<u>Supplementary Information</u> *for* Resonance Natural Bond Orbitals (RNBOs): Efficient Semi-Localized Orbitals for Computing and Visualizing Reactive Chemical Processes

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This supplement consists of *Gaussian 16*[1] and *NBOPro@Jmol*[2] input and output files for a particular value of the intrinsinc reaction coordinate (IRC = 1.455, near the transition state) for the Claisen rearrangement reaction (B3LYP/6-311++G** level) as described in the main article. Each such input file corresponds to the molecular geometry of a particular frame of the animated video that can be viewed at http://nbo7.chem.wisc.edu/claisen.ppsx.

The steps (program and I/O) to produce the frame of the video displaying RNBO #10 at IRC = 1.455 are summarized below:

1. Use program *Gaussian 16* with input file "claisen_55.gau" to produce output file "claisen_55.47" (wavefunction archive file).
2. Use program *Notepad* to edit "claisen_55.47" for RNBO output.
3. Use program *NBOPro@Jmol*[2] (RUN module) with edited input file "claisen.55.47" and keywords "NRT PLOT RNBO" to produce output file "claisen_55.nbo".
4. Use program *NBOPro@Jmol* (VIEW module) with edited input file "claisen_55.47" to select RNBO #10, then select "3D View" to generate the raytraced "claisen_55.bmp" file.

The successive I/O files (or relevant portions thereof) to complete these steps are shown below:

********** "claisen_55.gau" file **********

```
%mem=2gb
%nprocshared=8
%chk=claisen
#b3lyp/6-311++G** nosymm pop=nbo6read

IRC( 55) =  1.45532, E =  -270.55379 (dE =  -4.75 kcal/mol)

 0  1
C    -1.5414    0.8204   -0.2965
C    -1.3038   -0.3751    0.2843
O    -0.4688   -1.2835   -0.2177
C     1.1704   -0.9246    0.1685
C     1.3917    0.4225   -0.3038
C     0.8413    1.4662    0.3519
H    -2.2122    1.5318    0.1722
H    -1.1984    1.0375   -1.2985
H    -1.6988   -0.5786    1.2855
H     1.1746   -1.0671    1.2463
H     1.6617   -1.7308   -0.3640
H     1.7287    0.5495   -1.3281
H     0.8205    2.4634   -0.0733
H     0.5187    1.3834    1.3820

$nbo file=claisen_55 archive $end
```

********** "claisen_55.47" file (initial lines) **********

```
$GENNBO  NATOMS=14  NBAS=188  UPPER  BODM  FORMAT=PRECISE  $END
$NBO FILE=claisen_55  $END
$COORD
 IRC( 55) = 1.45532, E = -270.55379 (dE = -4.75 kcal/mol)
     6    6      -1.541400       0.820400      -0.296500
     6    6      -1.303800      -0.375100       0.284300
     8    8      -0.468800      -1.283500      -0.217700
     ....
```

********** edited "claisen_55.47" file **********

[The edits consist of the "NRT NRTCYC=0 PLOT RNBO" keywords of the $NBO...$END keylist (line 2) and the eight resonance structures of the $NRTSTR...$END keylist for the transition state structure (lines 3-44).]

```
$GENNBO  NATOMS=14  NBAS=188  UPPER  BODM  FORMAT=PRECISE  $END
$NBO NRT NRTCYC=0 PLOT RNBO
  FILE=claisen_55  $END
$NRTSTR
STR        ! Wgt=42.94%; rhoNL=1.12958; D(0)=0.07755
LONE 3 2 END
BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 S 4 5 S 4 10 S 4 11 D 5 6
S 5 12 S 6 13 S 6 14 END
END
STR        ! Wgt=38.46%; rhoNL=1.43080; D(0)
```

```
BOND S 1 2 S 1 6 S 1 7 S 1 8 D 2 3 S 2 9 D 4 5 S 4 10 S 4 11 S 5 6
S 5 12 S 6 13 S 6 14 END
END
STR        ! Wgt=6.25%; rhoNL=2.53390; D(0)=0.11612
LONE 3 1 9 1 END
BOND S 1 2 S 1 6 S 1 7 S 1 8 T 2 3 D 4 5 S 4 10 S 4 11 S 5 6 S 5 12
S 6 13 S 6 14 END
END
STR        ! Wgt=2.66%; rhoNL=3.00162; D(0)=0.12638
LONE 3 2 8 1 END
BOND T 1 2 S 1 7 S 2 3 S 3 4 S 4 5 S 4 10 S 4 11 D 5 6 S 5 12 S 6 13
S 6 14 END
END
STR        ! Wgt=2.66%; rhoNL=2.97878; D(0)=0.12590
LONE 3 2 12 1 END
BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 S 4 5 S 4 10 S 4 11 T 5 6
S 6 13 END
END
STR        ! Wgt=2.62%; rhoNL=2.97300; D(0)=0.12577
LONE 3 2 14 1 END
BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 S 4 5 S 4 10 S 4 11 T 5 6
S 6 13 END
END
STR        ! Wgt=2.36%; rhoNL=2.88481; D(0)=0.12390
LONE 3 2 4 1 END
BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 S 4 10 S 4 11 T 5 6 S 5 12
S 6 14 END
END
STR        ! Wgt=1.75%; rhoNL=2.57701; D(0)=0.11710
LONE 3 3 END
BOND T 1 2 S 1 8 S 2 9 S 3 4 S 4 5 S 4 10 S 4 11 D 5 6 S 5 12 S 6 13
S 6 14 END
END
$END
 $COORD
 IRC( 55) = 1.45532, E = -270.55379 (dE = -4.75 kcal/mol)
     6    6      -1.541400       0.820400      -0.296500
     6    6      -1.303800      -0.375100       0.284300
     8    8      -0.468800      -1.283500      -0.217700
     …
```

A portion of the "claisen_55.nbo" output file, showing full output for NRT and RNBO keyword modules, is displayed below:

********** "claisen_55.nbo" file (NRT section) **********

```
********************************** NBO 7.0 **********************************
            N A T U R A L   A T O M I C   O R B I T A L   A N D
         N A T U R A L   B O N D   O R B I T A L   A N A L Y S I S
 ************************ development version (D000000) ************************
  (c) Copyright 1996-2018 Board of Regents of the University of Wisconsin System
      on behalf of the Theoretical Chemistry Institute.  All rights reserved.

          Cite this program [NBO 7.0.0 (15-Nov-2018)] as:

          NBO 7.0.  E. D. Glendening, J. K. Badenhoop, A. E. Reed,
          J. E. Carpenter, J. A. Bohmann, C. M. Morales, P. Karafiloglou,
          C. R. Landis, and F. Weinhold, Theoretical Chemistry Institute,
          University of Wisconsin, Madison, WI (2018)
```

```
      /NRT    / : Natural Resonance Theory Analysis
      /RNBO   / : Write the AO to RNBO transformation to lfn44
      /PLOT   / : Write information for the orbital plotter
      /FILE   / : Set to claisen_55

Filename set to claisen_55

Job title:  IRC( 55) = 1.45532, E = -270.55379 (dE = -4.75 kcal/mol)
 .
 .
 .
NATURAL RESONANCE THEORY ANALYSIS:

   Parent structure threshold:  50% of leading weight
Delocalization list threshold:  1 kcal/mol

C1 symmetry, 1 symmetry operator(s), 1 unique atom permutation(s)
8 initial TOPO matrices: NRTSTR = 8; NBI = 0; SYM = 0

 cycle  structures    D(w)      kmax  CHOOSE   ION    E2   SYM   dbmax   dbrms
-------------------------------------------------------------------------------
   1       8/10    0.05005315     8      18     0    30     0   1.823   1.127
   2      18/73    0.04983204    11     114     0     0     0   0.040   0.020

QPNRT(18/73): D(0)=0.05974429; D(w)=0.04983204; dbmax=0.040; dbrms=0.020
Timing(sec): search=3.73; Gram matrix=0.37; minimize=0.00; other=0.23


TOPO matrix for the leading resonance structure:

    Atom  1   2   3   4   5   6   7   8   9  10  11  12  13  14
    ---- --- --- --- --- --- --- --- --- --- --- --- --- --- ---
  1.  C   0   2   0   0   0   0   1   1   0   0   0   0   0   0
  2.  C   2   0   1   0   0   0   0   0   1   0   0   0   0   0
  3.  O   0   1   2   1   0   0   0   0   0   0   0   0   0   0
  4.  C   0   0   1   0   1   0   0   0   0   1   1   0   0   0
  5.  C   0   0   0   1   0   2   0   0   0   0   0   1   0   0
  6.  C   0   0   0   0   2   0   0   0   0   0   0   0   1   1
  7.  H   1   0   0   0   0   0   0   0   0   0   0   0   0   0
  8.  H   1   0   0   0   0   0   0   0   0   0   0   0   0   0
  9.  H   0   1   0   0   0   0   0   0   0   0   0   0   0   0
 10.  H   0   0   0   1   0   0   0   0   0   0   0   0   0   0
 11.  H   0   0   0   1   0   0   0   0   0   0   0   0   0   0
 12.  H   0   0   0   0   1   0   0   0   0   0   0   0   0   0
 13.  H   0   0   0   0   0   1   0   0   0   0   0   0   0   0
 14.  H   0   0   0   0   0   1   0   0   0   0   0   0   0   0

        Resonance
   RS   Weight(%)                  Added(Removed)
---------------------------------------------------------------------------
    1     50.30
    2     23.56   ( C  1- C  2),  C  1- C  6,  C  2- O  3, ( O  3- C  4),
                   C  4- C  5, ( C  5- C  6)
    3      2.63   ( C  1- C  2),  C  2- O  3,  C  1, ( O  3)
    4      2.51    C  1- C  2, ( C  1- H  8), ( C  2- H  9),  H  8
    5      2.32   ( C  1- C  2),  C  1- C  6,  C  2- O  3,  C  2- O  3,
                  ( C  2- H  9), ( O  3- C  4),  C  4- C  5, ( C  5- C  6),
                  ( O  3),  H  9
    6      2.22    C  5- C  6, ( C  5- H 12), ( C  6- H 14),  H 14
    7      2.19    C  5- C  6, ( C  5- H 12), ( C  6- H 14),  H 12
```

```
    8      2.06    C  1- C  2, ( C  1- H  8), ( C  2- H  9),  H  9
    9      1.90    C  4- C  5, ( C  4- H 10), ( C  5- H 12),  H 10
   10      1.79    C  1- C  2, ( C  1- H  7), ( C  2- O  3),  O  3
   11      1.67   ( C  4- C  5),  C  5- C  6, ( C  6- H 13),  C  4
   12      1.44   ( C  4- C  5),  C  5- C  6, ( C  6- H 13),  H 13
   13      1.39    C  4- C  5, ( C  4- H 10), ( C  5- H 12),  H 12
   14      1.12    C  4- C  5, ( C  4- H 11), ( C  5- C  6),  H 11
   15      1.04    C  4- C  5, ( C  4- H 11), ( C  5- C  6),  C  6
   16      0.91    C  1- C  2, ( C  1- H  7), ( C  2- O  3),  H  7
   17      0.49   ( C  4- C  5), ( C  5- C  6),  C  4,  C  5
   18      0.49   ( C  4- C  5), ( C  5- C  6),  C  5,  C  6
 others    0.00
-------------------------------------------------------------------------
         100.00   * Total *


Natural Bond Order:  (total/covalent/ionic)

    Atom       1      2      3      4      5      6      7      8      9
    ----   ------ ------ ------ ------ ------ ------ ------ ------ ------
  1.  C  t 0.0263 1.7876 0.0000 0.0000 0.0000 0.2587 0.9729 0.9544 0.0000
         c   ---  1.7221 0.0000 0.0000 0.0000 0.2198 0.7796 0.7597 0.0000
         i   ---  0.0655 0.0000 0.0000 0.0000 0.0390 0.1934 0.1947 0.0000

  2.  C  t 1.7876 0.0000 1.2812 0.0000 0.0000 0.0000 0.0000 0.0000 0.9312
         c 1.7221   ---  0.7886 0.0000 0.0000 0.0000 0.0000 0.0000 0.7795
         i 0.0655   ---  0.4926 0.0000 0.0000 0.0000 0.0000 0.0000 0.1517

  3.  O  t 0.0000 1.2812 1.9684 0.7413 0.0000 0.0000 0.0000 0.0000 0.0000
         c 0.0000 0.7886   ---  0.4495 0.0000 0.0000 0.0000 0.0000 0.0000
         i 0.0000 0.4926   ---  0.2918 0.0000 0.0000 0.0000 0.0000 0.0000

  4.  C  t 0.0000 0.0000 0.7413 0.0216 1.2723 0.0000 0.0000 0.0000 0.0000
         c 0.0000 0.0000 0.4495   ---  1.1463 0.0000 0.0000 0.0000 0.0000
         i 0.0000 0.0000 0.2918   ---  0.1261 0.0000 0.0000 0.0000 0.0000

  5.  C  t 0.0000 0.0000 0.0000 1.2723 0.0097 1.7852 0.0000 0.0000 0.0000
         c 0.0000 0.0000 0.0000 1.1463   ---  1.6925 0.0000 0.0000 0.0000
         i 0.0000 0.0000 0.0000 0.1261   ---  0.0927 0.0000 0.0000 0.0000

  6.  C  t 0.2587 0.0000 0.0000 0.0000 1.7852 0.0152 0.0000 0.0000 0.0000
         c 0.2198 0.0000 0.0000 0.0000 1.6925   ---  0.0000 0.0000 0.0000
         i 0.0390 0.0000 0.0000 0.0000 0.0927   ---  0.0000 0.0000 0.0000

  7.  H  t 0.9729 0.0000 0.0000 0.0000 0.0000 0.0000 0.0091 0.0000 0.0000
         c 0.7796 0.0000 0.0000 0.0000 0.0000 0.0000   ---  0.0000 0.0000
         i 0.1934 0.0000 0.0000 0.0000 0.0000 0.0000   ---  0.0000 0.0000

  8.  H  t 0.9544 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0251 0.0000
         c 0.7597 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000   ---  0.0000
         i 0.1947 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000   ---  0.0000

  9.  H  t 0.0000 0.9312 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0437
         c 0.0000 0.7795 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000   ---
         i 0.0000 0.1517 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000   ---

 10.  H  t 0.0000 0.0000 0.0000 0.9672 0.0000 0.0000 0.0000 0.0000 0.0000
         c 0.0000 0.0000 0.0000 0.7797 0.0000 0.0000 0.0000 0.0000 0.0000
         i 0.0000 0.0000 0.0000 0.1875 0.0000 0.0000 0.0000 0.0000 0.0000
```

11.	H	t	0.0000	0.0000	0.0000	0.9785	0.0000	0.0000	0.0000	0.0000	0.0000
		c	0.0000	0.0000	0.0000	0.7754	0.0000	0.0000	0.0000	0.0000	0.0000
		i	0.0000	0.0000	0.0000	0.2031	0.0000	0.0000	0.0000	0.0000	0.0000
12.	H	t	0.0000	0.0000	0.0000	0.0000	0.9230	0.0000	0.0000	0.0000	0.0000
		c	0.0000	0.0000	0.0000	0.0000	0.7328	0.0000	0.0000	0.0000	0.0000
		i	0.0000	0.0000	0.0000	0.0000	0.1903	0.0000	0.0000	0.0000	0.0000
13.	H	t	0.0000	0.0000	0.0000	0.0000	0.0000	0.9689	0.0000	0.0000	0.0000
		c	0.0000	0.0000	0.0000	0.0000	0.0000	0.7724	0.0000	0.0000	0.0000
		i	0.0000	0.0000	0.0000	0.0000	0.0000	0.1965	0.0000	0.0000	0.0000
14.	H	t	0.0000	0.0000	0.0000	0.0000	0.0000	0.9559	0.0000	0.0000	0.0000
		c	0.0000	0.0000	0.0000	0.0000	0.0000	0.7673	0.0000	0.0000	0.0000
		i	0.0000	0.0000	0.0000	0.0000	0.0000	0.1886	0.0000	0.0000	0.0000

Atom			10	11	12	13	14
1.	C	t	0.0000	0.0000	0.0000	0.0000	0.0000
		c	0.0000	0.0000	0.0000	0.0000	0.0000
		i	0.0000	0.0000	0.0000	0.0000	0.0000
2.	C	t	0.0000	0.0000	0.0000	0.0000	0.0000
		c	0.0000	0.0000	0.0000	0.0000	0.0000
		i	0.0000	0.0000	0.0000	0.0000	0.0000
3.	O	t	0.0000	0.0000	0.0000	0.0000	0.0000
		c	0.0000	0.0000	0.0000	0.0000	0.0000
		i	0.0000	0.0000	0.0000	0.0000	0.0000
4.	C	t	0.9672	0.9785	0.0000	0.0000	0.0000
		c	0.7797	0.7754	0.0000	0.0000	0.0000
		i	0.1875	0.2031	0.0000	0.0000	0.0000
5.	C	t	0.0000	0.0000	0.9230	0.0000	0.0000
		c	0.0000	0.0000	0.7328	0.0000	0.0000
		i	0.0000	0.0000	0.1903	0.0000	0.0000
6.	C	t	0.0000	0.0000	0.0000	0.9689	0.9559
		c	0.0000	0.0000	0.0000	0.7724	0.7673
		i	0.0000	0.0000	0.0000	0.1965	0.1886
7.	H	t	0.0000	0.0000	0.0000	0.0000	0.0000
		c	0.0000	0.0000	0.0000	0.0000	0.0000
		i	0.0000	0.0000	0.0000	0.0000	0.0000
8.	H	t	0.0000	0.0000	0.0000	0.0000	0.0000
		c	0.0000	0.0000	0.0000	0.0000	0.0000
		i	0.0000	0.0000	0.0000	0.0000	0.0000
9.	H	t	0.0000	0.0000	0.0000	0.0000	0.0000
		c	0.0000	0.0000	0.0000	0.0000	0.0000
		i	0.0000	0.0000	0.0000	0.0000	0.0000
10.	H	t	0.0190	0.0000	0.0000	0.0000	0.0000
		c	---	0.0000	0.0000	0.0000	0.0000
		i	---	0.0000	0.0000	0.0000	0.0000

```
 11.  H  t 0.0000 0.0112 0.0000 0.0000 0.0000
         c 0.0000   ---  0.0000 0.0000 0.0000
         i 0.0000   ---  0.0000 0.0000 0.0000

 12.  H  t 0.0000 0.0000 0.0358 0.0000 0.0000
         c 0.0000 0.0000   ---  0.0000 0.0000
         i 0.0000 0.0000   ---  0.0000 0.0000

 13.  H  t 0.0000 0.0000 0.0000 0.0144 0.0000
         c 0.0000 0.0000 0.0000   ---  0.0000
         i 0.0000 0.0000 0.0000   ---  0.0000

 14.  H  t 0.0000 0.0000 0.0000 0.0000 0.0222
         c 0.0000 0.0000 0.0000 0.0000   ---
         i 0.0000 0.0000 0.0000 0.0000   ---


Natural Atomic Valencies and Electron Counts:

                     Co-    Electro- Electron
    Atom  Valency  Valency  Valency   Count
    ----  -------  -------  -------  -------
  1.  C    3.9737   3.4812   0.4925   8.0000
  2.  C    4.0000   3.2902   0.7098   8.0000
  3.  O    2.0225   1.2381   0.7843   7.9817
  4.  C    3.9592   3.1509   0.8084   7.9616
  5.  C    3.9806   3.5716   0.4090   7.9806
  6.  C    3.9688   3.4521   0.5167   7.9680
  7.  H    0.9729   0.7796   0.1934   1.9641
  8.  H    0.9544   0.7597   0.1947   1.9589
  9.  H    0.9312   0.7795   0.1517   1.9499
 10.  H    0.9672   0.7797   0.1875   1.9723
 11.  H    0.9785   0.7754   0.2031   1.9793
 12.  H    0.9230   0.7328   0.1903   1.9177
 13.  H    0.9689   0.7724   0.1965   1.9666
 14.  H    0.9559   0.7673   0.1886   1.9562


$NRTSTR
  STR        ! Wgt=50.30%; rhoNL=0.67004; D(0)=0.05974
    LONE 3 2 END
    BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 S 4 5 S 4 10 S 4 11 D 5 6
         S 5 12 S 6 13 S 6 14 END
  END
  STR        ! Wgt=23.56%; rhoNL=2.02207; D(0)=0.10374
    LONE 3 2 END
    BOND S 1 2 S 1 6 S 1 7 S 1 8 D 2 3 S 2 9 D 4 5 S 4 10 S 4 11 S 5 6
         S 5 12 S 6 13 S 6 14 END
  END
  STR        ! Wgt=2.63%; rhoNL=1.78597; D(0)=0.09749
    LONE 1 1 3 1 END
    BOND S 1 2 S 1 7 S 1 8 D 2 3 S 2 9 S 3 4 S 4 5 S 4 10 S 4 11 D 5 6
         S 5 12 S 6 13 S 6 14 END
  END
  STR        ! Wgt=2.51%; rhoNL=2.53323; D(0)=0.11610
    LONE 3 2 8 1 END
    BOND T 1 2 S 1 7 S 2 3 S 3 4 S 4 5 S 4 10 S 4 11 D 5 6 S 5 12 S 6 13
         S 6 14 END
  END
  STR        ! Wgt=2.32%; rhoNL=3.16575; D(0)=0.12979
    LONE 3 1 9 1 END
```

```
    BOND S 1 2 S 1 6 S 1 7 S 1 8 T 2 3 D 4 5 S 4 10 S 4 11 S 5 6 S 5 12
         S 6 13 S 6 14 END
  END
  STR        ! Wgt=2.22%; rhoNL=2.50783; D(0)=0.11552
    LONE 3 2 14 1 END
    BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 S 4 5 S 4 10 S 4 11 T 5 6
         S 6 13 END
  END
  STR        ! Wgt=2.19%; rhoNL=2.51520; D(0)=0.11569
    LONE 3 2 12 1 END
    BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 S 4 5 S 4 10 S 4 11 T 5 6
         S 6 13 END
  END
  STR        ! Wgt=2.06%; rhoNL=2.47614; D(0)=0.11479
    LONE 3 2 9 1 END
    BOND T 1 2 S 1 7 S 2 3 S 3 4 S 4 5 S 4 10 S 4 11 D 5 6 S 5 12 S 6 13
         S 6 14 END
  END
  STR        ! Wgt=1.90%; rhoNL=2.52591; D(0)=0.11594
    LONE 3 2 10 1 END
    BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 D 4 5 S 4 11 D 5 6 S 6 13
         S 6 14 END
  END
  STR        ! Wgt=1.79%; rhoNL=2.09269; D(0)=0.10553
    LONE 3 3 END
    BOND T 1 2 S 1 8 S 2 9 S 3 4 S 4 5 S 4 10 S 4 11 D 5 6 S 5 12 S 6 13
         S 6 14 END
  END
  STR        ! Wgt=1.67%; rhoNL=2.40838; D(0)=0.11321
    LONE 3 2 4 1 END
    BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 S 4 10 S 4 11 T 5 6 S 5 12
         S 6 14 END
  END
  STR        ! Wgt=1.44%; rhoNL=2.60640; D(0)=0.11777
    LONE 3 2 13 1 END
    BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 S 4 10 S 4 11 T 5 6 S 5 12
         S 6 14 END
  END
  STR        ! Wgt=1.39%; rhoNL=2.53923; D(0)=0.11624
    LONE 3 2 12 1 END
    BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 D 4 5 S 4 11 D 5 6 S 6 13
         S 6 14 END
  END
  STR        ! Wgt=1.12%; rhoNL=2.62415; D(0)=0.11817
    LONE 3 2 11 1 END
    BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 D 4 5 S 4 10 S 5 6 S 5 12
         S 6 13 S 6 14 END
  END
  STR        ! Wgt=1.04%; rhoNL=2.44056; D(0)=0.11396
    LONE 3 2 6 1 END
    BOND D 1 2 S 1 7 S 1 8 S 2 3 S 2 9 S 3 4 D 4 5 S 4 10 S 5 6 S 5 12
         S 6 13 S 6 14 END
  END
$END
```

********** “claisen_55.nbo” file (RNBO section) **********

```
RESONANCE NATURAL BOND ORBITAL (RNBO) ANALYSIS:

 Hybridization/Polarization Analysis of RNBOs in NAO Basis:
 RNBO / Occupancy / Atomic Hybrid Contributions
 -------------------------------------------------------------------------------
   1. (2.00000)  CR ( 1)  C  1
                           99.999%  C  1 s(100.00%)
   2. (2.00000)  CR ( 1)  C  2
                          100.000%  C  2 s(100.00%)
   3. (2.00000)  CR ( 1)  O  3
                          100.000%  O  3 s(100.00%)
   4. (2.00000)  CR ( 1)  C  4
                          100.000%  C  4 s(100.00%)
   5. (2.00000)  CR ( 1)  C  5
                           99.999%  C  5 s(100.00%)
   6. (2.00000)  CR ( 1)  C  6
                           99.999%  C  6 s(100.00%)
   7. (2.00000)  LP ( 1)  O  3
                            0.734%  C  1 s(  0.64%)p99.99( 99.26%)d 0.16(  0.10%)
                            1.050%  C  2 s(  5.07%)p18.07( 91.54%)d 0.67(  3.39%)
                           97.367%  O  3 s( 51.94%)p 0.93( 48.04%)d 0.00(  0.02%)
                            0.395%  C  4 s( 12.14%)p 6.87( 83.38%)d 0.37(  4.49%)
                            0.144%  C  5 s( 11.15%)p 7.88( 87.86%)d 0.09(  0.99%)
                            0.029%  C  6 s(  4.32%)p21.33( 92.19%)d 0.81(  3.49%)
                            0.016%  H  8 s( 99.16%)p 0.01(  0.84%)
                            0.161%  H  9 s( 99.52%)p 0.00(  0.48%)
                            0.027%  H 10 s( 95.85%)p 0.04(  4.15%)
                            0.071%  H 11 s( 97.71%)p 0.02(  2.29%)
   8. (2.00000)  LP ( 2)  O  3
                            0.424%  C  1 s( 65.75%)p 0.51( 33.28%)d 0.01(  0.98%)
                            1.220%  C  2 s(  0.61%)p99.99( 92.14%)d11.90(  7.25%)
                           96.543%  O  3 s(  4.26%)p22.44( 95.70%)d 0.01(  0.03%)
                            0.274%  C  4 s(  2.55%)p35.73( 91.12%)d 2.48(  6.33%)
                            0.341%  C  5 s( 15.29%)p 5.47( 83.59%)d 0.07(  1.12%)
                            0.187%  C  6 s(  3.89%)p24.66( 95.93%)d 0.05(  0.18%)
                            0.110%  H  7 s( 99.89%)p 0.00(  0.11%)
                            0.750%  H  9 s( 99.66%)p 0.00(  0.34%)
                            0.117%  H 10 s( 97.87%)p 0.02(  2.13%)
                            0.012%  H 14 s( 99.68%)p 0.00(  0.32%)
   9. (2.00000)  BD ( 1)  C  1- C  2
                           49.868%  C  1 s( 37.56%)p 1.66( 62.30%)d 0.00(  0.13%)
                           49.747%  C  2 s( 39.94%)p 1.50( 59.97%)d 0.00(  0.09%)
                            0.157%  O  3 s(  3.25%)p29.39( 95.54%)d 0.37(  1.21%)
                            0.029%  C  4 s(  5.37%)p17.49( 93.91%)d 0.13(  0.72%)
                            0.044%  C  5 s( 25.03%)p 2.98( 74.70%)d 0.01(  0.27%)
                            0.050%  C  6 s( 33.18%)p 2.00( 66.48%)d 0.01(  0.34%)
                            0.030%  H  7 s( 88.23%)p 0.13( 11.77%)
                            0.024%  H  8 s( 85.79%)p 0.17( 14.21%)
                            0.040%  H  9 s( 92.97%)p 0.08(  7.03%)
  10. (2.00000)  BD ( 2)  C  1- C  2
                           50.626%  C  1 s(  0.49%)p99.99( 99.45%)d 0.12(  0.06%)
                           41.752%  C  2 s(  0.20%)p99.99( 99.73%)d 0.33(  0.07%)
                            0.206%  O  3 s(  9.03%)p 9.63( 87.03%)d 0.44(  3.94%)
                            2.521%  C  4 s( 12.57%)p 6.95( 87.36%)d 0.01(  0.07%)
                            0.321%  C  5 s(  1.95%)p49.60( 96.84%)d 0.62(  1.21%)
                            4.506%  C  6 s(  1.00%)p98.93( 98.86%)d 0.14(  0.14%)
                            0.013%  H  7 s( 23.36%)p 3.28( 76.64%)
                            0.011%  H  9 s( 15.14%)p 5.60( 84.86%)
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                        0.013%  H 11 s( 95.42%)p 0.05(  4.58%)
                        0.016%  H 14 s( 70.13%)p 0.43( 29.87%)
11. (2.00000)  BD ( 1)  C  1- H  7
                       59.458%  C  1 s( 28.68%)p 2.48( 71.19%)d 0.00(  0.12%)
                        0.529%  C  2 s(  4.46%)p21.11( 94.17%)d 0.31(  1.37%)
                        0.196%  O  3 s( 36.68%)p 1.72( 63.04%)d 0.01(  0.28%)
                        0.015%  C  5 s( 11.28%)p 7.84( 88.36%)d 0.03(  0.36%)
                        0.013%  C  6 s(  1.93%)p49.69( 96.00%)d 1.07(  2.06%)
                       39.730%  H  7 s( 99.96%)p 0.00(  0.04%)
                        0.044%  H  9 s( 98.87%)p 0.01(  1.13%)
12. (2.00000)  BD ( 1)  C  1- H  8
                       59.795%  C  1 s( 29.75%)p 2.36( 70.13%)d 0.00(  0.12%)
                        0.480%  C  2 s(  2.95%)p32.60( 96.05%)d 0.34(  1.00%)
                        0.070%  O  3 s( 14.02%)p 6.11( 85.58%)d 0.03(  0.40%)
                        0.019%  C  5 s(  0.74%)p99.99( 96.74%)d 3.43(  2.52%)
                        0.038%  C  6 s(  5.90%)p15.31( 90.30%)d 0.64(  3.80%)
                        0.011%  H  7 s( 73.93%)p 0.35( 26.07%)
                       39.401%  H  8 s( 99.97%)p 0.00(  0.03%)
                        0.178%  H  9 s( 99.09%)p 0.01(  0.91%)
13. (2.00000)  BD ( 1)  C  2- O  3
                        0.112%  C  1 s(  1.63%)p59.91( 97.90%)d 0.29(  0.47%)
                       33.074%  C  2 s( 27.10%)p 2.68( 72.62%)d 0.01(  0.28%)
                       66.640%  O  3 s( 34.76%)p 1.87( 65.14%)d 0.00(  0.10%)
                        0.059%  C  4 s(  6.45%)p13.89( 89.59%)d 0.61(  3.96%)
                        0.013%  C  5 s( 36.36%)p 1.70( 61.94%)d 0.05(  1.70%)
                        0.060%  H  7 s( 99.37%)p 0.01(  0.63%)
                        0.011%  H  8 s( 96.43%)p 0.04(  3.57%)
                        0.012%  H 11 s( 98.31%)p 0.02(  1.69%)
14. (2.00000)  BD ( 1)  C  2- H  9
                        0.215%  C  1 s(  3.03%)p31.71( 96.23%)d 0.24(  0.74%)
                       57.552%  C  2 s( 30.13%)p 2.32( 69.75%)d 0.00(  0.13%)
                        0.149%  O  3 s(  7.43%)p12.24( 90.90%)d 0.22(  1.67%)
                        0.058%  C  4 s(  4.32%)p21.98( 94.93%)d 0.17(  0.75%)
                        0.012%  C  5 s( 43.28%)p 1.23( 53.10%)d 0.08(  3.62%)
                        0.015%  C  6 s( 14.67%)p 5.73( 84.07%)d 0.09(  1.26%)
                        0.026%  H  7 s( 98.53%)p 0.01(  1.47%)
                        0.375%  H  8 s( 99.89%)p 0.00(  0.11%)
                       41.586%  H  9 s( 99.96%)p 0.00(  0.04%)
15. (2.00000)  BD ( 1)  O  3- C  4
                        0.506%  C  1 s(  1.23%)p79.98( 98.59%)d 0.14(  0.17%)
                        4.077%  C  2 s(  1.03%)p94.90( 98.08%)d 0.85(  0.88%)
                       67.678%  O  3 s(  9.60%)p 9.42( 90.36%)d 0.00(  0.04%)
                       25.943%  C  4 s( 12.89%)p 6.75( 86.98%)d 0.01(  0.13%)
                        0.336%  C  5 s(  3.68%)p25.68( 94.51%)d 0.49(  1.80%)
                        1.396%  C  6 s(  0.89%)p99.99( 99.05%)d 0.07(  0.06%)
                        0.037%  H 10 s( 93.55%)p 0.07(  6.45%)
16. (2.00000)  BD ( 1)  C  4- C  5
                        0.030%  C  2 s( 36.00%)p 1.75( 62.85%)d 0.03(  1.15%)
                        0.062%  O  3 s(  5.80%)p15.90( 92.16%)d 0.35(  2.04%)
                       49.573%  C  4 s( 34.75%)p 1.87( 65.16%)d 0.00(  0.09%)
                       49.807%  C  5 s( 31.05%)p 2.22( 68.86%)d 0.00(  0.09%)
                        0.270%  C  6 s(  1.84%)p52.92( 97.26%)d 0.49(  0.90%)
                        0.016%  H 10 s( 82.06%)p 0.22( 17.94%)
                        0.017%  H 11 s( 83.48%)p 0.20( 16.52%)
                        0.027%  H 12 s( 86.26%)p 0.16( 13.74%)
                        0.159%  H 13 s( 99.62%)p 0.00(  0.38%)
                        0.028%  H 14 s( 98.70%)p 0.01(  1.30%)
17. (2.00000)  BD ( 1)  C  4- H 10
                        0.020%  C  2 s(  6.40%)p13.73( 87.92%)d 0.89(  5.67%)
                        0.050%  O  3 s( 13.26%)p 6.25( 82.85%)d 0.29(  3.89%)
                       59.260%  C  4 s( 27.31%)p 2.66( 72.54%)d 0.01(  0.14%)
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                         0.223%  C  5 s(  2.94%)p32.43( 95.30%)d 0.60(  1.76%)
                         0.069%  C  6 s( 21.59%)p 3.56( 76.98%)d 0.07(  1.43%)
                        40.097%  H 10 s( 99.96%)p 0.00(  0.04%)
                         0.251%  H 12 s( 99.69%)p 0.00(  0.31%)
18. (2.00000)  BD ( 1)  C  4- H 11
                         0.026%  C  1 s(  1.26%)p78.28( 98.31%)d 0.34(  0.43%)
                         0.090%  C  2 s( 21.85%)p 3.49( 76.33%)d 0.08(  1.82%)
                         0.060%  O  3 s( 44.19%)p 1.16( 51.20%)d 0.10(  4.61%)
                        60.011%  C  4 s( 27.24%)p 2.67( 72.62%)d 0.01(  0.14%)
                         0.221%  C  5 s(  3.58%)p26.44( 94.72%)d 0.47(  1.70%)
                         0.141%  C  6 s( 46.11%)p 1.14( 52.76%)d 0.02(  1.13%)
                         0.011%  H 10 s( 75.72%)p 0.32( 24.28%)
                        39.361%  H 11 s( 99.96%)p 0.00(  0.04%)
                         0.054%  H 12 s( 99.41%)p 0.01(  0.59%)
                         0.017%  H 13 s( 99.82%)p 0.00(  0.18%)
19. (2.00000)  BD ( 1)  C  5- C  6
                         0.034%  C  1 s( 29.81%)p 2.34( 69.84%)d 0.01(  0.36%)
                         0.012%  C  2 s( 45.94%)p 1.16( 53.47%)d 0.01(  0.58%)
                         0.215%  C  4 s(  3.14%)p30.39( 95.43%)d 0.45(  1.43%)
                        50.698%  C  5 s( 34.98%)p 1.86( 64.92%)d 0.00(  0.10%)
                        48.818%  C  6 s( 37.85%)p 1.64( 62.04%)d 0.00(  0.11%)
                         0.018%  H 10 s( 97.81%)p 0.02(  2.19%)
                         0.077%  H 11 s( 99.11%)p 0.01(  0.89%)
                         0.060%  H 12 s( 91.22%)p 0.10(  8.78%)
                         0.034%  H 13 s( 88.21%)p 0.13( 11.79%)
                         0.022%  H 14 s( 81.86%)p 0.22( 18.14%)
20. (2.00000)  BD ( 2)  C  5- C  6
                         0.111%  C  1 s(  9.98%)p 8.47( 84.53%)d 0.55(  5.49%)
                         1.387%  C  2 s(  1.39%)p70.69( 98.38%)d 0.16(  0.23%)
                         0.610%  O  3 s( 24.51%)p 3.07( 75.20%)d 0.01(  0.29%)
                         5.824%  C  4 s(  6.16%)p15.16( 93.43%)d 0.07(  0.40%)
                        51.543%  C  5 s(  0.18%)p99.99( 99.78%)d 0.26(  0.05%)
                        40.363%  C  6 s(  0.83%)p99.99( 99.09%)d 0.09(  0.08%)
                         0.013%  H  8 s( 88.01%)p 0.14( 11.99%)
                         0.073%  H 10 s( 97.28%)p 0.03(  2.72%)
                         0.035%  H 11 s( 97.93%)p 0.02(  2.07%)
                         0.015%  H 12 s( 45.43%)p 1.20( 54.57%)
21. (2.00000)  BD ( 1)  C  5- H 12
                         0.294%  C  4 s(  4.18%)p22.63( 94.53%)d 0.31(  1.30%)
                        59.715%  C  5 s( 26.17%)p 2.82( 73.71%)d 0.00(  0.11%)
                         0.440%  C  6 s(  2.23%)p43.49( 97.09%)d 0.30(  0.67%)
                         0.151%  H 10 s( 99.56%)p 0.00(  0.44%)
                         0.051%  H 11 s( 99.16%)p 0.01(  0.84%)
                        39.054%  H 12 s( 99.97%)p 0.00(  0.03%)
                         0.062%  H 13 s( 99.29%)p 0.01(  0.71%)
                         0.216%  H 14 s( 99.74%)p 0.00(  0.26%)
22. (2.00000)  BD ( 1)  C  6- H 13
                         0.029%  C  1 s(  5.02%)p18.55( 93.05%)d 0.39(  1.93%)
                         0.041%  C  2 s(  2.70%)p35.84( 96.90%)d 0.15(  0.39%)
                         0.181%  C  4 s( 39.37%)p 1.51( 59.61%)d 0.03(  1.02%)
                         0.338%  C  5 s(  1.28%)p76.14( 97.59%)d 0.88(  1.13%)
                        59.744%  C  6 s( 28.59%)p 2.49( 71.28%)d 0.00(  0.13%)
                         0.012%  H 11 s( 99.49%)p 0.01(  0.51%)
                         0.075%  H 12 s( 99.65%)p 0.00(  0.35%)
                        39.554%  H 13 s( 99.96%)p 0.00(  0.04%)
                         0.011%  H 14 s( 75.80%)p 0.32( 24.20%)
23. (2.00000)  BD ( 1)  C  6- H 14
                         0.014%  C  1 s( 15.46%)p 5.05( 78.00%)d 0.42(  6.55%)
                         0.050%  C  4 s( 29.60%)p 2.31( 68.28%)d 0.07(  2.12%)
                         0.251%  C  5 s(  5.68%)p16.32( 92.77%)d 0.27(  1.54%)
                        59.336%  C  6 s( 28.99%)p 2.45( 70.88%)d 0.00(  0.13%)
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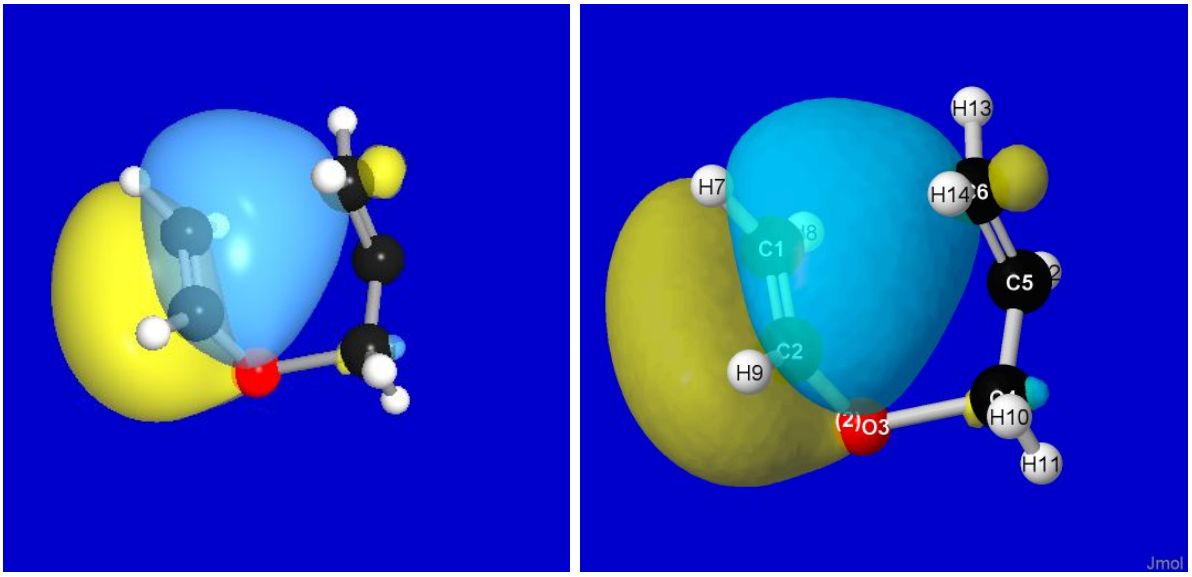
```
 0.375%  H 12 s( 99.63%)p 0.00(  0.37%)
 0.011%  H 13 s( 74.46%)p 0.34( 25.54%)
39.938%  H 14 s( 99.96%)p 0.00(  0.04%)
```

The final “claisen_55.bmp” image file is shown below (with corresponding *Jmol* rendering and atom numbering at the right):



As quantified in the RNBO output above, RNBO 10 has noticeable multi-center contributions at atoms C6 (4.5%) and C4 (2.5%) as well as the primary contributions at atoms C1 (50.6%) and C2 (41.8%).

References

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(2) Weinhold, F.; Phillips, D.; Foo, Z. Y.; Glendening, E. D.; Hanson, R. M. *NBOPro@Jmol*, Theoretical Chemistry Institute, University of Wisconsin-Madison, Madison WI, 2018.