Data file for LiH:

2 *number of atoms*

LiH

Li 0.000 0.00 0.00

H 1.610 0.00 0.00

1H = 2625.5 kJ/mol

1H = 627.52 kcal/mol

1H = 27.2116 eV

1H = 219,476.6 cm^{-1}

Output file for LiH

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

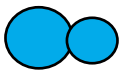
Atoms: 1 Li 2 H

1 Li 0.2361 3.0425 *3.043*0.529Å = 1.61Å*

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	0.392
1 Li2px	0.0	1.0	0.0	0.0	0.505
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	0.392	0.505	0.0	0.0	1.0

$\int$  $d\tau = 0.392$

2s 1s

Li H

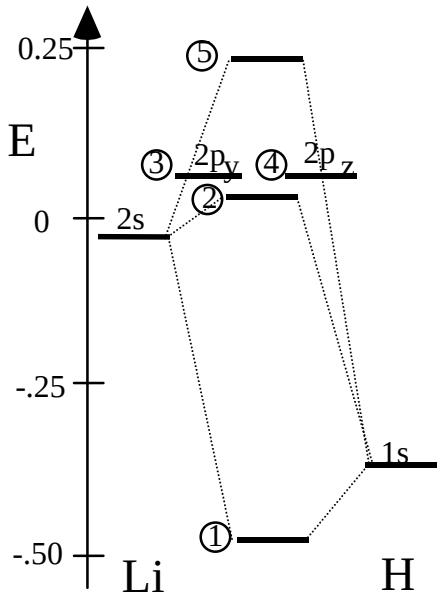
$\int$  $d\tau = 0.505$

$2p_x$ 1s

Li H

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
1 Li2s	0.424	0.823	0.0	0.0	0.379
1 Li2p_x	0.429	-0.551	0.0	0.0	0.716
1 Li2p_y	0.0	0.0	0.0	1.000	0.0
1 Li2p_z	0.0	0.0	1.000	0.0	0. 0
2 H1s	0.798	-0.141	0.0	0.0	-0.587



$\sigma_1 = 0.424\ 2s(Li) + 0.429\ 2p_x(Li) + 0.798\ 1s(H)$

$\sigma_2 = 0.823\ 2s(Li) - 0.551\ 2p_x(Li) - 0.141\ 1s(H)$

$$\text{fraction ionic} = \frac{\text{H coefficients}^2 - \text{Li coefficients}^2}{\text{H coefficients}^2 + \text{Li coefficients}^2}$$

$$\text{fraction ionic} = \frac{(0.798)^2 - (0.424)^2 - (0.429)^2}{(0.798)^2 + (0.424)^2 + (0.429)^2} = 0.272 = 27.2\% \quad Li^+ H^-$$

c_{ij} = coefficient for MO i and atomic orbital j

Electron Density *(CNDO version)*

$$d_a = \sum_{j \text{ on } a} \sum_{i=1}^{m} n_i \, c_{ij}^2$$

for atom a and MO i with n_i electrons

all MO's

j = all atomic orbitals on atom a

Bond Order

$$P_{ab} = \sum_{j \text{ on } a} \sum_{k \text{ on } b} \sum_{i=1}^{m} n_i \, 2 \, c_{ij} \, c_{ik} \, S_{jk}$$

for atoms a and b and MO i with n_i electrons

all MO's

j = all atomic orbitals on atom a

k = all atomic orbitals on atom b

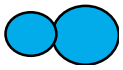
_____SCF Population Matrix_____

Sums over all MO's (but in this case only one MO is occupied)

k \ j	1 Li2s	1 Li2px	1 Li2py	1 Li2pz	2 H1s
	$c_{2s,Li}^2 * 2$	$c_{2s,Li} * c_{2px,Li} * 2$			$c_{2s,Li} * c_{1s,H} * 2$
1 Li2s	0.3596	0.3638	0.	0.	0.6764
	$c_{2px,Li} * c_{2s,Li} * 2$	$c_{2px}^2 * 2$			$c_{2px,Li} * c_{1s,H} * 2$
1 Li2px	0.3638	0.3681	0.	0.	0.6843
1 Li2py	0.	0.	0.	0.	0.
1 Li2pz	0.	0.	0.	0.	0.
	$c_{1s,H} * c_{2s,Li} * 2$	$c_{1s,H} * c_{2px,Li} * 2$			$c_{1s,H}^2 * 2$
2 H1s	0.6764	0.6843	0.	0.	1.272

Bond Orders with Overlap Included

Only one filled orbital, with two orbitals on Li



(with the size of the orbital ∝ orbital coefficient)

$c_{2s,Li} * c_{1s,H} * S_{2s,Li;1s,H} * 4 = 0.6764 * 0.392 = 0.530$

\+

$c_{2px,Li} * c_{1s,H} * S_{2s,Li;1s,H} * 4 = 0.6843 * 0.505 = 0.692$

1.222

Electronic energy = -1.4162 a.u. *in Hartrees*

Total energy = -1.0875 a.u. *in Hartrees with nuclear repulsion*

= -29.5923 eV *-1.0875*627.52 kcal/mol = -682.43 kcal/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	*sum of diagonal entries in bond order matrix*
1 Li	0.728	0.272	*electron density = $(c_{2s,Li}^2 + c_{2px,Li}^2)*2$*
2 H	1.272	-0.272	*electron density = $c_{1s,H}^2*2$ net negative charge on H of –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