INTERPRETATION OF ROTATIONAL STRUCTURE IN ZEKE SPECTRA OF MOLECULAR CLUSTERS

M. FORD, and KLAUS MÜLLER-DETHLEFS, *Department of Chemistry, University of York, Heslington, York Y010 5DD, U.K.*.

In large molecules and molecular clusters, the rotational structure in ZEKE spectra is not always fully resolved. However, the rotational structure, and hence rotational constants, can be obtained from deconvolution of the ZEKE band profile, provided the rotational states in the intermediate (neutral) state have been identified. In addition, we invoke a spectator model for the ZEKE transitions, which simplifies the selection rules to $—N^+ - N— \leq 10 \leq —N^+ + N—$ and $K^+ - K = -\lambda_0$, where $l_0(\lambda_0)$ is the angular momentum (projection) quantum number of the spectator electron. We present first results of a fitting procedure for comparison with experimental ZEKE spectra of phenol complexes.