

CHARMMRATE abstract

CHARMMRATE is a module of CHARMM for interfacing it with POLYRATE. The POLYRATE main program becomes a subprogram of CHARMM. POLYRATE can be called to carry out variational transition state theory calculations with multidimensional semiclassical tunneling contributions. When POLYRATE needs the value or gradient of the potential energy surface, it calls a set of interface routines called hooks. The hooks in turn call CHARMM routines for energies and gradients calculated by molecular mechanisms or QM/MM methods.