```
hydrogen-GS>matlab

                    < M A T L A B (R) >
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  To get started, type one of these commands: helpwin, helpdesk, or demo.
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>> H =[ 0 1; 1 0]
H =
     0     1
     1     0                              Ethylene

>> [C,E]=eig(H)
C =
    0.7071    0.7071
   -0.7071    0.7071
E =
   -1.0000         0
         0    1.0000
--------------------------------------------------------------------------------

>> H=[0 1 0; 1 0 1; 0 1 0]
H =
     0     1     0
     1     0     1                        Allyl
     0     1     0

>> [C,E]=eig(H)
C =
    0.5000   -0.7071   -0.5000
    0.7071    0.0000    0.7071
    0.5000    0.7071   -0.5000
E =
    1.4142         0         0
         0    0.0000         0
         0         0   -1.4142
>> H= [0 1 1 1 ; 1 0 0 0; 1 0 0 0; 1 0 0 0]
```

```
H =

     0     1     1     1
     1     0     0     0
     1     0     0     0
     1     0     0     0                    Trimethylenemethane
>> [C,E]=eig(H)
C =
         0       -0.7071   -0.0000    0.7071
    -0.7071   -0.4082    0.4082   -0.4082
     0.7071   -0.4082    0.4082   -0.4082
         0       -0.4082   -0.8165   -0.4082
E =
         0         0         0         0
         0    1.7321         0         0
         0         0         0         0
         0         0         0   -1.7321
--------------------------------------------------------------------------------
>> H = [0 1 0 0 0 1; 1 0 1 0 0 0; 0 1 0 1 0 0; 0 0 1 0 1 0; 0 0 0 1 0 1; 1 0 0 0 1 0]
H =
     0     1     0     0     0     1
     1     0     1     0     0     0
     0     1     0     1     0     0
     0     0     1     0     1     0                          Benzene
     0     0     0     1     0     1
     1     0     0     0     1     0
>> [C,E]=eig(H)
          C =
    -0.5000   -0.5000   -0.2887   -0.4082    0.2887    0.4082
    -0.5000    0.5000   -0.2887    0.4082   -0.2887    0.4082
     0.0000    0.0000    0.5774   -0.4082   -0.5774    0.4082
     0.5000   -0.5000   -0.2887    0.4082   -0.2887    0.4082
     0.5000    0.5000   -0.2887   -0.4082    0.2887    0.4082
         0         0         0.5774    0.4082    0.5774    0.4082
E =
    1.0000         0         0         0         0         0
         0   -1.0000         0         0         0         0
         0         0   -1.0000         0         0         0
         0         0         0   -2.0000         0         0
         0         0         0         0    1.0000         0
         0         0         0         0         0    2.0000
>> H=[0 1 1 ; 1 0 1; 1 1 0]
```

```
H =
     0     1     1
     1     0     1                                        #cyclopropenyl
     1     1     0
>> [C,E]=eig(H)                                          #diagonalize cyclopropenyl
C =
   -0.6133    0.5390    0.5774
    0.7734    0.2616    0.5774
   -0.1601   -0.8006    0.5774
E =
   -1.0000         0         0
         0   -1.0000         0
         0         0    2.0000
>> C1P=C(1,2)*C(:,1)-C(1,1)*C(:,2)      # C(:,1) and C(:,2) are degenerate
 C1P=                                      # pick a combo which has zero on atom #1
         0                                 # C1P= a * C(:,1) - b* C(:,2)
    0.5774
   -0.5774
>> C1P=C1P/norm(C1P)
C1P =
         0
    0.7071                 #normalize C2P this combo
   -0.7071
>> C2P=C(:,1)+C(:,2)*(C(1,2)/C(1,1))   #get second combo orthognal to first
C2P =
  -1.0870                  # C2P=  C(:,1) + c * C(:,2)       .
    0.5435                 # where (a/b)= - c guaranties orthog
    0.5435
>> C2P=C2P/norm(C2P)                                                              # normalize
C2P second new mo
C2p =
   -0.8165
    0.4082
    0.4082
>> CP= [ C1P C2P C(:,3)]               # make a new matrix with mo columns
CP =                                   # C1P C2P and C(:,3) original non-degenerate
         0       -0.8165    0.5774     # m.o.
    0.7071    0.4082    0.5774
   -0.7071    0.4082    0.5774
>> CP*CP'                               #check to see if this combo is
ans =                                   #unitary (orthonormal)

    1.0000   -0.0000         0
   -0.0000    1.0000   -0.0000
         0   -0.0000    1.0000
```