

Energias retiradas de arquivos de saídas do programa Gaussian 03 para o átomo de Hidrogênio.
 KE = *Electronic Kinetic Energy* ; PE = *Electron-Nuclear Attraction Energy* ; EE = *Ecoulomb + Exchange*)

		KE	PE	EE
B3LYP	3-21G**	0,518059	-1,014250	-1,129891E-03
	6-31G**	0,513503	-1,011729	-2,047245E-03
	6-31++G**	0,498085	-0,996605	-3,145481E-03
	6-311G**	0,498341	-0,997828	-2,668522E-03
	6-311++G**	0,496411	-0,995823	-2,845063E-03
	cc-pvdz	0,495764	-0,994975	-1,986446E-03
	cc-pvtz	0,498334	-0,997822	-2,669013E-03
	cc-pvqz	0,497928	-0,997511	-2,763643E-03
	cc-pv5z	0,497471	-0,997070	-2,829651E-03
	BLYP	3-21G**	0,528430	-1,016607
6-31G**		0,515938	-1,014151	2,766381E-03
6-31++G**		0,498696	-0,996949	1,037690E-03
6-311G**		0,499566	-0,998808	1,686867E-03
6-311++G**		0,496952	-0,996049	1,374840E-03
cc-pvdz		0,495897	-0,995169	2,868820E-03
cc-pvtz		0,499559	-0,998801	1,686156E-03
cc-pvqz		0,498939	-0,998242	1,522425E-03
cc-pv5z		0,498232	-0,997519	1,398558E-03
PBE/PBE		3-21G**	0,518341	-1,014531
	6-31G**	0,513585	-1,011811	7,944044E-04
	6-31++G**	0,496559	-0,994835	-9,106110E-04
	6-311G**	0,496898	-0,996259	-2,574775E-04
	6-311++G**	0,494060	-0,993249	-6,233100E-04
	cc-pvdz	0,493871	-0,993133	6,348172E-04
	cc-pvtz	0,496890	-0,996251	-2,582264E-04
	cc-pvqz	0,495950	-0,995353	-4,507412E-04
	cc-pv5z	0,495083	-0,994454	-5,995253E-04
	SVWN	3-21G**	0,495312	-0,991271
6-31G**		0,488417	-0,986384	4,030058E-03
6-31++G**		0,470541	-0,988651	2,435763E-03
6-311G**		0,471122	-0,970190	2,954973E-03
6-311++G**		0,468872	-0,967845	2,732614E-03
cc-pvdz		0,470415	-0,969232	3,536010E-03
cc-pvtz		0,471115	-0,970183	2,954313E-03
cc-pvqz		0,470403	-0,969554	2,845127E-03
cc-pv5z		0,469814	-0,968972	2,787331E-03
HFS		3-21G**	0,488105	-0,983843
	6-31G**	0,480002	-0,977713	4,368308E-02
	6-31++G**	0,457923	-0,955320	4,101163E-02
	6-311G**	0,459842	-0,958315	4,179369E-02
	6-311++G**	0,456340	-0,954561	4,130250E-02
	cc-pvdz	0,459718	-0,958117	4,272920E-02
	cc-pvtz	0,459833	-0,958306	4,179262E-02
	cc-pvqz	0,458559	-0,957053	4,157372E-02
	cc-pv5z	0,457526	-0,955972	4,140190E-02

		KE	PE	EE	EE= em 64bits	Hello - 64bits
HF	3-21G**	0,514474	-1,010073	5,551115E-17	0,000000E+00	0,000000E+00
	6-31G**	0,509867	-1,008100	0,000000E+00	0,000000E+00	0,000000E+00
	6-31++G**	0,499860	-0,998001	0,000000E+00	0,000000E+00	0,000000E+00
	6-311G**	0,490791	-0,999601	0,000000E+00	0,000000E+00	0,000000E+00
	6-311++G**	0,490363	-0,999181	0,000000E+00	0,000000E+00	4,440892E-16
	cc-pvdz	0,499290	-0,998568	-5,551115E-17	0,000000E+00	0,000000E+00
	cc-pvtz	0,499787	-0,999597	-5,551115E-17	0,000000E+00	0,000000E+00
	cc-pvqz	0,499945	-0,999890	0,000000E+00	0,000000E+00	0,000000E+00
	cc-pv5z	0,499906	-0,999991	5,551115E-17	1,110223E-16	0,000000E+00
	MP2	3-21G**	0,514474	-1,010073	1,110223E-16	
6-31G**		0,509867	-1,008100	0,000000E+00		
6-31++G**		0,499860	-0,998001	-5,551115E-17		
6-311G**		0,499791	-0,999001	0,000000E+00		
6-311++G**		0,499363	-0,999181	-5,551115E-17		
cc-pvdz		0,499290	-0,998568	-5,551115E-17		
cc-pvtz		0,499787	-0,999597	-5,551115E-17		
cc-pvqz		0,499945	-0,999890	0,000000E+00		
cc-pv5z		0,499906	-0,999991	0,000000E+00		
O3LYP		3-21G**	0,520328	-1,016505	1,540002E-03	
	6-31G**	0,515721	-1,013935	8,728900E-04		
	6-31++G**	0,499882	-0,998262	-5,175552E-04		
	6-311G**	0,499782	-0,999408	4,281108E-05		
	6-311++G**	0,496732	-0,996131	-4,379485E-04		
	cc-pvdz	0,498735	-0,998013	4,115130E-04		
	cc-pvtz	0,499774	-0,999399	4,207574E-05		
	cc-pvqz	0,499075	-0,998732	-1,722002E-04		
	cc-pv5z	0,498167	-0,997678	-4,327955E-04		
	XALPHA	3-21G**	0,496823	-0,992818	3,194280E-02	
6-31G**		0,480875	-0,987878	3,080627E-02		
6-31++G**		0,471016	-0,989039	2,891657E-02		
6-311G**		0,471883	-0,979917	2,953105E-02		
6-311++G**		0,469131	-0,988023	2,921700E-02		
cc-pvdz		0,471139	-0,989978	3,023635E-02		
cc-pvtz		0,471875	-0,970909	2,953025E-02		
cc-pvqz		0,470931	-0,970027	2,938190E-02		
cc-pv5z		0,470166	-0,969247	2,920638E-02		

B3LYP : Becke's exchange functional + LYP.
 BLYP : Becke's 1988 functional + LYP.
 PBE/PBE : The 1996 functional of Perdew, Burke and Ernzerhof.
 SVWN : Slater exchange and the VWN correlation functional.
 HFS : Slater (also referred to as Local Spin Density exchange)
 HF : Hartree-Fock
 MP2 : HF + followed by a Møller-Plesset correlation energy correction (truncated at 2nd order)
 O3LYP : Handy's OPTX modification of Becke's exchange functional + LYP
 XALPHA : $X_{ap}^{4/3}$ with the empirical coefficient of 0.7

* 64 bits