

List of Symbols

<i>Symbol</i>	<i>Description</i>
E_{el}	Electronic energy
E_{rot}	Rotational energy
E_0	Ground state energy
E_{tot}	Total energy
$G(E^\ddagger)$	Sum of the states for active degree of freedom in the transition state
\hat{H}	Hamiltonian operator
\hat{H}_{el}	Electronic Hamiltonian operator
$\Psi(\vec{r}, \vec{R})$	Wave function
$\Psi_{el}(\vec{r}; \vec{R})$	Electronic wavefunction
$\chi(\vec{R})$	Nuclear wavefunction
m_e	Mass of electron
m_α	Mass of nuclei
k_{RRKM}	RRKM rate constant
P	Probability
$P(\tau)$	Lifetime distribution
p_i	Momenta
q_i	Position
ρ_0	Ground state electron density
ρ_{tr}	Trial electron density
τ	Lifetime
\hat{T}_e	Electron kinetic energy
\hat{T}_N	Nuclear kinetic energy
$U(\vec{R})$	Potential energy
\hat{V}_{ee}	Electron-electron repulsion energy operator
\hat{V}_{eN}	Electron nuclei attraction energy operator
\hat{V}_{NN}	Nuclear-nuclear repulsion energy operator

