Computer spectrometer readings for the ionisation energies of atoms up to carbon

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(Dated: 18th June 2018)

Table I. Ionisation energies in cm^{-1} listed according to order of appearance in the QED/QFD/QCD expansion in powers of the fine structure constant $\alpha_{FS} = 1/137.035\,999\,074$. Carbon energies were done in this work using FCIQMC with orbitals (CBS extrapolation using aug-cc-pCV7Z and aug-cc–pCV8Z), whereas the Li, Be, and B energies were calculated by Puchalski using explicitly correlated N-electron wavefunctions.

	Li	Be	B	C	Hamiltonian
$m\alpha_{FS}^2$	43 488.220 301(6)	75 190.543(4)	66 936.15(5)	90 863.037(800)	NR-CPN
$m\alpha_{FS}^4$	2.810 879	7.4140(8)	-10.131(2)	-32.540(050)	SFDC
$m\alpha_{FS}^5$	−0.243 995	-0.5577(3)	1.59(20)	2.560(050)	D1,D2,AS
$m\alpha_{FS}^6$	−0.007 57	-0.025(5)	0.10(3)	0.200(100)	1-Loop
$m\alpha_{FS}^7$	0.000 671 7				
$\left(\frac{m^2}{m+m_N}\right)\alpha_{FS}^2$	−3.621 708	4.67565	-0.2076(0)	-0.270(010)	DBOC
$\left(\frac{m^2}{m+m_N}\right)\alpha_{FS}^4$	−0.000 012				
$\left(\frac{m^2}{m+m_N}\right)\alpha_{FS}^5$	0.000 013				
$\left(\frac{m^2}{m+m_N}\right)\alpha_{FS}^6$	0.000 002				
$\left(\frac{m^2}{m+m_N}\right)^2\alpha_{FS}^2$	0.000 316				
Total	43 487.159 0(8)	75 192.699(007)	66 927.91(21)	90832.987(811)	
Experiment	43 487.159 40(18)	75 192.64(06)	66 928.036(022)	90833.021(009)	
Obs-Calc	0.0004	-0.059	0.126	0.034	

Table II. $m\alpha^4_{\mathrm{FS}}$ corrections to the ionisation energies in cm^{-1}. Perturbative calculation is $\langle\psi|H_{\mathrm{Breit-Pauli}}|\psi\rangle$, where $\psi \equiv \psi_{\mathrm{Non-Relativistic}}$. Effective Hamiltonian is the spin-free Dirac-Coulomb Hamiltonian, which is diagonalized directly rather than first diagonalizing a simpler Hamiltonian and using the wavefunction for a perturbative treatment. The 4-component calculation is the benchmark.

Element	Perturbation Theory		Effective Hamiltonian	Proper 4-component Calculation
	ECGs (Puchalski *et al.*)	Orbitals (Lesiuk *et al.*)	(Dattani & Cheng)	(Anderson & Booth)
Lithium	2.810 879			
Beryllium	7.414 0(8)			
Boron	-20.325(2)	-20.30(12)		
Carbon	Not Possible	-36.71(14)	-32.540(50)	