Potential energy tables for HF molecule using different approximation methods

All the energies are in Hartrees and distances are in bohr units.

Distances	RHF	MP2	CCSD	CCSD(T)	CR-CC(2,3),D
0.8660	-98.98448	-99.07195	-99.07560	-99.07688	-99.07674
1.2996	-99.90504	-100.00983	-100.01260	-100.01378	-100.01364
1.7328	-100.02189	-100.14218	-100.14425	-100.14553	-100.14536
2.1660	-99.98552	-100.11929	-100.12161	-100.12320	-100.12297
2.5992	-99.92428	-100.07038	-100.07462	-100.07686	-100.07647
3.0324	-99.86585	-100.02426	-100.03254	-100.03601	-100.03521
3.4656	-99.81543	-99.98691	-100.00138	-100.00724	-100.00531
4.3320	-99.73865	-99.94032	-99.96941	-99.98605	-99.97657
5.1984	----------	----------	----------	----------	----------
6.9312	-99.63301	-99.96373	-99.68169	-99.67928	-99.68121
8.6630	----------	----------	----------	----------	----------

All the energies are in Hartrees and distances are in bohr units.

Distances	MP2 Correlation	CCSD Correlation	CCSD(T) Correlation	CR-CC(2,3),D Correlation
0.8660	-0.0874761567	-0.0911253629	-0.0924007539	-0.0922634839
1.2996	-0.1047928063	-0.1075694846	-0.1087485185	-0.1086026626
1.7328	-0.1202865355	-0.1223639867	-0.1236375493	-0.1234665160
2.1660	-0.1337690077	-0.1376847933	-0.1376091310	-0.1374544581
2.5992	-0.1461042056	-0.1503442316	-0.1525791441	-0.1521966298
3.0324	-0.1584097783	-0.1666890006	-0.1701573586	-0.1693555929
3.4656	-0.1714741740	-0.1859506827	-0.1918111421	-0.1898784876
4.3320	-0.2016714657	-0.2307652924	-0.2474046177	-0.2379197293
5.1984	----------	----------	----------	----------
6.9312	-0.3307133472	-0.0486789777	-0.0462634229	-0.0481997819
8.6630	----------	----------	----------	----------

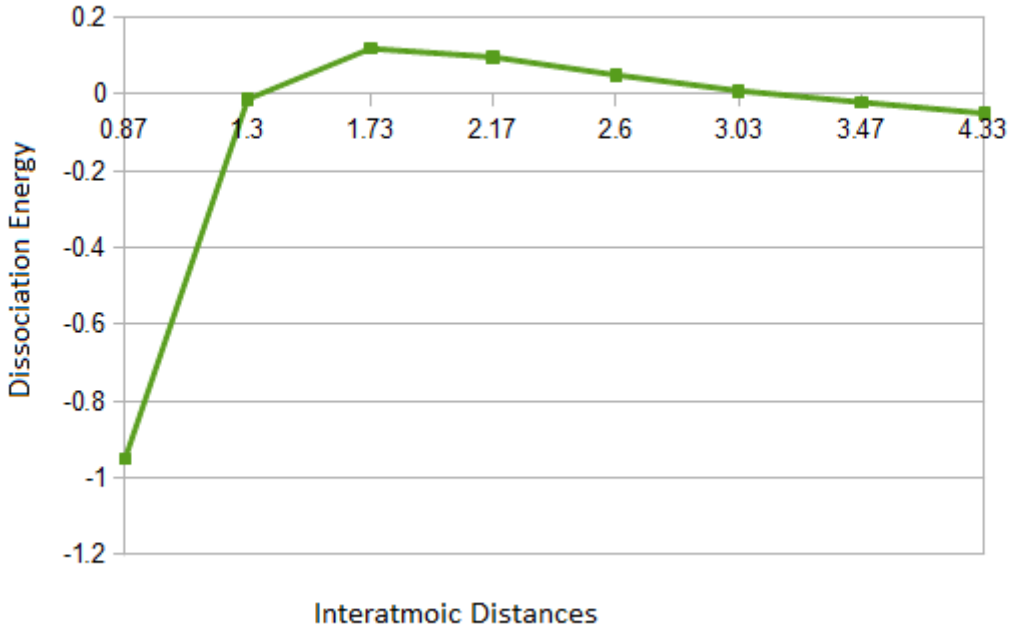
Dissociation energy calculations

Energy(Hartree) of Fluorine atom CR-CC(2,3),D = -99.5280620789

Energy(Hartree) of Hydrogen atom CR-CC(2,3),D = -0.4981890197

All the energies are in Hartrees and distances are in bohr units.

Distances	HF (CR-CC(2,3),D)	Dissociation Energy
0.8660	-99.07674	0.949511099
1.2996	-100.01364	0.012611098
1.7328	-100.14536	-0.119108901
2.1660	-100.12297	-0.096718901
2.5992	-100.07647	-0.050218901
3.0324	-100.03521	-0.008958901
3.4656	-100.00531	0.020941098
4.3320	-99.97657	0.049681098



Dissociation curve for CR-CC(2,3),D.

Best estimate for the energy of the system at internuclear distance R_e is for CR-CC(2,3),D which is equal to -100.14536 Hartrees.

Dissociation energy for the best approximation is -0.119108901 Hartrees and yes this is the lowest energy found.

RHF is a variational method.
MP-2 on the other hand improves the RHF method by adding electron co-relation effects effects by means of perturabation method. Hence Mp-2 is not a variational method.

CCSD, CCSD(T), and CR-CC(2,3),D are also improvement over the RHF thoery. These are also not variational methods. These methods takes the basic RHF molecular orbitals method and constructs multi-electron wavefunctions using the exponential cluster operator to account for electron co-relation. CCSD(T) and CR-CC(2,3),D differs from the CCSD due to the fact that they are more accurate methods and require more computational power than CCSD but they use the same construction of electron co-realtions and hence have a lot of similarties.