

### *Ab Initio* SCF Atomic Energies

	HF	MP2	B3LYP	B3LYP	B3LYP
	6-31G*	6-311G*	6-311G*	6-311+G*	cc-pVTZ
H	-0.4982329	-0.499809811	-0.502155915	-0.502155915	-0.5021563
Li	-7.4313723	-7.4320264	-7.4912968	-7.4913333	-7.4920159
Be	-14.5669444	-14.5985691	-14.6711842	-14.6713141	-14.6724455
B	-24.5220372	-24.5693278	-24.6618695	-24.6624669	-24.6637586
C	-37.6808603	-37.74502322	-37.8559888	-37.8572669	-37.8585746
N	-54.3854425	-54.4750512	-54.5985435	-54.6007232	-54.601781
O	-74.7839336	-74.9181455	-75.0853748	-75.0898713	-75.0918572
F	-99.3649569	-99.5541705	-99.7538101	-99.7605798	-99.7628675
Na	-161.841435	-161.845926	-162.286694	-162.286844	-162.296912
Mg	-199.5956109	-199.606556	-200.093098	-200.0932688	-200.0976386
Si	-288.8317857	-288.8921959	-289.393806	-289.3941537	-289.3963273
P	-340.6902044	-340.7671703	-341.2804859	-341.281716	-341.2858577
S	-397.4759577	-397.5807253	-398.1320492	-398.1330364	-398.1386911
Cl	-459.4479641	-459.5851374	-460.1661563	-460.1668773	-460.1746898

To Paste this data into Excel: Copy the values, without the column headings, onto the clipboard. In Excel pull down the “Paste” menu and choose “Use Text Import Wizard.” Choose the space delimited file type:

