DO WE REALLY KNOW THE STRUCTURE OF ANILINE-X (X=AR, NE) IN THE GROUND ELECTRONIC STATE S_0?

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We recently presented the rotational spectra of aniline, C_6H_7N, complexed with Ar, ^{20}Ne and ^{22}Ne [a].
Now we will describe the analysis of two additional isotopomer spectra of the ^{15}N-substituted aniline complexed with Ar and Ne. The very accurate values of the rotational constants for both the parent molecular cluster and its derivatives, obtained using a Fourier transform microwave spectrometer in the spectral region 1-18 GHz, now confirm that there is one structure compatible with the full set of moments of inertia obtained.
Due to large amplitude motions exhibited by rare gas atoms in weakly bounded van der Waals systems, it raises the question about the meaning of the rare gas coordinates obtained from such a study.
Hopefully, a global analysis of microwave and available UV results, supported by quantum calculations, will extract more information on the cluster structure and dynamics.

[a] D. Consalvo, V. Storm, and H. Dreizler, Chem. Phys. in press