In the first approximation a "diatomic approximation" may suffice. In the latter only the rotational-vibrational interaction associated with a rotation involving the two largest moments of inertia is considered and one may proceed as follows:

In this "diatomic approximation", the Schrodinger equation has a form permitting separation of variables according to the formalism described earlier. The wave equation is first separated into equations for the translational (center of mass), rotational and internal motions using this formalism. The equation for internal motion now contains a rotational constant of the motion, which appears in a centrifugal potential term. The sum of the potential energy and of this centrifugal potential has a saddle-point when the original potential energy function has one and when the centrifugal distortion is not too large. A suitable system of internal coordinates is then introduced to permit this effective potential energy surface to be approximated by a surface permitting separation of variables, as described previously. Thereby, the choice of the reaction coordinate will now depend on the rotational state of the activated complex. With this qualification in mind, Eqs. (21) and (22) again apply, but now the summation over the rotational α should be made only after the other summations and the integration have been performed.

A slightly more general approach would be to neglect the vibrational angular momentum as before and to treat the activated complex as a symmetric top. Although separation of rotational from internal motion does not fall within the previously described formalism, one can