

improved canonical variational transition-state theory (ICVTST)

A modification of canonical variational transition-state theory in which, for energies below the threshold energy, the position of the dividing surface is taken to be that of the microcanonical threshold energy. This forces the contributions to rate constants to be zero below the threshold energy. A compromise dividing surface is then chosen so as to minimize the contributions to the rate constant made by reactants having higher energies.

Source:

PAC, 1996, 68, 149 (*A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996)*) on page 168