$$E = U_\alpha(R_e) + (v+½)\nu_e - x_e\nu_e\,(v+½)^2 + y_e\nu_e\,(v+½)^3 + B_eJ(J+1) - D_e[J(J+1)]^2 - \alpha_e(v+½)J(J+1) + Y_{00}$$

where all spectroscopic quantities are expressed in energy units (or the corresponding frequency or wavenumbers). In energy units,

$$B_e \equiv \hbar^2 / 2\mu R_e^2$$

$$hx_e\nu_e \equiv ¼\, B_e^2/(h\nu_e)^2 \cdot \{ (^{10}/_3)B_e[U'''(R_e)R_e^3]^2/(h\nu_e)^2 - U^{iv}(R_e)R_e^4 \}$$

$$D_e \equiv 4\, B_e^3/(h\nu_e)^2$$

$$\alpha_e \equiv -2\, B_e^2/h\nu_e \cdot \{3 + 2\, B_e[U'''(R_e)R_e^3]^2/(h\nu_e)^2 \}$$

$$Y_{00} \equiv B_e^2/16(h\nu_e)^2 \cdot \{ U^{iv}(R_e)R_e^4 - (^{14}/_9)B_e[U'''(R_e)R_e^3]^2/(h\nu_e)^2 \}$$

$$h\nu_e \equiv (h/2\pi)[\, U''(R_e)/\mu \,]^{½}$$

Energy Conversion Factors 300 MHz = 0.01 cm^{-1}, 208.5 cm^{-1} = 300 K

		erg	eV	cm^{-1}
1 erg	=	1	6.2415×10^{11}	5.0340×10^{15}
1 eV	=	1.6022×10^{-12}	1	8065.5
1 cm^{-1}	=	1.9865×10^{-16}	1.23985×10^{-4}	1
1 kcal/mole	=	6.9478×10^{-14}	4.3364×10^{-2}	349.75
1 hartree	=	4.3598×10^{-11}	27.212	219,474.6

		kcal/mole	hartree
1 erg	=	1.4393×10^{13}	2.2937×10^{10}
1 eV	=	23.060	3.6749×10^{-2}
1 cm^{-1}	=	2.8591×10^{-3}	4.55634×10^{-6}
1 kcal/mole	=	1	1.5936×10^{-3}
1 hartree	=	627.51	1