THE ROTATIONAL SPECTRA OF THE WEAKLY BOUND He_1-C_5H_5N, He_2-C_5H_5N, and H_2-C_5H_5N COMPLEXES

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The rotational spectra of three very weakly bound complexes, He_1-C_5H_5N, He_2-C_5H_5N, and H_2-C_5H_5N, have been studied using a pulsed molecular beam microwave spectroscopic method. Analysis of the rotational and ^{14}N nuclear quadrupole coupling constants of these complexes shows that all three complexes possess the perpendicular geometric configuration. In this configuration, in the dimer, He and H_2 bind above the aromatic plan of C_5H_5N and are displaced by less than ten degrees away from the c-axis of the pyridine monomer, toward the nitrogen atom. In the trimer, the second helium atom preferentially binds below the aromatic plan of C_5H_5N, opposite of the first helium atom. An MP2 $ab\ initio$ interaction potential between He and C_5H_5N has been generated and the theoretical results are consistent with those from the experiment. The spectra, molecular structures, quadrupole coupling parameters, and interaction potentials will be discussed.[a]

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