Ionic vs. Covalent Charge Distributions

Concept. You will optimize the structures of some di-, tri-, and tetra-atomic molecules, and examine their Mulliken charge distributions, and compare to expectations for ionic vs. covalent behavior in the periodic table of elements.

Procedure. Use RHF/6-31G* methodology to build and optimize LiH, LiF, LiI, NaH, NaF, NaI, BeH_2, OH_2, OF_2, NH_3, NF_3, SO_2, FH, CO_2. Record the Mulliken charge distributions in the results section. Do the results correlate with your expectations based upon the periodic table of elements? The dipole moments for diatomics can be computed compared to experimental results from the literature.

Literature. Periodic table from standard texts have electronegativities. NIST and related THEOCHEM databases are most likely to have dipole data.

MOLECULE	CHARGE 1	CHARGE 2	CHARGE 3	CHARGE 4	DIPOLE	Exptl DIPOLE
Li(-)H(+)						
LiF						
LiI						
NaH						
NaF						
NaI						
BeH_2						
OH_2						
H_3N						
F_3N						
FH						
CO_2						
SO_2						