CALCULATION OF ENERGY LEVELS AND IR INTENSITIES OF CO_2 FOR HIGH TEMPERATURE APPLICATIONS

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In order to be able to predict radiative transfer in hot gases issued from combustion, a spectroscopic database including the hot band contributions is generated for $C^{12} * O^{16}{}_{*_2}$. The nuclear potential energy surface and the dipole moment surface are taken as expansions in normal coordinates and are determined by fitting selected experimental data. The energy levels are obtained using the Lanczos method with basis functions expressed as products of harmonic oscillator functions and a rotational function. The wave functions are also calculated iteratively using inverse iteration. These methods allow us to calculate energy levels and wave functions up to J=200 and a total energy varying from $13000 cm^{-1}$ to $18000 cm^{-1}$ according to J values.