Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Nonadiabatic photodynamics and UV absorption spectrum of all-trans-octatetraene: Supplementary Information

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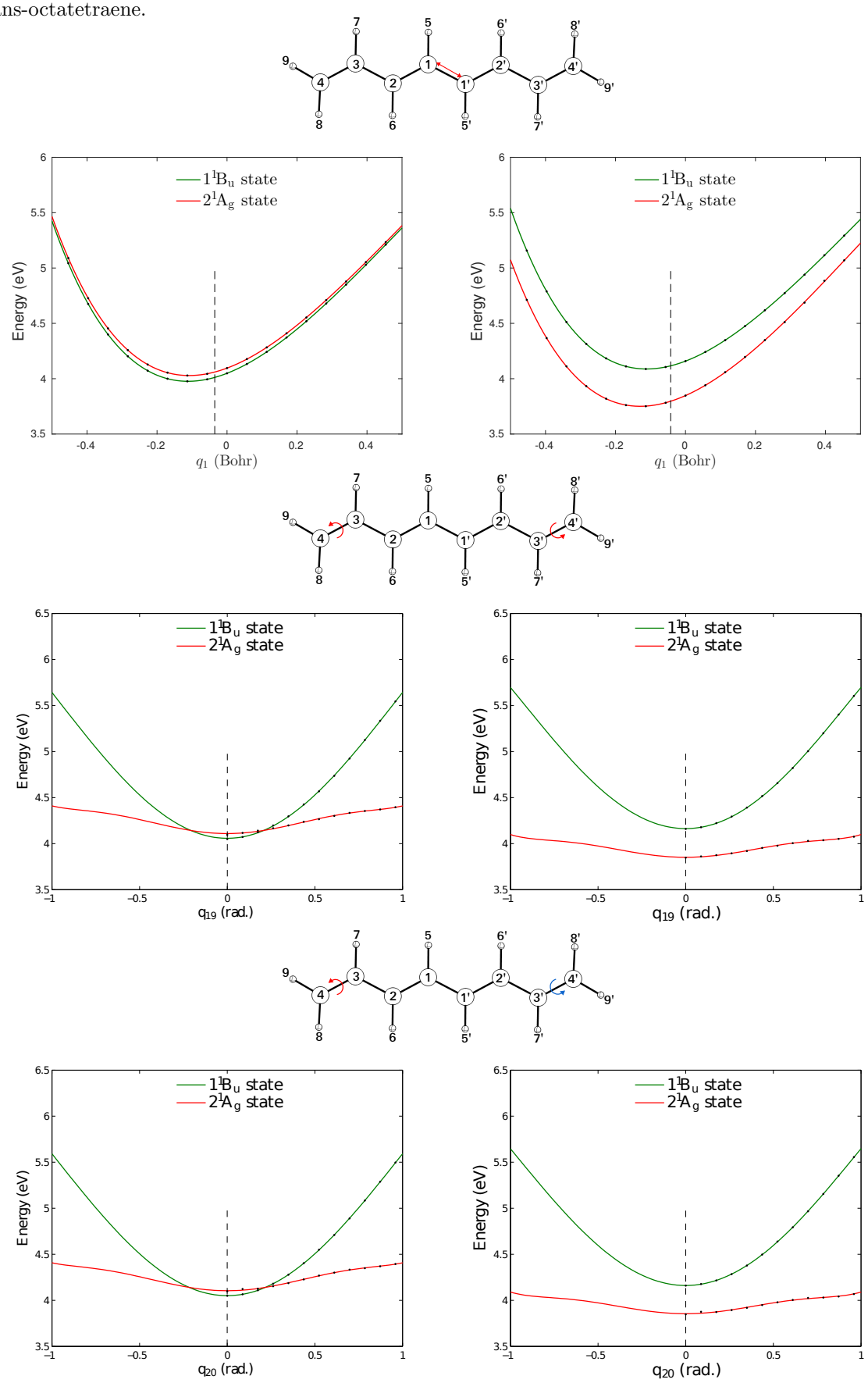
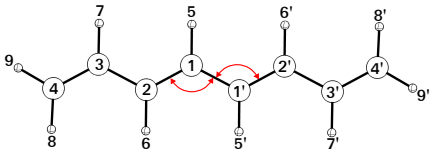
December 19, 2016

Figure 1: DFT/MRCI-R (left) and DFT/MRCI-S (right) 1D cuts of excited states potential energy surface for all-trans-octatetraene.

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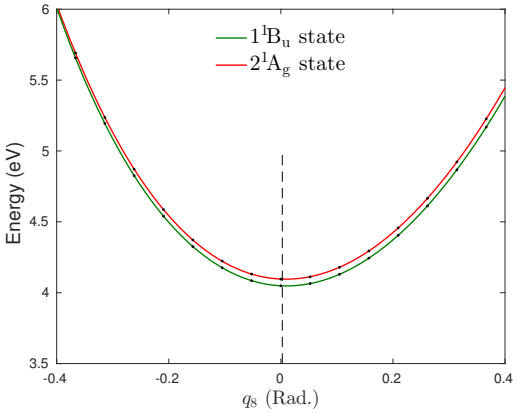
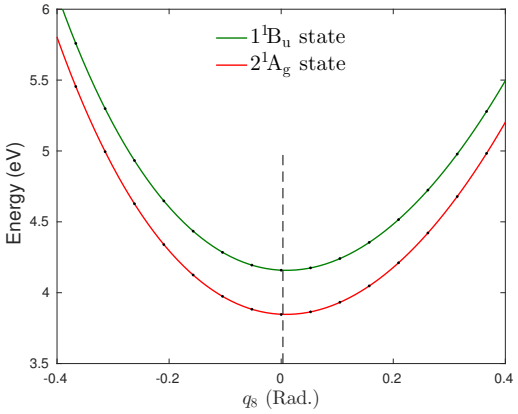
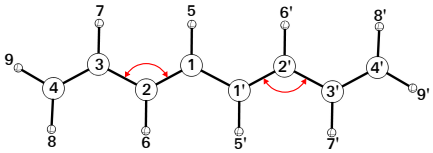

1^1B_u state
2^1A_g state
Energy (eV)
q_8 (Rad.)


1^1B_u state
2^1A_g state
Energy (eV)
q_8 (Rad.)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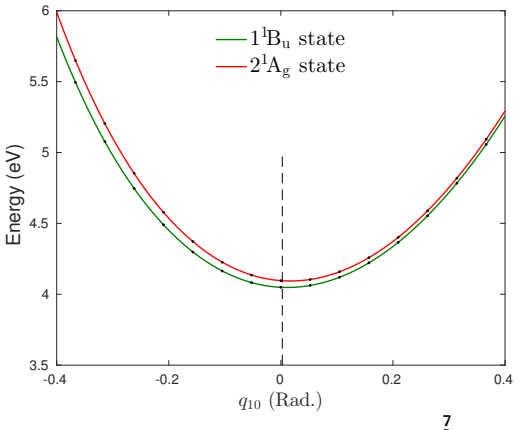
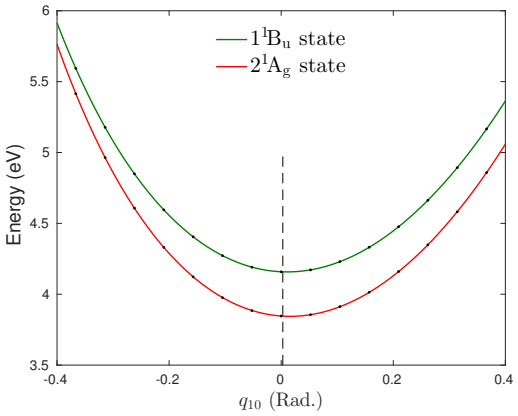
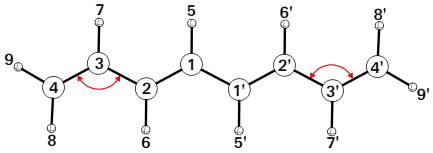

1^1B_u state
2^1A_g state
Energy (eV)
q_{10} (Rad.)


1^1B_u state
2^1A_g state
Energy (eV)
q_{10} (Rad.)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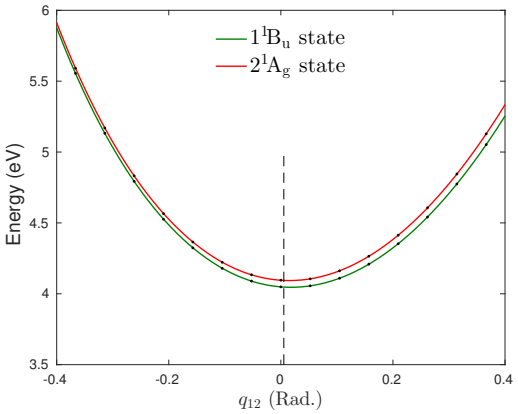
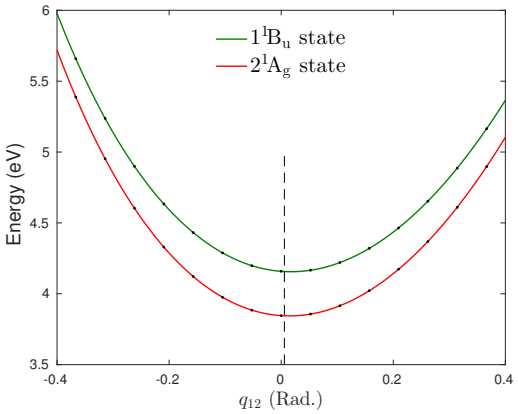
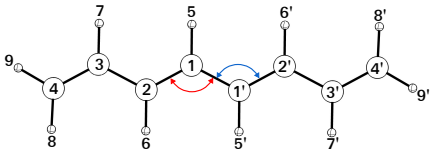

1^1B_u state
2^1A_g state
Energy (eV)
q_{12} (Rad.)


1^1B_u state
2^1A_g state
Energy (eV)
q_{12} (Rad.)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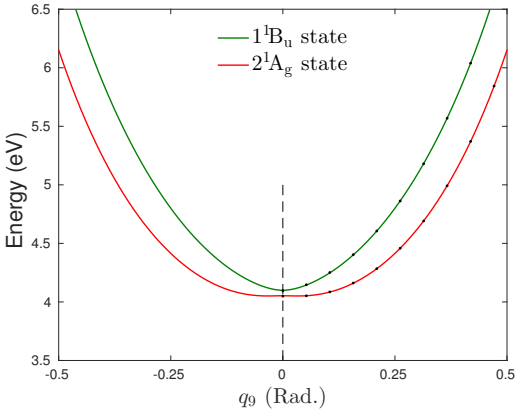
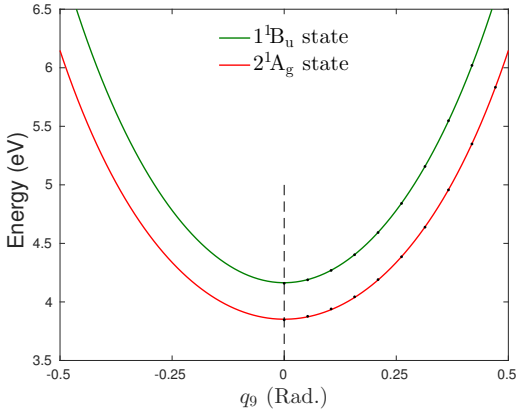
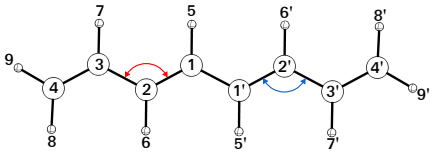

1^1B_u state
2^1A_g state
Energy (eV)
6.5
6
5.5
5
4.5
4
3.5
-0.5
-0.25
0
0.25
0.5
q_9 (Rad.)


1^1B_u state
2^1A_g state
Energy (eV)
6.5
6
5.5
5
4.5
4
3.5
-0.5
-0.25
0
0.25
0.5
q_9 (Rad.)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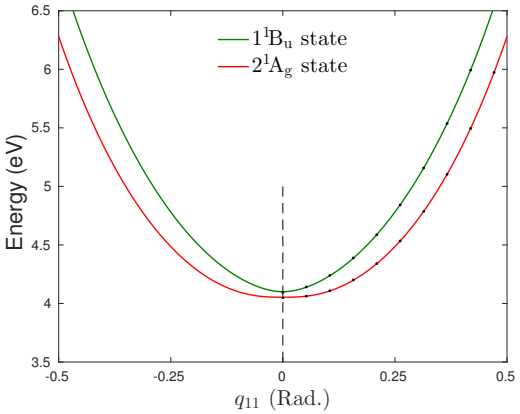
1^1B_u state
2^1A_g state
Energy (eV)
6.5
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5.5
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4.5
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3.5
-0.5
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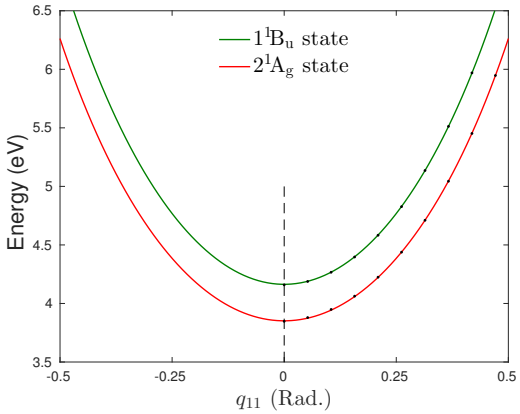
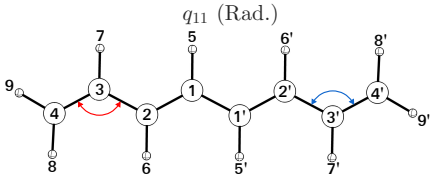
0.25
0.5
q_{11} (Rad.)


1^1B_u state
2^1A_g state
Energy (eV)
6.5
6
5.5
5
4.5
4
3.5
-0.5
-0.25
0
0.25
0.5
q_{11} (Rad.)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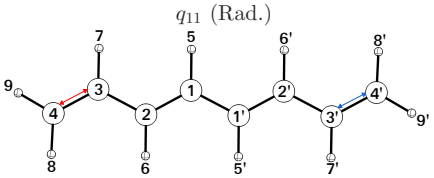
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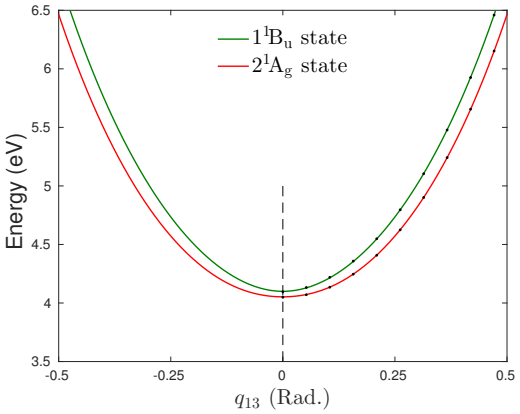
1^1B_u state
2^1A_g state
Energy (eV)
6.5
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5.5
5
4.5
4
3.5
-0.5
-0.25
0
0.25
0.5
q_{13} (Rad.)

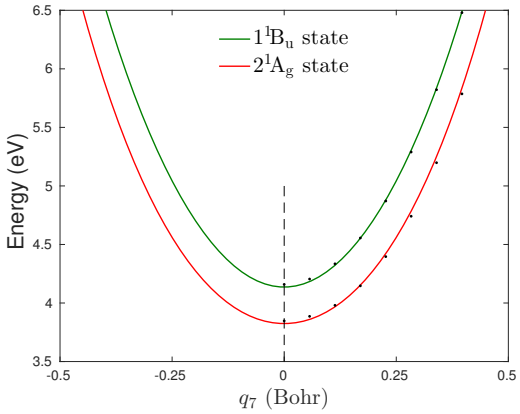
1^1B_u state
2^1A_g state
Energy (eV)
6.5
6
5.5
5
4.5
4
3.5
-0.5
-0.25
0
0.25
0.5
q_7 (Bohr)

Figure 2: Magnitude of the dipole moment of 1^1B_u and 2^1A_g states modulated by q_9 (b_u) and q_{15} (a_u) symmetry adapted distortions. For illustration, positive-negative combination indicates that two vectors are anticollinear near FC region.