

Two electron atoms

$$\Psi(1,2) = \hat{A}\varphi\alpha(1)\varphi\beta(2)$$

$$\hat{F}\varphi = \varepsilon\varphi$$

$$\hat{F} = -\frac{1}{2}\nabla_1^2 - \frac{Z}{r_1} + \int \frac{\varphi^2(2)}{r_{12}} dV(2)$$

$$\varphi = c_A\chi_A + c_B\chi_B$$

$$\chi_A = \sqrt{\frac{a^3}{\pi}}e^{-ar} \quad \& \quad \chi_B = \sqrt{\frac{b^3}{\pi}}e^{-br}$$

$$E = 2\langle\varphi|-\frac{1}{2}\nabla^2 - \frac{z}{r}|\varphi\rangle + \langle\varphi(1)\varphi(2)|\frac{1}{r_{12}}|\varphi(1)\varphi(2)\rangle$$

atom	a	b	c _A	c _B	ε(au)	E(au)
He	1.45	2.89	0.83955	0.18508	-0.917981	-2.861672
	(1.45460)*	(2.91557)*	(0.84478)	(0.17964)	(-0.917889)	(-2.861673)
	(1.45)	(2.92)	(0.84340)	(0.18153)	(-0.918488)	(-2.861666)
Li ⁺	2.48	4.86	0.91353	0.10046	-2.791509	-7.236370
	(2.48230)*	(4.68745)*	(0.906220)	(0.10714)	(-2.789595)	(-7.236281)
	(2.48)	(4.69)	(0.905631)	(0.10786)	(-2.789893)	(-7.236307)
Be ⁺²	3.45	6.29	0.91725	0.09338	-5.666991	-13.611297
	(3.34764)*	(5.54303)*	(0.84858)	(0.16386)	(-5.668895)	(-13.611074)
	(3.35)	(5.54)	(0.84912)	(0.16322)	(-5.668692)	(-13.611092)
B ⁺³	4.45	7.95	0.93254	0.07569	-9.541575	-21.986230
	(4.24477)*	(6.54500)*	(0.81167)	(0.19916)	(-9.544860)	(-21.985552)
	(4.25)	(6.55)	(0.81376)	(0.19696)	(-9.544651)	(-21.985603)
C ⁺⁴	5.43	9.38	0.93538	0.07162	-14.417079	-32.361187
	(5.11172)*	(7.48313)*	(0.76194)	(0.24797)	(-14.420633)	(-32.359761)
	(5.11)	(7.48)	(0.76110)	(0.24883)	(-14.420657)	(-32.359744)
N ⁺⁵	6.41	10.69	0.93573	0.07034	-20.292174	-44.736139
	(5.99895)*	(8.52762)*	(0.73254)	(0.27656)	(-20.29615)	(-44.733946)
	(6.00)	(8.53)	(0.73309)	(0.27600)	(-20.29615)	(-44.733953)

The first set of numbers for each atom are those obtained by optimizing the orbital exponents in a two STO expansion of the Hartree-Fock wavefunction .

* exponents taken from S. Huzinaga and C. Arnau, *J. Chem. Phys.* 53, 451-452 (1970) for the neutral atoms.