ANOMALOUS CENTRIFUGAL DISTORTION AND A GENERALIZED DEFINITION OF A QUASILINEAR MOLECULE

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Monodromy in the bending potential function is mapped into the rotation-bending spectrum, as shown in the previous talk. The form this takes in NCNCS for the parameter corresponding to D_J in an asymmetric rotor will be demonstrated. Years ago, extremely large values of D_{JK} and D_K , as well as higher order terms, were found for HNCO, HNCS, and most importantly, H₂O, and discussed as "anomalous centrifugal distortion". At that time no one understood the physical origin of the phenomenon, although we knew it must have something to do with the bending mode. Today we can correlate it directly with monodromy in the bending potential function. The early definition of a quasilinearity parameter^{*a*}, allowing us to classify molecules with a more or less large amplitude bending mode, limited the concept to those that were rather close to the linear limit, specifically with the ground state below or only just above the top of the barrier to linearity. Recent work has shown that a considerably larger group of molecules should actually be considered quasilinear. This talk will show why this is so, and conclude with the definition of a generalized quasilinearity parameter which can be used to implement such a classification.

^aK. Yamada and M. Winnewisser Z. Naturforsch. <u>31A</u> (139-144), 1976.