Towards Chemical Accuracy in Atomic Ionization Energies: The Case of H, C, N, O, F, P, and S Atoms

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Table S1. Spin-orbit corrections derived from the NIST fine-structure levels [48] for the C, N, O, F, P, and S atoms and their corresponding cations. The E_{LS} value was calculated using eq. (15). The ΔE_{SO} value represents the energy difference between E_{LS} and the lowest fine-structure level, as defined in eq. (16). The ΔIE_{SO} value was obtained as the difference between the cationic and neutral ΔE_{SO} values (eq. (17)). The SOC correction is reported in eV and was applied to the calculated ionization energies using eq. (18).

Atom	Neutral term	Cation term	ΔE_{SO} neutral (cm^{-1})	ΔE_{SO} cation (cm^{-1})	ΔIE_{SO} (cm^{-1})	ΔIE_{SO} (eV)
C	^3P	$^2P^\circ$	29.591	42.280	12.689	+0.0016
N	$^4S^\circ$	^3P	0.000	88.890	88.890	+0.0110
O	^3P	$^4S^\circ$	77.975	0.000	-77.975	-0.0097
F	$^2P^\circ$	^3P	134.714	168.123	33.409	+0.0041
P	$^4S^\circ$	^3P	0.000	315.589	315.589	+0.0391
S	^3P	$^4S^\circ$	195.756	0.000	-195.756	-0.0243

Academic Editors: Jean Paul Jay-Gerin and Jintana Meesungnoen

Received: 29 April 2026
Revised: 12 June 2026
Accepted: 17 June 2026
Published: 25 June 2026

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