ANALYSIS OF THE FIR CYANAMIDE SPECTRUM BY THE "MULTIMOLECULE" RITZ PROGRAM

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The multi-molecule version of the "Ritz" program, presented at the last Columbus Symposium, has been used for the investigation of the ground small-amplitude vibrational state of H_2NCN. The absorption spectrum between 20 and 985 cm^{-1} has been measured on the Bruker Fourier transform spectrometer at the Physikalisch-Chemisches Institut of the Justus Liebig University, Giessen. The resolution of the spectra was 0.00166 cm^{-1}, so that the spectrum is fully resolved. The sample was vaporized at 100 C in a slow flow through a three meter sample cell maintained at 130–140 C for the duration of the measurements. At the moment, the assignment database contains more than 18 800 assigned lines, corresponding to transitions between more than 3 900 energy levels of the inversion states with the quantum number $n = 0$ and 1. The cyanamide molecule has two identical H atoms in the NH_2 group. The total nuclear spin of the two H atoms can thus be either $I = 1$ or $I = 0$. This is reflected over the symmetry of the complete molecular wavefunction, which must be antisymmetrical under exchange of the two protons. Since radiation-induced transitions cannot change the nuclear-spin wavefunction, the levels of cyanamide belong to two different species, labeled by the nuclear spin. The same behavior is observed also in other molecules with two equivalent hydrogens, notably in water. The two species are called para (lower spin multiplicity, 1, corresponding to $I = 0$) and ortho (higher spin mutliplicity, 3, corresponding to $I = 1$), in analogy to the case of the hydrogen molecule. Transitions between the two species are forbidden. The levels assigned for the ortho species include levels with the quantum number K ranging from 0 to 12 for $n = 0$, and from 0 to 9 and 11 for $n = 1$. For the para species, the assigned levels have K ranging from 0 to 11 for $n = 0$, and from 0 to 8 and 10 for $n = 1$. The level sequences $(n = 1, K = 10)$ of the ortho species, and $(n = 1, K = 9)$ of the para species, probably affected by strong perturbations, are still under investigation. Important improvements have been introduced into the line-analysis routine, on which a new peak-finder program is based.