

# Calculated Mulliken Charges Using Different Pople Basis Sets

## Example Lithium Fluoride: Li-F

### Input

#P HF/STO-3G scf=tight

LiF: HF/STO-3G// HF/STO-3G

0 1

Li

F 1 1.3

Mulliken $q(\text{Li})/e$	Basis set
0.224096	STO-3G
0.702147	4-31G
0.726539	6-31G
0.614487	6-31G(d)
0.591135	6-311G(d)
0.567779	6-311+G(d)
0.643234	6-311+G(3df)
<b>NBO charge <math>q(\text{Li})/e</math></b>	
<b>0.96338</b>	6-311+G(3df)

Mulliken population analysis displays an **overestimation of the covalent character** of a bond and is **unduly sensitive to basis sets**.