

# On spectral sensitivity of the CO molecule to temporal variation of fundamental physical constants

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A comparison of laboratory and astronomical spectroscopic measurements are used for discovery of the fundamental effects not described in the framework of the Standard Model. Due to a high sensitivity of the vibrational and rotational kinetic energies of molecules to nuclear masses, the high-redshift quasar absorption spectra of H<sub>2</sub> and CO molecules are generally implied to probe a possible variation of the proton-to-electron mass ratio  $m_p/m_e$  on a cosmological time scale [1] while a temporal variation of the fine structure constant  $\alpha$  is normally investigated via measurements of the atomic lines shift. The unprecedented accurate spectroscopic measurement on the  $a^3\Pi \rightarrow X^1\Sigma^+$  band of various isotopologues of CO confirms the extreme sensitivity of electronic transitions involved nearly degenerate rovibronic levels for probing a variation of mass on a laboratory time scale [2]. The impact of relativistic interactions on the spectral characteristics of the ground  $X^1\Sigma^+$  state of CO molecule was theoretically studied as well [3].

At the present work we estimate a sensitivity of the spin-forbidden triplet-singlet  $a^3\Pi \rightarrow X^1\Sigma^+$  Cameron system of CO molecule onto a variation of the fine structure constant  $\alpha$  since the pronounced impact of the  $\alpha$ -value drifting on the spin-orbit splitting and relative intensity distribution into the intercombination transition should be expected. Therefore, both relativistic and mass effects could be treated simultaneously. The fully relativistic model of the electron system of the CO molecule was based on the Dirac-Coulomb-Gaunt approximation for the Hamiltonian which considered  $\alpha$  as a variable parameter and used the “exact” transformation to the two-component picture [4]. To describe the electron correlation we implied the large scale multi-reference configuration interaction (MRCI) method. To monitor of the energy convergence of the MRCI method the various compositions of reference wave function and active space were employed. The correlation consistent core-valence aug-cc-pCVQZ and d-aug-cc-pCV5Z atomic basis sets were used [5]. Potential energy curves of the excited states were obtained by adding the vertical excitation energies as functions of the internuclear distance to the accurate empirical ground state PEC [6]. The dependence of the calculated energies and transition dipole moments on the different values of the parameter  $\alpha$  was studied in details. All calculations were accomplished by the DIRAC17 code [7].

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