93805 | 282.40 | 281.197 | ±2. | | 20.786 | | 173.718 | | 6.197 | | † |
| MnO (S) | | 70.93745 | -385.221 |  |  | | 44.102 | | 59.71 | |  | |  |
| MnO2(S) | | 86.93685 | -520.029 |  |  | | 54.415 | | 53.049 | |  | |  |
| Mn2O3 (S) | | 157.8743 | -959.002 |  |  | | 99.034 | | 110.499 | |  | |  |
| Mn3O4 Solid-A | | 228.81175 | -1387.8 |  |  | | 140.515 | | 155.599 | |  | |  |
| Mn5N2(S) | | 302.70373 | -204.2 |  |  | | 175.724 | | 187.443 | |  | |  |
| MnS Solid | | 87.00405 | -214.2 |  |  | | 49.943 | | 78.199 | |  | |  |
| MnS2 (S) | | 119.07005 | -223.844 |  |  | | 70.075 | | 99.914 | |  | |  |
| Mo(cr) REFERENCE ELEMENT | | 95.94 | 0 | 0 |  | | 23.933 | | 28.605 | | 4.585 | | † |
| Mo | | 95.94 | 658.5 | 656.888 | ±2. | | 20.786 | | 181.953 | | 6.197 | | † |
| MoC Solid-C | | 107.951 | -28.451 |  |  | | 30.878 | | 36.652 | |  | |  |
| MoO2 Solid | | 127.9388 | -588.94 |  |  | | 55.982 | | 46.275 | |  | |  |
| MoO2 | | 127.9388 | -8.314 |  |  | | 34.002 | | 252.344 | |  | |  |
| Mo2C(S) | | 203.891 | -53.137 |  |  | | 60.207 | | 65.814 | |  | |  |
| N <^~> | | 14.00674 | 472.68 | 470.818 | ±0.024 | | 20.786 | | 153.302 | | 6.197 | | † |
| N+ <^> | | 14.00619 | 1881.903 | 1872.924 | ±0.024 | | 21.285 | | 159.799 | | 7.117 | | † |
| N- | | 14.00729 | 485.27 | 489.304 | ±4.10 | | 21.009 | | 159.930 | | 6.498 | | † |
| NBrH2 | | 95.92662 | 83.638 | 98.190 | ±8. | | 40.293 | | 252.579 | | 10.511 | | # |
| NBr2H DiBromoImide | | 174.82268 | 200.999 | 221.415 | ±8. | | 53.164 | | 299.353 | | 12.673 | | # |
| NBr3 | | 253.71874 | 316.310 | 341.044 | ±8. | | 72.068 | | 333.337 | | 16.382 | | # |
| NCLH2 | | 51.47532 | 55.438 | 62.472 | ±8. | | 39.112 | | 241.148 | | 10.360 | | # |
| NCL2H | | 85.92008 | 142.453 | 148.242 | ±8. | | 50.518 | | 276.325 | | 11.961 | | # |
| NCL3 | | 120.36484 | 228.237 | 231.594 | ±8. | | 68.029 | | 298.775 | | 14.749 | | # |
| ND | | 16.0208 | 355.739 | 355.710 | ±8. | | 29.159 | | 187.234 | | 8.648 | | † |
| NHD Radical | | 17.02878 | 178.165 | 181.106 | ±8. | | 33.703 | | 205.600 | | 9.912 | | # |
| ND2 | | 18.0349 | 181.937 | 184.878 | ±8. | | 34.415 | | 204.335 | | 9.962 | | † |
| ND2H | | 19.04288 | -52.748 | -45.684 |  | | 35.976 | | 209.279 | | 10.074 | | # |
| ND3 | | 20.04901 | -54.501 | -47.546 | ±0.4 | | 38.225 | | 203.931 | | 10.234 | | †# |
| NF | | 33.00514 | 232.99 | 233. | ±3. | | 30.228 | | 212.908 | | 8.738 | | † |
| NF2 | | 52.00355 | 34.421 | 37.000 | ±5. | | 41.058 | | 249.638 | | 10.582 | | † |
| NF3 <&> | | 71.00195 | -131.7 | -125.98 | ±1. | | 53.497 | | 260.812 | | 11.855 | | † |
| NH <~> | | 15.01468 | 358.792 | 358.76 | ±0.17d | | 29.193 | | 181.227 | | 8.601 | | † |
| NH singlet excited c | | 15.01468 | 509.39 | 509.342 | ±0.18 | | 29.147 | | 177.867 | | 8.617 | | # |
| NH triplet only | | 15.01468 | 358.79d | 354.74d | ±0.17d | |  | |  | |  | |  |
| NH+ Aminyliumyld | | 15.01413 | 1665.795 | 1658.98d | ±0.25d | | 32.775 | | 187.651 | | 9.495 | | † |
| NH- | | 15.01523 | 316.797 | 322.942 | ±0.17d | | 29.155 | | 172.482 | | 8.621 | |  |
| NHF | | 34.01308 | 112.0 | 114.952 | ±15 | | 35.234 | | 230.806 | | 10.030 | | † |
| NHF2 | | 53.01149 | -103 | -96.413 | ±15 | | 43.384 | | 252.814 | | 10.807 | | † |
| NOH Hydroxyimidogen | | 31.01408 | 214.51 | 217.414 | ±0.93 | | 34.989 | | 230.932 | | 10.006 | | # |
| NOH+Hydroxyaminiumyl | | 31.01353 | 1163.44 | 1160.18 | ±1.43 | | 34.380 | | 255.511 | | 9.973 | | # |
| NOH- | | 31.01463 | 224.03 | 232.7653 | ±2.4 | | 38.421 | | 230.823 | | 10.371 | | # |
| HOONO Peroxynitrous acid | | 63.01288 | -12.76d | -6.13d | ±0.38d | | 64.323 | | 280.522 | | 14.302 | | # |
| NH2 AMIDOGEN RADICAL<~> | | 16.02258 | 186.2 | 189.1 | ±0.15d | | 33.663 | | 194.868 | | 9.911 | | # |
| NH2+ Aminylium | | 16.02207 | 1269.973 | 1266.648 | ±0.169 | | 33.609 | | 189.481 | | 9.931 | | # |
| NH2- Amide | | 16.02316 | 105.910 | 114.987 | ±0.34d | | 33.460 | | 189.662 | | 9.924 | | # |
| NH2D | | 18.03672 | -48.697 | -41.627 |  | | 35.157 | | 205.591 | | 10.018 | | # |
| NH2F | | 35.02102 | -75 | -67.889 | ±15. | | 36.474 | | 229.534 | | 10.105 | | † |
| NH2O\* Nitroxyl | | 32.02202 | 64.730 | 71.385d | ±0.85d | | 39.380 | | 233.544 | | 10.488 | | # |
| H2NO+c | | 32.02147 | 945.38 | 946.32d | ±0.84d | | 34.901 | | 224.785 | | 9.993 | | # |
| H2NO-c | | 32.02257 | 36.12 | 49.3d | ±1.8d | | 37.347 | | 228.416 | | 10.167 | | # |
| HNOH *trans* & Equil  Hydroxyamidogend | | 32.02202 | 100.9c | 101.54d | ±0.98d | | 38.237 | | 233.511 | | 10.256 | | # |
| HNOH *cis* | | 32.02202 | 116.99 | 123.586 | ±1.31 | | 40.147 | | 234.976 | | 10.547 | | # |
| HNOH+ *trans* | | 32.02147 | 1019.22 | 1020.174 | ±1.87 | | 34.929 | | 225.030 | | 9.991 | | # |
| HNOH+ *cis* | | 32.02147 | 1048.3 | 1049.243 | ±2.0d | | 35.112 | | 225.166 | | 10.002 | | # |
| HNOH- Hydroxyamidogen | | 32.02257 | 79.15 | 91.2d | ±2.05 | | 44.952 | | 234.457 | | 11.171 | | # |
| NH3 AMONIA RRHO calc <^~> | | 17.03056 | -45.567 | -38.513 | ±0.03 | | 34.597 | | 192.475 | | 9.984 | | # |
| NH3 AMONIA Anharmonic calc | | 17.03056 | -45.567 | -38.946 | ±0.03 | | 35.630 | | 192.770 | | 10.043 | | † |
| NH3+ cation | | 17.03001 | 943.294 | 944.04 | ±0.03 | | 36.034 | | 198.847 | | 10.094 | | # |
| NH3- c | | 17.03111 | 25.2d | 38.3d | ±2.8 | | 36.089 | | 200.301 | | 10.067 | | # |
| NH2OH cr | | 33.02996 | -107.50 |  | ±0.65 | |  | |  | |  | | X |
| NH2OH Hydroxyl Amine *trans* | | 33.02996 | -43.95 | -33.809 | ±0.49d | | 46.472 | | 236.181 | | 11.236 | | †# |
| NH2OH Hydroxyl Amine *cis* | | 33.02996 | -25.23 | -14.618 | ±1.41 | | 42.636 | | 233.768 | | 10.765 | | # |
| NH2OH+ Hydroxyl Amine cation | | 33.02941 | 854.33 | 858.071 | ±1.75 | | 45.881 | | 241.982 | | 11.439 | | # |
| NH4+ AMONIUM ION | | 18.03795 | 637.9d | 642.995 | ±0.21d | | 34.764 | | 186.095 | | 9.979 | | #† |
| NH4Br crystal | | 97.9425 | -270.333 | -253.756 | ±0.15d | | 88.676 | | 112.842 | | 16.954 | | # |
| NH4Cl crystald | | 53.4912 | -314.553 | -311.389 | ±0.063 | | 86.441 | | 94.860 | | 22.698 | | † |
| NH4CLO4(I) | | 117.4888 | -295.767 | -277.78 |  | | 128.072 | | 184.18 | | 25.238 | | † |
| NO <^~> | | 30.00614 | 91.271 | 90.767 | ±0.064 | | 29.862 | | 210.748 | | 9.179 | | † |
| NO+ | | 30.00559 | 990.807 | 984.453d | ±0.064 | | 29.123 | | 198.234 | | 8.670 | | † |
| NO- Oxonitrate anion | | 30.00669 | 81.713 | 83.208 | ±0.12d | | 29.667 | | 210.274 | | 8.698 | | # |
| NOCL <^> | | 65.45884 | 52.524 | 54.425 | ±0.5 | | 44.623 | | 261.590 | | 11.364 | | † |
| NOF | | 49.00454 | -65 | -62.633 | ±2.0 | | 41.530 | | 248.224 | | 10.720 | | † |
| NOF3 | | 87.00135 | -187 | -178.78 | ±7. | | 68.067 | | 277.731 | | 13.698 | | † |
| NO2 <^~> | | 46.00554 | 34.193 | 37.0 | ±0.07 | | 37.177 | | 240.171 | | 10.208 | | † |
| NO2+ ONO+ | | 46.00499 | 964.409 | 961.75d | ±0.2 | | 37.791 | | 236.935 | | 10.318 | | # |
| NO2- | | 46.00609 | -191.518 | -182.482 | ±0.47 | | 37.215 | | 236.241 | | 10.177 | | † |
| N(OO) cyclo<~> | | 46.00554 | 351.69 | 354.309 | ±1.47 | | 39.519 | | 243.941 | | 10.396 | | # |
| N(OO)+ cyclo | | 46.00499 | 1364.94 | 1361.38 | ±1.94 | | 39.288 | | 237.329 | | 10.378 | | # |
| N(OO)- cyclo | | 46.00609 | 286.43 | 295.469 | ±1.6 | | 37.049 | | 237.163 | | 10.173 | | # |
| NOO Peroxyimidogend | | 46.00554 | 410.20 | 412.246 | ±1.7 | | 42.673 | | 252.496 | | 10.970 | | # |
| NOO+ | | 46.00499 | 1408.9 | 1405.34 | ±3.63 | | 39.287 | | 243.090 | | 10.378 | | # |
| NOO- | | 46.00609 | 154.11 | 162.726 | ±1.6 | | 40.910 | | 245.695 | | 10.597 | | # |
| NO2CL | | 81.45824 | 12.5 | 17.901 | ±1. | | 53.246 | | 272.128 | | 12.205 | | † |
| NO2F | | 65.00394 | -109 | -102.92 | ±20 | | 48.999 | | 259.287 | | 11.347 | | † |
| NO3 <~> | | 62.00494 | 74.628 | 79.35d | ±0.19d | | 46.935 | | 252.623 | | 10.959 | | † |
| NO3+ | | 62.00439 | 1292.57 | 1291.2 | ±0.86d | | 52.621 | | 255.193 | | 12.519 | | # |
| NO3- Nitrate | | 62.00549 | -312.185 | -299.405 | ±0.61d | | 44.724 | | 245.638 | | 10.733 | | †# |
| NO3Cl (See ClNO3) | |  |  |  |  | |  | |  | |  | | # |
| NO3F | | 81.00334 | 15. | 22.324 | ±3. | | 66.959 | | 293.171 | | 14.444 | | † |
| NS see SN | |  |  |  |  | |  | |  | |  | |  |
| NT | | 17.0227 | 519.487 | 519.377 | ±8. | | 29.208 | | 190.701 | | 8.652 | | # |
| NT3 Tritium Amonia (N3H3) | | 23.0548 | -76.178 | -69.32 | ±8. | | 39.222 | | 209.142 | | 10.331 | | # |
| N2 Reference Element <^!> | | 28.01348 | 0 | 0 |  | | 29.124 | | 191.607 | | 8.670 | | † |
| N2 excited, singlet | | 28.01348 | 99.73 | 99.73 |  | | 29.125 | | 197.375 | | 8.670 | |  |
| N2+ | | 28.01293 | 1509.509 | 1503.310 | 5.5∙104 | | 29.137 | | 197.663 | | 8.671 | | † |
| N2- | | 28.01403 | 189.84 | 196.033 | ±2.11 | | 29.194 | | 204.539 | | 8.674 | | #† |
| N2D2 Cis | | 32.0416 | 202.857 | 209.788 |  | | 39.025 | | 224.095 | | 10.308 | | †# |
| N2F2 | | 66.01029 | 62.374 | 67. | ±10 | | 56.569 | | 268.216 | | 12.869 | | † |
| N2F4 | | 104.00709 | -22 | -13.491 | ±10 | | 88.384 | | 317.531 | | 17.812 | | † |
| N2H Diazenyl <~> | | 29.02142 | 249.484 | 252.415 | ±0.74d | | 34.358 | | 224.507 | | 9.973 | | # |
| N2H+ Diazenylium NNH+ | | 29.02087 | 1045.33d | 1042.75d | ±0.74d | | 36.115 | | 202.514 | | 9.277 | | # |
| N2H- | | 29.02197 | 168.87 | 176.669 | ±2.12 | | 44.952 | | 233.124 | | 11.402 | | # |
| N2H2 equil *cis.trans iso 1,1* <~> | | 30.02936 | 200.219 | 207.36 | ±0.543 | | 35.045 | | 218.333 | | 9.997 | | #† |
| N2H2 *cis* Z-Diazene *cis* | | 30.02936 | 222.465 | 229.620 | ±0.81 | | 34.780 | | 218.417 | | 9.983 | | # |
| HN=NH+ Diazene equil cation g | | 30.02881 | 1125.67 | 1132.58 | ±0.67 | |  | |  | |  | | X |
| HN=NH- Diazene equil anion g | | 30.02991 | 262.4 | 269.3 | ±1.7 | |  | |  | |  | | X |
| H2NN Isodiazene | | 30.02936 | 300.938 | 308.022 | ±0.81d | | 35.747 | | 218.155 | | 10.054 | | # |
| H2NN+ Isodiazene cation c | | 30.02881 | 1144.42 | 1145.265 | ±1.46 | | 36.424 | | 224.153 | | 10.095 | | # |
| H2NN- Isodiazene anion c | | 30.02991 | 374.07 | 387.310 | ±1.71 | | 36.424 | | 237.522 | | 10.095 | | # |
| HNNH+ *trans* E-Diazene | | 30.02881 | 1131.88 | 1132.65 | ±0.72 | | 37.500 | | 222.857 | | 10.173 | | # |
| HNNH+ *cis* | | 30.02881 | 1156.7 | 1157.3 | ±1.29 | | 39.195 | | 223.35 | | 10.310 | | # |
| HNNH-  *trans* E-Diazene | | 30.02991 | 256.24 | 269.353 | ±1.62 | | 37.960 | | 226.896 | | 10.223 | | # |
| HNNH- *cis* | | 30.02991 | 271.42 | 284.179 | ±1.62 | | 40.324 | | 228.638 | | 10.577 | | # |
| HNNH- equil | | 30.02991 | 256.29 | 269.353 | ±1.62 | | 37.960 | | 226.896 | | 10.223 | | # |
| H2NN=O | | 46.02876 | 82.199 | 91.592 | ±8. | | 50.568 | | 249.708 | | 12.085 | | # |
| ND2NO2 NitrAmide-D2 | | 64.04048 | (see D2N2O2) | | |  | |  | |  | |  | | | # |
| NH2NO2 NITRAMIDE | | 62.02816 | 4.088 | 17.472 | ±8. | | 56.672 | | 268.548 | | 12.434 | | #† |
| H3N2 HYDRAZINE RAD <~> | | 31.03730 | 224.856 | 235.594 | ±0.91. | | 42.496 | | 236.791 | | 10.634 | | # |
| N2H3+ | | 31.03675 | 964.58 | 969.665 | ±1.13 | | 36.691 | | 227.297 | | 10.090 | | # |
| N2H3- | | 31.03785 | 236.8d | 252.9d | ±2.4 | | 46.079 | | 237.044 | | 11.403 | | # |
| N2H4(L) Hydrazin liq | | 32.04524 | 50.78d | 57.34d | ±0.18d | | 98.839 | | 121.545 | |  | | † |
| N2H4 HYDRAZIN <~> | | 32.04524 | 95.18  97.42 | 109.337  111.47p | ±0.2d  0.47p | | 48.43 | | 238.466 | | 11.449 | | † |
| N2H4+ | | 32.04469 | 879.85 | 887.768  886.6 | ±2.36  2.0p | | 50.089 | | 234.629 | | 11.491 | | # |
| N2H4- Hydrazin anion | | 32.04579 | 190.83 217.8. | 210.9d  232.2p | ±3.60  4.1 | | 47.923 | | 240.775 | | 11.579 | | # |
| NH4NO3 (solid) | | 80.04344 | -365.22 | -350.26 | ±0.19 | | 139.080 | | 150.810 | | 23.662 | | † |
| NH4NO3 gas | | 80.04344 | -230.6  -258.6 | -211.195 | ±3.  ±22. | | 93.110 | | 330.093 | | 19.221 | | #  X |
| N2O (NNO) Nitrous oxide <^~> | | 44.01288 | 81.6 | 85.029 | ±0.1 | | 38.628 | | 220.01 | | 9.581 | | † |
| N2O+ | | 44.01233 | 1333.399 | 1329.146 | ±0.12d | | 42.263 | | 233.859 | | 10.623 | | † |
| N2O- NNO- c | | 44.01343 | 91.52 | 100.3 | ±2.2d | |  | |  | |  | | X |
| N2O O(NN) cyclo c Oxadiazirine | | 44.01288 | 350.62 | 352.54 | ±1.69 | | 42.696 | | 240.866 | | 11.091 | | # |
| (NN)O+ cyclo cation | | 44.01233 | 1516.52 | 1512.823 | ±2.66 | | 40.254 | | 242.751 | | 10.509 | | # |
| (NN)O- cyclo anion c | | 44.01343 | 93.84 | 99.7d | ±2.54 | | 40.746 | | 244.447 | | 10.570 | | # |
| NON | | 44.01288 | 540.58 | 542.5 | ±1.76 | | 42.693 | | 240.863 | | 11.090 | | # |
| NON+ | | 44.01233 | 1450.5d | 1444.1d | ±2.7 | | 40.253 | | 242.749 | | 10.509 | | # |
| NON-c | | 44.01343 | 489.35 | 498.1d | ±2.7d | | 38.675 | | 241.062 | | 10.358 | | # |
| O=N-N=O *cis*d | | 60.01228 | 171.06d | 172.82d | ±0.14d | | 58.897 | | 282.895 | | 14.597 | | # |
| HN2O2 HN\*NO2 | | 61.02022 | 182.966 | 191.009 | ±100. | | 60.386 | | 287.102 | | 13.541 | | # |
| N2O3 O=N-NO2 | | 76.01168 | 86.631 | 91.2 | ±0.15d | | 72.733 | | 314.736 | | 17.121 | | † |
| N2O3+ O=N-NO2 N Sesquioxide | | 76.01113 | 1033.8d | 1031.0 | ±4.1d | |  | |  | |  | | X |
| N2O3+ | | 76.01113 | 1036.847 | 1033.763 | ±8.99 | | 76.843 | | 320.915 | | 18.577 | | # |
| N2O3- O=N-NO2- | | 76.01223 | -113.1d | -103.0d | ±2.9d | |  | |  | |  | | X |
| N2O3 ONONO Nitrosyl nitrite | | 76.01168 | 86.1d | 91.2d | ±1.6d | | 72.612 | | 294.381 | | 16.080 | | # |
| N2O3- ONONO- | | 76.01222 | -110.16 | -100.8]d | ±4.31 | | 73.720 | | 319.218 | | 16.458 | | # |
| N(O3)N | | 76.01168 | 593.3 | 602.76 | ±2.0 | | 60.123 | | 257.543 | | 12.231 | | # |
| N2O4 liq O2NNO2 liq | | 92.01108 | -27.10d | -37.96d | ±0.18d | |  | |  | |  | | X |
| N2O4 O2NNO2 <^> | | 92.01108 | 10.785 | 19.4 | ±0.13 | | 79.168 | | 304.451 | | 16.741 | | #† |
| N2O4 ONONO2 *cis* | | 92.01108 | 51.78 | 61.421 | ±2.10 | | 78.606 | | 314.338 | | 16.389 | | # |
| N2O5 O2NONO2 | | 108.01048 | 15.437 | 25.010 | ±0.35d | | 95.332 | | 355.717 | | 20.797 | | †# |
| N3 AZIDE RADICAL | | 42.02022 | 449.924 | 453.358 | ±0.71 | | 36.175 | | 223.072 | | 9.571 | | †# |
| N3+ | | 42.01967 | 1523.1 | 1519.52 | ±1.1 | | 41.979 | | 218.241 | | 10.388 | | # |
| N3- | | 42.02077 | 184.38 | 194.228 | ±1. | | 37.031 | | 212.443 | | 9.354 | | # |
| N3D Azidic Acid-d | | (see DN3) |  |  |  | |  | |  | |  | | # |
| N3H (s) Azidic Acid c | | 43.02816 | 261.701 |  | ±0.7 | |  | |  | |  | | X |
| N3H AZIDIC ACID | | 43.02816 | 291.826 | 298.118 | ±0.56 | | 44.219 | | 239.330 | | 10.947 | | †# |
| N3H+ | | 43.02761 | 1334.177 | 1333.176 | ±0.957 | | 47.155 | | 248.163 | | 11.158 | | # |
| N3H- c | | 43.02871 | 304.8d | 317.3d | ±2.5d | | 43.238 | | 249.912 | | 10.768 | | # |
| HN3O4 HN(NO2)2 | | 107.02576 | 109.491 | 125.715 | ±8. | | 92.101 | | 332.335 | | 18.376 | | # |
| N4 chain N=N-N=N | | 56.02696 | 686.6 | 684.814 | ±7.6 | | 66.451 | | 359.261 | | 19.126 | | # |
| N4 tetrahedral | | 56.02696 | 759.425 [757.4]d | 766.849 [763.9]d | ±1.98 ±1.6d | | 44.675 | | 232.489 | | 10.717 | | # |
| N4 Cyclo Tetrazete | | 56.02696 | 763.55d | 761.478d | ±2.4 | | 66.510 | | 380.611 | | 19.412 | | # |
| N4+ Cyclo | | 56.02641 | 1804.777 | 1803.46 | ±8. | | 53.671 | | 253.142 | | 12.460 | |  |
| N4- tetrahedral | | 56.02751 | 752.592 | 764.147 | ±8. | | 52.194 | | 246.694 | | 11.983 | | # |
| N4H4 NH4N3 (cr) | |  | 114.14 |  | ±0.94 | |  | |  | |  | | X |
| N4H4 NH4N3 (g) | |  | 179.7 | Doubtful |  | |  | | existence | |  | | X |
| N4H4O4 NH4N(NO2)2 solid | | 124.06 | -149.8 |  |  | |  | |  | |  | | X |
| N4H4O4 NH4N(NO2)2 gas | | 124.06 | Does not | existingas | phase | | (see | | Burcat.thr | | ) | | X |
| Na(cr) REFERENCE ELEMENT | | 22.98977 | 0. | 0. |  | | 28.230 | | 51.300 | | 6.460 | | † |
| Na(g) <^> | | 22.98977 | 107.5 | 107.763 | ±0.7 | | 20.786 | | 153.719 | | 6.197 | | † |
| Na+ | | 22.98922 | 609.34 |  |  | | 20.785 | | 147.953 | | 6.197 | | † |
| NaBH4 Solid | | 37.83253 | see | BH4Na |  | |  | |  | |  | | # |
| NaCN (cr,l) see CNNa | | 49.00721 |  |  |  | |  | |  | |  | | † |
| NaCl(cr) cubic Sodium Chloride | | 58.44247 | -411.260 | -410.809 | ±0.12 | | 50.500 | | 72.150 | | 10.600 | | † |
| NaCl(g) | | 58.44247 | -181.545 | -180.109 | ±0.2 | | 35.798 | | 229.798 | | 9.615 | | † |
| NaOH(cr) Sodium Hydroxide | | 39.99711 | -425.8 | -421.384 | ±0.2 | | 59.650 | | 64.445 | | 10.487 | | † |
| NaOH(l) Sodium Hydroxide | | 39.99711 | -416.878 | -412.331 | ±12.7 | |  | |  | |  | | † |
| NaOH(g) Sodium Hydroxide | | 39.99711 | -191.000 | -187.684 | ±8. | | 45.057 | | 237.036 | | 11.718 | | #† |
| NaOH+ Sodium Hydroxide cation | | 39.99656 | 683.886 | 681.004 |  | | 49.257 | | 242.630 | | 11.695 | | † |
| NaNO3(s) Sodium Nitrate | | 84.99471 | -467.700 | -461.115 | ±0.5 | | 93.050 | | 116.400 | | 17.230 | | † |
| NaNO3 (g) | | 84.99471 | -285.529 | -277.115 | ±5. | | 67.667 | | 300.084 | | 15.401 | | † |
| NaO2(cr) | | 54.98857 | -261. | -264.16 | ±3. | | 72.130 | | 115.900 | | 18.300 | | † |
| Na2CO3(s) | | 105.98844 | -1129.355 | -1122.946 | ±0.26 | | 112.300 | | 135.000 | | 20.750 | | † |
| Na2O(cr) | | 61.97894 | -414.57 | -409.71 | ±4.2 | | 69.120 | | 75.040 | | 12.400 | | † |
| Na2O(liq) | | 61.97894 | -372.843 |  |  | | 104.600 | | 91.607 | |  | | † |
| Na2O (g) | | 61.97894 | -16.56 | -13.710 | ±10. | | 56.773 | | 271.324 | | 14.410 | | † |
| Na2O2(cr) | | 77.97834 | -512. | -506.074 | ±5. | | 89.330 | | 94.770 | | 15.694 | | † |
| Na2O2(g) | | 77.97834 | -123.93 | -117.895 | ±30. | | 68.503 | | 289.595 | | 15.565 | | † |
| Ne REFERENCE ELEMENT<^> | | 20.1797 | 0 | 0 |  | | 20.786 | | 146.33 | | 6.197 | | † |
| Ne+ | | 20.17915 | 2086.966 | 2080.66 | ±0.001 | | 22.120 | | 158.310 | | 6.304 | | † |
| NeH radical | | 21.18764 | 212.715 | 212.674 | ±8. | | 38.706 | | 209.838 | | 10.472 | | # |
| NeH+ | | 21.18709 | 1338.395 | 1333.952 | ±8. | | 29.104 | | 175.879 | | 8.676 | | # |
| Ni(cr) REFERENCE ELEMENT | | 58.6934 | 0 | 0 |  | | 25.987 | | 29.87 | | 4.786 | | † |
| Ni | | 58.6954 | 434.903 | 428.078 | ±2.1 | | 23.361 | | 182.193 | | 6.825 | | † |
| Ni+ | | 58.69285 | 1172.6 | 1165. |  | | 20.990 | | 174.574 | | 6.206 | | † |
| Ni- | | 58.69395 | 311.764 | 316.541 |  | | 21.018 | | 174.580 | | 6.207 | | † |
| NiO Solid-A | | 74.6928 | -239.7 |  | ±0.5 | | 44.309 | | 37.991 | |  | |  |
| NiS(a) Crystal | | 90.7594 | -87.864 | -87.131 | ±6.3 | | 47.112 | | 52.992 | | 8.465 | | † |
| NiS2(s) | | 122.8254 | -131.378 |  | ±16.7 | | 70.627 | | 71.966 | |  | | † |
| Ni3S2(a) | | 240.2122 | -217.986 | -215.96 | ±5 | | 117.65 | | 133.888 | | 21.156 | | † |
| Ni3S4(s) | | 304.3442 | -301.115 |  | ±25.1 | | 164.808 | | 186.481 | |  | | † |
| Np(s) Neptunium REF.ELEMENT | | 237.0482 | 0. | 0. |  | | 29.624 | | 50.460 | |  | | X |
| Np g | | 237.0482 | 465.100 | 465.407 | ±3.0 | | 20.816 | | 197.719 | | 6.198 | | # |
| Np+3 | |  | -512.866 |  | ±2.092 | |  | | 193.584 | |  | | X |
| O <^!> | | 15.99940 | 249.175 | 246.79 | ±0.002 | | 21.912 | | 161.06 | | 6.725 | | † |
| O singlet (excited) <~> | | 15.99940 | 438.523 | 436.666 | ±0.002 | | 20.786 | | 156.816 | | 6.197 | | # |
| O triplet only (excited) | | 15.99940 | 249.229d | 246.844d | ±0.002 | |  | |  | |  | | X |
| O+ | | 15.99885 | 1568.787 | 1560.752 | ±0.002 | | 20.786 | | 154.961 | | 6.197 | | † |
| O- | | 15.99995 | 101.846 | 105.813 | ±0.002 | | 21.685 | | 157.797 | | 6.571 | | † |
| OT Tritium Oxide | | 19.0154 | 36.364 | 35.942 |  | | 29.370 | | 193.115 | | 9.067 | | # |
| T2O Tritium Water (3H2O) | | 22.0315 | -252.303 | -249.369 |  | | 34.958 | | 204.132 | | 10.016 | | # |
| O2 REFERENCE ELEMENT <^!> | | 31.99880 | 0 | 0 |  | | 29.378 | | 205.147 | | 8.680 | | † |
| O2 singlet (excited)d | | 31.99880 | 94.418 | 94.409 | ±0.001 | | 29.485 | | 201.915 | | 8.689 | | # |
| O2 triplet only c | | 31.99880 | 0.0000 | 0.000 | ±1.2E-5 | | Like | | REF | | Elemen | | X |
| O2+ | | 31.99825 | 1171.828 | 1165. [170.782]d | ±0.009 | | 30.67 | | 205.393 | | 9.311 | | † |
| O2- Superoxide anion | | 31.99935 | -48.028 [-48.92]d | -42.5 | ±0.18 | | 31.422 | | 209.336 | | 9.350 | | † |
| O2Pt see PtO2 | |  |  |  |  | |  | |  | |  | | # |
| O3 OZONE <~> | | 47.9982 | 141.8 | 144.454 | ±0.04d | | 39.378 | | 239.011 | | 10.366 | | † |
| O3+ | | 47.99765 | 1356.140 | 1352.45 | ±0.042 | | 40.631 | | 239.385 | | 10.511 | | † |
| O3- Ozone Anion | | 47.99875 | -67.049 | -58.463 | ±0.203 | | 41.790 | | 247.593 | | 10.631 | | # |
| O3 cyclo O(OO) Trioxirane | | 47.9982 | 272.46 | 275.188 | ±1.55 | | 38.788 | | 230.192 | | 10.292 | | # |
| O3+ cyclo O(OO) | | 47.99765 | 1503.8d | 1500.4d | ±4.4d | | 38.728 | | 233.057 | | 10.342 | | # |
| O3- cyclo O(OO) | | 47.99875 | -62.957 | -54.283 | ±8. | | 40.789 | | 238.085 | | 10.543 | | # |
| O4 | | 63.99760 | 397.672 | 403.426 | ±8. | | 51.050 | | 246.600 | | 11.607 | | # |
| O4+ | | 63.99705 | 1443.9 | 1443.5 | ±8. | | 49.235 | | 251.642 | | 11.557 | | # |
| O4- | | 63.99815 | -96.985 | -87.148 | ±8. | | 58.601 | | 264.132 | | 13.721 | | # |
| Os (S) REFERENCE ELEMENT | | 190.230 | 0. | 0. |  | | 24.660 | | 32.552 | | 4.987 | | # |
| Os Osmium | | 190.230 | 788.002 | 786.792 |  | | 20.786 | | 192.577 | | 6.197 | | # |
| P(cr,white) REF. ELEMENT | | 30.97376 | 0. | 0. |  | | 23.824 | | 41.090 | | 5.360 | | † |
| P(cr,red) | | 30.97376 | -17.460 | -15.707 |  | | 21.187 | | 22.853 | | 3.607 | |  |
| P <&> | | 30.97376 | 316.5 | 315.663 | ±1 | | 20.786 | | 163.2 | | 6.197 | | † |
| P+ | | 30.97321 | 1335.46 | 1337.47 |  | | 25.859 | | 166.971 | | 8.142 | | † |
| P- | | 30.97431 | 238.827 | 243.636 |  | | 22.169 | | 169.126 | | 6.748 | | † |
| PBr3 see Br3P | |  |  |  |  | |  | |  | |  | | # |
| PBr3+ see Br3P | | 270.68521 |  |  |  | |  | |  | |  | | # |
| PCL | | 66.42646 | 134.615 | 135.275 | ±42. | | 33.991 | | 236.883 | | 9.291 | | † |
| PCLF | | 85.42486 | -269.299 | -266.832 | ±8 | | 48.058 | | 282.105 | | 11.897 | | #† |
| PClF+ | | 85.42431 | 583.900 | 580.583 | ±8 | | 45.924 | | 272.646 | | 11.482 | | # |
| PCLF- | | 85.42541 | -392.945. | -384.986 | ±8 | | 50.850 | | 282.679 | | 12.602 | | #† |
| PCLF2 | | 104.42327 | -735.077 | -730.177 | ±30. | | 63.101 | | 295.068 | | 13.876 | | † |
| PCLF4 | | 142.42007 | -1364.91 | -1355.629 | ±100. | | 93.005 | | 326.834 | | 18.321 | | † |
| PCl=O | | 82.42586 | -269.299 | -266.701 | ±8. | | 46.371 | | 273.016 | | 11.692 | | # |
| PCl=O+ | | 82.42531 | 807.056 | 803.261 | ±8. | | 46.585 | | 278.187 | | 11.802 | | # |
| PCl=O- | | 82.42641 | -403.342 | -395.522 | ±8. | | 49.085 | | 287.415 | | 12.587 | | # |
| PCL2 | | 101.87916 | -72.371 | -70.405. | ±8. | | 51.418 | | 288.492 | | 12.576 | | #† |
| PCL2+ | | 101.87861 | 763.869 | 759.999 | ±8. | | 49.425 | | 278.685 | | 12.110 | | # |
| PCL2- | | 101.87971 | -242.605 | -235.283 | ±8. | | 53.786 | | 289.569 | | 13.304 | | #† |
| PCL2F | | 120.87756 | -511.925 | -507.839 | ±30. | | 67.435 | | 307.925 | | 14.868 | | † |
| PCL2F3 | | 158.87437 | -1122.02 | -1113.29 | ±100. | | 97.348 | | 335.435 | | 19.047 | | † |
| PCL3 <&> | | 137.33186 | -267.9 | -264.98 | ±8. | | 72.507 | | 314.278 | | 16.215 | | #† |
| PCL3+ | | 137.33131 | 688.85 | 685.904 | ±8. | | 70.031 | | 316.536 | | 15.664 | | # |
| PCL3- anion | | 137.33241 | -400.9 | -394.863 | ±8. | | 78.257 | | 347.604 | | 19.101 | | # |
| PCL3F2 | | 175.32867 | -878.875 | -870.953 | ±100. | | 102.183 | | 338.132 | | 20.165 | | † |
| PCL3O | | 153.33126 | -539.200 | -533.679 | ±8. | | 85.194 | | 326.492 | | 17.950 | | #† |
| PCL3O+ | | 153.33071 | 655.529 | 652.231 | ±8. | | 90.618 | | 356.318 | | 20.301 | | # |
| PCL3O- | | 153.33181 | -692.919 | -685.394 | ±8. | | 93.745 | | 383.585 | | 22.175 | | # |
| PCL4F | | 191.78296 | -635.016 | -628.616 | ±100. | | 107.850 | | 358.036 | | 21.734 | | † |
| PCL5 | | 208.23726 | -376. | -370.993 | ±2.0 | | 113.318 | | 367.208 | | 23.305 | | † |
| PD | | 32.98786 | 229.55 | 230.536 | ±8. | | 29.323 | | 201.925 | | 8.659 | | # |
| PD3 Phosphine-D3 | | 37.01607 | -4.971 | +2.641 | ±8. | | 42.333 | | 221.724 | | 10.602 | | # |
| PF <&> | | 49.97216 | -47.945 | -47.063 | ±20.9 | | 31.619 | | 225.006 | | 8.891 | | † |
| PF+ | | 49.97161 | 901.518 | 895.663 | ±37.7 | | 33.429 | | 224.038 | | 9.430 | | † |
| PF- | | 49.97271 | -164.046 | -157.592 | ±69. | | 34.786 | | 225.221 | | 9.516 | | † |
| PF2 | | 68.97057 | -465.014 | -462.066. | ±8. | | 44.599 | | 263.662 | | 11.237 | | #† |
| PF2+ | | 68.97002 | 399.769 | 396.722 | ±8. | | 42.598 | | 255.256 | | 10.962 | | # |
| PF2- | | 68.97112 | -548.657 | -540.112. | ±8.. | | 47.696 | | 262.085 | | 11.733 | | #† |
| PF3 | | 87.96897 | -934.304 | -928.864 | ±8. | | 59.278 | | 274.890 | | 13.157 | | #† |
| PF3+ | | 87.96842 | 180.159 | 179.159 | ±8. | | 57.568 | | 280.230 | | 13.051 | | # |
| PF3O | | 103.96837 | -1237.359 | -1228.96 | ±8. | | 70.364 | | 288.186 | | 14.542 | | # |
| PF3O+ | | 103.96782 | -8.142 | -7.732 | ±8. | | 73.155 | | 310.717 | | 16.093 | | # |
| PF5 | | 125.96578 | -1558.050 | -1547.48 | ±8 | | 86.198 | | 303.235 | | 16.852 | | #† |
| PH | | 31.9817 | 230.752 | 231.698 | ±33.5 | | 29.175 | | 196.381 | | 8.648 | | † |
| PH+ | | 31.98115 | 1224.9 | 1219.62 |  | | 29.116 | | 192.853 | | 8.677 | | # |
| PH- | | 31.98225 | 138.69 | 145.81 | ±8. | | 29.127 | | 193.088 | | 8.677 | | # |
| PH2 Phosphonium Radical | | 32.98964 | 135.474 | 139.333 | ±8. | | 34.272 | | 212.710 | | 9.969 | | #† |
| PH2+ Phosphonium cation | | 32.98909 | 1089.1 | 1086.764 | ±8. | | 34.234 | | 206.917 | | 9.967 | | # |
| PH2- Phosphonium anion | | 32.99019 | 7.07 | 17.10 | ±8. | | 34.441 | | 207.306 | | 9.978 | | #† |
| PH3 PHOSPHINE RRHO <&> | | 33.99758 | 11.786 | 19.712 | ±8. | | 37.102 | | 210.245 | | 10.137 | | #† |
| PH3+ | | 33.99703 | 965.537 | 967.081 | ±8. | | 39.053 | | 216.361 | | 10.321 | | # |
| PH3- | | 33.99812 | 160.870 | 174.515 | ±8. | | 41.962 | | 213.382 | | 10.533 | | # |
| P(OH)3 Metaphosphoric acid | | See | H3PO3 |  |  | |  | |  | |  | |  |
| O=P(OH)3 Orthophosphoric acid | | See | H3PO4 |  |  | |  | |  | |  | |  |
| PH4+ Phosphonium cation | | 35.00497 | 769.973 | 775.749 | ±8. | | 40.122 | | 203.417 | | 10.322 | | # |
| PN <&> | | 44.98050 | 171.487 | 172.48 | ±15. | | 29.691 | | 211.135 | | 8.702 | | † |
| PN+ | | 44.97995 | 1334.964 | 1329.755 | ±8. | | 29.630 | | 216.813 | | 8.701 | | # |
| PN- | | 44.98105 | 159.226 | 166.373 | ±8. | | 30.189 | | 217.871 | | 8.736 | | # |
| PO <&> | | 46.97316 | -27.344 | -27.548 | ±3. | | 31.761 | | 222.744 | | 9.390 | | † |
| PO+ | | 46.97261 | 785.860 | 780.668 | ±8. | | 29.519 | | 211.765 | | 8.695 | | # |
| PO- | | 46.97371 | -140.067 | -132.948 | ±1. | | 30.759 | | 222.403 | | 8.778 | | † |
| PO2 | | 62.97256 | -269.299 | -266.701 | ±8. | | 46.371 | | 273.016 | | 11.692 | | #† |
| PO2- | | 62.97311 | -625.25 | -615.76 | ±8. | | 40.983 | | 250.195 | | 10.698 | | #† |
| PO3 | | 78.97196 | -450.6 | -446.5 | ±8.4 | | 59.116 | | 287.252 | | 14.228 | | # |
| PO3+ | | 78.97141 | 790.317 | 788.91 | ±8. | | 56.270 | | 268.961 | | 12.907 | | # |
| PO3- | | 78.97251 | -930.37 | -917.965 | ±8. | | 52.739 | | 265.321 | | 12.022 | | # |
| H2PO4- Phosphoric acid anion | | 96.98779 | -1277.667 | -1270.378 | ±8. | | 85.475 | | 313.507 | | 16.200 | | # |
| HPO4 Phosphoric acid radical | | 95.97930 | -642.688 | -631.222 | ±8. | | 77.479 | | 306.278 | | 15.488 | | # |
| HPO4-2 Phosphoric acid bianion | | 95.98039 | -911.188 | -921.660 | ±8. | | 78.569 | | 290.824 | | 15.376 | | # |
| PO4-3 Phosphate triple anion | | 94.97301 | -31.365 | -4.067 | ±8. | | 68.472 | | 287.400 | | 13.740 | | # |
| PS <&> | | 63.03976 | 159.83 | 159.985 | ±2.2 | | 35.242 | | 234.068 | | 9.616 | | #† |
| PT Tritium Phosphor | | 33.9898 | 227.92 | 228.8 | ±8. | | 29.552 | | 205.501 | | 8.696 | | # |
| P2 <&> | | 61.94752 | 144. | 145.816 | ±2.0 | | 32.032 | | 218.124 | | 8.904 | | † |
| P2H radical | | 62.95546 | 223.873 | 228.183 | ±8. | | 41.163 | | 255.618 | | 10.644 | | # |
| P2H+ cation | | 62.95491 | 1031.9 | 1030.3 | ±8. | | 38.583 | | 246.799 | | 10.315 | | # |
| P2H- anion | | 62.95601 | 70.006 | 80.575 | ±8. | | 40.146 | | 249.465 | | 10.523 | | # |
| P2H2 Diphosphene HP=PH *trans* | | 63.96340 | 126.378 | 134.640 | ±8. | | 45.355 | | 248.821 | | 10.926 | | # |
| P2H2+ HP=PH+ cation | | 63.96285 | 1058.465 | 1058.879 | ±8. | | 52.732 | | 262.452 | | 12.440 | | # |
| P2H2- HP=PH- anion | | 63.96395 | 25.777 | 39.350 | ±8. | | 50.003 | | 259.425 | | 11.679 | | # |
| P2H4 H2P-PH2 | | 65.97928 | 38.828 | 52.863 | ±8. | | 61.236 | | 265.919 | | 13.621 | | # |
| P2H4+ H2P-PH2+ | | 65.97873 | 904.045 | 911.899 | ±8. | | 63.517 | | 265.943 | | 13.371 | | # |
| P2H4- H2P-PH2- | | 65.97983 | 63.980 | 82.918 | ±8. | | 78.702 | | 308.306 | | 18.040 | | # |
| P2O3 | | 109.94572 | -684.645 | -677. | ±15. | | 73.927 | | 312.698 | | 16.095 | | † |
| P2O4 | | 125.94512 | -933.755 | -923. | ±25. | | 85.131 | | 312.913 | | 17.326 | | † |
| P2O5 | | 141.94452 | -1124.37 | -1114. | ±30. | | 105.936 | | 366.58 | | 22.050 | | † |
| P3 | | 92.92128 | 210. | 214.074 | ±20. | | 51.873 | | 263.529 | | 12.006 | | † |
| P3O6 | | 188.91768 | -1575.68 | -1557. | ±35. | | 135.741 | | 376.077 | | 23.439 | | † |
| P4 tetrahedral <&> | | 123.89504 | 74.931 | 82.263 | ±0.4 | | 67.081 | | 279.930 | | 14.109 | | #† |
| P4O6 (P2O3)2 | | 219.89144 | -1606. | -1583.317 | ±40. | | 148.611 | | 356.395 | | 24.798 | | † |
| P4O7 | | 235.89084 | -1984.45 | -1959. | ±15. | | 159.256 | | 379.867 | | 26.372 | | † |
| P4O10(s) | | 283.88904 | -3010.10 | -2979.479 | ±3.2 | | 215.569 | | 231.000 | | 34.220 | | † |
| P4O10 (P2O5)2 | | 283.88904 | -2906.22 | -2872.479 | ±5. | | 191.196 | | 402.094 | | 31.097 | | † |
| Pb (cr) Reference Element | | 207.2 | 0. | 0. |  | | 24.430 | | 36.899 | | 6.870 | | † |
| Pb (gas) | | 207.2 | 195.2 | 195.88 | ±0.8 | | 20.786 | | 175.377 | | 6.197 | | † |
| Pb+ | | 207.19945 | 916.997 | 910.799 |  | | 20.786 | | 181.140 | | 6.197 | | † |
| Pb- | | 207.20054 | 153.882 | 160.752 |  | | 20.786 | | 186.903 | | 6.197 | | † |
| PbBr | | 287.1040 | 64.821 | 73.805 | ±20 | | 36.916 | | 272.744 | | 10.146 | | † |
| PbBr2 | | 367.0080 | -103.908 | -87.54 | ±7. | | 56.966 | | 339.673 | | 15.022 | | † |
| PbBr3 | | 446.9120 | -104.011 | -80.330 | ±80. | | 80.540 | | 385.255 | | 19.969 | | † |
| PbBr4 | | 526.8260 | -182.436 | -152.4 | ±80. | | 104.468 | | 427.724 | | 25.871 | | † |
| PbCl | | 242.65270 | 8.819 | 10.493 | ±12. | | 36.215 | | 261.306 | | 9.787 | | † |
| PbCl2 | | 278.10540 | -175.046 | -173.5 | ±5. | | 55.299 | | 315.621 | | 14.003 | | † |
| PbCl3 | | 313.55810 | -177.654 | -175.27 | ±80. | | 77.918 | | 351.604 | | 18.256 | | † |
| PbCl4 | | 349.0108 | -327.43 | -325.65 | ±80. | | 100.537 | | 381.682 | | 23.449 | | † |
| PbF | | 226.19840 | -98.072 | -96.853 | ±10. | | 34.401 | | 249.962 | | 9.268 | | † |
| PbF2 | | 245.19681 | -443.427 | -440.30 | ±11. | | 50.981 | | 291.532 | | 12.573 | | † |
| PbF3 | | 264.19521 | -489.573 | -485.0 | ±60. | | 70.582 | | 316.287 | | 15.535 | | † |
| PbF4 | | 283.1936 | -799.925 | -795.03 | ±60. | | 90.232 | | 331.825 | | 19.626 | | † |
| PbH | | 208.20794 | 236.19 | 238.605 | ±19.2 | | 29.409 | | 220.699 | | 8.689 | | # |
| PbI | | 344.10447 | 108.904 | 112.033 | ±4. | | 37.152 | | 280.413 | | 10.339 | | † |
| PbI2 | | 461.00894 | -10.253 | -5434 | ±5. | | 57.182 | | 352.613 | | 15.247 | | † |
| PbI3 | | 587.91341 | 21.755 | 27.35 | ±80. | | 81.624 | | 411.532 | | 21.065 | | † |
| PbI4 | | 714.81788 | -41.281 | -35.485 | ±80. | | 106.276 | | 463.806 | | 27.521 | | † |
| PbN6 solid Lead Azide | |  | 483.7 |  |  | |  | |  | |  | | X |
| PbN6(S) Lead Azidew | | 291.3 | 462.3 |  |  | |  | |  | |  | | X |
| PbO(S) | | 223.19940 | -218.6 | -216.61 | ±0.5 | | 46.414 | | 67.840 | | 9.225 | | † |
| PbO | | 223.19940 | 68.187 | 70.385 | ±4.5 | | 32.513 | | 240.045 | | 8.962 | | † |
| PbO2(S) | | 239.19880 | -276.0 | -271.41 | ±1.5 | | 60.997 | | 71.920 | | 10.962 | | † |
| PbO2 | | 239.19880 | 136.153 | 139.452 | ±100. | | 51.721 | | 261.093 | | 12.251 | | † |
| PbS(S) Galena | | 239.2660 | -99.475 | -99.703 | ±1.5 | | 49.499 | | 91.200 | | 11.510 | | † |
| PbS | | 239.2660 | 127.945 | 129.797 | ±1.5 | | 35.085 | | 251.414 | | 9.430 | | † |
| PbS2 | | 271.3320 | 244.049 | 245.722 | ±10. | | 57.511 | | 286.141 | | 14.021 | | † |
| PbTe (S)(L) | | 334.80000 | -70.7 |  |  | | 50.551 | | 110.039 | |  | |  |
| PbTe | | 334.80000 | 393. |  |  | | 36.732 | | 271.391 | | 10.103 | | # |
| Pd(S) REFERENCE ELEMENT | | 106.420 | 0. | 0. |  | | 25.891 | | 37.602 | | 5.439 | | # |
| Pd Paladium (gas) | | 106.420 | 375.999 | 375.242 |  | | 20.786 | | 167.063 | | 6.196 | | # |
| Pd+ Paladium Cation | | 106.41945 | 1186.591 | 1179.63 |  | | 20.786 | | 181.962 | | 6.197 | | # |
| Po(cr) Polonium REF. ELEMENT | | 208.98240 | 0. | 0. |  | | 25.999 | | 61.999 | | 6.699 | | # |
| Po Polonium (gas) | | 208.98240 | 182.017 | 182.52 |  | | 20.786 | | 188.811 | | 6.197 | | # |
| Po+ Polonium cation | | 208.98185 | 1000.83 | 994.637 |  | | 20.786 | | 187.067 | | 6.197 | | # |
| Po- Polonium anion | | 208.98295 | -7.18 | -13.376 |  | | 20.786 | | 187.067 | | 6.197 | | # |
| Po2 DiPolonium (gas) | | 417.9648 | 180.0 | 183.04 |  | | 37.171 | | 274.943 | | 10.360 | | # |
| Pt(S) REFERENCE ELEMENT | | 195.078 | 0. | 0. |  | | 25.640 | | 41.568 | | 5.707 | | # |
| Pt Platinum | | 195.078 | 564.999 | 558.422 |  | | 25.531 | | 192.410 | | 6.577 | | # |
| Pt+ Platinum cation | | 195.07745 | 1431.815 | 1425.129 |  | | 20.786 | | 189.518 | | 6.197 | | # |
| Pt- Platinum anion | | 195.07855 | 353.121 | 358.828 |  | | 20.826 | | 180.385 | | 6.197 | | # |
| PtH radical | | 196.08594 | N/A | N/A |  | | 29.723 | | 216.963 | | 8.681 | | # |
| PtO2 solid anhydrous | | 227.07680 | ~80.0 |  |  | |  | |  | |  | | X |
| PtO2 PlatinumDioxide | | 227.07680 | 170.707 |  |  | | 43.118 | | 259.626 | |  | | # |
| Pu cr Plutonium REF. ELEMENT | | 239.05216 | 0. | 0. |  | | 31.490 | | 54.460 | |  | | X |
| Pu (g) Plutonium | | 239.05216 | 349.000 | 348.710 |  | | 20.854 | | 177.055 | | 6.199 | | # |
| Pu+ Plutonium cation | |  | 939.198 | 833.710 |  | | 20.880 | | 182.822 | | 6.200 | | # |
| PuH2 (s) | | 246.080 | -139.327 |  |  | | 39.018 | | 59.831 | |  | | X |
| PuO (s) | | 260.064 | -564.840 |  |  | | 51.269 | | 70.710 | |  | | X |
| PuO2 (s) | | 278.073 | -1055.832 |  |  | | 66.242 | | 66.128. | |  | | X |
| Pu(SO4)2 (s) | | 428.191 | -2200.784 |  |  | | 181.815 | | 163.176 | |  | | X |
| Ra Radium (cr) Reference Element | | 226.02540 | 0. | 0. |  | | 28.999 | | 68.998 | | 7.201 | | # |
| Ra Radium (g) | | 226.02540 | 160. | 161. |  | | 20.786 | | 138.168 | | 5.862 | | # |
| Ra+(g) Radium cation | | 226.02485 | 675.524 | 670.293 |  | | 20.786 | | 182.222 | | 6.197 | | # |
| Rn REFERENCE ELEMENT | | 222.01760 | 0. | 0. |  | | 20.786 | | 176.238 | | 6.197 | | † |
| Rn+ Radon Cation | | 222.01705 | 1043.3 | 1037.1 |  | | 20.786 | | 187.761 | | 6.197 | | † |
| S(S) REFERENCE ELEMENT | | 32.066 | 0. | 0. |  | | 22.690 | | 33.070 | | 4.412 | | † |
| S \*\*\*\*\* <~> | | 32.066 | 277.17 | 274.925 | ±0.25 | | 23.674 | | 167.832 | | 6.657 | | † |
| S+ | | 32.06545 | 1282.496 | 1274.514 |  | | 20.786 | | 163.632 | | 6.197 | | † |
| S- | | 32.06655 | 70.369 | 74.513 |  | | 22.783 | | 164.923 | | 6.465 | | † |
| SBr | | See BrS |  |  |  | |  | |  | |  | |  |
| SBr2 | | See Br2S |  |  |  | |  | |  | |  | |  |
| SCL | | 67.5187 | 156.47 | 155.648 | ±16.7 | | 37.542 | | 237.328 | | 9.819 | | † |
| SCL2 | | 102.9714 | -17.573 | -16.425 | ±3.3 | | 50.896 | | 281.633 | | 12.445 | | † |
| SCL2+ | | 102.97085 | 901.383 | 896.326 | ±2. | | 50.861 | | 287.327 | | 12.453 | | † |
| SCL2- | | 102.97195 | -210.857 | -205.528 | ±8. | | 56.219 | | 301.415 | | 14.462 | | # |
| SF | | 51.0644 | 15.446 | 14.8 | ±6.3 | | 35.180 | | 225.282 | | 9.470 | | † |
| SF+ | | 51.06385 | 994.570 | 988.333 | ±10. | | 31.679 | | 225.410 | | 8.864 | | † |
| SF- | | 51.06495 | -231.347 | -225.2 | ±50. | | 31.787 | | 216.351 | | 8.875 | | † |
| SF2 | | 70.06281 | -293.189 | -291. | ±10. | | 44.415 | | 256.582 | | 11.048 | | † |
| SF2+ | | 70.06226 | 706.016 | 701.821 |  | | 44.937 | | 263.528 | | 11.234 | | † |
| SF2- | | 70.06336 | -394.795 | -387.485 | ±42. | | 50.165 | | 267.450 | | 12.125 | | † |
| SF3 | | 89.06121 | -504.101 | -500. | ±20. | | 63.148 | | 285.616 | | 13.548 | | † |
| SF3+ | | 89.06066 | 393.583 | 392.627 | ±33.5 | | 56.224 | | 268.977 | | 12.409 | | † |
| SF3- | | 89.06176 | -790.124 | -780. | ±7. | | 64.068 | | 281.593 | | 13.773 | | † |
| SF4 | | 108.05961 | -760. | -753.321 | ±20. | | 76.673 | | 296.714 | | 15.383 | | † |
| SF4+ | | 108.05906 | 416.112 | 415.471 | ±50. | | 80.396 | | 311.676 | | 16.506 | | † |
| SF4- | | 108.06016 | -887.464 | -877.685 | ±33.5 | | 89.189 | | 312.967 | | 18.480 | | † |
| SF5 | | 127.05802 | -902.663 | -895. | ±10. | | 100.085 | | 322.275 | | 18.811 | | † |
| SF5+ | | 127.05746 | 172.644 | 176.574 | ±20.9 | | 89.844 | | 298.157 | | 16.347 | | † |
| SF5- | | 127.05856 | -1204.62 | -1191. | ±10. | | 101.065 | | 317.070 | | 19.050 | | † |
| SF5Br | | 206.96202 | -972.8 | -953.5 | ±59 | | 107.075 | | 333.654 | | 19.433 | | # |
| SF5CL | | 162.51072 | -1038.9 | -1026.293 | ±10.5 | | 104.344 | | 323.589 | | 18.458 | | # |
| SF6 <^> | | 146.05642 | -1219.4 | -1205.453 | ±1.5 | | 97.069 | | 291.678 | | 16.940 | | † |
| SF6- | | 146.05697 | -1341.88 | -1322.282 | ±29.3 | | 99.986 | | 302.865 | | 17.491 | | † |
| SN | | 46.07274 | 279.45 | 278.427 | ±2.1 | | 31.795 | | 222.096 | | 9.393 | | #† |
| SO <~> | | 48.06540 | 4.760 | 4.714 | ±0.18 | | 30.176 | | 221.942 | | 8.798 | | † |
| SO- | | 48.06595 | -105.968 | -100.486 | ±5.0 | | 34.425 | | 223.679 | | 9.467 | | † |
| SOF2 | | 86.06221 | -584.952 | -580. | ±50. | | 57.095 | | 279.138 | | 12.625 | | † |
| SO2 <^~> | | 64.0648 | -296.81 | -294.266 | ±0.21 | | 39.842 | | 248.222 | | 10.548 | | † |
| SO2+ cation | | 64.06425 | 914.506 | 910.559 | ±8. | | 41.696 | | 255.018 | | 10.842 | | # |
| SO2- | | 64.06535 | -408.606 | -400.066 | ±3.5 | | 41.795 | | 256.027 | | 10.749 | | † |
| SO2CLF | | 118.5159 | -556.472 | -549.070 | ±21 | | 71.593 | | 302.854 | | 14.701 | | † |
| SO2CL2 | | 134.9702 | -354.802 | -348.559 | ±2.1 | | 77.096 | | 311.101 | | 16.029 | | † |
| SO2F2 | | 102.06161 | -760. | -751.573 | ±8.4 | | 65.776 | | 283.543 | | 13.490 | | † |
| SO3 <~> | | 80.06420 | -395.9 | -390.156 | ±0.71 | | 50.619 | | 256.547 | | 11.688 | | † |
| SO3- | | 80.06475 | -595.95 | -584.378 | ±8. | | 53.666 | | 265.328 | | 12.057 | | # |
| SO4 | | 96.06360 | -241.124 | -233.251 | ±8. | | 67.566 | | 278.915 | | 13.899 | | # |
| SO4- Sulfate anion | | 96.06414 | -743.8 | -729.975 | ±8. | | 69.442 | | 297.636 | | 14.145 | | # |
| ST Sulfur Tritium | | 35.08982 | 135.022 | 142.899 | ±8. | | 32.656 | | 204.812 | | 9.237 | | # |
| ST2 | | 38.098 | -34.016 | -31.221 | ±8. | | 36.819 | | 220.562 | | 10.186 | | # |
| S2 <~> | | 64.13200 | 128.60 | 128.292 | ±0.3 | | 32.505 | | 228.167 | | 9.132 | | † |
| S2- | | 64.13255 | -37.132 | -31.708 | ±4.0 | | 37.193 | | 228.430 | | 9.597 | | † |
| S2CL | | 99.58470 | 78.6 | 79.540 | ± | | 50.968 | | 292.162 | | 12.474 | | † |
| S2CL2 | | 135.0374 | -16.736 | -16.734 | ±4.2 | | 72.776 | | 327.237 | | 16.521 | | † |
| S2F2 (S=SF2) Thiothionyl fluoride | | 102.12881 | -331.8 | -327.869 | ±2.1 | | 63.128 | | 292.833 | | 13.718 | | #† |
| FS2F (FSSF) Fluorodisulfane | | 102.12881 | -322.2 | -319.146 | ±2.1 | | 66.042 | | 294.088 | | 14.595 | | #† |
| S2F10 | | 254.11603 | -2064.39 |  | ±29.3 | | 176.702 | | 397.041 | |  | |  |
| S2O SSO | | 80.13140 | -56.035 | -54. | ±1.4 | | 44.114 | | 266.968 | | 11.129 | | † |
| S2O+ SSO+ cation | | 80.13085 | 976.948 | 972.108 | ±8. | | 46.704 | | 272.463 | | 11.807 | | # |
| S2O- SOS anion | | 80.13195 | -246.800 | -239.309 | ±1.6 | | 48.457 | | 273.597 | | 11.871 | | # |
| SOS cyclo | | 80.13140 | 134.306 | 136.383 | ±4.2 | | 45.310 | | 261.411 | | 11.087 | | # |
| S2O+ SOS cyclo cation | | 80.13085 | 1057.414 | 1052.393 | ±8. | | 47.592 | | 273.147 | | 11.988 | | # |
| S3 | | 96.19800 | 144.738 | 146. | ±4. | | 48.964 | | 276.296 | | 11.974 | | † |
| S3- | | 96.19855 | -81.5 | -74.4 | ±2.5 | | 50.769 | | 286.108 | | 12.370 | | # |
| S4 | | 128.2640 | 135.632 | 139. | ±3. | | 65.944 | | 293.565 | | 14.280 | | † |
| S5 | | 160.3300 | 132.993 | 136. | ±4. | | 87.870 | | 354.088 | | 19.053 | | † |
| S6 | | 192.3960 | 101.315 | 105. | ±3. | | 113.165 | | 357.812 | | 22.787 | | † |
| S7 | | 224.4620 | 111.890 | 116.5 | ±3. | | 133.866 | | 404.855 | | 26.274 | | † |
| S8 | | 256.528 | 101.277 | 105. | ±2. | | 156.503 | | 432.546 | | 31.573 | | † |
| Sb(s) REFERENCE ELEMENT | | 121.760 | 0 | 0 |  | | 25.301 | | 45.080 | | 5.822 | | # |
| Sb(g) | | 121.760 | 264.588 |  |  | | 20.786 | | 180.264 | | 6.197 | | # |
| Sb-W | | 121.761 | 161. |  | ±6.3 | |  | |  | |  | | X |
| SbBr3 TriBromoAntimon | | 361.4720 | -120.123 |  | ±21. | | 79.632 | | 377.075 | | 19.762 | | # |
| SbCl singlet | | 157.21270 | 177.820 |  | ±11.4 | | 37.948 | | 248.179 | | 9.750 | | # |
| SbCl2 DichloroAntimon Radical | | 192.66540 | -98.742 | -97.32 | ±4.27 | | 43.229 | | 280.788 | | 11.032 | | # |
| SbCl3 TrichloroAntimon. | | 228.11810 | -313.382 | -312.0 | ±4.48 | | 77.389 | | 341.080 | | 18.207 | | # |
| SbCl5 PentachloroAntimon | | 299.0235 | -433.044 |  | ±9.12 | | 122.115 | | 422.234 | | 27.003 | | # |
| SbF | | 140.7584 | -74.128 |  |  | | 35.992 | | 236.617 | | 9.301 | | # |
| SbF3 TriFluoroAntimon | | 178.75521 | -812.533 |  |  | | 68.256 | | 303.031 | |  | | # |
| SbOH singlet | | 138.76734 | 68.199 |  | ±19.8 | | 39.595 | | 273.714 | | 10.471 | | # |
| SbOH triplet | | 138.76734 | 21.34 |  | ±6.4 | | 40.422 | | 263.403 | | 10.573 | | # |
| Sb(OH)2 | | 155.77468 | -279.073 |  | ±6.3 | | 66.186 | | 308.869 | | 14.798 | | # |
| SbH3 Antimonium Hydride | | 124.78382 | 144.766 | 153.218 | ±4.2 | | 41.217 | | 232.745 | | 10.493 | | # |
| Sb(OH)3 | | 172.78202 | -638.478 |  | ±4.5 | | 97.581 | | 333.671 | | 19.140 | | # |
| Sb2(g) | | 243.520 | 236. |  |  | | 36.412 | | 255.882 | | 9.894 | | # |
| Sb2H4 (g) DiStibane | | 247.552 | 239.3 |  |  | |  | |  | |  | | X |
| Sb4(g) | | 487.04000 | 205. |  |  | | 79.318 | | 354.711 | | 18.880 | | # |
| Si(cr) REFERENCE ELEMENT | | 28.0855 | 0. | 0. |  | | 19.789 | | 18.81 | | 3.217 | | † |
| Si <~> | | 28.0855 | 450. | 448.32 | ±0.84 | | 22.251 | | 167.982 | | 7.550 | | † |
| Si+ | | 28.08495 | 1242.5 | 1232.185 |  | | 24.336 | | 163.429 | | 7.343 | | † |
| Si- SG | | 28.08605 | 308.817 |  | ±14. | | 20.786 | | 187.196 | |  | | X |
| SiC(b) Silicon carbide | | 40.09620 | 734.946 | 730. | ±20. | | 31.032 | | 226.213 | | 9.217 | | † |
| SiC2 | | 52.10690 | 631.361 | 625.0 | ±12. | | 44.227 | | 252.239 | | 11.685 | | † |
| SiCl <&> | | 63.53820 | 142.363 | 140.327 | ±40. | | 35.783 | | 237.840 | | 9.884 | | † |
| SiCl2 | | 98.99090 | -163.069 | -163.2 | ±4.2 | | 51.274 | | 281.618 | | 12.529 | | † |
| SiCl3 | | 134.44360 | -336.272 | -335. | ±10. | | 70.563 | | 316.646 | | 15.717 | | † |
| SiHCl3 | | 135.45154 | -496.222 | -491.150 | ±4.2 | | 75.457 | | 313.722 | | 16.152 | | † |
| SiCl4 <^> | | 169.89630 | -662.2 | -660.076 | ±0.8 | | 90.406 | | 331.452 | | 19.455 | | † |
| SiF MonofluoroSilicone radical | | 47.08390 | -62.555 | -63.776 | ±8. | | 31.551 | | 220.615 | | 8.851 | | #† |
| SiF+ MonofluoroSilicone cation | | 47.08335 | 657.491 | 650.143 | ±8. | | 30.593 | | 214.001 | | 8.765 | | # |
| SiF- MonofluoroSilicone anion | | 47.08445 | -87.869 | -83036 | ±8. | | 32.550 | | 216.367 | | 8.968 | | # |
| SIF2 DifluoroSilylene | | 66.08231 | -630.625 | -629.8 | ±8 | | 44.396 | | 262.954 | | 11.231 | | # |
| SiF2+ Difluorosilane cation | | 66.08176 | 429.400 | 423.96 | ±8. | | 43.488 | | 261.852 | | 11.247 | | # |
| SiF2- Difluorosilane anion | | 66.08285 | -661.0 | -654.7 | ±8. | | 47.004 | | 266.168 | | 11.614 | | # |
| SiOF2 O=SiF2 DiFluorooxySilane | | 82.08171 | -899.008 | -895.734 | ±8. | | 57.762 | | 277.687 | | 13.109 | | # |
| SiOF2+ O=SiF2 cation | | 82.08116 | 247.409 | 243.780 | ±8. | | 59.201 | | 281.730 | | 13.649 | | # |
| SiOF2- O=SiF2 anion | | 82.08225 | -1056.075 | -1047.142 | ±8. | | 60.504 | | 279.970 | | 13.461 | | # |
| SiF3 TrifluoroSilyl Radical | | 85.08071 | -993.365 | -990.4 | ±8. | | 59.613 | | 282.433 | | 13.398 | | # |
| SiHF3 TriFluoroSilane | | 86.08865 | -1207.67 | -1200.5 | ±5.4 | | 63.486 | | 277.351 | | 13.545 | | # |
| SiHF3+ Trifluorosilane cation | | 86.08810 | 73.200 | 71.550 | ±8. | | 74.988 | | 291.332 | | 15.874 | | # |
| SiF4 TetrafluoroSilane <^~> | | 104.07911 | -1614.98 | -1609.4 | ±4.2 | | 73.534 | | 282.615 | | 15.325 | | # |
| SiF4+ TetrafluoroSilane cation | | 104.07856 | -81.09 | -83.341 | ±8.0 | | 79.002 | | 297.107 | | 16.636 | | # |
| SiF4- TetrafluoroSilane anion | | 104.07966 | -1544.08 | -1534.93 | ±8. | | 82.680 | | 317.359 | | 18.190 | | # |
| SiH | | 29.09344 | 376.560 | 375.355 | ±8. | | 29.209 | | 192.745 | | 8.656 | | # |
| SiH+ | | 29.09289 | 1144.5 | 1136.9 | ±8. | | 29.555 | | 192.472 | | 8.686 | | # |
| SiH- | | 29.09399 | 298.812 | 303.800 | ±8. | | 29.259 | | 187.615 | | 8.660 | | # |
| SiHT3 TritritiumSilane | | 38.14159 | 27.610 | 36.134 | ±10. | | 53.868 | | 234.262 | | 11.781 | | # |
| SiH2  singlete radical | | 30.10138 | 263.843 | 265.527 | ±8. | | 34.742 | | 207.584 | | 10.001 | | # |
| SiH2  triplete radical | | 30.10138 | 354.623 | 356.244 | ±8. | | 35.460 | | 215.360 | | 10.065 | | # |
| SiH2+ cation | | 30.10083 | 1156.920 | 1152.340 | ±8. | | 35.343 | | 211.902 | | 10.054 | | # |
| SiH2- anion | | 30.10193 | 153.720 | 161.565 | ±8. | | 35.067 | | 213.949 | | 10.023 | | # |
| SiH2T2 DiTritiumSilane | | 36.13348 | 30.086 | 39.077 | ±10. | | 49.675 | | 226.033 | | 11.263 | | # |
| SiT2HD Silane T2 D | | 37.13964 | 10.150 | 18.873 | ±10. | | 52.372 | | 241.100 | | 11.582 | | # |
| SiH3 Silyl <~> | | 31.10932 | 195.569 | 201.090 | ±8. | | 40.077 | | 217.058 | | 10.398 | | #† |
| SiH3+ Silyl cation | | 31.10877 | 988.889 | 988.206 | ±8. | | 39.544 | | 210.564 | | 10.342 | | # |
| SiH3- Silyl anion | | 31.10987 | 52.253 | 64.053 | ±8. | | 38.758 | | 211.838 | | 10.260 | | # |
| SiH3T MonoTritiumSilane | | 34.89487 | 32.451 | 41.815 | ±10. | | 45.939 | | 222.416 | | 10.840 | | # |
| SiH4 Silane <^~> | | 32.11726 | 34.7 | 44.319 | ±8.2 | | 42.787 | | 204.208 | | 10.535 | | † |
| SiH4+ cation | | 32.11671 | 1144.596 | 1147.027 | ±8. | | 51.119 | | 215.286 | | 11.525 | | # |
| SiH3OH Silanol | | 48.11666 | -282.000 | -294.462 | ±8. | | 56.981 | | 247.425 | | 12.462 | | # |
| SiO gas | | 44.08490 | -102.223 | -103.381 | ±8. | | 29.899 | | 211.591 | | 8.715 | | # |
| SiO+ cation | | 44.08435 | 1020.495 | 1013.110 | ±8. | | 30.185 | | 217.702 | | 8.734 | | # |
| SiO- anion | | 44.08545 | -117.002 | -112.018 | ±8. | | 30.459 | | 218.277 | | 8.754 | | # |
| SiO2(Lqz) Quarz | | 60.08430 | -910.7 | -905.718 | ±1.0 | | 44.602 | | 41.460 | | 9.916 | | † |
| SiO2 gas | | 60.08430 | -322.070 | -321.432 | ±10. | | 45.674 | | 233.390 | | 11.260 | | # |
| SiO2- anion | | 60.08485 | -488.386 | -481398 | ±8. | | 42.656 | | 256.257 | | 11.039 | | # |
| SiS2 Solid | | 92.2175 | -213.384 |  |  | | 77.482 | | 80.333 | |  | | # |
| SiT Silicone Tritium | | 31.10155 | 369.096 | 367.882 |  | | 29.982 | | 201.971 | | 8.716 | | # |
| SIT+ Silicone Tritium cation | | 31.10100 | 1131.270 | 1123.810 | ±20. | | 29.775 | | 195.962 | | 8.702 | | # |
| SIT- Silicone tritium anion | | 31.10205 | 294.695 | 299.582 | ±20. | | 30.382 | | 196.679 | | 8.744 | | # |
| SiT4 TetraTritium Silane | | 40.14970 | 17.344 | 25.330 | ±8. | | 58.469 | | 226.904 | | 12.370 | | # |
| SiT4- TetraTritium Silane anion | | 40.15020 | 138.147 | 151.239 | ±20. | | 64.317 | | 238.121 | | 12.994 | | # |
| Si2F6 HexaFluoroDisilan | | 170.16142 | -2346.722 | -2340.593 | ±8. | | 128.567 | | 404.351 | | 26.782 | | # |
| Si2F6+ HexaFluoroDisilan cation | | 170.16087 | -1205.088 | -1207.485 | ±8. | | 130.849 | | 433.135 | | 28.747 | | # |
| Si2F6- HexaFluoroDisilan anion | | 170.16197 | -2401.735 | -2391.386 | ±8. | | 136.436 | | 411.445 | | 28.461 | | # |
| Si2OF6 F3Si-O-SiF3 | | 186.16082 | -2865.848 | -2857.612 | ±8. | | 138.522 | | 446.199 | | 29.015 | | # |
| Si2H HSi≡Si radical | | 57.17894 | 492.176 | 492.246 | ±8. | | 40.409 | | 254.305 | | 10.599 | | # |
| Si2H2 HSi≡SiH | | 58.18688 | 452.119 | 453.439 | ±8. | | 57.192 | | 262.489 | | 13.583 | | # |
| Si2H2+ HSi≡SiH+ cation | | 58.18633 | 1267.000 | 1261.208 | ±8. | | 59.584 | | 276.578 | | 14.357 | | # |
| Si2H4 H2Si=SiH2 | | 60.20276 | 273.136 | 282.273 | ±8. | | 70.016 | | 262.567 | | 14.234 | | # |
| Si2H4+ H2Si=SiH2  cation | | 60.20221 | 1066.000 | 1068.288 | ±8. | | 71.846 | | 265.111 | | 14.613 | | # |
| Si2H4 H3Si-SiH | | 60.20276 | 304.231 | 312.848 | ±8. | | 69.895 | | 280.449 | | 14.754 | | # |
| Si2H4+ H3Si-SiH+ cation | | 60.20276 | 1121.250 | 1122.709 | ±8. | | 72.353 | | 286.811 | | 14.975 | | # |
| Si2H4- H3Si-SiH- anion | | 60.20331 | 138.975 | 153.737 | ±8. | | 69.440 | | 284.039 | | 14.468 | | # |
| Si2H5 H3Si-SiH2\* | | 61.21070 | 227.220 | 239.884 | ±8. | | 76.052 | | 295.764 | | 14.942 | | # |
| Si2H5- H3Si-SiH2\*- anion | | 61.21125 | 39.329 | 57.710 | ±8. | | 75.852 | | 295.424 | | 14.810 | | # |
| Si2H6 Disilan H3Si-SIH3 <~> | | 62.21864 | 80.3 | 96.502 | ±1.5 | | 77.260 | | 274.605 | | 15.638 | | # |
| Si2H6+ cation H3Si-SiH3 | | 62.21809 | 1016.014 | 1022.833 | ±8. | | 90.949 | | 302.371 | | 17.963 | | # |
| Si2N2O(s) Silicon Oxynitride solid | | 100.18388 | -947.711 |  |  | | 65.56 | | 45.350 | |  | | † |
| Si3H5 SiH2=SiH-SiH2 | | 89.29620 | 433..257 | 444.025 | ±8. | | 103.073 | | 336.958 | | 20.055 | | # |
| Si3H5+ SiH2=SiH-SiH2  cation | | 89.29565 | 1107.610 | 1111.848 | ±8. | | 100.783 | | 340.465 | | 19.973 | | # |
| Si3H5- SiH2=SiH-SiH2 anion | | 89.29675 | 209.000 | 225.513 | ±8. | | 101.867 | | 331.845 | | 20.079 | | # |
| Si3H5 CycloTriSilane radical | | 89.29620 | 387.024 | 399.641 | ±8. | | 99.539 | | 314.302 | | 18.206 | | # |
| Si3H5+ CycloTriSilane cation | | 89.29565 | 1096.095 | 1101.488 | ±8. | | 98.930 | | 318.325 | | 18.785 | | # |
| Si3H5- CycloTriSilane anion | | 89.29675 | 147.948 | 166.494 | ±8. | | 98.121 | | 307.705 | | 18.005 | | # |
| Si3H6 CycloTriSilan | | 90.30414 | 257.314 | 273.626 | ±8. | | 105.306 | | 304.512 | | 18.965 | | # |
| Si3H6+ CycloTriSilan cation | | 90.30359 | 1063.513 | 1071.472 | ±8. | | 111.575 | | 319.427 | | 20.369 | | # |
| Si3H6- CycloTriSilan anion | | 90.30469 | 289.248 | 310.386 | ±8. | | 108.758 | | 314.228 | | 19.588 | | # |
| Si3H7 n-SiH3-SiH2-SiH2\* | | 91.31208 | 262.379 | 280.452 | ±8. | | 114.942 | | 354.048 | | 21.217 | | # |
| Si3H7+ n-SiH3-SiH2-SiH2\*+ | | 91.31153 | 985.767 | 996.160 | ±8. | | 116.509 | | 347.994 | | 21.336 | | # |
| Si3H7- n-SiH3-SiH2-SiH2\*- | | 91.31263 | 56.170 | 79.445 | ±8. | | 113.947 | | 346.165 | | 20.944 | | # |
| Si3H7 i-SiH3-SiH\*-SiH3 | | 91.31208 | 251.718 | 269.829 | ±8. | | 113.162 | | 339.966 | | 21.188 | | # |
| Si3H7+ i-SiH3-SiH\*-SiH3+ | | 91.31153 | 977.584 | 987.432 | ±8. | | 115.382 | | 344.968 | | 22.331 | | # |
| Si3H7- i-SiH3-SiH\*-SiH3- | | 91.31263 | 28.806 | 52.471 | ±8. | | 110.578 | | 334.645 | | 21.152 | | # |
| Si3H8 Tri Silan | | 92.32002 | 109.228 | 131.052 | ±8. | | 112.552 | | 343.103 | | 21.700 | | # |
| Si3H8- TriSilan anion | | 92.32057 | 122.122 | 147.101 | ±8. | | 123.630 | | 346.629 | | 23.036 | | # |
| Si3N4(a) Silicon Nitride | | 140.28346 | -787.8 | -772.921 | ±3. | | 93.010 | | 66.065 | | 12.113 | | † |
| Si4H7 cyclotetrasilane radical | | 119.39758 | 339.182 | 358.382 | ±8. | | 132.552 | | 360.528 | | 23.309 | | # |
| Si4H7+ cytetrasilane radical cation | | 119.39703 | 1026.227 | 1038.433 | ±8. | | 134.837 | | 350.763 | | 23.408 | | # |
| Si4H7- cytetrasilane radical anion | | 119.39813 | 108.800 | 133.735 | ±8. | | 131.810 | | 351.163 | | 23.105 | | # |
| Si4H8 cyclotetrasilane | | 120.40552 | 201.058 | 224.213 | ±8. | | 137.843 | | 342.156 | | 23.587 | | # |
| Si4H8+ cyclotetrasilane cation | | 120.40497 | 1062.080 | 1075.116 | ±8. | | 147.644 | | 385.233 | | 26.790 | | # |
| Si4H9 SiH3-SiH2-SiH2-SiH2\* | | 121.41346 | 293.750 | 317.669 | ±8. | | 149.814 | | 409.481 | | 27.658 | | # |
| Si4H9+ SiH3-SiH2-SiH2-SiH2+ | | 121.41291 | 939.986 | 958.090 | ±8. | | 146.722 | | 380.952 | | 25.276 | | # |
| Si4H9- SiH3-SiH2-SiH2-SiH2- | | 121.41401 | 77.123 | 105.169 | ±8. | | 149.771 | | 394.291 | | 27.658 | | # |
| Si4H9 SiH3-SiH\*-SiH2-SiH3 | | 121.41346 | 285.869 | 309.074 | ±8. | | 151.369 | | 405.267 | | 27.761 | | # |
| Si4H9+ SiH3-SiH\*-SiH2-SiH3+ | | 121.41291 | 984.922 | 1006.100 | ±8. | | 147.899 | | 399.839 | | 28.157 | | # |
| Si4H9- SiH3-SiH\*-SiH2-SiH3- | | 121.41401 | 47.910 | 76.253 | ±8. | | 148.389 | | 386.626 | | 27.427 | | # |
| Si4H9 (SiH3)2-SiH-SiH2\* | | 121.41346 | 287.550 | 310.681 | ±8. | | 153.868 | | 403.944 | | 27.845 | | # |
| Si4H9+ (SiH3)2-SiH-SiH2\*+ | | 121.41291 | 993.951 | 1008.415 | ±8. | | 151.507 | | 404.473 | | 28.292 | | # |
| Si4H9- (SiH3)2-SiH-SiH2\*- | | 121.41401 | 66.328 | 93.914 | ±8. | | 153.044 | | 397.181 | | 27.769 | | # |
| Si4H9 (SiH3)3Si\* | | 121.41346 | 270.596 | 293.485 | ±8. | | 148.452 | | 398.748 | | 28.087 | | # |
| Si4H9- (SiH3)3Si\*- anion | | 121.41401 | 17.653 | 46.024 | ±8. | | 150.442 | | 381.591 | | 27.264 | | # |
| Si4H10 n-Tetrasilane | | 122.42140 | 142.863 | 170.592 | ±8. | | 152.455 | | 407.440 | | 27.482 | | # |
| Si4H10- n-Tetrasilane anion | | 122.42195 | 128.330 | 159.870 | ±8. | | 159.029 | | 430.902 | | 29.868 | | # |
| Si5H9 cyclopentasilane radical | | 149.49896 | 327.406 | 352.193 | ±8. | | 168.977 | | 414.872 | | 29.407 | | # |
| Si5H9+ cyclopentasilane radical | | 149.49841 | 1027.423 | 1044.105 | ±8. | | 172.120 | | 421.981 | | 30.445 | | # |
| Si5H9- cyclopentasilane radical | | 149.49951 | 79.813 | 109.943 | ±8. | | 168.489 | | 408.458 | | 29.396 | | # |
| Si5H10 cyclo | | 150.50690 | 189.397 | 218.051 | ±8. | | 173.967 | | 401.697 | | 29.774 | | # |
| Si5H10+ cyclo cation | | 150.50635 | 1058.569 | 1076.882 | ±8. | | 185.851 | | 430.374 | | 32.990 | | # |
| Si5H12 n-PentaSilane | | 152.52278 | 177.37 | 210.79 | ±8. | | 178.296 | | 488.638 | | 33.477 | | # |
| Si5H12- n-PentaSilane anion | | 152.52333 | 144.50 | 181.94 | ±8. | | 184.268 | | 508.548 | | 35.649 | | # |
| Si6H11 cyclo radical | | 179.60034 | 351.611 | 381.832 | ±8. | | 205.391 | | 465.188 | | 35.658 | | # |
| Si6H11+ cyclo radical cation | | 179.59979 | 1039.444 | 1061.152 | ±8. | | 208.642 | | 468.661 | | 36.538 | | # |
| Si6H11- cyclo radical anion | | 179.60089 | 99.118 | 134.541 | ±8. | | 204.763 | | 457.281 | | 35.598 | | # |
| Si6H12 cycloHexaSilane | | 180.60828 | 212.476 | 246.543 | ±8. | | 210.583 | | 447.199 | | 36.045 | | # |
| Si6H12+ cyHexaSilane cation | | 180.60773 | 1074.209 | 1098.128 | ±8. | | 222.369 | | 474.835 | | 38.858 | | # |
| Si6H12- cyHexaSilane anion | | 180.60883 | 204.191 | 241.492 | ±8. | | 216.896 | | 465.731 | | 37.900 | | # |
| Sn (cr) REFERENCE ELEMENT | | 118.710 | 0.0 | 0.0 |  | | 27.112 | | 51.179 | | 6.322 | | X |
| Sn | | 118.710 | 301.2 | 301.308 | ±1.5 | | 21.260 | | 168.495 | | 6.216 | | † |
| Sn+ | | 118.70945 | 1015.95 | 1009.878 |  | | 20.786 | | 174.193 | | 6.197 | | † |
| Sn- | | 118.71055 | 179.496 | 185.526 |  | | 24.464 | | 181.197 | | 6.490 | | † |
| SnCl4 TetraChloroStanum <&> | | 260.52080 | -478.650 | -476.30 | ±4.2 | | 98.459 | | 364.549 | | 22.340 | | †# |
| SnH3 TriHydroStanum Radical | | 121.73382 | 258.153 | 266.252 | ±4.2 | | 44.818 | | 240.204 | | 10.926 | | # |
| SnD4 TetrahydroStanum-d4 | | 126.76640 | 167.218. | 177.203 | ±6. | | 62.794 | | 248.508 | | 13.476 | | # |
| SnH4 TetraHydroStanum | | 122.74176 | 162.758 | 174.594 | ±4.2 | | 51.108 | | 228.991 | | 11.423 | | # |
| T Tritium (3H) gas | | 3.01605 | 223.371 | 221.148 |  | | 20.786 | | 128.386 | | 6.197 | | # |
| T2 Tritium (3H)2 n REF.ELEMENT | | 6.0321 | 0. | 0. |  | | 29.200 | | 153.327 | | 8.611 | | # |
| 98Tc(cr)Technetium Ref.Element | | 97.9072 | 0 | 0 |  | | 24.698 | | 32.999 | | 5.200 | | # |
| 98Tc(gas) Technetium | | 97.9072 | 635.00 | 634.00 |  | | 20.794 | | 181.050 | | 6.097 | | # |
| 98Tc+ Technetium cation | | 97.90665 | 709.594 | 702.4 |  | | 20.786 | | 182.331 | | 6.197 | | # |
| Te(s) Telurium Ref. Element | | 127.60 | 0 | 0 |  | | 25.723 | | 49.409 | | 6.100 | | # |
| Te Telurium | | 127.60 | 209.459 | 209.363 |  | | 20.786 | | 182.711 | | 6.197 | | # |
| Te+ Telurium cation | | 127.59945 | 1085.355 | 1079.062 |  | | 20.786 | | 180.853 | | 6.197 | | # |
| Te- Telurium anion | | 127.60055 | 14.253 | 20.363 |  | | 20.786 | | 180.853 | | 6.197 | | # |
| Th(S) Thorium Reference Element | | 232.038 | 0. | 0. |  | | 26.230 | | 51.830 | | 6.350 | | †? |
| Th (g) | | 232.038 | 602.000 | 602.158 |  | | 20.789 | | 190.058 | | 6.197 | | # |
| Th+ Thorium cation | |  | 1193.218 | 1187.153 |  | | 21.304 | | 188.281 | | 6.218 | | # |
| ThO Thorium Monooxide | | 248.03750 | -25.104 |  |  | | 31.266 | | 240.062 | |  | | # |
| ThO2 (s) Thorium Dioxide | | 264.03690 | -1226.414 |  | ±3.5 | | 61.798 | | 65.229 | |  | | # |
| ThO2 (g) | | 264.03690 | -497.896 |  |  | | 47.354 | | 287.601 | |  | | # |
| V (S) Vanadium REF. ELEMENT | | 50.94150 | 0. | 0. |  | | 24.896 | | 28.936 | | 4.640 | | †X |
| V gas | | 50.94150 | 517.267 | 514.000 | ±2. | | 26.012 | | 182.302 | | 7.907 | | † |
| V+ | | 50.94095 | 1173.745 | 1165.848 |  | | 23.150 | | 183.378 | | 7.898 | | †X |
| V- | | 50.94205 | 460.386 | 463.345 |  | | 23.049 | | 183.438 | | 7.878 | | †X |
| W(cr) Reference Element | | 183.84 | 0 | 0 |  | | 35.378 | | 32.374 | | 4.973 | | † |
| W | | 183.84 | 851.244 | 850. | ±5. | | 21.306 | | 173.957 | | 6.217 | | † |
| W+ Tungsten cation | | 183.83945 | 1627.841 | 1620.395 |  | | 21.392 | | 179.739 | | 6.221 | | † |
| W- Tungsten anion | | 183.84055 | 770.6 | 775.6 | ±2.1 | | 20.786 | | 188.782 | | 6.197 | | #† |
| WBr | | 263.74400 | 586.2 | 593.7 | ±84. | | 35.945 | | 272.568 | | 9.716 | | # |
| WC6O6 W(CO)6 | | 351.90060 | 879.1 | 875.443 | ±1.8 | | 208.755 | | 444.175 | | 40.991 | | # |
| WCl | | 219.29270 | 553.54 | 553.74 | ±41.8 | | 34.772 | | 261.860 | | 9.364 | | # |
| WCl2O2 solid | | 286.74420 | -780.316 |  | ±5.9 | | 104.408 | | 200.832 | |  | | † |
| WCl2O2 | | 286.74420 | -671.5 | -668.20 | ±25. | | 87.200 | | 353.932 | | 19.504 | | † |
| WCL4O solid | | 341.65020 | -671.14 |  | ±8.4 | | 146.248 | | 172.799 | |  | | † |
| WCl4O | | 341.65020 | -573.5 | -568.09 | ±20.9 | | 106.140 | | 377.084 | | 22.271 | | † |
| WCl6 Solid | | 396.55620 | -593.71 |  | ±25.1 | | 175.418 | | 238.488 | |  | | † |
| WCl6 | | 396.55620 | -493.7 | -491.987 | ±25.1 | | 143.943 | | 419.172 | | 30.791 | | † |
| WF Rad. | | 202.83840 | 386.18 |  |  | | 34.020 | | 251.1 | |  | |  |
| WF2 | | 221.83681 | -86.19 | -84.946 | ±13.4 | | 51.838 | | 263.815 | | 12.554 | | # |
| WF3 Rad. | | 240.83521 | -507.1 | -503.5 | ±12. | | 66.246 | | 306.787 | | 14.575 | | # |
| WF4 | | 259.83361 | -928.85 | -925.19 | ±10.5 | | 85.689 | | 325.365 | | 18.965 | | # |
| WF5 Rad. | | 278.83202 | -1293.3 | -1286.9 | ±8.5 | | 103.140 | | 345.821 | | 20.685 | | # |
| WF6 | | 297.83041 | -1721.72 | -1744.427 | ±1.7 | | 118.841 | | 340.971 | | 22.711 | | # |
| WO | | 199.83940 | 401.73 | 402.29 | ±62.8 | | 30.434 | | 245.768 | | 8.754 | | † |
| WO2 solid | | 215.83880 | -588.1 | -583.16 | ±1.5 | | 55.780 | | 50.640 | | 8.711 | | X† |
| WO2 | | 215.83880 | 29.062 | 32.00 | ±15. | | 41.980 | | 271.487 | | 10.715 | | † |
| WO3 (cr) | | 231.83820 | -841.300 | -836.587 | ±2.0 | | 79.705 | | 81.640 | | 13.280 | | X† |
| WO3 gas | | 231.83820 | -319.725 | -315.000 | ±15. | | 59.164 | | 283.127 | | 13.268 | | † |
| WO3- anion | | 231.83875 | -650.5 | -640.0 | ±30. | | 61.174 | | 291.664 | | 13.715 | | † |
| W2O6 (WO3)2 | | 463.67640 | -1210.8 | -1200.0 | ±35. | | 128.395 | | 395.245 | | 25.543 | | † |
| W3O9 (WO3)3 | | 695.51460 | -2013.3 | -2000. | ±50. | | 204.304 | | 518.322 | | 40.688 | | † |
| W4O12 (WO3)4 | | 927.3528 | -2817.4 | -2800. | ±60. | | 276.407 | | 618.888 | | 54.539 | | † |
| W5O15 (WO3)5 | | 1159.1910 | -3551.5 | -3530. | ±100. | | 349.313 | | 717.875 | | 68.473 | | † |
| Xe REFERENCE ELEMENT <^> | | 131.29 | 0 | 0 |  | | 20.786 | | 169.686 | | 6.197 | | † |
| Xe+ | | 131.28945 | 1176.552 | 1170.35 | ±0.006 | | 20.786 | | 181.212 | | 6.197 | | † |
| XeF4 wk Xenon Tetrafluoride | | 207.28361 | -182.00 | -177.2 | ±4.2 | | 89.998 | | 323.6±5. | | 19.058 | | # |
| XeH+ | | 132.29739 | 1042.79d | 1038.36d | ±0.94d | | 29.125 | | 206.925 | | 8.677 | | # |
| Zn(cr) REFERENCE ELEMENT | | 65.39 | 0 | 0 |  | | 25.390 | | 41.630 | | 5.657 | | † |
| Zn <&> | | 65.39 | 130.4 | 129.86 |  | | 20.786 | | 160.993 | | 6.197 | | † |
| Zn+ | | 65.38945 | 1043. | 1036.26 |  | | 20.786 | | 166.756 | | 6.197 | | † |
| ZnCO3 Zinc Carbonate | | 125.3989 | -812.78 |  |  | | 80.077 | | 82.400 | |  | |  |
| ZnCL2 | | 136.29540 | -265.684 |  |  | | 56.902 | | 276.672 | |  | |  |
| Zn(NO3)2 (S) | |  | -483.66 |  |  | |  | | 193.7 | |  | | X |
| Zn(NO3)2.6H2O(cr) | |  | -2305.05 |  |  | |  | |  | |  | | X |
| ZnO (S) | | 81.3894 | -350.460 | -347.433 | ±0.24 | | 41.089 | | 43.640 | | 6.970 | | # |
| ZnO Zinc Oxide | | 81.3894 | 110.424 | 111.544 |  | | 31.804 | | 223.654 | | 8.877 | | # |
| ZnO- Zinc Oxide anionw | |  | 53.1 |  | ±4.2 | |  | |  | |  | | X |
| ZnS (cr) Wurzite | | 97.4560 | -194.800 | -193.582 |  | | 45.880 | | 58.840 | | 8.851 | | # |
| ZnS (cr) Zinc Sulphide | | 97.4560 | -200.500 | -199.249 |  | | 45.760 | | 58.660 | | 8.818 | | # |
| ZnS (g) | | 97.4560 | 183.935 | 184.545 |  | | 35.245 | | 237.200 | | 9.459 | | # |
| ZnSO4 (cr) | | 161.4536 | -980.144 | -969.95 | ±4.2 | | 99.035 | | 110.541 | | 17.238 | | † |
| Zn3N2 (S) Zinc Nitride | | 224.18348 | -22.602 |  |  | | 109.334 | | 108.784 | |  | |  |
| Zr(cr) REFERENCE ELEMENT | | 91.2240 | 0. | 0. |  | | 25.202 | | 38.869 | | 5.497 | | † |
| Zr | | 91.2240 | 599.319 | 598.0 | ±20.9 | | 26.642 | | 181.346 | | 6.816 | | † |
| Zr+ | | 91.2234 | 1246.25 | 1238.07 | ±20.9 | | 28.283 | | 183.642 | | 7.472 | | † |
| Zr- | | 91.22455 | 552.952 | 556.897 |  | | 28.693 | | 185.765 | | 7.749 | | † |
| ZrCl2 | | 162.12940 | -185.750 | -185.316 | ±20.9 | | 57.677 | | 292.562 | | 14.244 | | # |
| ZrCl4 | | 233.0348 | -869.980 | -868.682 | ±2.1 | | 98.234 | | 367.710 | | 22.561 | | # |
| ZrF | | 110.22240 | 82.84 | 83.666 | ±20.9 | | 33.420 | | 243.7 | | 9.084 | | # |
| ZrF2 | | 129.22080 | -558.150 | -555.657 | ±20.9 | | 48.652 | | 283.430 | | 11.829 | | # |
| ZrF4 | | 167.21762 | -1673.6 | -1669.395 | ±3.3 | | 86.810 | | 319.300 | | 18.942 | | # |
| ZrN(cr) | | 105.23074 | -371.238 | -367.996 |  | | 40.443 | | 38.861 | | 6.590 | | † |
| ZrN | | 105.23074 | 713.372 | 714.341 |  | | 31.661 | | 233.491 | | 8.863 | | † |
| ZrO | | 107.22340 | 83.923 | 84.790 |  | | 34.374 | | 228.400 | | 8.970 | | † |
| ZrO2(cr) | | 123.22280 | -1100.3 | -1094.874 | ±0.7 | | 55.920 | | 50.390 | | 8.751 | | † |
| ZrO2 | | 123.22280 | -317.043 | -314.874 | ±>15. | | 46.062 | | 273.750 | | 12.008 | | † |

a  Values from Active Thermochemical Tables ATcT A (2005). Not published.

b  Values from Active Thermochemical Tables ATcT B 30.5.2010

<http://atct.anl.gov>

c Values from Active Thermochemical Tables ATcT C ver. 1.112 May 2011.

d Values from Active Thermochemical Tables ATcT D ver. 1.110 December 2013

as posted in http://atct.anl.gov/ThermochemicaData/version1.110/index.html

f  Active Thermochemical Tables ATcT F ver. 1.118 December 2015

g Active Thermochemical Tables ATcT G ver 1.122 2017

h Active Thermochemical Tables ATcT H ver 1.122p 2020

W Webbook NIST Database

# 9 term NASA polynomials are available in the NEWNASA.TXT file for this species.

† 9-term NASA polynomials are available in

http://www.grc.nasa.gov/WWW/CEAWeb/ceaThermoBuild.htm

X Polynomials not available

[ ] values in square brackets are from ATcT D see d above

<!> Transport properties are available at <http://melchior.usc.edu/JetSurF/JetSurF1.0>

<~> Transport properties available at T. Noto, V. Babushok, A. Hamins, and W. Tsang. Combust. Flame, 112:147-160, 1998.

[http://dx.doi.org/10.1016/S0010-2180(97)81763-4](https://webmail.technion.ac.il/horde/util/go.php?url=http%3A%2F%2Fdx.doi.org%2F10.1016%2FS0010-2180%2897%2981763-4&Horde=590873676a70382cc5bc251efa7b3ba2)

<^> NASA Transport properties in polynomial form. Available at

<ftp://ftp.grc.nasa.gov/users/mzehe/trans.inp>

<&> NASA Transport properties in polynomial form. Calculated by Sanford Gordon

in the publications: NASA TM-4513 (1993) and NASA TM-4647 (1995) by R.A Svehla. .