THE COUPLED-CHANNEL DEPERTURBATION ANALYSIS OF THE A~B~X STATES MANIFOLD OF CN WITH ALMOST SPECTROSCOPIC ACCURACY

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A direct deperturbation analysis for the experimental rovibronic term values belonging to the first three electronic states of the CN radical has been performed using an iterative solution of the inverse spectroscopic problem based on a rigorous coupled-channel approximation. Besides potential energy curves (PECs), the non-adiabatic energy matrix explicitly included the spin-orbit and Coriolis coupling functions between the $X^2\Sigma^+$, $A^2\Pi$ and $B^2\Sigma^+$ states. The regular perturbation caused by the remote doublet states was taken into account by the introduction of so-called Λ-doubling parameters as an implicit function of the interatomic distance. The initial set of the deperturbed PECs was defined in analytical extended Morse oscillator (EMO) form while the non-adiabatic coupling functions were given as the properly morphed *ab initio* electronic matrix elements [a]. The resulting PECs and non-adiabatic parameters reproduce the overall set of experimental energy levels with an accuracy of about 0.01-0.02 cm^{-1}, which is almost comparable with their uncertainty of measurement.[b] .

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[a]V. A. Terashkevich, E.A. Pazyuk, and A.V. Stolyarov. *Journal of Quantitative Spectroscopy and Radiative Transfer*, **276**, 107916, 2021