Erratum: Explicitly correlated wave functions of the ground state and the lowest quintuplet state of the carbon atom [Phys. Rev. A **99**, 052512 (2019)]

Krzysztof Strasburger

(Received 4 June 2019; published 21 June 2019)

DOI: [10.1103/PhysRevA.99.069901](https://doi.org/10.1103/PhysRevA.99.069901)

The orbit-orbit magnetic interaction integrals in our work were symmetrized incorrectly. This error was affecting, among others, the wave functions with symmetries used for the considered states of the carbon atom. Correct values of the orbit-orbit term and whole relativistic shifts are given in Table I. Consequently, the orbit-orbit energies are converged within a few nanohartrees. In the paragraph before the last paragraph of Sec. III, corrected energies of ^{12}C have to be changed to $E(^3P_g) = -37.857\,269$ and $E(^5S_u) = -37.703\,662$. Their difference amounts to $0.153\,607$ hartree or $33\,713\text{ cm}^{-1}$. The missing contribution amounts to, at least, 6 cm^{-1} . In the last sentence of Sec. III: The orbit-orbit term contributes nearly 16 cm^{-1} to the excitation energy—almost 15% of the total contribution of relativistic corrections, amounting to 108 cm^{-1} .

These changes do not affect other conclusions of the paper.

TABLE I. Orbit-orbit term and relativistic shift for ^{12}C .

K	3P_g		5S_u	
	$\langle \hat{H}_4 \rangle$	$\langle \hat{H}_{RS} \rangle$	$\langle \hat{H}_4 \rangle$	$\langle \hat{H}_{RS} \rangle$
88	−0.000016296	−0.013968250	0.000056199	−0.013531324
129	−0.000015900	−0.014003954	0.000056148	−0.013547045
189	−0.000015467	−0.014029658	0.000056189	−0.013561152
277	−0.000015362	−0.014041825	0.000056205	−0.013570427
406	−0.000015335	−0.014053920	0.000056184	−0.013574362
595	−0.000015304	−0.014061628	0.000056167	−0.013578169
872	−0.000015264	−0.014067879	0.000056169	−0.013580168
1278	−0.000015230	−0.014070071	0.000056165	−0.013580265
1873	−0.000015222	−0.014072572	0.000056165	−0.013582685
2745	−0.000015209	−0.014073117	0.000056165	−0.013582669
4023	−0.000015203	−0.014074637	0.000056164	−0.013583055
5896	−0.000015200	−0.014074667		