# Supporting information for: Computational study of one-step polar Diels-Alder reactions using the NEB method for the minimum energy paths search

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All normal modes associated to the imaginary and the lowest positive real vibration frequencies are presented here at the M06-2X/6-31++G** level. Also, we present all contour maps of the laplacian of the electronic density in the plane formed by the approaching carbon atoms, in the transition states at the same theory level, where nuclear, bonding and ring critical points are drawn in black, gray and blue, respectively; atomic interaction lines are drawn in red, the limit of atomic basins in gray and isolines in black, were positive values correspond to the continuous lines, the negative ones to the dashed lines and 0 value to the bold continuous lines.

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Table S1: Imaginary and lowest positive real wavenumbers ($cm^{-1}$) for each transition state found.

| System | B3LYP/6-31+G* | | B3LYP/6-31++G** | | M06-2X/6-31+G* | | M06-2X/6-31++G** | |
|---|---|---|---|---|---|---|---|---|
| | $i\bar{\nu}^{\ddagger}$ | $\bar{\nu}_1$ | $i\bar{\nu}^{\ddagger}$ | $\bar{\nu}_1$ | $i\bar{\nu}^{\ddagger}$ | $\bar{\nu}_1$ | $i\bar{\nu}^{\ddagger}$ | $\bar{\nu}_1$ |
| 1-*endo* | -447.332 | 87.061 | -451.073 | 87.915 | -461.617 | 89.798 | -464.678 | 88.977 |
| 1-*exo* | -446.442 | 102.075 | -448.183 | 101.533 | -467.720 | 98.760 | -472.334 | 99.721 |
| 2 | -429.625 | 86.357 | -443.003 | 85.715 | -409.144 | 83.791 | -412.490 | 84.068 |
| 3-*endo* | -445.059 | 73.608 | -448.238 | 73.663 | -426.227 | 73.533 | -428.011 | 76.120 |
| 3-*exo* | -442.773 | 79.793 | -446.026 | 79.790 | -421.955 | 84.258 | -424.810 | 84.665 |
| 4 | -346.292 | 73.226 | -348.788 | 74.156 | -393.456 | 83.553 | -396.721 | 84.989 |
| 5-*endo* | -350.398 | 68.473 | -354.864 | 65.622 | -373.766 | 78.251 | -376.449 | 78.665 |
| 5-*exo* | -349.756 | 77.933 | -352.828 | 75.328 | -376.261 | 75.700 | -379.834 | 77.197 |
| 6 | -340.759 | 67.715 | -340.468 | 67.938 | -312.301 | 69.085 | -328.574 | 68.100 |

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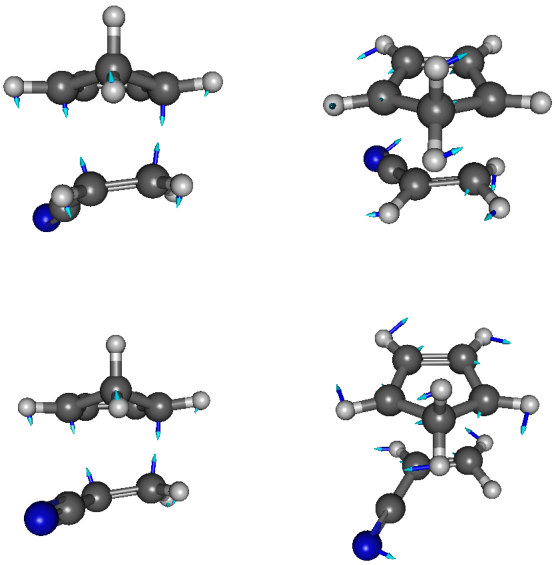

Figure S1: Normal modes associated to the imaginary and the lowest positive real vibration frequencies in the transition states of system 1.

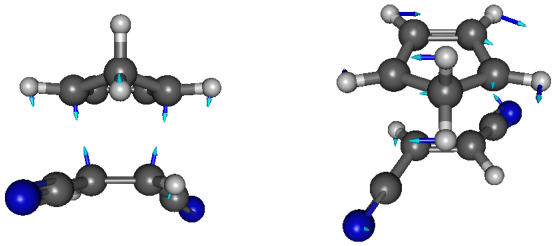

Figure S2: Normal modes associated to the imaginary and the lowest positive real vibration frequencies in the transition state of system 2.

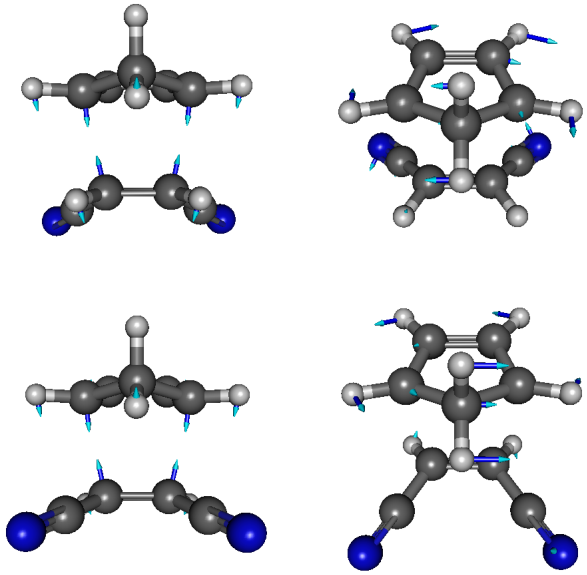

Figure S3: Normal modes associated to the imaginary and the lowest positive real vibration frequencies in the transition states of system 3.

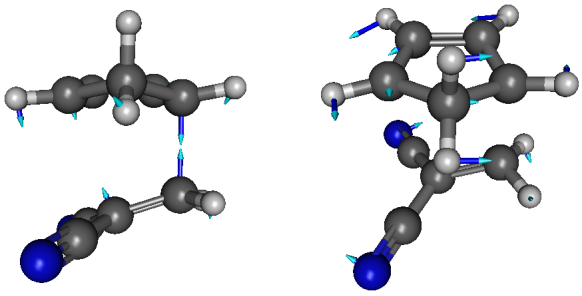

Figure S4: Normal modes associated to the imaginary and the lowest positive real vibration frequencies in the transition state of system 4.

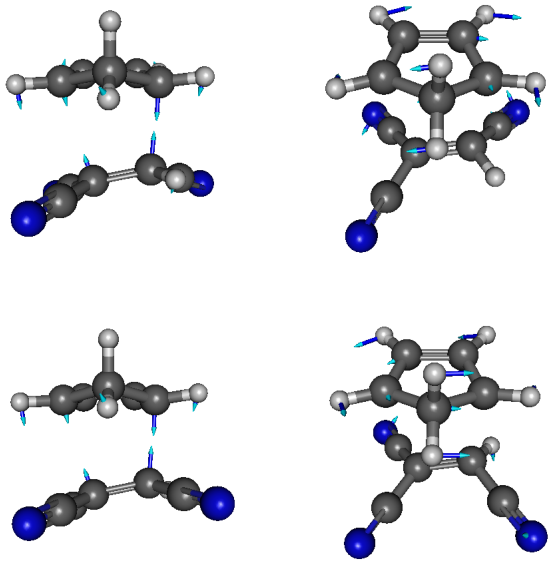

Figure S5: Normal modes associated to the imaginary and the lowest positive real vibration frequencies in the transition states of system 5.

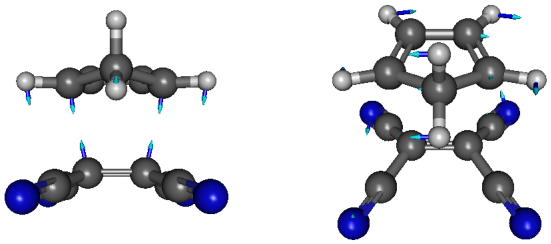

Figure S6: Normal modes associated to the imaginary and the lowest positive real vibration frequencies in the transition state of system 6.

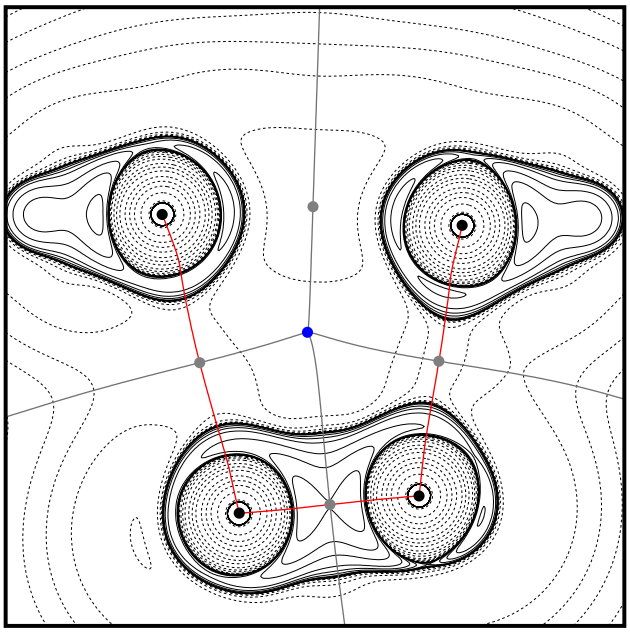

Figure S7: Contour map of the laplacian of the electronic density in the plane formed by the approaching carbon atoms, in the transition state of system 1-*endo*.

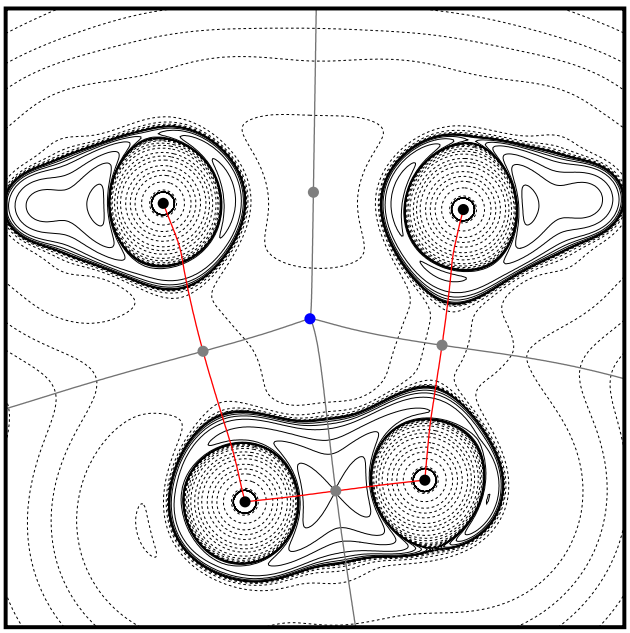

Figure S8: Contour map of the laplacian of the electronic density in the plane formed by the approaching carbon atoms, in the transition state of system 1-*exo*.

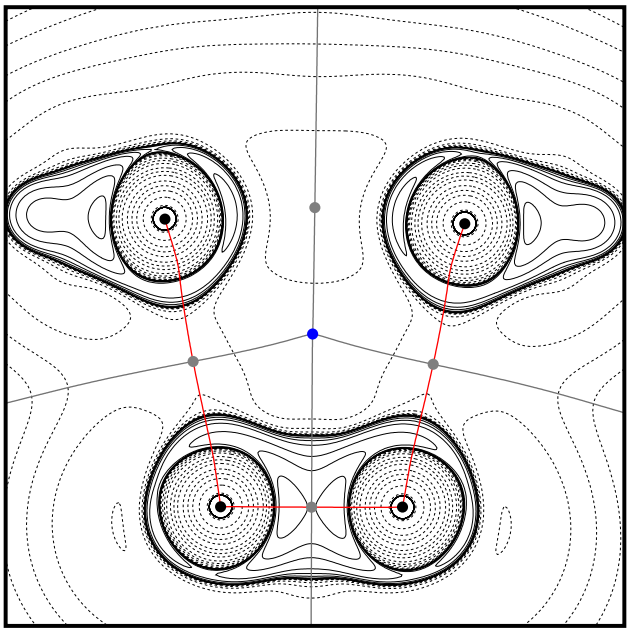

Figure S9: Contour map of the laplacian of the electronic density in the plane formed by the approaching carbon atoms, in the transition state of system 2.

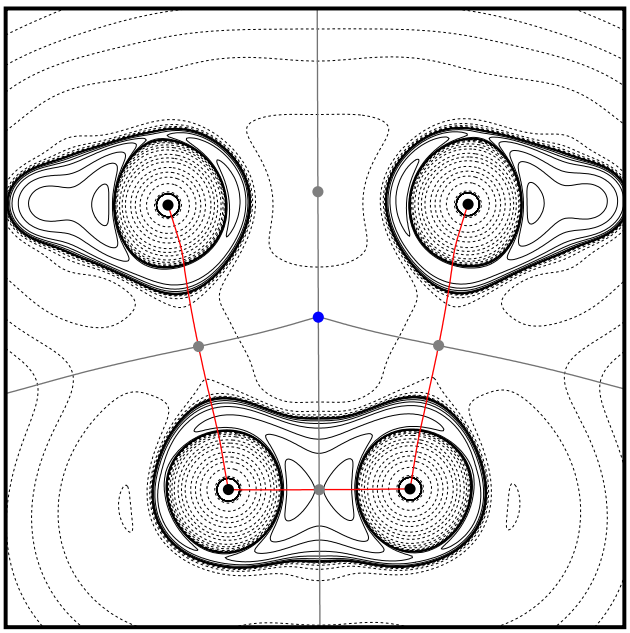

Figure S10: Contour map of the laplacian of the electronic density in the plane formed by the approaching carbon atoms, in the transition state of system 3-*endo*.

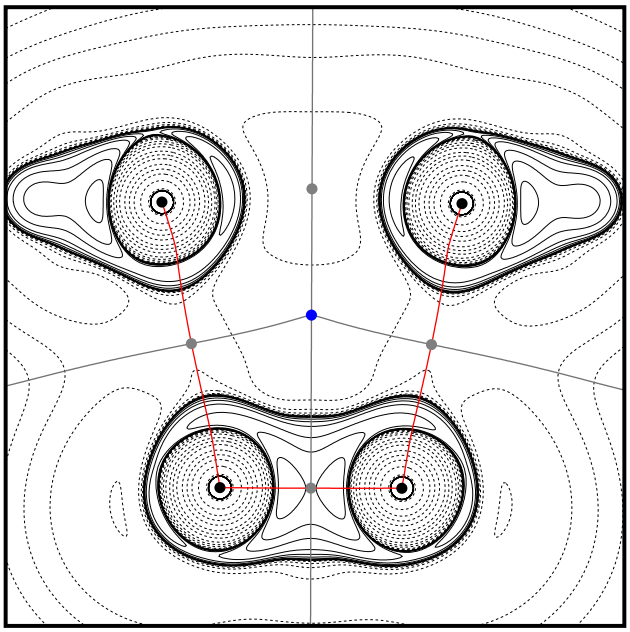

Figure S11: Contour map of the laplacian of the electronic density in the plane formed by the approaching carbon atoms, in the transition state of system 3-*exo*.

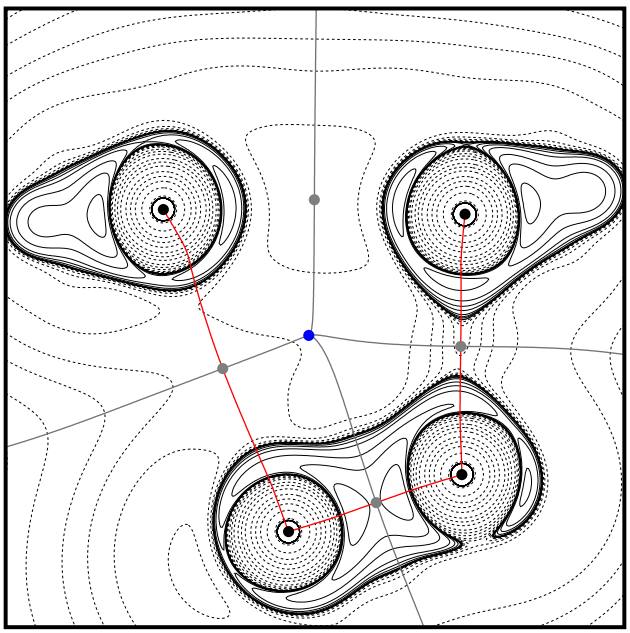

Figure S12: Contour map of the laplacian of the electronic density in the plane formed by the approaching carbon atoms, in the transition state of system 4.

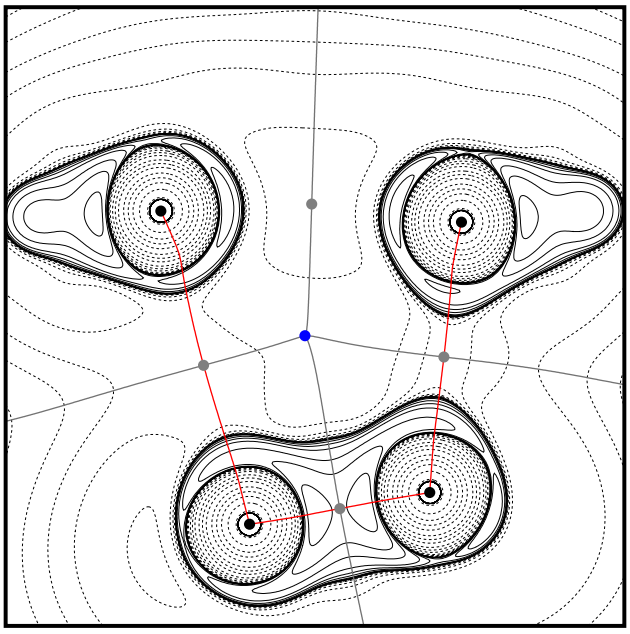

Figure S13: Contour map of the laplacian of the electronic density in the plane formed by the approaching carbon atoms, in the transition state of system 5-*endo*.

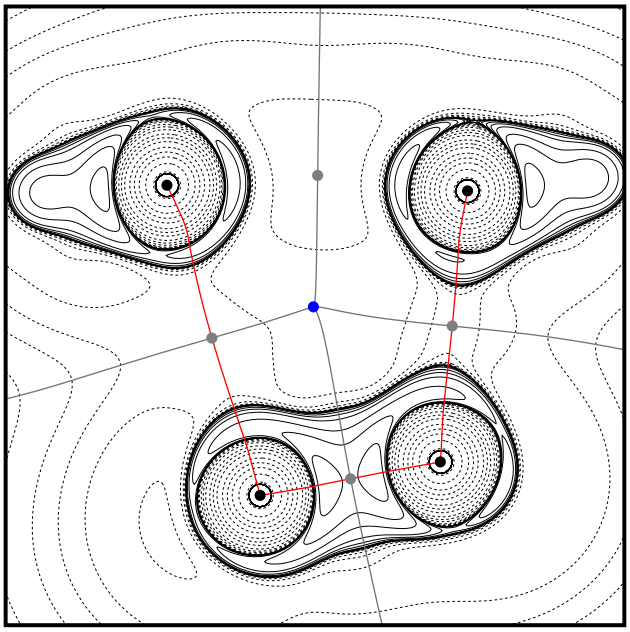

Figure S14: Contour map of the laplacian of the electronic density in the plane formed by the approaching carbon atoms, in the transition state of system 5-*exo*.

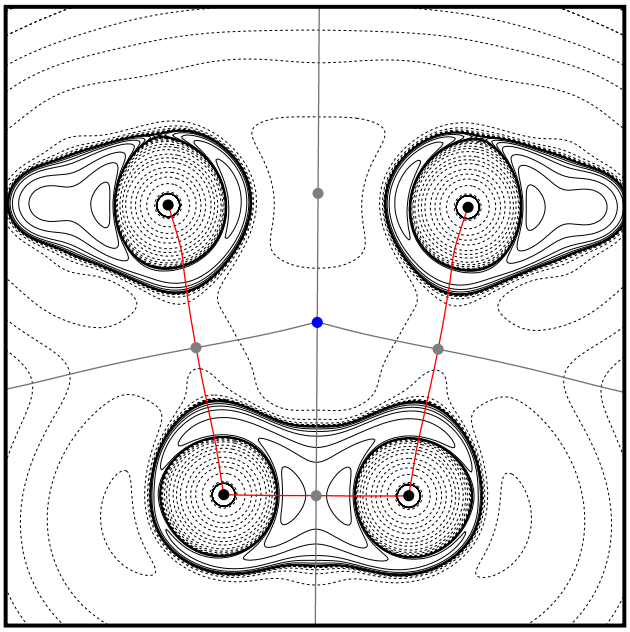

Figure S15: Contour map of the laplacian of the electronic density in the plane formed by the approaching carbon atoms, in the transition state of system 6.