Supporting Information

High-Multiplicity Natural Orbitals in Multireference Configuration Interaction for Excited States

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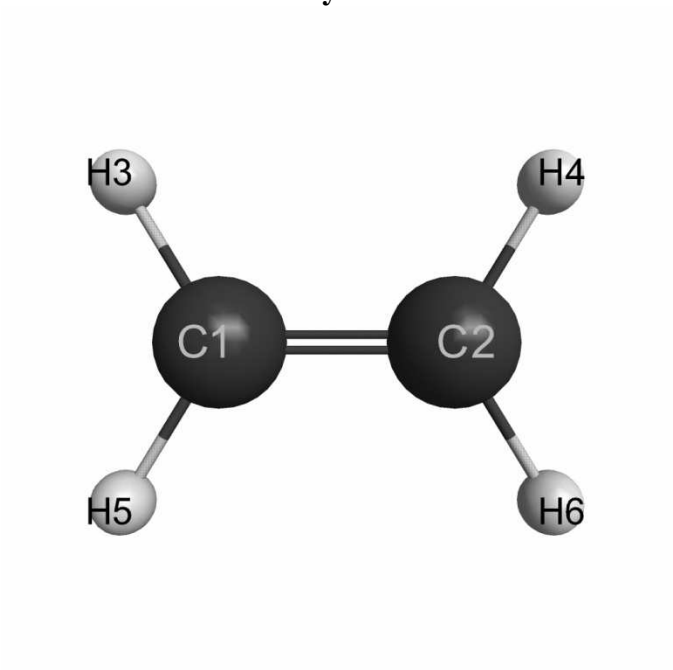
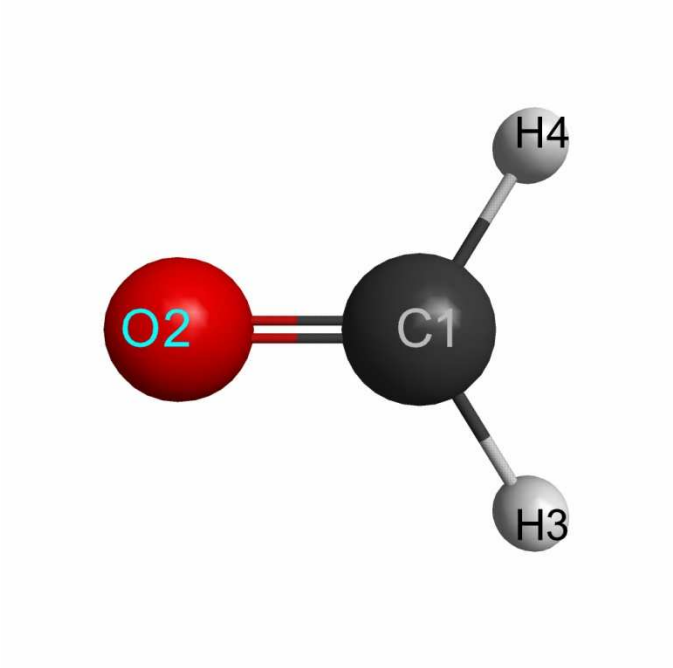
General Remarks. Here we give structures for all of the molecules studied in their equilibrium geometries.

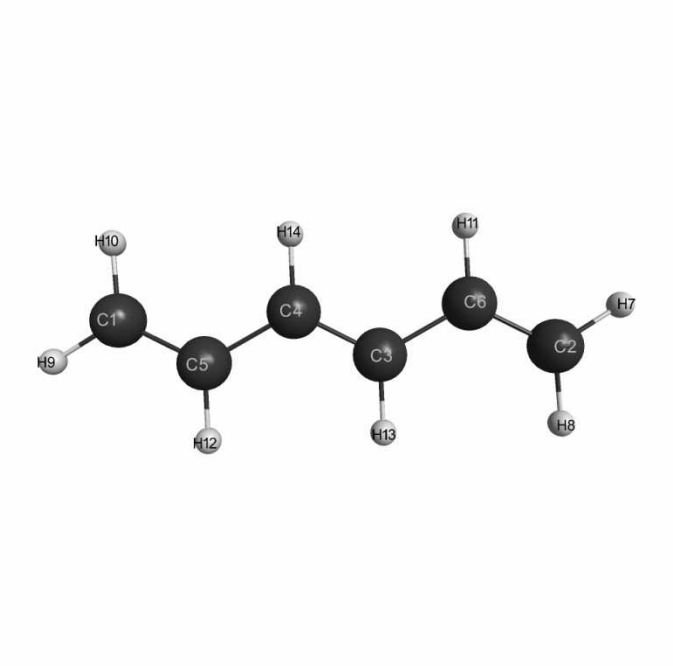
ethylene



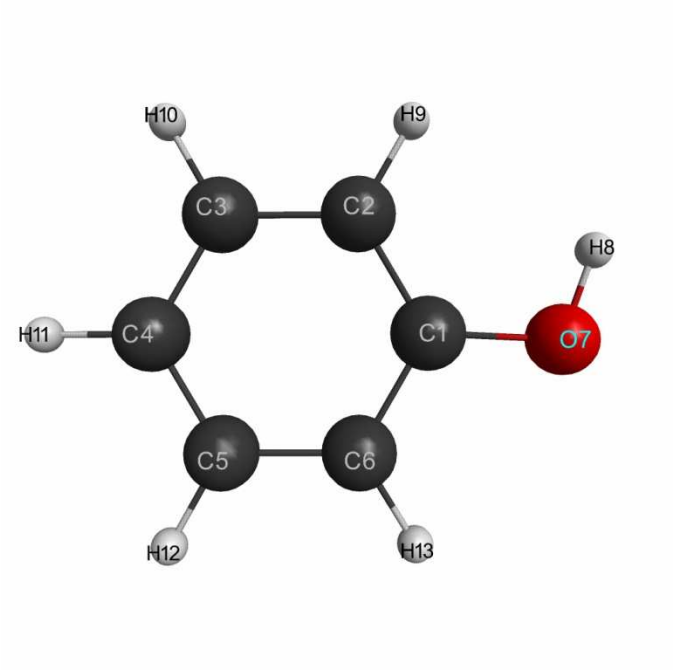
Formaldehyde



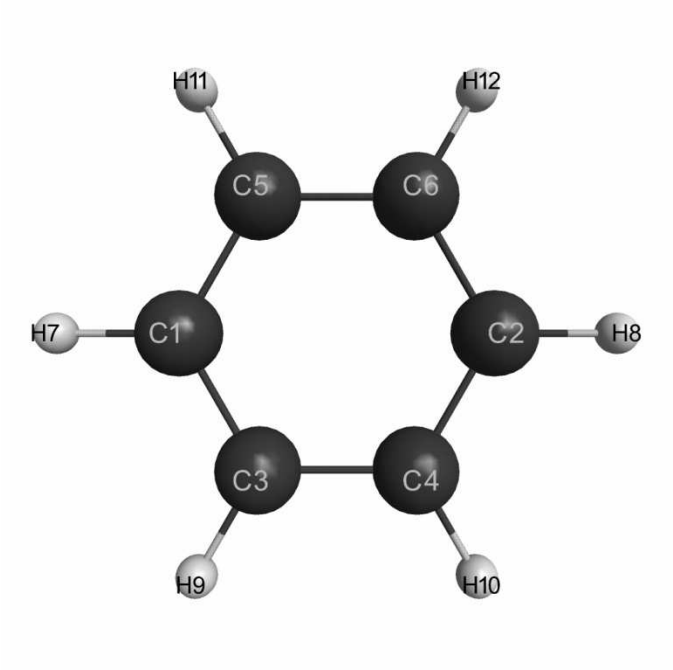
Hexatriene



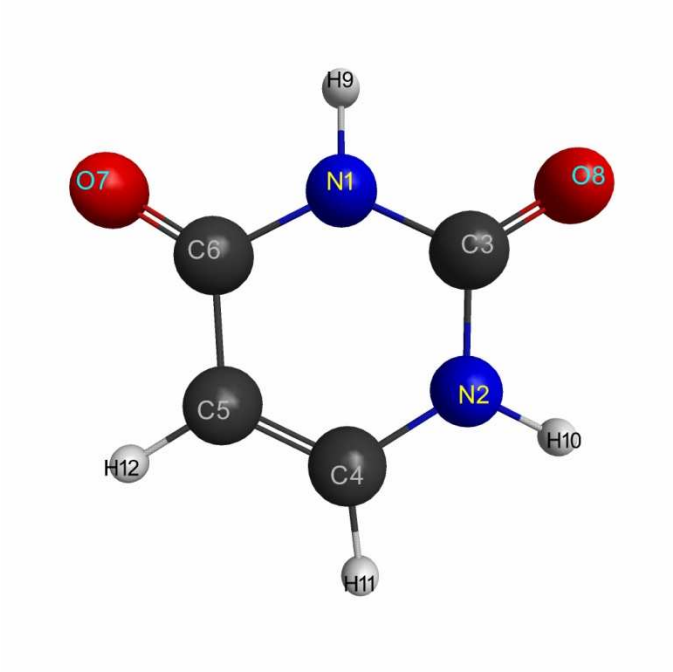
Phenol



Benzene



Uracil


H9
O7
N1
O8
C6
C3
C5
N2
H10
H12
C4
H11