LiH CNDO Calculations

charge=0 multiplicity=1
filled alpha orbitals=1

_____Atomic Coordinates (Å)_____

Atom	x	y	z
1 Li	0.0	0.0	0.0
2 H	1.61	0.0	0.0

Coulombic repulsion integrals (bottom triangle)(a.u.)
_____ and internuclear distances (top triangle)(a.u.)_____

Atoms:	1 Li	2 H
1Li	0.2361	3.0425
2 H	0.254	0.75

_____ Overlap Matrix _____

	1 Li2s	1 Li2px	1 Li2py	1 Li2pz	2 H1s
1 Li2s	1.0	0.0	0.0	0.0	0.3917
1 Li2px	0.0	1.0	0.0	0.0	0.5051
1 Li2py	0.0	0.0	1.0	0.0	0.0
1 Li2pz	0.0	0.0	0.0	1.0	0.0
2 H1s	0.3917	0.5051	0.0	0.0	1.0

SCF eigenvalues (a.u.) and eigenvectors
_____(eigenvectors listed in columns)_____

E(i)	-0.4818	0.0322	0.0767	0.0767	0.2186
vector	1	2	3	4	5
atom:					
1 Li2s	0.424	0.8225	0.0	0.0	0.379
1 Li2px	0.429	-0.551	0.0	0.0	0.7158
1 Li2py	0.0	0.0	0.0	1.0	0.0
1 Li2pz	0.0	0.0	1.0	0.0	0.0
2 H1s	0.7976	-0.1409	0.0	0.0	-0.5865

_____SCF Population matrix_____

	1 Li2s	1 Li2px	1 Li2py	1 Li2pz	2 H1s
1 Li2s	0.3596	0.3638	0.0	0.0	0.6764
1 Li2px	0.3638	0.3681	0.0	0.0	0.6843
1 Li2py	0.0	0.0	0.0	0.0	0.0
1 Li2pz	0.0	0.0	0.0	0.0	0.0
2 H1s	0.6764	0.6843	0.0	0.0	1.2724

_____Total Bond Order (including overlap integrals)_____

Atoms:	1 Li
2 H	0.611

Electronic energy = -1.4162 a.u.
Total energy = -1.0875 a.u.
= -29.5923 eV
= -682.421 kcal/mol
= -2855.203 kJ/mol
(the total energy includes nuclear-nuclear repulsion)
Total bond dissociation energy, Do = 9.0279 eV = 871.059 kJ/mol

Total atom electron densities and atomic charges

atom	density	charge
1 Li	0.7276	0.272
2 H	1.2724	-0.272

Dipole from atom densities

x	y	z
-2.11	0.0	0.0

Complete dipole (including atomic polarization)

x	y	z
-6.21	0.0	0.0

H_2O – Bent: 90 deg.

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charge=0   multiplicity=1
filled alpha orbitals=4

_______Atomic Coordinates (Å)______
Atom      x       y       z
 1  O   0.0     0.0     0.0
 2  H   0.96    0.0     0.0
 3  H  -0.0     0.96    0.0

        Coulombic repulsion integrals (bottom triangle)(a.u.)
_________ and internuclear distances (top triangle)(a.u.)_________
Atoms:  1  O    2  H    3  H
 1 O   0.8265  1.8142  1.8142
 2 H   0.4999  0.75    2.5656
 3 H   0.4999  0.3756  0.75

_____________________________________ Overlap Matrix _____________________________________
          1  O2s    1  O2px   1  O2py   1  O2pz   2  H1s    3  H1s
 1  O2s    1.0       0.0       0.0       0.0       0.4777    0.4777
 1  O2px   0.0       1.0       0.0       0.0       0.382    -0.0
 1  O2py   0.0       0.0       1.0       0.0       0.0       0.382
 1  O2pz   0.0       0.0       0.0       1.0       0.0       0.0
 2  H1s    0.4777    0.382     0.0       0.0       1.0       0.3331
 3  H1s    0.4777   -0.0       0.382     0.0       0.3331    1.0
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                      SCF eigenvalues (a.u.) and eigenvectors
_____________________________(eigenvectors listed in columns)_____________________________

E(i)    -1.498    -0.755    -0.7378   -0.657     0.319     0.3557
vector     1         2         3         4         5         6
atom:
 1  O2s    0.8547   -0.0      -0.3547    0.0      -0.0      -0.3791
 1  O2px   0.0623   -0.5498    0.579     0.0       0.4447   -0.4012
 1  O2py   0.0623    0.5498    0.579     0.0      -0.4447   -0.4012
 1  O2pz   0.0       0.0       0.0       1.0       0.0       0.0
 2  H1s    0.3617   -0.4447    0.3192    0.0      -0.5498    0.5169
 3  H1s    0.3617    0.4447    0.3192    0.0       0.5498    0.5169
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_____________________________SCF Population matrix_____________________________________
          1  O2s    1  O2px   1  O2py   1  O2pz   2  H1s    3  H1s
 1  O2s    1.7126   -0.3041   -0.3041    0.0       0.3919    0.3919
 1  O2px  -0.3041    1.2827    0.0736    0.0       0.9037   -0.0742
 1  O2py  -0.3041    0.0736    1.2827    0.0      -0.0742    0.9037
 1  O2pz   0.0       0.0       0.0       2.0       0.0       0.0
 2  H1s    0.3919    0.9037   -0.0742    0.0       0.861     0.0701
 3  H1s    0.3919   -0.0742    0.9037    0.0       0.0701    0.861
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_____________________________Total Bond Order (including overlap integrals)_______________
Atoms:  1  O   2  H
 2  H   0.532
 3  H   0.532  0.023

Electronic energy = -26.8647 a.u.
Total energy =   -19.8604 a.u.
             =  -540.4322 eV
             = -12462.775 kcal/mol
             = -52143.382 kJ/mol
  (the total energy includes nuclear-nuclear repulsion)
Total bond dissociation energy, Do = 19.6869 eV = 1899.494 kJ/mol

Total atom electron densities and atomic charges
atom   density   charge
 1  O  6.2781   -0.278
 2  H  0.861     0.139
 3  H  0.861     0.139

Dipole from atom densities
    x      y      z
   0.64   0.64   0.0

Complete dipole (including atomic polarization)
    x      y      z
   1.62   1.62   0.0
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H_2O – Linear: 180deg.

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charge=0   multiplicity=1
filled alpha orbitals=4

_______Atomic Coordinates (Å)______
Atom      x       y       z
 1  O   0.0     0.0     0.0
 2  H   0.96    0.0     0.0
 3  H  -0.96   -0.0     0.0

        Coulombic repulsion integrals (bottom triangle)(a.u.)
_________ and internuclear distances (top triangle)(a.u.)_________
Atoms:  1  O    2  H    3  H
 1 O   0.8265  1.8142  1.8142
 2 H   0.4999  0.75    3.6283
 3 H   0.4999  0.274   0.75

_____________________________________ Overlap Matrix _____________________________________
          1  O2s    1  O2px   1  O2py   1  O2pz   2  H1s    3  H1s
 1  O2s    1.0       0.0       0.0       0.0       0.4777    0.4777
 1  O2px   0.0       1.0       0.0       0.0       0.382    -0.382
 1  O2py   0.0       0.0       1.0       0.0       0.0      -0.0
 1  O2pz   0.0       0.0       0.0       1.0       0.0       0.0
 2  H1s    0.4777    0.382     0.0       0.0       1.0       0.1501
 3  H1s    0.4777   -0.382    -0.0       0.0       0.1501    1.0
_____________________________________________________________________________________

                      SCF eigenvalues (a.u.) and eigenvectors
_____________________________(eigenvectors listed in columns)_____________________________

E(i)    -1.3959   -0.8174   -0.5872   -0.5872    0.2322    0.4767
vector     1         2         3         4         5         6
atom:
 1  O2s    0.8585   -0.0       0.0       0.0      -0.5127   -0.0
 1  O2px  -0.0       0.7134    0.0       0.0      -0.0      -0.7008
 1  O2py   0.0       0.0       0.0       1.0       0.0       0.0
 1  O2pz   0.0       0.0       1.0       0.0       0.0       0.0
 2  H1s    0.3626    0.4955    0.0       0.0       0.6071    0.5044
 3  H1s    0.3626   -0.4955    0.0       0.0       0.6071   -0.5044
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_________________________________SCF Population matrix_________________________________
          1  O2s    1  O2px   1  O2py   1  O2pz   2  H1s    3  H1s
 1  O2s    1.4742   -0.0       0.0       0.0       0.6226    0.6226
 1  O2px  -0.0       1.0178    0.0       0.0       0.707    -0.707
 1  O2py   0.0       0.0       2.0       0.0       0.0       0.0
 1  O2pz   0.0       0.0       0.0       2.0       0.0       0.0
 2  H1s    0.6226    0.707     0.0       0.0       0.754    -0.2282
 3  H1s    0.6226   -0.707     0.0       0.0      -0.2282    0.754
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_____________________________Total Bond Order (including overlap integrals)_____________
Atoms:  1  O   2  H
 2  H   0.567
 3  H   0.567 -0.034

Electronic energy = -26.6887 a.u.
Total energy =   -19.7985 a.u.
             =  -538.7496 eV
             = -12423.971 kcal/mol
             = -51981.031 kJ/mol
  (the total energy includes nuclear-nuclear repulsion)
Total bond dissociation energy, Do = 18.0043 eV = 1737.142 kJ/mol

Total atom electron densities and atomic charges
atom   density   charge
 1  O  6.492    -0.492
 2  H  0.754     0.246
 3  H  0.754     0.246

Dipole from atom densities
    x      y      z
  -0.0   -0.0    0.0

Complete dipole (including atomic polarization)
    x      y      z
  -0.0   -0.0    0.0
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http://www.colby.edu/chemistry/PChem/scripts/cndo.html

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