**A STUDY OF ETHYL BROMIDE PYROLYSIS**

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SCF energy, zero-point corrected electronic energy, frequencies and geometry of molecules, radicals and transition states, calculated at the CBS-QB3 level of theory.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Species** | **E(SCF)** | **CBSQB3 (0K)** | **Frequencies** | **Geometry** | | |
| **N°** | **Atom N°** | **XYZ Coordinates** |
|  | **[Hartrees]** | **[Hartrees]** | **[cm-1]** |  |  | **[Angstroms]** |
|  | -2651.052202 | -2651.917070 | |  |  |  | | --- | --- | --- | | 258.4893 | 283.0501 | 542.4294 | | 776.2100 | 971.5209 | 1032.3173 | | 1077.6864 | 1264.2882 | 1275.2492 | | 1415.3554 | 1485.2176 | 1488.5036 | | 1501.4431 | 3025.4179 | 3087.9685 | | 3102.5488 | 3114.6267 | 3160.5934 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -3.073710 | 0.641458 | -0.004216 | | 2 | 1 | -2.731105 | -0.394422 | -0.028154 | | 3 | 1 | -2.731431 | 1.138670 | -0.913420 | | 4 | 1 | -4.169568 | 0.639677 | -0.006836 | | 5 | 6 | -2.581249 | 1.357849 | 1.236646 | | 6 | 1 | -2.885127 | 2.401624 | 1.267450 | | 7 | 1 | -2.885690 | 0.862874 | 2.155916 | | 8 | 35 | -0.596696 | 1.406636 | 1.322311 | | | |
|  | -78.625522 | -78.971549 | |  |  |  | | --- | --- | --- | | 109.3765 | 477.8501 | 813.2088 | | 980.1624 | 1061.9807 | 1191.6457 | | 1401.0624 | 1465.1176 | 1482.6691 | | 1482.9581 | 2941.0498 | 3033.8239 | | 3077.1239 | 3138.7127 | 3238.3470 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | 0.686049 | -0.013854 | 0.000000 | | 2 | 1 | 1.102969 | -0.502495 | -0.886121 | | 3 | 1 | 1.102969 | -0.502495 | 0.886121 | | 4 | 1 | 1.080795 | 1.016085 | 0.000000 | | 5 | 6 | -0.801451 | -0.039441 | 0.000000 | | 6 | 1 | -1.359195 | 0.021100 | 0.926318 | | 7 | 1 | -1.359195 | 0.021100 | -0.926318 | | | |
|  | -2572.960559 | -2573.469171 | 2617.2601 | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 35 | -1.158889 | 0.342466 | 0.000000 | | 2 | 1 | -2.582480 | 0.342466 | 0.000000 | | | |
|  | -2650.422381 | -2651.259517 | |  |  |  | | --- | --- | --- | | 148.7480 | 289.7664 | 362.8044 | | 616.3973 | 999.0287 | 1012.6646 | | 1107.7940 | 1268.3297 | 1406.3405 | | 1461.6623 | 1480.3024 | 2969.5144 | | 3046.4393 | 3088.5327 | 3213.4501 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | 0.300460 | 2.163774 | 0.032202 | | 2 | 1 | 0.844808 | 2.228101 | -0.921887 | | 3 | 1 | 1.050744 | 2.082000 | 0.824120 | | 4 | 1 | -0.243599 | 3.103391 | 0.166198 | | 5 | 6 | -0.651006 | 1.026482 | 0.060350 | | 6 | 1 | -1.671014 | 1.088979 | -0.290791 | | 7 | 35 | 0.009024 | -0.742136 | 0.129807 | | | |
|  | -1.132955 | -1.166083 | 4419.2598 | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 1 | -0.730352 | 0.274390 | 0.000000 | | 2 | 1 | -1.474526 | 0.274390 | 0.000000 | | | |
|  | -2650.420208 | -2651.259524 | |  |  |  | | --- | --- | --- | | 214.0578 | 279.4293 | 349.6206 | | 753.1439 | 788.5224 | 988.9257 | | 1084.6433 | 1166.2658 | 1242.1535 | | 1464.2556 | 1514.4726 | 3131.4038 | | 3147.7701 | 3206.5203 | 3253.8201 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -2.950026 | 0.328810 | 0.606210 | | 2 | 1 | -2.718312 | -0.542232 | 1.205881 | | 3 | 1 | -3.210353 | 0.174778 | -0.433267 | | 4 | 6 | -2.708369 | 1.642484 | 1.108327 | | 5 | 1 | -3.202004 | 2.455856 | 0.588577 | | 6 | 1 | -2.721043 | 1.756705 | 2.186456 | | 7 | 35 | -0.659781 | 2.136962 | 0.707480 | | | |
|  | -40.355896 | -40.465297 | |  |  |  | | --- | --- | --- | | 1341.6165 | 1341.6165 | 1341.6165 | | 1563.5772 | 1563.5772 | 3039.2754 | | 3153.2315 | 3153.2315 | 3153.2315 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | 0.000000 | 0.000000 | 0.000000 | | 2 | 1 | 0.630364 | 0.630364 | 0.630364 | | 3 | 1 | -0.630364 | -0.630364 | 0.630364 | | 4 | 1 | -0.630364 | 0.630364 | -0.630364 | | 5 | 1 | 0.630364 | -0.630364 | -0.630364 | | | |
|  | -2612.134904 | -2613.493977 | |  |  |  | | --- | --- | --- | | 591.6799 | 963.6906 | 963.7752 | | 1329.7894 | 1473.4907 | 1473.6733 | | 3087.9305 | 3198.8159 | 3199.5547 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -0.709971 | -0.054214 | 0.000000 | | 2 | 1 | -0.331744 | 0.430141 | 0.897350 | | 3 | 1 | -0.331744 | 0.430141 | -0.897350 | | 4 | 1 | -1.797000 | -0.087793 | 0.000000 | | 5 | 35 | -0.057346 | -1.899993 | 0.000000 | | | |
|  | -5144.738328 | -5145.731399 | 310.4402 | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 35 | -1.077664 | -2.331461 | 0.000000 | | 2 | 35 | -3.421437 | -2.331461 | 0.000000 | | | |
|  | -76.848481 | -77.187452 | |  |  |  | | --- | --- | --- | | 642.7642 | 642.7642 | 773.3899 | | 773.3899 | 2070.0035 | 3420.0722 | | 3523.0666 |  |  | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | 0.402063 | 0.872576 | 0.000000 | | 2 | 1 | -0.660868 | 0.872576 | 0.000000 | | 3 | 6 | 1.600153 | 0.872576 | 0.000000 | | 4 | 1 | 2.663085 | 0.872576 | 0.000000 | | | |
|  | -78.062182 | -78.416642 | |  |  |  | | --- | --- | --- | | 835.1085 | 973.1495 | 973.8676 | | 1066.7693 | 1238.8140 | 1379.7025 | | 1472.2799 | 1692.0617 | 3120.7298 | | 3135.8768 | 3191.9421 | 3220.4129 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | 0.000000 | -0.663451 | 0.000000 | | 2 | 1 | 0.922646 | -1.234599 | 0.000000 | | 3 | 1 | -0.922646 | -1.234599 | 0.000000 | | 4 | 6 | 0.000000 | 0.663451 | 0.000000 | | 5 | 1 | -0.922646 | 1.234599 | 0.000000 | | 6 | 1 | 0.922646 | 1.234599 | 0.000000 | | | |
| \* | -2651.533754 | -2652.406819 | |  |  |  | | --- | --- | --- | | -529.6476 | 37.8810 | 112.8832 | | 245.3696 | 262.0922 | 527.7380 | | 760.8823 | 959.2181 | 972.9720 | | 1064.4791 | 1222.1966 | 1249.2799 | | 1410.7560 | 1480.5538 | 1481.8074 | | 1497.9982 | 3015.7511 | 3084.5628 | | 3105.7973 | 3115.9907 | 3175.3266 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -1.652731 | 0.037875 | -0.001095 | | 2 | 1 | -1.355402 | -1.012064 | -0.016823 | | 3 | 1 | -1.256005 | 0.524103 | -0.893979 | | 4 | 1 | -2.747892 | 0.081060 | -0.049793 | | 5 | 6 | -1.187261 | 0.727333 | 1.258189 | | 6 | 1 | -1.411958 | 1.790100 | 1.288014 | | 7 | 1 | -1.510548 | 0.239500 | 2.174497 | | 8 | 35 | 0.868775 | 0.668896 | 1.411543 | | 9 | 1 | 2.868949 | 0.966306 | 1.331798 | | | |
| \* | -2651.516508 | -2652.400160 | |  |  |  | | --- | --- | --- | | -1284.3099 | 224.2664 | 287.2504 | | 310.4155 | 350.2606 | 570.1292 | | 844.7000 | 991.5761 | 1035.3271 | | 1078.5102 | 1215.8055 | 1270.3329 | | 1282.9413 | 1408.3742 | 1472.7573 | | 1486.8012 | 1513.1396 | 3022.3896 | | 3081.5699 | 3104.4220 | 3136.8539 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -1.706846 | 0.305212 | -0.000319 | | 2 | 1 | -1.423006 | -0.749941 | -0.057346 | | 3 | 1 | -1.347393 | 0.804943 | -0.901889 | | 4 | 1 | -2.800064 | 0.363823 | 0.016909 | | 5 | 6 | -1.154837 | 0.950246 | 1.240520 | | 6 | 1 | -1.516531 | 0.554314 | 2.186463 | | 7 | 35 | 0.783697 | 1.028466 | 1.323785 | | 8 | 1 | -1.565519 | 2.200454 | 1.254841 | | 9 | 1 | -1.946761 | 3.081626 | 1.236574 | | | |
| \* | -2651.514200 | -2652.395517 | |  |  |  | | --- | --- | --- | | -1215.2836 | 138.8437 | 249.2241 | | 342.2487 | 533.5858 | 579.2901 | | 800.8179 | 973.8126 | 994.5748 | | 1069.2235 | 1183.6102 | 1190.0871 | | 1203.9976 | 1274.2029 | 1445.3923 | | 1473.0509 | 1718.3770 | 3068.8300 | | 3079.4636 | 3132.6024 | 3169.7903 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -0.039990 | -0.012453 | 0.001982 | | 2 | 1 | 0.052621 | -1.070489 | -0.232068 | | 3 | 1 | -0.026626 | 0.580381 | -1.236176 | | 4 | 1 | -1.031773 | 0.264108 | 0.361910 | | 5 | 6 | 1.075407 | 0.579433 | 0.800134 | | 6 | 1 | 0.995295 | 1.660361 | 0.897720 | | 7 | 1 | 1.159770 | 0.134076 | 1.792245 | | 8 | 35 | 2.852057 | 0.253221 | -0.029526 | | 9 | 1 | -0.012968 | 1.003326 | -2.048601 | | | |
| \* | -2650.349282 | -2651.198454 | |  |  |  | | --- | --- | --- | | -272.4148 | 162.7134 | 226.4973 | | 349.3164 | 597.4135 | 628.1823 | | 927.1730 | 966.5244 | 1020.0647 | | 1280.3084 | 1395.7602 | 1622.0389 | | 3144.9352 | 3213.1091 | 3240.4827 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -4.604163 | 0.338033 | 0.024098 | | 2 | 1 | -4.788454 | 1.161739 | -0.656464 | | 3 | 1 | -3.656335 | 0.314484 | 0.545652 | | 4 | 1 | -5.189376 | 1.863244 | 1.647182 | | 5 | 6 | -5.496329 | -0.642356 | 0.116801 | | 6 | 1 | -6.439400 | -0.663772 | -0.410976 | | 7 | 35 | -5.261364 | -2.166877 | 1.232195 | | | |
| \* | -2650.342603 | -2651.192630 | |  |  |  | | --- | --- | --- | | -764.3201 | 331.1583 | 357.9851 | | 410.1913 | 589.1410 | 594.3135 | | 901.9156 | 982.0765 | 1016.3304 | | 1265.8074 | 1386.1020 | 1577.7346 | | 3143.6111 | 3212.6427 | 3242.6190 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -2.636969 | 0.218918 | 0.005085 | | 2 | 1 | -1.999526 | -0.635927 | 0.187911 | | 3 | 1 | -3.663771 | 0.037290 | -0.292867 | | 4 | 6 | -2.223951 | 1.476945 | 0.199382 | | 5 | 1 | -2.794838 | 2.351682 | -0.076837 | | 6 | 1 | -2.965520 | 1.901202 | 1.973298 | | 7 | 35 | -0.396869 | 1.902737 | 0.592573 | | | |
| \* | -2650.952453 | -2651.826248 | |  |  |  | | --- | --- | --- | | -1364.0968 | 230.0857 | 293.3669 | | 310.3455 | 665.0101 | 830.6337 | | 1023.8685 | 1049.8026 | 1213.6105 | | 1256.6727 | 1270.0906 | 1404.6794 | | 1469.1504 | 1588.5263 | 3112.3243 | | 3166.9514 | 3201.6595 | 3268.4717 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -1.612198 | 0.088121 | 0.002365 | | 2 | 1 | -1.597360 | -0.996818 | -0.044700 | | 3 | 1 | -0.454296 | 0.438529 | -0.318312 | | 4 | 1 | -2.261734 | 0.594943 | -0.705255 | | 5 | 6 | -1.363357 | 0.702221 | 1.232011 | | 6 | 1 | -1.569801 | 1.752641 | 1.395067 | | 7 | 1 | -0.907543 | 0.164562 | 2.054016 | | 8 | 35 | 1.225759 | 1.350623 | 0.189841 | | | |
| \* | -2649.727609 | -2650.591916 | |  |  |  | | --- | --- | --- | | -1367.3974 | 218.6298 | 331.4005 | | 571.681 | 689.8017 | 759.5657 | | 867.9008 | 942.0512 | 1572.1645 | | 1836.5455 | 3262.7484 | 3420.8643 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | 0.962732 | 0.796679 | 0.003005 | | 2 | 1 | 1.571000 | 1.720196 | -0.525889 | | 3 | 1 | 0.261318 | 0.172849 | -0.527084 | | 4 | 6 | 1.450038 | 0.930528 | 1.144361 | | 5 | 1 | 1.900179 | 1.092962 | 2.099488 | | 6 | 35 | 2.898880 | 3.104131 | -0.055113 | | | |
| \* | -2650.416349 | -2651.255654 | |  |  |  | | --- | --- | --- | | -133.4366 | 195.9816 | 394.9172 | | 820.0730 | 879.3459 | 949.9664 | | 996.7829 | 1237.4716 | 1254.9926 | | 1469.5327 | 1551.5087 | 3148.3131 | | 3158.9666 | 3235.0947 | 3259.9255 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | 0.062899 | 1.972694 | -0.002413 | | 2 | 1 | 0.358627 | 1.101890 | 0.567651 | | 3 | 1 | -0.129902 | 1.806578 | -1.054130 | | 4 | 6 | -0.510114 | 3.052947 | 0.640061 | | 5 | 1 | -0.944592 | 3.871140 | 0.079024 | | 6 | 1 | -0.450734 | 3.158529 | 1.716218 | | 7 | 35 | 2.290329 | 2.751642 | -0.333565 | | | |
| \* | -5223.371674 | -5224.732419 | |  |  |  | | --- | --- | --- | | -112.9760 | 53.2789 | 55.2992 | | 263.5756 | 389.9772 | 440.8409 | | 580.5577 | 652.8595 | 782.5167 | | 814.2657 | 1013.1657 | 1091.4188 | | 1187.7536 | 1253.5512 | 1464.6149 | | 1500.0569 | 1655.5721 | 3121.6204 | | 3131.4398 | 3191.6483 | 3235.2679 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | 1.004920 | 1.387964 | 0.022892 | | 2 | 1 | 1.101735 | 0.308090 | -0.001260 | | 3 | 6 | 1.320087 | 2.099977 | 1.256545 | | 4 | 1 | 1.023325 | 3.143912 | 1.267390 | | 5 | 1 | 1.021070 | 1.588004 | 2.165647 | | 6 | 35 | 3.362453 | 2.186672 | 1.411608 | | 7 | 1 | 1.101681 | 1.906937 | -0.924419 | | 8 | 35 | -2.243869 | 1.395513 | 0.039779 | | 9 | 1 | -0.746844 | 1.391244 | 0.030394 | | | |
| \* | -5223.337930 | -5224.689505 | |  |  |  | | --- | --- | --- | | -259.3465 | 30.9804 | 66.0876 | | 82.7041 | 159.5714 | 247.0212 | | 398.6551 | 706.3395 | 832.6428 | | 969.1841 | 1082.4315 | 1193.0297 | | 1394.0328 | 1476.6911 | 1478.4075 | | 1504.3939 | 2943.1829 | 3071.1075 | | 3125.9919 | 3189.1278 | 3296.7146 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -1.839888 | 1.320225 | 0.000000 | | 2 | 1 | -2.302176 | 2.301803 | -0.133343 | | 3 | 1 | -2.568270 | 0.536793 | -0.223735 | | 4 | 1 | -1.052756 | 1.242173 | -0.772948 | | 5 | 6 | -1.240339 | 1.162025 | 1.336573 | | 6 | 1 | -0.911724 | 2.017665 | 1.910356 | | 7 | 1 | -1.207156 | 0.199786 | 1.828697 | | 8 | 35 | 1.520528 | 0.747861 | 0.575298 | | 9 | 35 | 1.827225 | 0.578391 | 3.049279 | | | |
| \* | -2690.583670 | -2691.641592 | |  |  |  | | --- | --- | --- | | -1635.7947 | 32.5787 | 90.7531 | | 159.7532 | 232.2634 | 284.3691 | | 427.2857 | 534.8506 | 566.5247 | | 594.8249 | 888.1874 | 994.4664 | | 1082.8365 | 1096.6859 | 1144.6951 | | 1265.4241 | 1375.0198 | 1396.1127 | | 1409.0059 | 1441.3929 | 1445.8665 | | 1476.8198 | 1491.4687 | 3017.8501 | | 3059.3102 | 3075.4063 | 3096.9668 | | 3127.9234 | 3193.0223 | 3196.2303 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -0.331445 | 0.034460 | -0.000170 | | 2 | 1 | 0.007973 | 0.454365 | -0.944701 | | 3 | 6 | 0.198248 | 0.714557 | 1.234003 | | 4 | 1 | 1.293324 | 0.690895 | 1.217140 | | 5 | 1 | -0.116382 | 1.761404 | 1.284940 | | 6 | 1 | -0.142523 | 0.213119 | 2.142386 | | 7 | 35 | -2.282745 | -0.056267 | -0.078779 | | 8 | 6 | 0.577004 | -2.504653 | -0.003988 | | 9 | 1 | 0.192787 | -2.929761 | -0.927540 | | 10 | 1 | 1.659373 | -2.405186 | 0.023627 | | 11 | 1 | 0.147038 | -2.940363 | 0.894331 | | 12 | 1 | 0.082519 | -1.209406 | -0.011499 | | | |
| \* | -2690.582731 | -2691.642461 | |  |  |  | | --- | --- | --- | | -1588.4914 | 25.4371 | 68.6888 | | 93.9093 | 222.3644 | 385.9944 | | 461.1380 | 509.7963 | 608.2085 | | 697.5906 | 797.2609 | 1042.2486 | | 1044.8231 | 1093.6510 | 1140.1972 | | 1242.1810 | 1268.5188 | 1377.0762 | | 1382.8089 | 1438.6135 | 1439.0766 | | 1471.4017 | 1491.7604 | 3060.1153 | | 3084.2018 | 3104.4425 | 3149.4005 | | 3174.8199 | 3196.2135 | 3198.4137 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -0.169412 | 1.955097 | 0.005892 | | 2 | 1 | 0.117012 | 2.442541 | -0.922450 | | 3 | 6 | 0.304688 | 2.668823 | 1.221242 | | 4 | 1 | 0.060259 | 3.729865 | 1.245993 | | 5 | 1 | 0.054507 | 2.177032 | 2.160256 | | 6 | 35 | -2.190309 | 1.905541 | -0.089142 | | 7 | 1 | 0.111980 | 0.905483 | -0.017941 | | 8 | 6 | 3.017326 | 2.669466 | 1.241605 | | 9 | 1 | 3.302277 | 3.222645 | 0.350376 | | 10 | 1 | 3.250375 | 3.176563 | 2.174056 | | 11 | 1 | 3.296613 | 1.619130 | 1.223973 | | 12 | 1 | 1.612852 | 2.653197 | 1.203178 | | | |
| \* | -2690.591593 | -2691.643368 | |  |  |  | | --- | --- | --- | | -355.8987 | 21.3034 | 65.1660 | | 73.0499 | 208.5529 | 208.5529 | | 339.7438 | 656.8781 | 657.7284 | | 692.1605 | 865.1652 | 917.2759 | | 1019.6574 | 1051.5680 | 1118.3495 | | 1229.4865 | 1403.6235 | 1432.0864 | | 1432.3152 | 1475.8079 | 1477.4930 | | 1492.7109 | 2989.5394 | 3071.2397 | | 3091.9679 | 3109.2772 | 3116.2937 | | 3200.2111 | 3244.2104 | 3244.4431 | | |  |  |  |  |  | | --- | --- | --- | --- | --- | | 1 | 6 | -1.318740 | 0.279366 | 0.026880 | | 2 | 1 | -1.004498 | 1.005046 | -0.726038 | | 3 | 1 | -1.254973 | 0.750677 | 1.009751 | | 4 | 1 | -2.376215 | 0.043292 | -0.160363 | | 5 | 6 | -0.500777 | -0.975577 | -0.039023 | | 6 | 1 | -0.663702 | -1.697212 | 0.755397 | | 7 | 1 | -0.406084 | -1.435880 | -1.017588 | | 8 | 6 | 3.856877 | 0.101125 | 0.755758 | | 9 | 1 | 4.361457 | -0.311275 | -0.109174 | | 10 | 1 | 3.815605 | 1.182291 | 0.802347 | | 11 | 1 | 4.052422 | -0.400843 | 1.695218 | | 12 | 35 | 1.663454 | -0.455653 | 0.352397 | | | |

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