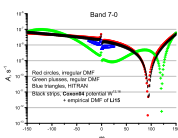


MODELLING THE DIPOLE MOMENT FUNCTION OF CARBON MONOXIDE CAPABLE OF PREDICTING THE ROTATIONAL DISTRIBUTION IN THE 7-0 BAND

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The rotational distributions of the intensities in the low- v vibrational bands are nearly insensitive to the specific forms of the PEFs and DMFs based on the experimental and/or *ab initio* data. This is not the case for the higher overtone bands. We discuss the problem: Which properties should the model PEF and DMF possess in order to be capable of predicting the intensities of the yet unobserved lines? Arguments are presented that the Born-Oppenheimer PEF and DMF should possess some features following from their properties as functions of the inter-atomic separation as a complex variable. In particular, they must contain branch points associated with the crossings between the ground and excited electronic states. This approach implies that both functions are to be fitted simultaneously to the common data set including both the line positions and the intensities. However, such a problem is very difficult to solve. Here and in Ref. (1), in application to CO, we assume that the PEF is given (2), and we develop an irregular DMF form containing two branch points corresponding to the expected crossings in the complex plane near 0.4 and 2.2 Å. We compare it with an alternative regular function (1) and find that the rotational distribution in the vibrational 7-0 band predicted by the former is very stable with respect to small variations in the data base, as opposed to the regular DMF showing strong instability. The predicted intensities (see figure) are stronger than the HITRAN values calculated by Li et al. (3) with a combined empirical/spline-interpolated *ab initio* DMF but are close to the ones calculated by us with the purely empirical DMF of Li et al. The irregular function is expected to provide for a reliable prediction of the ro-vibrational line intensities in the 7-0 band.

This work was performed in accordance with the state task, state registration No. AAAA-A19-119071190017-7.

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