Theoretical study of hyperfine structure of ground state in neutral Carbon

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In this work, hyperfine constants are reported for $1s^22s^22p^2\ ^3P_{1,2}$ states of C I using multiconfiguration Hartree-Fock (MCHF) [1] and a (deconstrained) partitioned correlation function interaction ((D)PCFI) [2–3] method. Systematic calculations were performed with the principal quantum number $n = 4...8$ and with orbital quantum numbers up to $l = l_{max}$. Configuration state functions (CSFs) were constructed by allowing single- (S) and double- (D) substitutions from a multireference (MR) set. Present calculations were performed with a MR set consisting of CSFs belonging to 11 configurations.

The PCFI [2–3] method was applied using three PCFs: 1) the first one, $\Lambda_{1s-1s1s}$, targets SD excitations from the core ($1s$) orbital; 2) a second one, Λ_{1s-nl}, targets S excitations from the $1s$ core shell and S excitation from the valence (nl) orbital; 3) a third one, $\Lambda_{nl-nlnl}$, targets SD excitations from the valence (nl) orbitals (where $n = 2, 3$ and $l = s, p, d$). The wave-function for $1s^22s^22p^2\ ^3P$ would be

$$|\Psi(1s^22s^22p^2\ ^3P)\rangle = |\Psi^{\rm MR}(^3P)\rangle + \alpha_{\rm CC}\ |\Lambda_{1s-1s1s}\rangle + \alpha_{\rm CV}\ |\Lambda_{1s-nl}\rangle + \alpha_{\rm VV}\ |\Lambda_{nl-nlnl}\rangle. \quad (1)$$

Also performed were calculations where the $\Lambda_{1s-1s1s}$ PCF was split into two subspaces ($\Lambda_{1s-1s1s} \to \Lambda_{1s} + \Lambda_{1s1s}$). The Λ_{1s} PCF focusing on the S excitations is dedicated to capture core-polarization (CP) effects. The many-electron wave-function is then written as the MR function corrected by four different PCFs.

From Table 1 it is seen that splitting of $\Lambda_{1s-1s1s}$ PCF in the two groups improves the hyperfine structure results. The results are in better agreement with the experiment. Results are compared with previous theoretical data and with experimental results. Calculations are in progress, additional schemes of calculations (choosing different MR set, etc.) are tested to improve the results.

Method	A (J=1)				A (J=2)				Reference
n	6	7	8		6	7	8		
MCHF	3.017	2.461	2.339		147.831	147.842	148.365		this work
DPCFI	−1.861	7.415			145.984	152.384			this work
CP-PCFI	3.559	4.229	4.083		148.444	148.958	148.900		this work
CP-DPCFI	1.962	3.917	2.665		147.608	149.440	148.079		this work
Unrestricted HF				13.7				160.6	[4]
MCHF				2.36				147.9	[5]
SD-MR-CI				2.28				148.1	[6]
MCHF				3.225				148.747	[7]
CI(CIV3)				7.63				152.0	[8]
Experiment				2.838(17)				149.055(10)	[9]
Experiment								149.0(3)	[10]

Table 1: *Comparison of the magnetic dipole constants (in MHz) for the* $1s^22s^22p^2\ ^3P_{1,2}$ *states in C I.*

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