***Supporting Information***

***for***

**Epoxidation of alkenes by peracids: From textbook mechanisms to a quantum mechanically derived curly-arrow depiction**

Johannes E. M. N. Klein,a,\* Gerald Kniziab and Henry S. Rzepac,\*

a *Molecular Inorganic Chemistry, Stratingh Institute for Chemistry, Faculty of Science and Engineering, University of Groningen, Nijenborgh 4, 9747 AG Groningen (The Netherlands). email:* *j.e.m.n.klein@rug.nl*

b *Department of Chemistry, Pennsylvania State University, 401A Chemistry Bldg; University Park, PA 16802 (USA).*

*c Department of Chemistry, Imperial College London, MSRH, 80 Wood Lane, London, W12 0BZ, (UK). email:* *rzepa@imperial.ac.uk*

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**1. Data for plots shown in Figure 1**

**Table S1:** Data for plots shown in Figure 1.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Reaction Coordinate[bohr amu1/2]** | **E [hartree]** | **ΔE [kcal mol-1]a** | **RMS Gradient Norm [hartree bohr-1]** | **Dipole Moment****[debye]** |
| -5.98506 | -422.12048 | 0.36216 | 4.0714E-5 | 2.33573 |
| -5.88684 | -422.12048 | 0.36276 | 3.2348E-5 | 2.33191 |
| -5.78897 | -422.12048 | 0.3636 | 4.0047E-5 | 2.32672 |
| -5.69041 | -422.12048 | 0.3648 | 3.7827E-5 | 2.32082 |
| -5.59078 | -422.12047 | 0.36662 | 2.1183E-5 | 2.31512 |
| -5.49144 | -422.12047 | 0.36939 | 4.3466E-5 | 2.31005 |
| -5.39215 | -422.12046 | 0.37292 | 5.0189E-5 | 2.30471 |
| -5.2928 | -422.12046 | 0.37719 | 5.0849E-5 | 2.30021 |
| -5.19348 | -422.12045 | 0.38209 | 5.3418E-5 | 2.2963 |
| -5.09371 | -422.12044 | 0.38728 | 2.8758E-5 | 2.293 |
| -4.99444 | -422.12043 | 0.39277 | 5.7811E-5 | 2.29037 |
| -4.89514 | -422.12042 | 0.3982 | 5.4821E-5 | 2.28758 |
| -4.79572 | -422.12041 | 0.4041 | 4.984E-5 | 2.28559 |
| -4.69615 | -422.1204 | 0.41098 | 4.2701E-5 | 2.28461 |
| -4.59636 | -422.12039 | 0.41931 | 2.5948E-5 | 2.28466 |
| -4.49663 | -422.12037 | 0.42966 | 3.9411E-5 | 2.28567 |
| -4.39679 | -422.12035 | 0.44266 | 4.0343E-5 | 2.2877 |
| -4.29688 | -422.12032 | 0.45899 | 4.5561E-5 | 2.29027 |
| -4.19695 | -422.12029 | 0.47892 | 5.2234E-5 | 2.2937 |
| -4.09699 | -422.12026 | 0.50239 | 5.5878E-5 | 2.29775 |
| -3.99704 | -422.12021 | 0.52932 | 6.5968E-5 | 2.30236 |
| -3.89708 | -422.12016 | 0.55956 | 7.2694E-5 | 2.30741 |
| -3.79713 | -422.12011 | 0.59287 | 7.8977E-5 | 2.3128 |
| -3.69717 | -422.12005 | 0.62898 | 8.4715E-5 | 2.3182 |
| -3.5972 | -422.11999 | 0.66758 | 8.7279E-5 | 2.32339 |
| -3.49725 | -422.11993 | 0.70858 | 9.4896E-5 | 2.32848 |
| -3.39731 | -422.11986 | 0.75202 | 1.00791E-4 | 2.3333 |
| -3.29738 | -422.11978 | 0.79821 | 1.07569E-4 | 2.33771 |
| -3.19746 | -422.11971 | 0.84766 | 1.15629E-4 | 2.34193 |
| -3.09754 | -422.11962 | 0.90107 | 1.21871E-4 | 2.34592 |
| -2.99764 | -422.11953 | 0.95936 | 1.37117E-4 | 2.34977 |
| -2.89774 | -422.11943 | 1.0236 | 1.50843E-4 | 2.35333 |
| -2.79784 | -422.11931 | 1.09547 | 1.68527E-4 | 2.35702 |
| -2.69794 | -422.11918 | 1.17701 | 1.91083E-4 | 2.36093 |
| -2.59801 | -422.11903 | 1.27047 | 2.1785E-4 | 2.36542 |
| -2.49807 | -422.11886 | 1.37843 | 2.53356E-4 | 2.37053 |
| -2.39812 | -422.11866 | 1.50384 | 2.94178E-4 | 2.37703 |
| -2.29817 | -422.11843 | 1.64971 | 3.41214E-4 | 2.38544 |
| -2.1982 | -422.11816 | 1.81851 | 3.93022E-4 | 2.396 |
| -2.09823 | -422.11785 | 2.01223 | 4.48857E-4 | 2.40917 |
| -1.99827 | -422.1175 | 2.23303 | 5.10359E-4 | 2.42538 |
| -1.8983 | -422.1171 | 2.48346 | 5.78184E-4 | 2.44535 |
| -1.79834 | -422.11665 | 2.76729 | 6.55674E-4 | 2.46974 |
| -1.69838 | -422.11613 | 3.08956 | 7.45325E-4 | 2.49913 |
| -1.59843 | -422.11555 | 3.45629 | 8.4873E-4 | 2.53369 |
| -1.49848 | -422.11488 | 3.87466 | 9.69826E-4 | 2.57257 |
| -1.39853 | -422.11412 | 4.35318 | 0.00111 | 2.61415 |
| -1.29857 | -422.11325 | 4.90103 | 0.00127 | 2.65861 |
| -1.19862 | -422.11225 | 5.5282 | 0.00145 | 2.70591 |
| -1.09866 | -422.1111 | 6.24653 | 0.00167 | 2.75477 |
| -0.99874 | -422.10979 | 7.07099 | 0.00192 | 2.80036 |
| -0.89883 | -422.10828 | 8.02003 | 0.00222 | 2.84994 |
| -0.79896 | -422.10651 | 9.13064 | 0.00263 | 2.87606 |
| -0.69915 | -422.10438 | 10.46478 | 0.00321 | 2.89974 |
| -0.5995 | -422.10169 | 12.15528 | 0.00426 | 2.84735 |
| -0.49986 | -422.09781 | 14.58622 | 0.0064 | 2.61556 |
| -0.3999 | -422.09234 | 18.01996 | 0.0083 | 2.10608 |
| -0.29993 | -422.08604 | 21.9718 | 0.00855 | 1.31514 |
| -0.19996 | -422.08025 | 25.60403 | 0.00693 | 0.59041 |
| -0.1 | -422.07623 | 28.12761 | 0.00386 | 1.66644 |
| 0 | -422.07478 | 29.03669 | 6.225E-6 | 3.33241 |
| 0.1 | -422.0763 | 28.08446 | 0.00413 | 5.10402 |
| 0.19996 | -422.08081 | 25.25231 | 0.00811 | 6.8052 |
| 0.29993 | -422.08807 | 20.70224 | 0.0115 | 8.27118 |
| 0.39991 | -422.09744 | 14.81989 | 0.01384 | 9.37126 |
| 0.49988 | -422.10812 | 8.12039 | 0.01505 | 10.06743 |
| 0.59986 | -422.11928 | 1.11212 | 0.01517 | 10.40763 |
| 0.69983 | -422.13016 | -5.71347 | 0.01427 | 10.46871 |
| 0.79981 | -422.14004 | -11.91487 | 0.0125 | 10.32015 |
| 0.89975 | -422.14838 | -17.14432 | 0.01011 | 10.02135 |
| 0.99962 | -422.15487 | -21.21915 | 0.00761 | 9.62525 |
| 1.09927 | -422.15972 | -24.26276 | 0.00573 | 9.1936 |
| 1.19893 | -422.16353 | -26.65294 | 0.00479 | 8.75635 |
| 1.29869 | -422.16695 | -28.8015 | 0.00462 | 8.31878 |
| 1.39857 | -422.17041 | -30.97282 | 0.00486 | 7.83096 |
| 1.49851 | -422.17415 | -33.31626 | 0.00536 | 7.26942 |
| 1.59843 | -422.17836 | -35.95597 | 0.0061 | 6.61521 |
| 1.69838 | -422.18308 | -38.91906 | 0.0067 | 5.93054 |
| 1.79834 | -422.18801 | -42.01499 | 0.00659 | 5.26194 |
| 1.8983 | -422.1925 | -44.83299 | 0.0055 | 4.66439 |
| 1.9982 | -422.19595 | -46.99397 | 0.00396 | 4.20861 |
| 2.09793 | -422.19849 | -48.59271 | 0.00305 | 4.01333 |
| 2.19776 | -422.2005 | -49.85473 | 0.00246 | 3.92471 |
| 2.29762 | -422.20215 | -50.88865 | 0.00204 | 3.88073 |
| 2.39753 | -422.20353 | -51.75313 | 0.00172 | 3.84679 |
| 2.49744 | -422.20469 | -52.48383 | 0.00146 | 3.83185 |
| 2.59735 | -422.20569 | -53.10624 | 0.00125 | 3.81793 |
| 2.69727 | -422.20654 | -53.6403 | 0.00108 | 3.81536 |
| 2.79719 | -422.20728 | -54.10371 | 9.40567E-4 | 3.81971 |
| 2.89712 | -422.20793 | -54.5112 | 8.32303E-4 | 3.83106 |
| 2.99707 | -422.2085 | -54.87407 | 7.46119E-4 | 3.84778 |
| 3.09702 | -422.20903 | -55.20169 | 6.77494E-4 | 3.86766 |
| 3.19699 | -422.2095 | -55.49984 | 6.16857E-4 | 3.89064 |
| 3.29696 | -422.20993 | -55.77051 | 5.58091E-4 | 3.91412 |
| 3.39694 | -422.21032 | -56.01461 | 5.02031E-4 | 3.93785 |
| 3.49692 | -422.21067 | -56.23425 | 4.524E-4 | 3.96123 |
| 3.5969 | -422.21099 | -56.4317 | 4.05028E-4 | 3.98377 |
| 3.69687 | -422.21127 | -56.60792 | 3.60627E-4 | 4.00534 |
| 3.79685 | -422.21152 | -56.76379 | 3.17226E-4 | 4.02444 |
| 3.89682 | -422.21173 | -56.90014 | 2.76579E-4 | 4.0419 |
| 3.99678 | -422.21192 | -57.01873 | 2.41434E-4 | 4.05885 |
| 4.09673 | -422.21209 | -57.12228 | 2.09937E-4 | 4.07606 |
| 4.19669 | -422.21223 | -57.21219 | 1.82426E-4 | 4.09485 |
| 4.29663 | -422.21235 | -57.28945 | 1.57264E-4 | 4.1154 |
| 4.39655 | -422.21246 | -57.35551 | 1.3729E-4 | 4.139 |
| 4.49646 | -422.21255 | -57.41271 | 1.22142E-4 | 4.16599 |
| 4.59635 | -422.21263 | -57.46257 | 1.02571E-4 | 4.1957 |
| 4.69627 | -422.2127 | -57.50613 | 9.6642E-5 | 4.22754 |
| 4.79613 | -422.21276 | -57.54471 | 8.8362E-5 | 4.25898 |
| 4.89597 | -422.21281 | -57.57929 | 8.2673E-5 | 4.28981 |
| 4.99577 | -422.21287 | -57.61095 | 8.0727E-5 | 4.32013 |
| 5.09556 | -422.21291 | -57.64089 | 6.7048E-5 | 4.34894 |
| 5.19548 | -422.21296 | -57.66963 | 7.5527E-5 | 4.37873 |
| 5.29531 | -422.213 | -57.69759 | 7.4275E-5 | 4.4074 |
| 5.39513 | -422.21305 | -57.72481 | 7.2824E-5 | 4.43566 |
| 5.49496 | -422.21309 | -57.75126 | 7.0959E-5 | 4.46368 |
| 5.59479 | -422.21313 | -57.77693 | 5.892E-5 | 4.49014 |
| 5.69473 | -422.21317 | -57.80154 | 6.8384E-5 | 4.518 |
| 5.79454 | -422.21321 | -57.82514 | 6.6058E-5 | 4.54477 |
| 5.89435 | -422.21324 | -57.84764 | 6.4201E-5 | 4.57075 |
| 5.99415 | -422.21328 | -57.86904 | 6.1957E-5 | 4.59613 |
| 6.09396 | -422.21331 | -57.88943 | 4.8416E-5 | 4.61981 |
| 6.19388 | -422.21334 | -57.90875 | 6.0146E-5 | 4.64461 |
| 6.29366 | -422.21337 | -57.92729 | 5.8334E-5 | 4.66834 |
| 6.39344 | -422.2134 | -57.94511 | 5.7232E-5 | 4.6913 |
| 6.49321 | -422.21343 | -57.96228 | 5.5487E-5 | 4.71346 |
| 6.593 | -422.21345 | -57.97888 | 4.0843E-5 | 4.73381 |
| 6.69292 | -422.21348 | -57.99473 | 5.3012E-5 | 4.75492 |
| 6.79269 | -422.2135 | -58.00995 | 5.1159E-5 | 4.77512 |
| 6.89246 | -422.21352 | -58.02446 | 5.0557E-5 | 4.79464 |
| 6.9922 | -422.21355 | -58.03822 | 4.9667E-5 | 4.8135 |
| 7.09193 | -422.21357 | -58.0512 | 3.3338E-5 | 4.83043 |
| 7.19185 | -422.21359 | -58.06313 | 4.6557E-5 | 4.84815 |
| 7.29157 | -422.2136 | -58.07405 | 4.494E-5 | 4.86517 |
| 7.39128 | -422.21362 | -58.08381 | 4.3909E-5 | 4.88127 |
| 7.49096 | -422.21363 | -58.09229 | 4.2095E-5 | 4.89657 |
| 7.5906 | -422.21364 | -58.09942 | 2.324E-5 | 4.9102 |
| 7.69045 | -422.21365 | -58.10501 | 3.7761E-5 | 4.92428 |
| 7.78998 | -422.21366 | -58.10932 | 3.3769E-5 | 4.93685 |
| 7.88943 | -422.21366 | -58.11262 | 3.2145E-5 | 4.94704 |
| 7.98881 | -422.21367 | -58.11517 | 3.4196E-5 | 4.95468 |
| 8.08802 | -422.21367 | -58.11717 | 1.3424E-5 | 4.95923 |

aReferenced to -422.121056397 hartree.

**2. Data for plots shown in Figure 2**

**Table S2:** Data for plots shown in Figure 2.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Reaction Coordinate[bohr amu1/2]** |  |  |  |  |  |  |  |
| -5.98506 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| -5.88684 | 1.2E-5 | 1.4E-5 | 6E-6 | 3.4E-5 | 4.1E-5 | 8E-6 | 1.3E-5 |
| -5.78897 | 4.9E-5 | 4.7E-5 | 4E-6 | 3.9E-5 | 6.9E-5 | 4E-6 | 1.8E-5 |
| -5.69041 | 1.17E-4 | 9.1E-5 | 1.2E-5 | 8.6E-5 | 1.38E-4 | 1.1E-5 | 4.9E-5 |
| -5.59078 | 2.03E-4 | 1.55E-4 | 1.5E-5 | 1.18E-4 | 2E-4 | 1.5E-5 | 7.9E-5 |
| -5.49144 | 2.77E-4 | 2.2E-4 | 1.9E-5 | 1.81E-4 | 2.77E-4 | 2.9E-5 | 1.18E-4 |
| -5.39215 | 3.63E-4 | 2.83E-4 | 2.6E-5 | 2.11E-4 | 3.36E-4 | 3.5E-5 | 1.51E-4 |
| -5.2928 | 4.34E-4 | 3.49E-4 | 3.2E-5 | 2.52E-4 | 4E-4 | 4.7E-5 | 1.89E-4 |
| -5.19348 | 5.05E-4 | 4.16E-4 | 3.6E-5 | 2.89E-4 | 4.61E-4 | 6.8E-5 | 2.31E-4 |
| -5.09371 | 5.7E-4 | 4.87E-4 | 3.9E-5 | 3.32E-4 | 5.34E-4 | 1.05E-4 | 2.79E-4 |
| -4.99444 | 6.36E-4 | 5.56E-4 | 4.4E-5 | 3.93E-4 | 6.08E-4 | 1.51E-4 | 3.26E-4 |
| -4.89514 | 7.45E-4 | 6.25E-4 | 5.1E-5 | 4.35E-4 | 6.7E-4 | 2.06E-4 | 3.75E-4 |
| -4.79572 | 8.74E-4 | 6.9E-4 | 5.9E-5 | 4.7E-4 | 7.19E-4 | 2.71E-4 | 4.28E-4 |
| -4.69615 | 0.00102 | 7.49E-4 | 6.7E-5 | 5.02E-4 | 7.61E-4 | 3.44E-4 | 4.87E-4 |
| -4.59636 | 0.0012 | 7.98E-4 | 7.4E-5 | 5.21E-4 | 7.89E-4 | 4.23E-4 | 5.52E-4 |
| -4.49663 | 0.00139 | 8.29E-4 | 8.1E-5 | 5.45E-4 | 8.02E-4 | 5.12E-4 | 6.18E-4 |
| -4.39679 | 0.0016 | 8.43E-4 | 8.4E-5 | 5.46E-4 | 7.93E-4 | 5.98E-4 | 6.88E-4 |
| -4.29688 | 0.00182 | 8.45E-4 | 8.6E-5 | 5.4E-4 | 7.69E-4 | 6.88E-4 | 7.59E-4 |
| -4.19695 | 0.00205 | 8.37E-4 | 8.6E-5 | 5.29E-4 | 7.38E-4 | 7.81E-4 | 8.28E-4 |
| -4.09699 | 0.00229 | 8.21E-4 | 8.5E-5 | 5.11E-4 | 6.98E-4 | 8.72E-4 | 9.01E-4 |
| -3.99704 | 0.00252 | 7.9E-4 | 8.3E-5 | 4.96E-4 | 6.49E-4 | 9.66E-4 | 9.68E-4 |
| -3.89708 | 0.00275 | 7.56E-4 | 7.9E-5 | 4.75E-4 | 5.97E-4 | 0.00106 | 0.00104 |
| -3.79713 | 0.00299 | 7.13E-4 | 7.3E-5 | 4.53E-4 | 5.41E-4 | 0.00115 | 0.00111 |
| -3.69717 | 0.00321 | 6.65E-4 | 6.7E-5 | 4.24E-4 | 4.78E-4 | 0.00125 | 0.00117 |
| -3.5972 | 0.00344 | 6.2E-4 | 5.8E-5 | 3.96E-4 | 4.26E-4 | 0.00136 | 0.00122 |
| -3.49725 | 0.00365 | 5.63E-4 | 5.2E-5 | 3.72E-4 | 3.66E-4 | 0.00147 | 0.00126 |
| -3.39731 | 0.00385 | 5E-4 | 4.9E-5 | 3.4E-4 | 3.08E-4 | 0.00159 | 0.00129 |
| -3.29738 | 0.00403 | 4.25E-4 | 5.9E-5 | 3E-4 | 2.48E-4 | 0.00171 | 0.00132 |
| -3.19746 | 0.00419 | 3.35E-4 | 8.7E-5 | 2.52E-4 | 1.88E-4 | 0.00182 | 0.00134 |
| -3.09754 | 0.00434 | 2.24E-4 | 1.33E-4 | 1.76E-4 | 1.36E-4 | 0.00192 | 0.00137 |
| -2.99764 | 0.00446 | 8.6E-5 | 1.95E-4 | 1E-4 | 1.46E-4 | 0.002 | 0.00139 |
| -2.89774 | 0.00456 | 1.09E-4 | 2.68E-4 | 3.2E-5 | 2.32E-4 | 0.00206 | 0.00141 |
| -2.79784 | 0.00465 | 3.01E-4 | 3.68E-4 | 1.32E-4 | 3.58E-4 | 0.0021 | 0.00144 |
| -2.69794 | 0.00472 | 5.26E-4 | 4.86E-4 | 2.7E-4 | 5.13E-4 | 0.00212 | 0.00148 |
| -2.59801 | 0.00479 | 7.73E-4 | 6.18E-4 | 4.33E-4 | 6.9E-4 | 0.00213 | 0.00153 |
| -2.49807 | 0.00486 | 0.00104 | 7.68E-4 | 5.98E-4 | 8.8E-4 | 0.00212 | 0.00159 |
| -2.39812 | 0.00495 | 0.00133 | 9.36E-4 | 7.94E-4 | 0.0011 | 0.00211 | 0.00166 |
| -2.29817 | 0.00506 | 0.00164 | 0.00112 | 0.00101 | 0.00135 | 0.00208 | 0.00176 |
| -2.1982 | 0.0052 | 0.00198 | 0.00132 | 0.00124 | 0.00163 | 0.00203 | 0.00188 |
| -2.09823 | 0.00537 | 0.00234 | 0.00153 | 0.0015 | 0.00196 | 0.00197 | 0.00204 |
| -1.99827 | 0.00558 | 0.00276 | 0.00177 | 0.00179 | 0.00234 | 0.00187 | 0.00226 |
| -1.8983 | 0.00583 | 0.00323 | 0.00202 | 0.00213 | 0.00282 | 0.00172 | 0.00254 |
| -1.79834 | 0.00612 | 0.00379 | 0.00229 | 0.00254 | 0.00341 | 0.00149 | 0.00292 |
| -1.69838 | 0.00646 | 0.00448 | 0.00259 | 0.00303 | 0.00415 | 0.00117 | 0.00342 |
| -1.59843 | 0.00683 | 0.0053 | 0.00291 | 0.00361 | 0.00502 | 7.46E-4 | 0.00405 |
| -1.49848 | 0.00724 | 0.00629 | 0.00326 | 0.00427 | 0.00605 | 2.65E-4 | 0.00481 |
| -1.39853 | 0.00768 | 0.00741 | 0.00363 | 0.00502 | 0.0072 | 5E-4 | 0.0057 |
| -1.29857 | 0.00815 | 0.00869 | 0.00404 | 0.00585 | 0.00848 | 0.00124 | 0.00673 |
| -1.19862 | 0.00866 | 0.01015 | 0.00448 | 0.00677 | 0.00987 | 0.00213 | 0.00791 |
| -1.09866 | 0.00921 | 0.01175 | 0.00497 | 0.00776 | 0.0113 | 0.00319 | 0.00924 |
| -0.99874 | 0.00989 | 0.01379 | 0.00549 | 0.00882 | 0.01278 | 0.00449 | 0.01074 |
| -0.89883 | 0.01058 | 0.01548 | 0.00619 | 0.00972 | 0.01397 | 0.00592 | 0.0124 |
| -0.79896 | 0.01177 | 0.01834 | 0.00695 | 0.01083 | 0.01525 | 0.00773 | 0.01425 |
| -0.69915 | 0.01318 | 0.02087 | 0.00781 | 0.01131 | 0.01577 | 0.0095 | 0.01621 |
| -0.5995 | 0.0165 | 0.02713 | 0.009 | 0.01205 | 0.01666 | 0.01145 | 0.01837 |
| -0.49986 | 0.02434 | 0.03977 | 0.01072 | 0.01439 | 0.0193 | 0.01361 | 0.02072 |
| -0.3999 | 0.03961 | 0.05918 | 0.01296 | 0.02031 | 0.02507 | 0.01586 | 0.02317 |
| -0.29993 | 0.0644 | 0.08557 | 0.01654 | 0.0294 | 0.03352 | 0.01809 | 0.026 |
| -0.19996 | 0.10206 | 0.12245 | 0.0221 | 0.04155 | 0.04417 | 0.02038 | 0.02933 |
| -0.1 | 0.15739 | 0.17674 | 0.0303 | 0.05661 | 0.05756 | 0.0231 | 0.03317 |
| 0 | 0.23736 | 0.25445 | 0.04166 | 0.07398 | 0.07275 | 0.02676 | 0.03757 |
| 0.1 | 0.33682 | 0.34505 | 0.0565 | 0.09338 | 0.08944 | 0.03169 | 0.04265 |
| 0.19996 | 0.42834 | 0.42269 | 0.07506 | 0.11395 | 0.10683 | 0.03791 | 0.04836 |
| 0.29993 | 0.49849 | 0.48014 | 0.0975 | 0.13469 | 0.1241 | 0.04523 | 0.05469 |
| 0.39991 | 0.55196 | 0.5226 | 0.12415 | 0.15416 | 0.14011 | 0.05323 | 0.06147 |
| 0.49988 | 0.59758 | 0.55428 | 0.1581 | 0.17107 | 0.15393 | 0.06148 | 0.06843 |
| 0.59986 | 0.65398 | 0.57727 | 0.21734 | 0.18443 | 0.16484 | 0.06943 | 0.0752 |
| 0.69983 | 0.73879 | 0.59297 | 0.31355 | 0.19457 | 0.17349 | 0.07715 | 0.08186 |
| 0.79981 | 0.78567 | 0.60281 | 0.36939 | 0.20205 | 0.17997 | 0.08519 | 0.08859 |
| 0.89975 | 0.80364 | 0.60888 | 0.39781 | 0.2073 | 0.18506 | 0.09358 | 0.09554 |
| 0.99962 | 0.81165 | 0.61251 | 0.41777 | 0.21163 | 0.18956 | 0.10256 | 0.10329 |
| 1.09927 | 0.81561 | 0.61462 | 0.43315 | 0.21516 | 0.19347 | 0.11217 | 0.11251 |
| 1.19893 | 0.81731 | 0.61591 | 0.44452 | 0.22033 | 0.19897 | 0.12302 | 0.12407 |
| 1.29869 | 0.81717 | 0.61672 | 0.45184 | 0.22754 | 0.20641 | 0.13582 | 0.1384 |
| 1.39857 | 0.81566 | 0.61726 | 0.45773 | 0.23504 | 0.2143 | 0.15174 | 0.15633 |
| 1.49851 | 0.81331 | 0.61759 | 0.46364 | 0.24343 | 0.22318 | 0.17118 | 0.17772 |
| 1.59843 | 0.81023 | 0.61767 | 0.47001 | 0.25257 | 0.233 | 0.19459 | 0.20262 |
| 1.69838 | 0.80693 | 0.61757 | 0.47631 | 0.26181 | 0.24297 | 0.21938 | 0.22786 |
| 1.79834 | 0.80364 | 0.61727 | 0.48235 | 0.27069 | 0.25256 | 0.24371 | 0.25161 |
| 1.8983 | 0.80062 | 0.61679 | 0.48782 | 0.27862 | 0.26118 | 0.26598 | 0.27241 |
| 1.9982 | 0.79816 | 0.61611 | 0.49226 | 0.2846 | 0.26783 | 0.28449 | 0.2887 |
| 2.09793 | 0.79678 | 0.61537 | 0.4947 | 0.28686 | 0.27076 | 0.29567 | 0.29844 |
| 2.19776 | 0.79594 | 0.61476 | 0.49607 | 0.28786 | 0.27251 | 0.30302 | 0.30473 |
| 2.29762 | 0.79535 | 0.61425 | 0.497 | 0.28842 | 0.27385 | 0.30844 | 0.30926 |
| 2.39753 | 0.79487 | 0.61379 | 0.49775 | 0.28903 | 0.27522 | 0.31301 | 0.31287 |
| 2.49744 | 0.79452 | 0.6134 | 0.49827 | 0.28944 | 0.27634 | 0.31656 | 0.3156 |
| 2.59735 | 0.79425 | 0.61305 | 0.49868 | 0.28987 | 0.27743 | 0.31966 | 0.31782 |
| 2.69727 | 0.79408 | 0.61275 | 0.49894 | 0.29014 | 0.27826 | 0.32214 | 0.3195 |
| 2.79719 | 0.79398 | 0.61252 | 0.49907 | 0.29031 | 0.27891 | 0.3242 | 0.32077 |
| 2.89712 | 0.79395 | 0.61235 | 0.49911 | 0.29039 | 0.27938 | 0.32588 | 0.3217 |
| 2.99707 | 0.79397 | 0.61223 | 0.49906 | 0.2904 | 0.2797 | 0.32727 | 0.32238 |
| 3.09702 | 0.79402 | 0.61215 | 0.49897 | 0.29037 | 0.27992 | 0.32849 | 0.32289 |
| 3.19699 | 0.7941 | 0.61211 | 0.49885 | 0.29029 | 0.28004 | 0.32958 | 0.32328 |
| 3.29696 | 0.79422 | 0.61207 | 0.4986 | 0.28951 | 0.27958 | 0.33062 | 0.32379 |
| 3.39694 | 0.7943 | 0.61205 | 0.49848 | 0.28941 | 0.27964 | 0.33162 | 0.32411 |
| 3.49692 | 0.79437 | 0.61204 | 0.49837 | 0.28933 | 0.27968 | 0.33262 | 0.32443 |
| 3.5969 | 0.79443 | 0.61203 | 0.49829 | 0.28926 | 0.27974 | 0.33365 | 0.32478 |
| 3.69687 | 0.79444 | 0.61204 | 0.49836 | 0.28985 | 0.28031 | 0.33469 | 0.32499 |
| 3.79685 | 0.79447 | 0.61203 | 0.49832 | 0.28983 | 0.28039 | 0.33579 | 0.32541 |
| 3.89682 | 0.79449 | 0.61201 | 0.49831 | 0.28983 | 0.28049 | 0.33691 | 0.32588 |
| 3.99678 | 0.7945 | 0.61199 | 0.49832 | 0.28985 | 0.28061 | 0.33803 | 0.32638 |
| 4.09673 | 0.79449 | 0.61197 | 0.49835 | 0.28991 | 0.28074 | 0.33914 | 0.3269 |
| 4.19669 | 0.79448 | 0.61196 | 0.49838 | 0.28995 | 0.28087 | 0.34016 | 0.3274 |
| 4.29663 | 0.79446 | 0.61194 | 0.49841 | 0.28998 | 0.28098 | 0.34109 | 0.32786 |
| 4.39655 | 0.79445 | 0.61192 | 0.49843 | 0.29 | 0.28107 | 0.34189 | 0.32824 |
| 4.49646 | 0.79444 | 0.6119 | 0.49844 | 0.29 | 0.28114 | 0.34255 | 0.32856 |
| 4.59635 | 0.79444 | 0.61189 | 0.49845 | 0.29 | 0.28119 | 0.3431 | 0.32883 |
| 4.69627 | 0.79444 | 0.61188 | 0.49844 | 0.28999 | 0.28124 | 0.3435 | 0.32904 |
| 4.79613 | 0.79443 | 0.61187 | 0.49844 | 0.29 | 0.28129 | 0.34381 | 0.32922 |
| 4.89597 | 0.7944 | 0.61186 | 0.49845 | 0.29003 | 0.28134 | 0.34396 | 0.32938 |
| 4.99577 | 0.79438 | 0.61185 | 0.49846 | 0.29005 | 0.28137 | 0.34393 | 0.32946 |
| 5.09556 | 0.79434 | 0.61185 | 0.49848 | 0.29007 | 0.28138 | 0.3437 | 0.32948 |
| 5.19548 | 0.79432 | 0.61185 | 0.49848 | 0.29008 | 0.28138 | 0.34331 | 0.32942 |
| 5.29531 | 0.7943 | 0.61186 | 0.49847 | 0.29007 | 0.28136 | 0.34284 | 0.32932 |
| 5.39513 | 0.79429 | 0.61186 | 0.49846 | 0.29006 | 0.28133 | 0.34231 | 0.32919 |
| 5.49496 | 0.79428 | 0.61187 | 0.49844 | 0.29005 | 0.2813 | 0.34175 | 0.32905 |
| 5.59479 | 0.79427 | 0.61187 | 0.49842 | 0.29004 | 0.28126 | 0.34119 | 0.32891 |
| 5.69473 | 0.79427 | 0.61188 | 0.49838 | 0.29002 | 0.28123 | 0.34062 | 0.32876 |
| 5.79454 | 0.79427 | 0.61189 | 0.49835 | 0.28999 | 0.28119 | 0.34007 | 0.32861 |
| 5.89435 | 0.79427 | 0.61189 | 0.49832 | 0.28998 | 0.28117 | 0.33955 | 0.32849 |
| 5.99415 | 0.79427 | 0.6119 | 0.4983 | 0.28996 | 0.28114 | 0.33906 | 0.32837 |
| 6.09396 | 0.79426 | 0.6119 | 0.49829 | 0.28997 | 0.28114 | 0.33865 | 0.32831 |
| 6.19388 | 0.79426 | 0.6119 | 0.49826 | 0.28996 | 0.28113 | 0.33825 | 0.32824 |
| 6.29366 | 0.79425 | 0.61191 | 0.49824 | 0.28996 | 0.28113 | 0.33789 | 0.32818 |
| 6.39344 | 0.79424 | 0.61191 | 0.49823 | 0.28997 | 0.28114 | 0.33759 | 0.32816 |
| 6.49321 | 0.79423 | 0.61191 | 0.49823 | 0.28999 | 0.28116 | 0.33735 | 0.32817 |
| 6.593 | 0.79422 | 0.61191 | 0.49824 | 0.29002 | 0.28118 | 0.33717 | 0.32821 |
| 6.69292 | 0.79421 | 0.6119 | 0.49823 | 0.29004 | 0.28121 | 0.33695 | 0.32823 |
| 6.79269 | 0.79421 | 0.6119 | 0.49822 | 0.29006 | 0.28123 | 0.3367 | 0.32823 |
| 6.89246 | 0.79424 | 0.61188 | 0.49809 | 0.28941 | 0.28073 | 0.33643 | 0.32838 |
| 6.9922 | 0.79424 | 0.61188 | 0.49807 | 0.28942 | 0.28074 | 0.33614 | 0.32836 |
| 7.09193 | 0.79424 | 0.61188 | 0.49806 | 0.28944 | 0.28075 | 0.33586 | 0.32835 |
| 7.19185 | 0.7942 | 0.6119 | 0.49816 | 0.29015 | 0.28129 | 0.33554 | 0.32815 |
| 7.29157 | 0.7942 | 0.61189 | 0.49813 | 0.29016 | 0.2813 | 0.33522 | 0.3281 |
| 7.39128 | 0.7942 | 0.61189 | 0.49809 | 0.29016 | 0.2813 | 0.33492 | 0.32806 |
| 7.49096 | 0.79425 | 0.61187 | 0.49793 | 0.28945 | 0.28077 | 0.33463 | 0.32819 |
| 7.5906 | 0.79424 | 0.61187 | 0.4979 | 0.28946 | 0.28079 | 0.33441 | 0.32819 |
| 7.69045 | 0.7942 | 0.61188 | 0.498 | 0.29018 | 0.28134 | 0.3342 | 0.32801 |
| 7.78998 | 0.79424 | 0.61186 | 0.49784 | 0.28947 | 0.28082 | 0.33402 | 0.32816 |
| 7.88943 | 0.79424 | 0.61186 | 0.49781 | 0.28948 | 0.28083 | 0.3339 | 0.32816 |
| 7.98881 | 0.79424 | 0.61186 | 0.49779 | 0.28948 | 0.28085 | 0.3338 | 0.32817 |
| 8.08802 | 0.79419 | 0.61187 | 0.49791 | 0.29023 | 0.28141 | 0.33376 | 0.32804 |

**3. Data for plots shown in Figures 3 and 4**

**Table S3:** Data shown in Figures 3 and 4 for *trans* dicyanopropene.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Reaction Coordinate[bohr amu1/2]** | **E [hartree]** | **ΔE [kcal mol-1]a** | **IBO Changes for π-Bond Olefin** | **IBO Changes for Lone Pair on Oxygen** | **Dipole Moment****[debye]** |
| -20.1808 | -606.62532 | 0.67136 | 0 | 0 | 3.75643 |
| -20.00126 | -606.62531 | 0.67551 | 8.9E-5 | 8E-5 | 3.75182 |
| -19.82546 | -606.62531 | 0.67813 | 2.83E-4 | 4.3E-5 | 3.77233 |
| -19.64596 | -606.6253 | 0.68578 | 1.74E-4 | 3.57E-4 | 3.77259 |
| -19.477 | -606.62527 | 0.70105 | 0.00119 | 8E-5 | 3.78863 |
| -19.30058 | -606.62525 | 0.71221 | 2.8E-4 | 3.06E-4 | 3.81892 |
| -19.12039 | -606.62526 | 0.71049 | 8.4E-4 | 3.8E-4 | 3.83557 |
| -18.93907 | -606.62526 | 0.71051 | 9.87E-4 | 1.76E-4 | 3.84761 |
| -18.75717 | -606.62524 | 0.71898 | 0.00145 | 4.55E-4 | 3.87877 |
| -18.56684 | -606.62525 | 0.71418 | 0.00158 | 3.83E-4 | 3.88544 |
| -18.37 | -606.62524 | 0.72332 | 0.00206 | 4.85E-4 | 3.89992 |
| -18.17119 | -606.62521 | 0.74266 | 0.00252 | 5.4E-4 | 3.90885 |
| -17.97218 | -606.62516 | 0.76936 | 0.00301 | 5.94E-4 | 3.92672 |
| -17.77346 | -606.62512 | 0.7982 | 0.00346 | 6.27E-4 | 3.9433 |
| -17.57431 | -606.62508 | 0.82487 | 0.00395 | 6.45E-4 | 3.9612 |
| -17.38237 | -606.62502 | 0.85675 | 0.00442 | 6.45E-4 | 3.93957 |
| -17.18854 | -606.62499 | 0.87762 | 0.0046 | 6.74E-4 | 3.98683 |
| -16.99053 | -606.62494 | 0.90697 | 0.00517 | 6.6E-4 | 3.96819 |
| -16.79245 | -606.62488 | 0.94466 | 0.00527 | 7.2E-4 | 3.99091 |
| -16.59322 | -606.62482 | 0.98403 | 0.00589 | 7.15E-4 | 3.99181 |
| -16.39482 | -606.62476 | 1.0254 | 0.00605 | 7.32E-4 | 4.01532 |
| -16.19546 | -606.62469 | 1.06466 | 0.00637 | 6.92E-4 | 4.02078 |
| -15.99645 | -606.62463 | 1.10318 | 0.00647 | 6.79E-4 | 4.02555 |
| -15.79689 | -606.62457 | 1.14223 | 0.007 | 6.36E-4 | 4.02782 |
| -15.59739 | -606.62451 | 1.17945 | 0.00707 | 6.13E-4 | 4.03014 |
| -15.40359 | -606.62444 | 1.2225 | 0.00764 | 5.22E-4 | 4.02376 |
| -15.21078 | -606.62438 | 1.26036 | 0.00752 | 9.92E-4 | 4.03883 |
| -15.01591 | -606.62433 | 1.29149 | 0.00808 | 5.2E-4 | 4.03372 |
| -14.82068 | -606.62429 | 1.3203 | 0.00789 | 9.4E-4 | 4.04638 |
| -14.62256 | -606.62424 | 1.34622 | 0.00842 | 9.46E-4 | 4.04852 |
| -14.42538 | -606.6242 | 1.37511 | 0.00826 | 9.02E-4 | 4.05798 |
| -14.22675 | -606.62416 | 1.3987 | 0.00864 | 9.12E-4 | 4.0636 |
| -14.02902 | -606.62413 | 1.42086 | 0.00882 | 8.57E-4 | 4.06762 |
| -13.83053 | -606.6241 | 1.43932 | 0.00896 | 8.58E-4 | 4.07166 |
| -13.63209 | -606.62407 | 1.45595 | 0.00913 | 8.35E-4 | 4.0743 |
| -13.44199 | -606.62403 | 1.48219 | 0.00948 | 6.25E-4 | 4.066 |
| -13.24804 | -606.62402 | 1.48932 | 0.00943 | 7.96E-4 | 4.08656 |
| -13.05085 | -606.62399 | 1.5031 | 0.00967 | 8.27E-4 | 4.07625 |
| -12.85329 | -606.62397 | 1.51917 | 0.00965 | 5.7E-4 | 4.08573 |
| -12.65539 | -606.62394 | 1.53628 | 0.00988 | 5.86E-4 | 4.08059 |
| -12.45754 | -606.62391 | 1.55454 | 0.01002 | 5.5E-4 | 4.08776 |
| -12.26043 | -606.62389 | 1.57133 | 0.01014 | 5.1E-4 | 4.07775 |
| -12.06434 | -606.62386 | 1.58532 | 0.01033 | 5.33E-4 | 4.08971 |
| -11.86775 | -606.62384 | 1.59699 | 0.01031 | 4.99E-4 | 4.07892 |
| -11.67326 | -606.62383 | 1.60889 | 0.01057 | 5.63E-4 | 4.09001 |
| -11.49356 | -606.62377 | 1.64268 | 0.01055 | 4.45E-4 | 4.06247 |
| -11.30793 | -606.62377 | 1.64233 | 0.01051 | 5.41E-4 | 4.09086 |
| -11.12094 | -606.62376 | 1.65173 | 0.01065 | 7.34E-4 | 4.05459 |
| -10.93174 | -606.62374 | 1.66254 | 0.01067 | 4.85E-4 | 4.06901 |
| -10.73816 | -606.62373 | 1.66817 | 0.01063 | 4.92E-4 | 4.05573 |
| -10.54733 | -606.62371 | 1.68065 | 0.01093 | 5.11E-4 | 4.05163 |
| -10.35858 | -606.62368 | 1.6978 | 0.01054 | 6.4E-4 | 4.05038 |
| -10.17149 | -606.62366 | 1.71082 | 0.01087 | 5.47E-4 | 4.04106 |
| -9.98352 | -606.62364 | 1.7244 | 0.01037 | 6.74E-4 | 4.03961 |
| -9.79199 | -606.62363 | 1.73486 | 0.01072 | 5.96E-4 | 4.03049 |
| -9.60809 | -606.62357 | 1.76881 | 0.01022 | 5.55E-4 | 4.03995 |
| -9.42739 | -606.62354 | 1.78594 | 0.01045 | 5.64E-4 | 4.0007 |
| -9.24497 | -606.62353 | 1.79741 | 0.01039 | 5.48E-4 | 4.01147 |
| -9.06076 | -606.62351 | 1.80805 | 0.01046 | 6.56E-4 | 3.97125 |
| -8.87577 | -606.62348 | 1.82624 | 0.01062 | 6.48E-4 | 3.97977 |
| -8.68537 | -606.62346 | 1.83921 | 0.01047 | 6.05E-4 | 3.93123 |
| -8.48879 | -606.62345 | 1.84588 | 0.01068 | 6.3E-4 | 3.92972 |
| -8.28989 | -606.62341 | 1.86735 | 0.01057 | 5.95E-4 | 3.90127 |
| -8.09186 | -606.62338 | 1.8915 | 0.01057 | 7.1E-4 | 3.88102 |
| -7.89297 | -606.62334 | 1.91484 | 0.01034 | 6.27E-4 | 3.8627 |
| -7.7039 | -606.62328 | 1.95055 | 0.0103 | 5.15E-4 | 3.83382 |
| -7.51697 | -606.62326 | 1.96577 | 0.01001 | 5.71E-4 | 3.8351 |
| -7.32731 | -606.62325 | 1.97248 | 0.01004 | 5.75E-4 | 3.81018 |
| -7.13582 | -606.62323 | 1.98265 | 0.00994 | 5.62E-4 | 3.78742 |
| -6.94559 | -606.6232 | 2.00229 | 0.01002 | 5.06E-4 | 3.76782 |
| -6.76058 | -606.62314 | 2.0366 | 0.00972 | 4.68E-4 | 3.72735 |
| -6.5719 | -606.62315 | 2.03595 | 0.00989 | 5.32E-4 | 3.72774 |
| -6.38208 | -606.62313 | 2.04285 | 0.00939 | 4.62E-4 | 3.69358 |
| -6.19867 | -606.62308 | 2.07666 | 0.00878 | 5.27E-4 | 3.69173 |
| -6.02301 | -606.62303 | 2.10603 | 0.00934 | 4.81E-4 | 3.63584 |
| -5.83994 | -606.62297 | 2.14874 | 0.00806 | 4.55E-4 | 3.65048 |
| -5.65955 | -606.6229 | 2.19039 | 0.00857 | 4.02E-4 | 3.62062 |
| -5.46895 | -606.62295 | 2.16024 | 0.00765 | 3.75E-4 | 3.60954 |
| -5.27989 | -606.6229 | 2.18814 | 0.00792 | 3.78E-4 | 3.59221 |
| -5.09489 | -606.62283 | 2.23333 | 0.00754 | 3.48E-4 | 3.56247 |
| -4.90226 | -606.62281 | 2.24517 | 0.00743 | 3.42E-4 | 3.55401 |
| -4.706 | -606.62277 | 2.27043 | 0.00755 | 3.35E-4 | 3.51299 |
| -4.50864 | -606.62271 | 2.30941 | 0.00748 | 3.54E-4 | 3.48168 |
| -4.31199 | -606.62262 | 2.36362 | 0.0076 | 4.33E-4 | 3.44468 |
| -4.11287 | -606.62251 | 2.43684 | 0.00774 | 5.26E-4 | 3.40628 |
| -3.91412 | -606.62234 | 2.54266 | 0.00816 | 5.74E-4 | 3.35954 |
| -3.71515 | -606.62211 | 2.68508 | 0.00843 | 8.93E-4 | 3.31106 |
| -3.51568 | -606.6218 | 2.87963 | 0.00879 | 0.00122 | 3.26175 |
| -3.31752 | -606.62139 | 3.1387 | 0.00897 | 0.00185 | 3.22911 |
| -3.12014 | -606.62086 | 3.46751 | 0.00926 | 0.00219 | 3.23058 |
| -2.94401 | -606.61947 | 4.34537 | 0.00942 | 0.00313 | 3.29706 |
| -2.76376 | -606.61855 | 4.92048 | 0.00928 | 0.00307 | 3.45137 |
| -2.56957 | -606.61768 | 5.46266 | 0.00925 | 0.00405 | 3.72775 |
| -2.37281 | -606.6151 | 7.08387 | 0.00911 | 0.00453 | 4.01225 |
| -2.17412 | -606.61069 | 9.84939 | 0.00911 | 0.00618 | 4.42933 |
| -1.97565 | -606.60385 | 14.14102 | 0.00937 | 0.00964 | 4.97886 |
| -1.77946 | -606.59799 | 17.82175 | 0.01023 | 0.01542 | 5.5609 |
| -1.58351 | -606.59427 | 20.15629 | 0.01159 | 0.02027 | 6.00015 |
| -1.38553 | -606.59206 | 21.54406 | 0.01281 | 0.02605 | 6.37526 |
| -1.18694 | -606.59021 | 22.70599 | 0.01498 | 0.0288 | 6.63147 |
| -0.98978 | -606.58825 | 23.93594 | 0.01691 | 0.03471 | 6.87655 |
| -0.79477 | -606.5858 | 25.46857 | 0.02071 | 0.03327 | 7.06364 |
| -0.59931 | -606.58266 | 27.44075 | 0.02216 | 0.04342 | 7.33184 |
| -0.39989 | -606.578 | 30.36436 | 0.03408 | 0.04362 | 7.44815 |
| -0.2 | -606.5694 | 35.76119 | 0.07127 | 0.05537 | 6.81691 |
| 7E-5 | -606.56423 | 39.00338 | 0.16599 | 0.09104 | 5.27237 |
| 0.2 | -606.57131 | 34.56557 | 0.30951 | 0.14429 | 3.40565 |
| 0.39993 | -606.59168 | 21.77853 | 0.43957 | 0.21433 | 2.58915 |
| 0.59986 | -606.61973 | 4.1811 | 0.69649 | 0.46812 | 2.65452 |
| 0.7998 | -606.64821 | -13.69311 | 0.74068 | 0.50953 | 2.63214 |
| 0.99973 | -606.67018 | -27.48187 | 0.7506 | 0.52002 | 2.45674 |
| 1.19874 | -606.67959 | -33.38131 | 0.75604 | 0.52422 | 2.30778 |
| 1.39317 | -606.68304 | -35.54874 | 0.75687 | 0.5233 | 2.37007 |
| 1.59109 | -606.68472 | -36.60035 | 0.75632 | 0.5249 | 2.41513 |
| 1.78239 | -606.68632 | -37.60967 | 0.75846 | 0.52206 | 2.51014 |
| 1.97063 | -606.68817 | -38.76603 | 0.7582 | 0.52353 | 2.46069 |
| 2.16676 | -606.68962 | -39.6768 | 0.75867 | 0.52268 | 2.4993 |
| 2.36667 | -606.69081 | -40.42677 | 0.75911 | 0.52217 | 2.51158 |
| 2.56655 | -606.69184 | -41.07343 | 0.75956 | 0.52169 | 2.52008 |
| 2.76643 | -606.69274 | -41.63717 | 0.76006 | 0.52118 | 2.53027 |
| 2.96632 | -606.69353 | -42.12817 | 0.76057 | 0.52067 | 2.54195 |
| 3.16621 | -606.69421 | -42.55897 | 0.76104 | 0.52019 | 2.5545 |
| 3.36608 | -606.6948 | -42.93021 | 0.76146 | 0.51975 | 2.56703 |
| 3.56593 | -606.69529 | -43.23366 | 0.76182 | 0.51937 | 2.58069 |
| 3.76567 | -606.69567 | -43.47426 | 0.76209 | 0.51909 | 2.59371 |
| 3.96543 | -606.69598 | -43.66561 | 0.76241 | 0.51877 | 2.60826 |
| 4.16474 | -606.69622 | -43.81828 | 0.76281 | 0.51844 | 2.62483 |
| 4.36455 | -606.69641 | -43.93786 | 0.76309 | 0.51823 | 2.64481 |
| 4.56388 | -606.69656 | -44.03009 | 0.76331 | 0.5181 | 2.67088 |
| 4.76279 | -606.69665 | -44.08981 | 0.76345 | 0.51803 | 2.68814 |
| 4.95958 | -606.69671 | -44.12798 | 0.76346 | 0.51801 | 2.69063 |
| 5.15645 | -606.69676 | -44.1609 | 0.76355 | 0.51788 | 2.6873 |
| 5.3539 | -606.69681 | -44.18701 | 0.76357 | 0.51782 | 2.68911 |
| 5.54889 | -606.69679 | -44.17455 | 0.76358 | 0.51773 | 2.68283 |
| 5.73165 | -606.6968 | -44.18619 | 0.76357 | 0.51769 | 2.66923 |
| 5.91147 | -606.69685 | -44.21243 | 0.7637 | 0.51753 | 2.70183 |
| 6.09091 | -606.69693 | -44.26409 | 0.7637 | 0.51741 | 2.66951 |
| 6.28765 | -606.69696 | -44.28383 | 0.7636 | 0.51743 | 2.64583 |
| 6.48409 | -606.697 | -44.31002 | 0.76365 | 0.51723 | 2.62089 |
| 6.68248 | -606.69705 | -44.33836 | 0.76364 | 0.51713 | 2.59229 |
| 6.87889 | -606.69709 | -44.36671 | 0.76359 | 0.51708 | 2.56635 |
| 7.07483 | -606.69711 | -44.37963 | 0.76352 | 0.51706 | 2.54222 |
| 7.26315 | -606.69714 | -44.39781 | 0.76352 | 0.51689 | 2.51447 |
| 7.45078 | -606.69709 | -44.36449 | 0.76349 | 0.51692 | 2.49261 |
| 7.63105 | -606.69717 | -44.41378 | 0.76348 | 0.51696 | 2.49877 |
| 7.8085 | -606.69727 | -44.47668 | 0.76347 | 0.51669 | 2.44332 |
| 7.99423 | -606.69734 | -44.52461 | 0.76349 | 0.51654 | 2.42382 |
| 8.19028 | -606.6974 | -44.56157 | 0.76347 | 0.51641 | 2.38191 |
| 8.38725 | -606.69745 | -44.59154 | 0.76344 | 0.51623 | 2.34329 |
| 8.5808 | -606.69747 | -44.60572 | 0.76339 | 0.51617 | 2.30997 |
| 8.76877 | -606.69754 | -44.6472 | 0.76335 | 0.51603 | 2.29349 |
| 8.95512 | -606.69765 | -44.71477 | 0.76332 | 0.51591 | 2.23791 |
| 9.14626 | -606.69773 | -44.76438 | 0.76331 | 0.51574 | 2.22334 |
| 9.33524 | -606.69783 | -44.83157 | 0.7633 | 0.51563 | 2.16326 |
| 9.52606 | -606.69791 | -44.87963 | 0.7633 | 0.51543 | 2.16702 |
| 9.71373 | -606.69804 | -44.96093 | 0.76332 | 0.51532 | 2.10221 |
| 9.9052 | -606.69818 | -45.04797 | 0.7633 | 0.51513 | 2.09472 |
| 10.10355 | -606.69828 | -45.10993 | 0.76332 | 0.51493 | 2.07433 |
| 10.30209 | -606.69836 | -45.162 | 0.76335 | 0.51463 | 2.06031 |
| 10.49945 | -606.69841 | -45.19086 | 0.76334 | 0.51457 | 2.06266 |
| 10.6927 | -606.69842 | -45.19974 | 0.76331 | 0.51437 | 2.06073 |
| 10.87792 | -606.69847 | -45.23067 | 0.76335 | 0.51435 | 2.06107 |
| 11.0651 | -606.69852 | -45.26028 | 0.76325 | 0.51446 | 2.09079 |
| 11.25479 | -606.69853 | -45.2677 | 0.76335 | 0.51426 | 2.07473 |
| 11.44328 | -606.6985 | -45.25232 | 0.76338 | 0.51424 | 2.09232 |
| 11.62406 | -606.69857 | -45.295 | 0.76323 | 0.51448 | 2.11372 |
| 11.80802 | -606.69863 | -45.32885 | 0.76331 | 0.5144 | 2.11763 |
| 12.00736 | -606.69866 | -45.34922 | 0.76329 | 0.51444 | 2.12914 |
| 12.20624 | -606.69869 | -45.3714 | 0.76326 | 0.51447 | 2.1396 |
| 12.40509 | -606.69873 | -45.39448 | 0.76325 | 0.51447 | 2.14727 |
| 12.60379 | -606.69877 | -45.41841 | 0.76325 | 0.51445 | 2.15081 |
| 12.80221 | -606.69881 | -45.44423 | 0.76326 | 0.51441 | 2.15371 |
| 13.00026 | -606.69885 | -45.47108 | 0.7633 | 0.51432 | 2.15056 |
| 13.19479 | -606.69887 | -45.4833 | 0.7633 | 0.51429 | 2.16398 |
| 13.38267 | -606.69881 | -45.44706 | 0.76333 | 0.51425 | 2.1461 |
| 13.5626 | -606.69881 | -45.44648 | 0.76341 | 0.51412 | 2.13931 |
| 13.73237 | -606.699 | -45.56512 | 0.76342 | 0.51398 | 2.13738 |
| 13.92119 | -606.69904 | -45.58872 | 0.76348 | 0.51415 | 2.15998 |
| 14.10872 | -606.69909 | -45.62111 | 0.76343 | 0.51412 | 2.15975 |
| 14.30066 | -606.69913 | -45.64656 | 0.76347 | 0.51416 | 2.16247 |
| 14.4926 | -606.69916 | -45.66521 | 0.76346 | 0.51414 | 2.16802 |
| 14.68183 | -606.69918 | -45.67812 | 0.76352 | 0.51414 | 2.17147 |
| 14.86875 | -606.6992 | -45.68878 | 0.76347 | 0.51417 | 2.17768 |
| 15.05367 | -606.6992 | -45.69175 | 0.76363 | 0.51396 | 2.19453 |
| 15.23702 | -606.69922 | -45.69872 | 0.76359 | 0.51402 | 2.1839 |
| 15.41871 | -606.69921 | -45.69277 | 0.76367 | 0.51381 | 2.17751 |
| 15.58854 | -606.69928 | -45.7414 | 0.76366 | 0.51386 | 2.17635 |
| 15.77283 | -606.69928 | -45.74192 | 0.76371 | 0.51387 | 2.19834 |
| 15.95077 | -606.69929 | -45.74678 | 0.76371 | 0.51377 | 2.13766 |
| 16.13318 | -606.6993 | -45.74883 | 0.7638 | 0.51362 | 2.14525 |
| 16.31635 | -606.6993 | -45.74892 | 0.76375 | 0.51369 | 2.09941 |
| 16.49914 | -606.69926 | -45.72636 | 0.76384 | 0.51347 | 2.11296 |
| 16.67875 | -606.69922 | -45.70141 | 0.76388 | 0.51362 | 2.06986 |
| 16.8546 | -606.69925 | -45.71747 | 0.76385 | 0.51354 | 2.08609 |
| 17.03071 | -606.69927 | -45.73591 | 0.76392 | 0.51351 | 2.0446 |
| 17.21184 | -606.69926 | -45.72757 | 0.76399 | 0.51333 | 2.02705 |
| 17.38432 | -606.69932 | -45.76141 | 0.76399 | 0.51341 | 2.02364 |
| 17.58077 | -606.69932 | -45.76614 | 0.76406 | 0.51326 | 2.01054 |
| 17.77621 | -606.69933 | -45.76818 | 0.7641 | 0.51332 | 2.01775 |

aReferenced to -606.626389823 hartree.

**Table S4:** Data shown in Figures 3 and 4 for *cis* dicyanopropene.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Reaction Coordinate[bohr amu1/2]** | **E [hartree]** | **ΔE [kcal mol-1]a** | **IBO Changes for π-Bond Olefin** | **IBO Changes for Lone Pair on Oxygen** | **Dipole Moment****[debye]** |
| -16.09258 | -606.62463 | 0.51047 | 0 | 0 | 10.5509 |
| -15.89501 | -606.62463 | 0.51056 | 4.4E-5 | 6.4E-5 | 10.55121 |
| -15.70956 | -606.62463 | 0.51022 | 6.3E-5 | 4.9E-5 | 10.55089 |
| -15.51574 | -606.62462 | 0.51363 | 3.1E-4 | 5.7E-5 | 10.55334 |
| -15.33522 | -606.62459 | 0.53827 | 9.49E-4 | 5.9E-5 | 10.57581 |
| -15.15635 | -606.62459 | 0.53841 | 5.52E-4 | 7.5E-5 | 10.53643 |
| -14.97923 | -606.62458 | 0.54129 | 6.2E-5 | 4.4E-5 | 10.55825 |
| -14.8011 | -606.62459 | 0.53651 | 2.14E-4 | 8.9E-5 | 10.5511 |
| -14.61149 | -606.6246 | 0.53001 | 8.94E-4 | 9.1E-5 | 10.54518 |
| -14.4137 | -606.62458 | 0.54238 | 0.00115 | 1.46E-4 | 10.53825 |
| -14.21634 | -606.62454 | 0.56445 | 0.00174 | 1.48E-4 | 10.52973 |
| -14.01901 | -606.62451 | 0.58829 | 0.00214 | 1.92E-4 | 10.51416 |
| -13.82998 | -606.62444 | 0.62695 | 0.00248 | 1.79E-4 | 10.4966 |
| -13.64808 | -606.62439 | 0.66185 | 0.00375 | 2.49E-4 | 10.47971 |
| -13.46884 | -606.62429 | 0.72167 | 0.00299 | 1.63E-4 | 10.52526 |
| -13.28508 | -606.6243 | 0.71876 | 0.00424 | 3.56E-4 | 10.44902 |
| -13.09617 | -606.62427 | 0.73535 | 0.00417 | 3.25E-4 | 10.46469 |
| -12.90627 | -606.62421 | 0.77436 | 0.00495 | 3.57E-4 | 10.44376 |
| -12.71418 | -606.62414 | 0.81565 | 0.00521 | 3.92E-4 | 10.42202 |
| -12.52126 | -606.62408 | 0.85399 | 0.00585 | 4.31E-4 | 10.41577 |
| -12.32342 | -606.62403 | 0.88569 | 0.00594 | 4.34E-4 | 10.38934 |
| -12.1256 | -606.62397 | 0.92632 | 0.00638 | 4.41E-4 | 10.37048 |
| -11.9262 | -606.6239 | 0.96867 | 0.00667 | 4.61E-4 | 10.34467 |
| -11.72737 | -606.62383 | 1.01253 | 0.00713 | 4.7E-4 | 10.32342 |
| -11.53958 | -606.62373 | 1.07496 | 0.00741 | 5E-4 | 10.28419 |
| -11.35146 | -606.62368 | 1.10961 | 0.00779 | 4.99E-4 | 10.28868 |
| -11.15541 | -606.62364 | 1.13087 | 0.00805 | 5.3E-4 | 10.24925 |
| -10.95727 | -606.62358 | 1.16672 | 0.00839 | 5.33E-4 | 10.22543 |
| -10.75797 | -606.62352 | 1.20758 | 0.00864 | 5.33E-4 | 10.19211 |
| -10.55882 | -606.62345 | 1.24926 | 0.00885 | 5.41E-4 | 10.16188 |
| -10.35936 | -606.62339 | 1.29121 | 0.00906 | 5.21E-4 | 10.1287 |
| -10.15986 | -606.62332 | 1.33321 | 0.0092 | 5.08E-4 | 10.09526 |
| -9.96039 | -606.62326 | 1.37319 | 0.00933 | 4.69E-4 | 10.0615 |
| -9.76082 | -606.6232 | 1.40958 | 0.00939 | 4.53E-4 | 10.02742 |
| -9.5674 | -606.62313 | 1.44858 | 0.00961 | 4.8E-4 | 9.97865 |
| -9.37874 | -606.62308 | 1.48224 | 0.00933 | 4.27E-4 | 9.97712 |
| -9.18973 | -606.62304 | 1.50899 | 0.00976 | 4.83E-4 | 9.91756 |
| -9.00002 | -606.623 | 1.53157 | 0.00935 | 4.68E-4 | 9.91509 |
| -8.81012 | -606.62296 | 1.55568 | 0.0098 | 4.58E-4 | 9.86804 |
| -8.62171 | -606.62292 | 1.58521 | 0.00949 | 4.49E-4 | 9.84212 |
| -8.4307 | -606.62289 | 1.59984 | 0.01005 | 4.54E-4 | 9.80016 |
| -8.23352 | -606.62288 | 1.61119 | 0.00986 | 4.3E-4 | 9.76553 |
| -8.03601 | -606.62284 | 1.63183 | 0.01002 | 4.21E-4 | 9.72329 |
| -7.83718 | -606.62281 | 1.65427 | 0.00999 | 4.19E-4 | 9.68155 |
| -7.64777 | -606.62275 | 1.6893 | 0.00994 | 4.02E-4 | 9.64108 |
| -7.4588 | -606.62272 | 1.71169 | 0.01005 | 4.32E-4 | 9.6107 |
| -7.27344 | -606.62266 | 1.74473 | 0.01006 | 4.07E-4 | 9.57363 |
| -7.09516 | -606.62258 | 1.79969 | 0.00998 | 4.69E-4 | 9.52887 |
| -6.91414 | -606.62257 | 1.80507 | 0.00964 | 2.69E-4 | 9.53068 |
| -6.72861 | -606.62259 | 1.79364 | 0.00989 | 4.53E-4 | 9.47216 |
| -6.54714 | -606.62252 | 1.83585 | 0.00918 | 2.33E-4 | 9.46068 |
| -6.35922 | -606.62253 | 1.82606 | 0.01018 | 4.32E-4 | 9.40177 |
| -6.16326 | -606.62251 | 1.84139 | 0.00948 | 4.1E-4 | 9.38626 |
| -5.96787 | -606.62246 | 1.8694 | 0.00965 | 4.02E-4 | 9.34964 |
| -5.78088 | -606.62238 | 1.92367 | 0.00904 | 6.29E-4 | 9.3434 |
| -5.59458 | -606.62236 | 1.93423 | 0.00911 | 3.71E-4 | 9.31138 |
| -5.4104 | -606.62231 | 1.96872 | 0.00873 | 4.43E-4 | 9.29919 |
| -5.23349 | -606.62221 | 2.02608 | 0.00838 | 3.68E-4 | 9.2928 |
| -5.05565 | -606.62219 | 2.03977 | 0.00857 | 4.63E-4 | 9.2602 |
| -4.87488 | -606.62219 | 2.04186 | 0.00748 | 2.97E-4 | 9.25675 |
| -4.69346 | -606.62218 | 2.04507 | 0.00821 | 4.03E-4 | 9.22811 |
| -4.50298 | -606.6222 | 2.03756 | 0.00719 | 4.02E-4 | 9.21964 |
| -4.30885 | -606.62217 | 2.05391 | 0.00702 | 3.85E-4 | 9.20892 |
| -4.11044 | -606.62213 | 2.07665 | 0.00635 | 3.78E-4 | 9.20633 |
| -3.93393 | -606.62199 | 2.16516 | 0.00577 | 3.4E-4 | 9.20669 |
| -3.73812 | -606.62205 | 2.13118 | 0.00526 | 3.64E-4 | 9.20729 |
| -3.54656 | -606.62201 | 2.15253 | 0.00502 | 4.38E-4 | 9.19735 |
| -3.35008 | -606.62195 | 2.19203 | 0.00492 | 5.84E-4 | 9.17992 |
| -3.15122 | -606.62183 | 2.26484 | 0.00477 | 8.02E-4 | 9.16205 |
| -2.95169 | -606.62165 | 2.38036 | 0.00474 | 0.00108 | 9.14269 |
| -2.75204 | -606.62139 | 2.54529 | 0.00472 | 0.00142 | 9.12201 |
| -2.55234 | -606.62103 | 2.7694 | 0.00463 | 0.00182 | 9.10205 |
| -2.3528 | -606.62056 | 3.06643 | 0.00457 | 0.0023 | 9.08958 |
| -2.15323 | -606.61993 | 3.4576 | 0.00438 | 0.00294 | 9.09092 |
| -1.96013 | -606.61901 | 4.03388 | 0.00457 | 0.00356 | 9.12467 |
| -1.77211 | -606.61775 | 4.82789 | 0.00469 | 0.00455 | 9.17269 |
| -1.58428 | -606.61608 | 5.87638 | 0.00512 | 0.00564 | 9.28262 |
| -1.3899 | -606.61446 | 6.88989 | 0.00605 | 0.00655 | 9.30188 |
| -1.19277 | -606.61175 | 8.59426 | 0.00653 | 0.00893 | 9.50738 |
| -0.99688 | -606.60786 | 11.03125 | 0.00964 | 0.01029 | 9.64147 |
| -0.79867 | -606.60301 | 14.07675 | 0.00918 | 0.01441 | 9.93493 |
| -0.5998 | -606.59583 | 18.5853 | 0.01826 | 0.01877 | 10.09008 |
| -0.39991 | -606.58206 | 27.22414 | 0.04823 | 0.0271 | 9.67124 |
| -0.2 | -606.56723 | 36.53159 | 0.12202 | 0.04661 | 8.68699 |
| 9E-5 | -606.56096 | 40.46577 | 0.27834 | 0.08252 | 7.72514 |
| 0.2 | -606.56773 | 36.21581 | 0.44976 | 0.13446 | 7.69452 |
| 0.39992 | -606.58608 | 24.70375 | 0.57164 | 0.22277 | 8.23534 |
| 0.59984 | -606.6097 | 9.88052 | 0.74442 | 0.4149 | 8.40075 |
| 0.79974 | -606.63259 | -4.48533 | 0.76953 | 0.46218 | 8.23746 |
| 0.9994 | -606.65201 | -16.66889 | 0.77152 | 0.48919 | 8.12331 |
| 1.19903 | -606.66687 | -25.99545 | 0.76855 | 0.5063 | 8.27224 |
| 1.39811 | -606.67369 | -30.278 | 0.76564 | 0.51515 | 8.54025 |
| 1.59243 | -606.67797 | -32.96086 | 0.76653 | 0.51532 | 8.58029 |
| 1.78633 | -606.68104 | -34.88635 | 0.76546 | 0.51357 | 8.7827 |
| 1.97835 | -606.68395 | -36.7128 | 0.76478 | 0.51829 | 8.8723 |
| 2.17338 | -606.68622 | -38.14091 | 0.76437 | 0.51818 | 8.94009 |
| 2.37297 | -606.68793 | -39.21018 | 0.76412 | 0.51861 | 8.97684 |
| 2.57268 | -606.68932 | -40.08603 | 0.76401 | 0.51887 | 8.99907 |
| 2.77252 | -606.69049 | -40.81809 | 0.76401 | 0.51897 | 9.01236 |
| 2.97241 | -606.69148 | -41.43745 | 0.76406 | 0.51896 | 9.02173 |
| 3.17233 | -606.69233 | -41.96991 | 0.76414 | 0.51888 | 9.03154 |
| 3.37225 | -606.69307 | -42.43377 | 0.76424 | 0.51879 | 9.04657 |
| 3.57217 | -606.6937 | -42.83448 | 0.76426 | 0.51885 | 9.06619 |
| 3.77209 | -606.69425 | -43.1751 | 0.7643 | 0.51883 | 9.08979 |
| 3.972 | -606.6947 | -43.45721 | 0.76437 | 0.51878 | 9.11409 |
| 4.17185 | -606.69506 | -43.68421 | 0.76445 | 0.51868 | 9.13677 |
| 4.37175 | -606.69534 | -43.86132 | 0.76458 | 0.51853 | 9.16047 |
| 4.5715 | -606.69556 | -43.99911 | 0.76462 | 0.51852 | 9.18402 |
| 4.7711 | -606.69573 | -44.10839 | 0.7647 | 0.51845 | 9.20765 |
| 4.9706 | -606.69587 | -44.19296 | 0.76483 | 0.51834 | 9.23126 |
| 5.16963 | -606.69596 | -44.25017 | 0.7649 | 0.51822 | 9.2492 |
| 5.3674 | -606.69602 | -44.28661 | 0.76494 | 0.51809 | 9.26207 |
| 5.56404 | -606.69606 | -44.31023 | 0.76494 | 0.51802 | 9.26813 |
| 5.75863 | -606.69609 | -44.32877 | 0.76496 | 0.51802 | 9.275 |
| 5.94922 | -606.69608 | -44.32401 | 0.76493 | 0.51795 | 9.25453 |
| 6.13656 | -606.69617 | -44.38138 | 0.76498 | 0.51793 | 9.25171 |
| 6.33606 | -606.6962 | -44.40345 | 0.76495 | 0.51791 | 9.24125 |
| 6.53376 | -606.69623 | -44.42228 | 0.7649 | 0.51788 | 9.22497 |
| 6.73207 | -606.69626 | -44.43833 | 0.76485 | 0.51788 | 9.20484 |
| 6.93023 | -606.69628 | -44.45231 | 0.76484 | 0.51782 | 9.18622 |
| 7.12728 | -606.69629 | -44.45949 | 0.76472 | 0.518 | 9.16541 |
| 7.3194 | -606.69629 | -44.45747 | 0.76488 | 0.51768 | 9.16619 |
| 7.50191 | -606.69627 | -44.44497 | 0.76475 | 0.51799 | 9.12506 |
| 7.68269 | -606.69614 | -44.3628 | 0.76454 | 0.5178 | 9.14604 |
| 7.86031 | -606.69615 | -44.36711 | 0.7648 | 0.51776 | 9.09629 |
| 8.03246 | -606.69632 | -44.47582 | 0.7647 | 0.51787 | 9.07723 |
| 8.23064 | -606.69632 | -44.47752 | 0.76474 | 0.5177 | 9.06365 |

aReferenced to -606.625443349 hartree.

**Table S5:** Data shown in Figures 3 and 4 for cyanoethene.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Reaction Coordinate[bohr amu1/2]** | **E [hartree]** | **ΔE [kcal mol-1]a** | **IBO Changes for π-Bond Olefin** | **IBO Changes for Lone Pair on Oxygen** | **Dipole Moment****[debye]** |
| -9.77059 | -475.06128 | -0.00412 | 0 | 0 | 7.24273 |
| -9.67136 | -475.06128 | -0.00306 | 2.9E-5 | 1E-6 | 7.24235 |
| -9.57241 | -475.06128 | -0.00155 | 5.7E-5 | 4.54E-4 | 7.24195 |
| -9.47435 | -475.06127 | -2.9493E-5 | 1.2E-4 | 4.02E-4 | 7.23818 |
| -9.37568 | -475.06127 | 0.00193 | 1.85E-4 | 3.51E-4 | 7.2342 |
| -9.2767 | -475.06127 | 0.00452 | 2.68E-4 | 0.00184 | 7.2276 |
| -9.1776 | -475.06126 | 0.00794 | 3.7E-4 | 0.00189 | 7.21922 |
| -9.07793 | -475.06125 | 0.01221 | 4.69E-4 | 0.00196 | 7.20869 |
| -8.97887 | -475.06125 | 0.0177 | 5.49E-4 | 0.00202 | 7.19793 |
| -8.87956 | -475.06124 | 0.02389 | 6.44E-4 | 0.00208 | 7.18355 |
| -8.78016 | -475.06122 | 0.031 | 7.2E-4 | 0.00213 | 7.16724 |
| -8.68067 | -475.06121 | 0.03904 | 7.85E-4 | 0.00217 | 7.15071 |
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| 13.96184 | -475.14412 | -51.98558 | 0.8205 | 0.53346 | 3.83535 |
| 14.06148 | -475.14415 | -52.0076 | 0.82052 | 0.53343 | 3.82036 |
| 14.16117 | -475.14419 | -52.03003 | 0.82055 | 0.53339 | 3.80653 |
| 14.26087 | -475.14422 | -52.05268 | 0.82056 | 0.53335 | 3.79372 |
| 14.36063 | -475.14426 | -52.07532 | 0.82058 | 0.5333 | 3.78219 |
| 14.46033 | -475.1443 | -52.09814 | 0.82059 | 0.53325 | 3.77237 |
| 14.56023 | -475.14433 | -52.1209 | 0.8206 | 0.5332 | 3.76532 |
| 14.65994 | -475.14437 | -52.1441 | 0.82061 | 0.53315 | 3.76037 |
| 14.75969 | -475.14441 | -52.16794 | 0.82062 | 0.53311 | 3.75736 |
| 14.85941 | -475.14445 | -52.19256 | 0.82062 | 0.53306 | 3.75571 |
| 14.95916 | -475.14449 | -52.21793 | 0.82063 | 0.53301 | 3.75529 |
| 15.05887 | -475.14453 | -52.24409 | 0.82063 | 0.53296 | 3.75543 |
| 15.15877 | -475.14457 | -52.27034 | 0.82063 | 0.53288 | 3.75747 |
| 15.25848 | -475.14461 | -52.29688 | 0.82062 | 0.53283 | 3.76047 |
| 15.35823 | -475.14466 | -52.32376 | 0.82061 | 0.53277 | 3.76539 |
| 15.45798 | -475.1447 | -52.35121 | 0.8206 | 0.5327 | 3.77191 |
| 15.55777 | -475.14475 | -52.37925 | 0.8206 | 0.53263 | 3.77994 |
| 15.65754 | -475.14479 | -52.40792 | 0.82058 | 0.53255 | 3.78843 |
| 15.75744 | -475.14484 | -52.43687 | 0.82056 | 0.53247 | 3.79878 |
| 15.85716 | -475.14488 | -52.46652 | 0.82054 | 0.53238 | 3.80986 |
| 15.95694 | -475.14493 | -52.49723 | 0.82052 | 0.53229 | 3.82277 |
| 16.05671 | -475.14498 | -52.52944 | 0.8205 | 0.53221 | 3.83757 |
| 16.15653 | -475.14504 | -52.56297 | 0.82047 | 0.53212 | 3.85418 |
| 16.25635 | -475.14509 | -52.59748 | 0.82044 | 0.53202 | 3.8719 |
| 16.35627 | -475.14515 | -52.63234 | 0.82041 | 0.53193 | 3.89167 |
| 16.45608 | -475.1452 | -52.66774 | 0.82037 | 0.53183 | 3.91229 |
| 16.55591 | -475.14526 | -52.70366 | 0.82033 | 0.53173 | 3.93379 |
| 16.65574 | -475.14532 | -52.74045 | 0.82029 | 0.53162 | 3.95621 |
| 16.75557 | -475.14538 | -52.77825 | 0.82024 | 0.53151 | 3.97973 |
| 16.85539 | -475.14544 | -52.81746 | 0.82019 | 0.53139 | 4.00474 |
| 16.95533 | -475.14551 | -52.85837 | 0.82014 | 0.53127 | 4.03233 |
| 17.05516 | -475.14558 | -52.90163 | 0.82008 | 0.53114 | 4.06085 |
| 17.15501 | -475.14565 | -52.94659 | 0.82002 | 0.531 | 4.0898 |
| 17.25486 | -475.14572 | -52.99207 | 0.81996 | 0.53086 | 4.11823 |
| 17.35472 | -475.14579 | -53.03759 | 0.8199 | 0.53071 | 4.14713 |
| 17.45457 | -475.14587 | -53.08369 | 0.81982 | 0.53054 | 4.17741 |
| 17.55452 | -475.14594 | -53.13042 | 0.81975 | 0.53037 | 4.20954 |
| 17.65437 | -475.14602 | -53.17668 | 0.81968 | 0.53019 | 4.24113 |
| 17.75422 | -475.14609 | -53.22073 | 0.81961 | 0.53001 | 4.27094 |
| 17.85407 | -475.14615 | -53.2627 | 0.81953 | 0.52982 | 4.30176 |
| 17.95393 | -475.14622 | -53.30234 | 0.81946 | 0.52963 | 4.33261 |
| 18.05376 | -475.14628 | -53.34113 | 0.81937 | 0.52943 | 4.36579 |
| 18.15371 | -475.14634 | -53.37855 | 0.81928 | 0.52923 | 4.3997 |
| 18.25354 | -475.14639 | -53.41348 | 0.8192 | 0.52903 | 4.43061 |
| 18.35337 | -475.14644 | -53.4452 | 0.81912 | 0.52884 | 4.46008 |
| 18.45314 | -475.14649 | -53.47297 | 0.81903 | 0.52867 | 4.48608 |
| 18.55283 | -475.14653 | -53.4971 | 0.81895 | 0.52851 | 4.50926 |
| 18.65241 | -475.14656 | -53.51825 | 0.81888 | 0.52837 | 4.52899 |
| 18.75222 | -475.14659 | -53.53609 | 0.81882 | 0.52826 | 4.54348 |
| 18.85155 | -475.14661 | -53.55143 | 0.81876 | 0.52817 | 4.55152 |
| 18.95067 | -475.14663 | -53.56473 | 0.81872 | 0.52811 | 4.55558 |
| 19.04962 | -475.14665 | -53.57642 | 0.81869 | 0.52806 | 4.55728 |
| 19.14854 | -475.14667 | -53.58658 | 0.81865 | 0.52801 | 4.5572 |
| 19.24741 | -475.14668 | -53.59582 | 0.81864 | 0.528 | 4.55651 |
| 19.34679 | -475.1467 | -53.60287 | 0.81861 | 0.52796 | 4.55928 |
| 19.44514 | -475.1467 | -53.60903 | 0.81858 | 0.52791 | 4.56434 |
| 19.54339 | -475.14671 | -53.61397 | 0.81854 | 0.52786 | 4.57235 |
| 19.64138 | -475.14672 | -53.61803 | 0.8185 | 0.5278 | 4.58412 |
| 19.73904 | -475.14672 | -53.62121 | 0.81847 | 0.52775 | 4.59936 |
| 19.83621 | -475.14673 | -53.62371 | 0.81846 | 0.52774 | 4.61437 |

aReferenced to -475.06127353 hartree.

**Table S6:** Data shown in Figures 3 and 4 for prop-1-ene.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Reaction Coordinate[bohr amu1/2]** | **E [hartree]** | **ΔE [kcal mol-1]a** | **IBO Changes for π-Bond Olefin** | **IBO Changes for Lone Pair on Oxygen** | **Dipole Moment****[debye]** |
| -5.98506 | -422.12048 | 0.36216 | 0 | 0 | 2.33573 |
| -5.88684 | -422.12048 | 0.36276 | 1.2E-5 | 6E-6 | 2.33191 |
| -5.78897 | -422.12048 | 0.3636 | 4.9E-5 | 4E-6 | 2.32672 |
| -5.69041 | -422.12048 | 0.3648 | 1.17E-4 | 1.2E-5 | 2.32082 |
| -5.59078 | -422.12047 | 0.36662 | 2.03E-4 | 1.5E-5 | 2.31512 |
| -5.49144 | -422.12047 | 0.36939 | 2.77E-4 | 1.9E-5 | 2.31005 |
| -5.39215 | -422.12046 | 0.37292 | 3.63E-4 | 2.6E-5 | 2.30471 |
| -5.2928 | -422.12046 | 0.37719 | 4.34E-4 | 3.2E-5 | 2.30021 |
| -5.19348 | -422.12045 | 0.38209 | 5.05E-4 | 3.6E-5 | 2.2963 |
| -5.09371 | -422.12044 | 0.38728 | 5.7E-4 | 3.9E-5 | 2.293 |
| -4.99444 | -422.12043 | 0.39277 | 6.36E-4 | 4.4E-5 | 2.29037 |
| -4.89514 | -422.12042 | 0.3982 | 7.45E-4 | 5.1E-5 | 2.28758 |
| -4.79572 | -422.12041 | 0.4041 | 8.74E-4 | 5.9E-5 | 2.28559 |
| -4.69615 | -422.1204 | 0.41098 | 0.00102 | 6.7E-5 | 2.28461 |
| -4.59636 | -422.12039 | 0.41931 | 0.0012 | 7.4E-5 | 2.28466 |
| -4.49663 | -422.12037 | 0.42966 | 0.00139 | 8.1E-5 | 2.28567 |
| -4.39679 | -422.12035 | 0.44266 | 0.0016 | 8.4E-5 | 2.2877 |
| -4.29688 | -422.12032 | 0.45899 | 0.00182 | 8.6E-5 | 2.29027 |
| -4.19695 | -422.12029 | 0.47892 | 0.00205 | 8.6E-5 | 2.2937 |
| -4.09699 | -422.12026 | 0.50239 | 0.00229 | 8.5E-5 | 2.29775 |
| -3.99704 | -422.12021 | 0.52932 | 0.00252 | 8.3E-5 | 2.30236 |
| -3.89708 | -422.12016 | 0.55956 | 0.00275 | 7.9E-5 | 2.30741 |
| -3.79713 | -422.12011 | 0.59287 | 0.00299 | 7.3E-5 | 2.3128 |
| -3.69717 | -422.12005 | 0.62898 | 0.00321 | 6.7E-5 | 2.3182 |
| -3.5972 | -422.11999 | 0.66758 | 0.00344 | 5.8E-5 | 2.32339 |
| -3.49725 | -422.11993 | 0.70858 | 0.00365 | 5.2E-5 | 2.32848 |
| -3.39731 | -422.11986 | 0.75202 | 0.00385 | 4.9E-5 | 2.3333 |
| -3.29738 | -422.11978 | 0.79821 | 0.00403 | 5.9E-5 | 2.33771 |
| -3.19746 | -422.11971 | 0.84766 | 0.00419 | 8.7E-5 | 2.34193 |
| -3.09754 | -422.11962 | 0.90107 | 0.00434 | 1.33E-4 | 2.34592 |
| -2.99764 | -422.11953 | 0.95936 | 0.00446 | 1.95E-4 | 2.34977 |
| -2.89774 | -422.11943 | 1.0236 | 0.00456 | 2.68E-4 | 2.35333 |
| -2.79784 | -422.11931 | 1.09547 | 0.00465 | 3.68E-4 | 2.35702 |
| -2.69794 | -422.11918 | 1.17701 | 0.00472 | 4.86E-4 | 2.36093 |
| -2.59801 | -422.11903 | 1.27047 | 0.00479 | 6.18E-4 | 2.36542 |
| -2.49807 | -422.11886 | 1.37843 | 0.00486 | 7.68E-4 | 2.37053 |
| -2.39812 | -422.11866 | 1.50384 | 0.00495 | 9.36E-4 | 2.37703 |
| -2.29817 | -422.11843 | 1.64971 | 0.00506 | 0.00112 | 2.38544 |
| -2.1982 | -422.11816 | 1.81851 | 0.0052 | 0.00132 | 2.396 |
| -2.09823 | -422.11785 | 2.01223 | 0.00537 | 0.00153 | 2.40917 |
| -1.99827 | -422.1175 | 2.23303 | 0.00558 | 0.00177 | 2.42538 |
| -1.8983 | -422.1171 | 2.48346 | 0.00583 | 0.00202 | 2.44535 |
| -1.79834 | -422.11665 | 2.76729 | 0.00612 | 0.00229 | 2.46974 |
| -1.69838 | -422.11613 | 3.08956 | 0.00646 | 0.00259 | 2.49913 |
| -1.59843 | -422.11555 | 3.45629 | 0.00683 | 0.00291 | 2.53369 |
| -1.49848 | -422.11488 | 3.87466 | 0.00724 | 0.00326 | 2.57257 |
| -1.39853 | -422.11412 | 4.35318 | 0.00768 | 0.00363 | 2.61415 |
| -1.29857 | -422.11325 | 4.90103 | 0.00815 | 0.00404 | 2.65861 |
| -1.19862 | -422.11225 | 5.5282 | 0.00866 | 0.00448 | 2.70591 |
| -1.09866 | -422.1111 | 6.24653 | 0.00921 | 0.00497 | 2.75477 |
| -0.99874 | -422.10979 | 7.07099 | 0.00989 | 0.00549 | 2.80036 |
| -0.89883 | -422.10828 | 8.02003 | 0.01058 | 0.00619 | 2.84994 |
| -0.79896 | -422.10651 | 9.13064 | 0.01177 | 0.00695 | 2.87606 |
| -0.69915 | -422.10438 | 10.46478 | 0.01318 | 0.00781 | 2.89974 |
| -0.5995 | -422.10169 | 12.15528 | 0.0165 | 0.009 | 2.84735 |
| -0.49986 | -422.09781 | 14.58622 | 0.02434 | 0.01072 | 2.61556 |
| -0.3999 | -422.09234 | 18.01996 | 0.03961 | 0.01296 | 2.10608 |
| -0.29993 | -422.08604 | 21.9718 | 0.0644 | 0.01654 | 1.31514 |
| -0.19996 | -422.08025 | 25.60403 | 0.10206 | 0.0221 | 0.59041 |
| -0.1 | -422.07623 | 28.12761 | 0.15739 | 0.0303 | 1.66644 |
| 0 | -422.07478 | 29.03669 | 0.23736 | 0.04166 | 3.33241 |
| 0.1 | -422.0763 | 28.08446 | 0.33682 | 0.0565 | 5.10402 |
| 0.19996 | -422.08081 | 25.25231 | 0.42834 | 0.07506 | 6.8052 |
| 0.29993 | -422.08807 | 20.70224 | 0.49849 | 0.0975 | 8.27118 |
| 0.39991 | -422.09744 | 14.81989 | 0.55196 | 0.12415 | 9.37126 |
| 0.49988 | -422.10812 | 8.12039 | 0.59758 | 0.1581 | 10.06743 |
| 0.59986 | -422.11928 | 1.11212 | 0.65398 | 0.21734 | 10.40763 |
| 0.69983 | -422.13016 | -5.71347 | 0.73879 | 0.31355 | 10.46871 |
| 0.79981 | -422.14004 | -11.91487 | 0.78567 | 0.36939 | 10.32015 |
| 0.89975 | -422.14838 | -17.14432 | 0.80364 | 0.39781 | 10.02135 |
| 0.99962 | -422.15487 | -21.21915 | 0.81165 | 0.41777 | 9.62525 |
| 1.09927 | -422.15972 | -24.26276 | 0.81561 | 0.43315 | 9.1936 |
| 1.19893 | -422.16353 | -26.65294 | 0.81731 | 0.44452 | 8.75635 |
| 1.29869 | -422.16695 | -28.8015 | 0.81717 | 0.45184 | 8.31878 |
| 1.39857 | -422.17041 | -30.97282 | 0.81566 | 0.45773 | 7.83096 |
| 1.49851 | -422.17415 | -33.31626 | 0.81331 | 0.46364 | 7.26942 |
| 1.59843 | -422.17836 | -35.95597 | 0.81023 | 0.47001 | 6.61521 |
| 1.69838 | -422.18308 | -38.91906 | 0.80693 | 0.47631 | 5.93054 |
| 1.79834 | -422.18801 | -42.01499 | 0.80364 | 0.48235 | 5.26194 |
| 1.8983 | -422.1925 | -44.83299 | 0.80062 | 0.48782 | 4.66439 |
| 1.9982 | -422.19595 | -46.99397 | 0.79816 | 0.49226 | 4.20861 |
| 2.09793 | -422.19849 | -48.59271 | 0.79678 | 0.4947 | 4.01333 |
| 2.19776 | -422.2005 | -49.85473 | 0.79594 | 0.49607 | 3.92471 |
| 2.29762 | -422.20215 | -50.88865 | 0.79535 | 0.497 | 3.88073 |
| 2.39753 | -422.20353 | -51.75313 | 0.79487 | 0.49775 | 3.84679 |
| 2.49744 | -422.20469 | -52.48383 | 0.79452 | 0.49827 | 3.83185 |
| 2.59735 | -422.20569 | -53.10624 | 0.79425 | 0.49868 | 3.81793 |
| 2.69727 | -422.20654 | -53.6403 | 0.79408 | 0.49894 | 3.81536 |
| 2.79719 | -422.20728 | -54.10371 | 0.79398 | 0.49907 | 3.81971 |
| 2.89712 | -422.20793 | -54.5112 | 0.79395 | 0.49911 | 3.83106 |
| 2.99707 | -422.2085 | -54.87407 | 0.79397 | 0.49906 | 3.84778 |
| 3.09702 | -422.20903 | -55.20169 | 0.79402 | 0.49897 | 3.86766 |
| 3.19699 | -422.2095 | -55.49984 | 0.7941 | 0.49885 | 3.89064 |
| 3.29696 | -422.20993 | -55.77051 | 0.79422 | 0.4986 | 3.91412 |
| 3.39694 | -422.21032 | -56.01461 | 0.7943 | 0.49848 | 3.93785 |
| 3.49692 | -422.21067 | -56.23425 | 0.79437 | 0.49837 | 3.96123 |
| 3.5969 | -422.21099 | -56.4317 | 0.79443 | 0.49829 | 3.98377 |
| 3.69687 | -422.21127 | -56.60792 | 0.79444 | 0.49836 | 4.00534 |
| 3.79685 | -422.21152 | -56.76379 | 0.79447 | 0.49832 | 4.02444 |
| 3.89682 | -422.21173 | -56.90014 | 0.79449 | 0.49831 | 4.0419 |
| 3.99678 | -422.21192 | -57.01873 | 0.7945 | 0.49832 | 4.05885 |
| 4.09673 | -422.21209 | -57.12228 | 0.79449 | 0.49835 | 4.07606 |
| 4.19669 | -422.21223 | -57.21219 | 0.79448 | 0.49838 | 4.09485 |
| 4.29663 | -422.21235 | -57.28945 | 0.79446 | 0.49841 | 4.1154 |
| 4.39655 | -422.21246 | -57.35551 | 0.79445 | 0.49843 | 4.139 |
| 4.49646 | -422.21255 | -57.41271 | 0.79444 | 0.49844 | 4.16599 |
| 4.59635 | -422.21263 | -57.46257 | 0.79444 | 0.49845 | 4.1957 |
| 4.69627 | -422.2127 | -57.50613 | 0.79444 | 0.49844 | 4.22754 |
| 4.79613 | -422.21276 | -57.54471 | 0.79443 | 0.49844 | 4.25898 |
| 4.89597 | -422.21281 | -57.57929 | 0.7944 | 0.49845 | 4.28981 |
| 4.99577 | -422.21287 | -57.61095 | 0.79438 | 0.49846 | 4.32013 |
| 5.09556 | -422.21291 | -57.64089 | 0.79434 | 0.49848 | 4.34894 |
| 5.19548 | -422.21296 | -57.66963 | 0.79432 | 0.49848 | 4.37873 |
| 5.29531 | -422.213 | -57.69759 | 0.7943 | 0.49847 | 4.4074 |
| 5.39513 | -422.21305 | -57.72481 | 0.79429 | 0.49846 | 4.43566 |
| 5.49496 | -422.21309 | -57.75126 | 0.79428 | 0.49844 | 4.46368 |
| 5.59479 | -422.21313 | -57.77693 | 0.79427 | 0.49842 | 4.49014 |
| 5.69473 | -422.21317 | -57.80154 | 0.79427 | 0.49838 | 4.518 |
| 5.79454 | -422.21321 | -57.82514 | 0.79427 | 0.49835 | 4.54477 |
| 5.89435 | -422.21324 | -57.84764 | 0.79427 | 0.49832 | 4.57075 |
| 5.99415 | -422.21328 | -57.86904 | 0.79427 | 0.4983 | 4.59613 |
| 6.09396 | -422.21331 | -57.88943 | 0.79426 | 0.49829 | 4.61981 |
| 6.19388 | -422.21334 | -57.90875 | 0.79426 | 0.49826 | 4.64461 |
| 6.29366 | -422.21337 | -57.92729 | 0.79425 | 0.49824 | 4.66834 |
| 6.39344 | -422.2134 | -57.94511 | 0.79424 | 0.49823 | 4.6913 |
| 6.49321 | -422.21343 | -57.96228 | 0.79423 | 0.49823 | 4.71346 |
| 6.593 | -422.21345 | -57.97888 | 0.79422 | 0.49824 | 4.73381 |
| 6.69292 | -422.21348 | -57.99473 | 0.79421 | 0.49823 | 4.75492 |
| 6.79269 | -422.2135 | -58.00995 | 0.79421 | 0.49822 | 4.77512 |
| 6.89246 | -422.21352 | -58.02446 | 0.79424 | 0.49809 | 4.79464 |
| 6.9922 | -422.21355 | -58.03822 | 0.79424 | 0.49807 | 4.8135 |
| 7.09193 | -422.21357 | -58.0512 | 0.79424 | 0.49806 | 4.83043 |
| 7.19185 | -422.21359 | -58.06313 | 0.7942 | 0.49816 | 4.84815 |
| 7.29157 | -422.2136 | -58.07405 | 0.7942 | 0.49813 | 4.86517 |
| 7.39128 | -422.21362 | -58.08381 | 0.7942 | 0.49809 | 4.88127 |
| 7.49096 | -422.21363 | -58.09229 | 0.79425 | 0.49793 | 4.89657 |
| 7.5906 | -422.21364 | -58.09942 | 0.79424 | 0.4979 | 4.9102 |
| 7.69045 | -422.21365 | -58.10501 | 0.7942 | 0.498 | 4.92428 |
| 7.78998 | -422.21366 | -58.10932 | 0.79424 | 0.49784 | 4.93685 |
| 7.88943 | -422.21366 | -58.11262 | 0.79424 | 0.49781 | 4.94704 |
| 7.98881 | -422.21367 | -58.11517 | 0.79424 | 0.49779 | 4.95468 |
| 8.08802 | -422.21367 | -58.11717 | 0.79419 | 0.49791 | 4.95923 |

aReferenced to -422.121056397 hartree.

**Table S7:** Data shown in Figures 3 and 4 for hydroxyethene.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Reaction Coordinate[bohr amu1/2]** | **E [hartree]** | **ΔE [kcal mol-1]a** | **IBO Changes for π-Bond Olefin** | **IBO Changes for Lone Pair on Oxygen** | **Dipole Moment****[debye]** |
| -8.66429 | -458.04696 | 0.00464 | 0 | 0 | 1.9069 |
| -8.56616 | -458.04696 | 0.00556 | 8E-5 | 3E-6 | 1.89505 |
| -8.46786 | -458.04696 | 0.00652 | 1.77E-4 | 8E-6 | 1.88202 |
| -8.36967 | -458.04696 | 0.00793 | 2.32E-4 | 1.1E-5 | 1.87126 |
| -8.2708 | -458.04695 | 0.01002 | 3.27E-4 | 1.5E-5 | 1.86257 |
| -8.17185 | -458.04695 | 0.01299 | 4E-4 | 1.7E-5 | 1.85777 |
| -8.07226 | -458.04694 | 0.0165 | 4.92E-4 | 1.8E-5 | 1.85632 |
| -7.97324 | -458.04694 | 0.02046 | 4.94E-4 | 1.7E-5 | 1.85752 |
| -7.87422 | -458.04693 | 0.02387 | 5.52E-4 | 2E-5 | 1.85634 |
| -7.77514 | -458.04693 | 0.02644 | 6.24E-4 | 2.7E-5 | 1.85425 |
| -7.67555 | -458.04692 | 0.02813 | 7.4E-4 | 2.4E-5 | 1.8513 |
| -7.57685 | -458.04692 | 0.02963 | 8.14E-4 | 1.51E-4 | 1.8492 |
| -7.47766 | -458.04692 | 0.03121 | 9.09E-4 | 1.5E-4 | 1.84374 |
| -7.3786 | -458.04692 | 0.03337 | 9.82E-4 | 1.49E-4 | 1.83964 |
| -7.27898 | -458.04691 | 0.03599 | 0.00105 | 1.48E-4 | 1.83852 |
| -7.17991 | -458.04691 | 0.03927 | 0.00102 | 1.48E-4 | 1.84024 |
| -7.08075 | -458.0469 | 0.04276 | 9.97E-4 | 1.47E-4 | 1.84632 |
| -6.98168 | -458.0469 | 0.04624 | 9.59E-4 | 1.47E-4 | 1.85385 |
| -6.88215 | -458.04689 | 0.0491 | 9.64E-4 | 1.46E-4 | 1.8648 |
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aReferenced to -458.046969109 hartree.