Electronic Supplementary Information for

Accurate measurement of sequential Ar desorption energies from the dispersion-dominated Ar_{1-3} complexes of aromatic molecule

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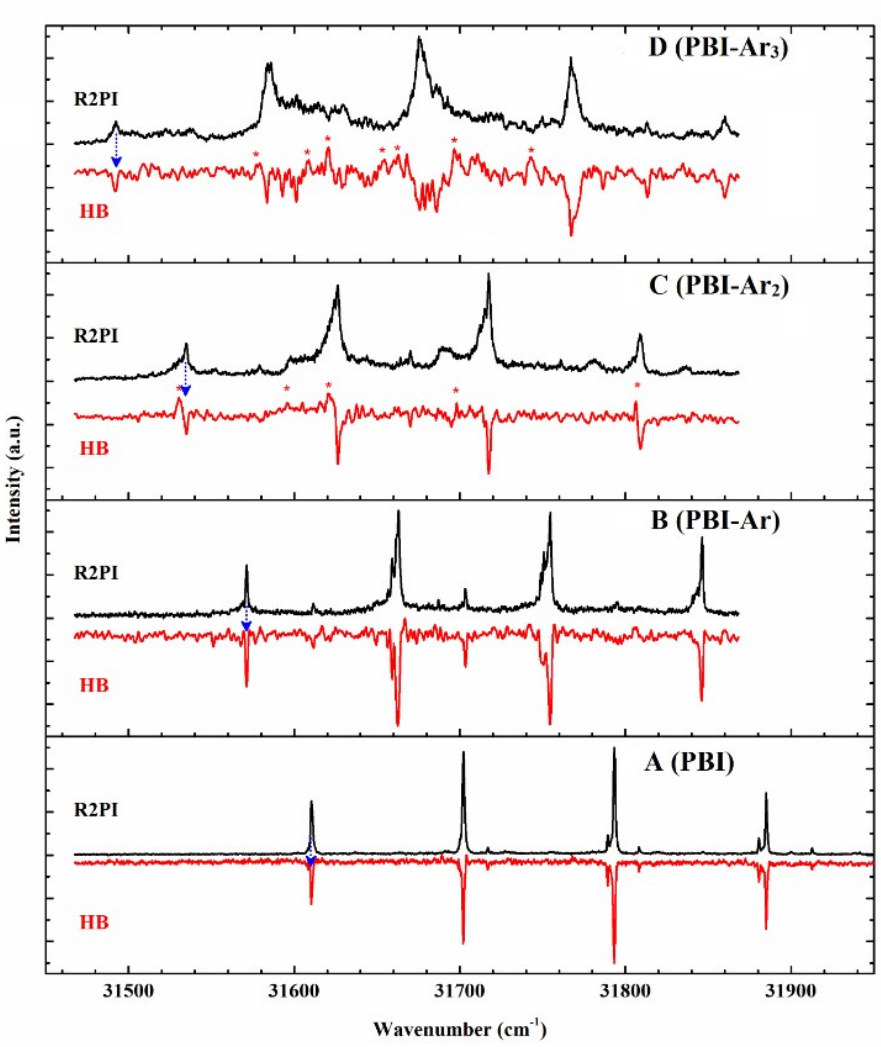
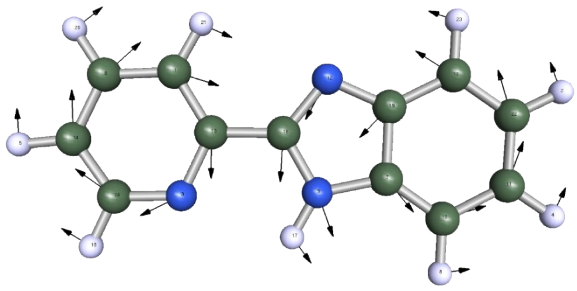
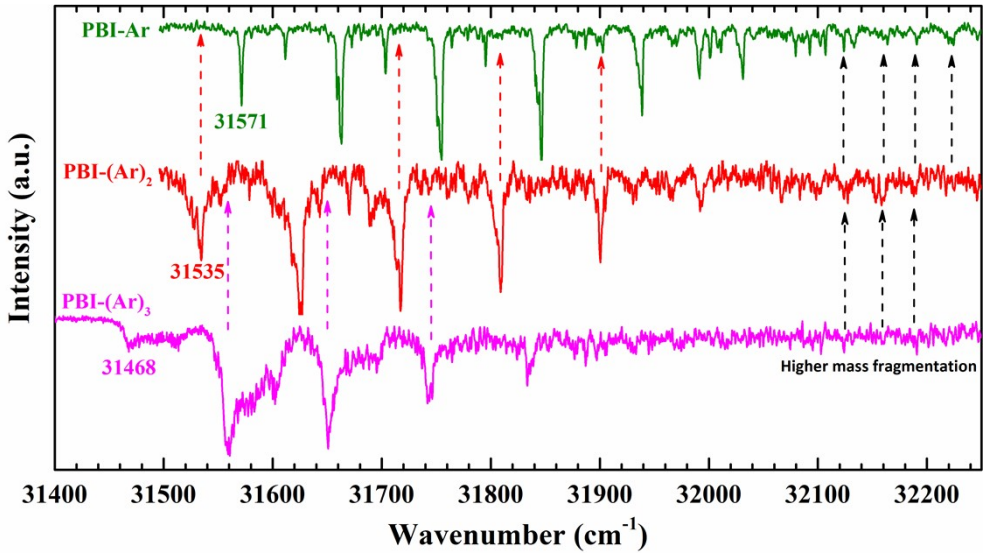


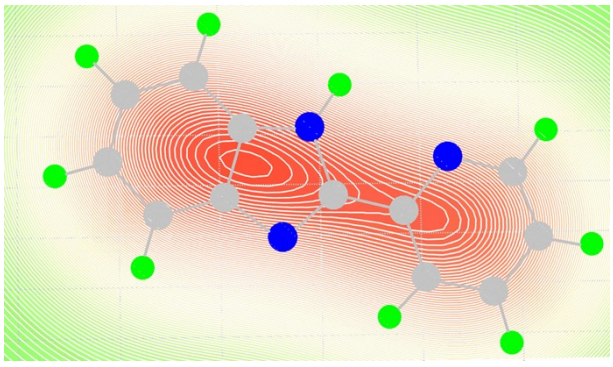
SI Figure S1. The difference spectra (HB) of PBI-Ar_n complexes were recorded by subtracting the R2PI spectra recorded with and without the hole-burning laser. The dotted arrows indicate the wavenumbers of the hole-burning laser positions. The * indicates contributions from low-energy isomers in the PBI-$Ar_{2/3}$ systems.



SI Figure S2. The ν_{45} vibrational modes corresponding to symmetric in-plane bending with respect to the C–C linkage between the pyridyl and imidazolyl groups.



SI Figure S3. Comparison of R2PI spectrum of PBI-Ar, PBI-Ar_2 and PBI-Ar_3 highlighting the fragmentation of higher masses



SI Figure S4. The dispersion contours of the Ar atom above the PBI molecular plane were calculated using the B3LYP-D3(BJ) method. The dispersion energies were calculated by placing the Ar atom on a plane parallel to the σ plane of the PBI molecule separated by 3.4 Å.