

GLOBAL ANALYSIS OF A-, B- AND C-TYPE TRANSITIONS INVOLVING TUNNELING COMPONENTS OF $K = 0$ AND 1 STATES OF THE METHANOL DIMER

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Spectral data on $K = 0$ and 1 levels of the methanol dimer available from previous and present Fourier transform microwave measurements have been interpreted globally, using a group-theoretically derived effective Hamiltonian and corresponding tunneling matrix elements to describe the splittings arising from a large number of tunneling motions. In the present work 302 new transitions (40 $K = 1 - 1$ a-type, 78 $K = 1 - 0$ b-type and 184 $K = 1 - 0$ c-type transitions) were added to the previous data set to give a total of 584 assigned transitions with $J \leq 6$. As a result of the complete $K = 0, 1$ data set for $J \leq 4$, the lone-pair-exchange tunneling splittings were obtained experimentally. Matrix element expansions in $J(J+1)$ used in the previous $K = 0$ formalism were modified to apply to $K > 0$, essentially by making a number of real coefficients complex, as required by the generalized internal-axis-method tunneling formalism. To reduce the number of adjustable parameters to an acceptable level in both the $K = 0$ and 1 effective Hamiltonians (used in separate $K = 0$ and $K = 1$ least-squares fits), a rather large number of assumptions concerning probably negligible parameters had to be made. The present fitting results should thus be considered as providing assurance for the group-theoretical line assignments as well as a nearly quantitative global interpretation of the tunneling splittings, even though they do not yet unambiguously determine the relative contributions from all 25 group-theoretically inequivalent tunneling motions in this complex, nor do they permit quantitative extrapolation to higher K levels.