Supporting Information

1,3-Bis(pyren-1-yl)imidazolium chloride (IPyr·HCl)

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Spectroscopic data of the title compound is reported for $^1$H-NMR, $^{13}$C-NMR, 2D-NMR experiments and for UV-spectra.

$^1$H-NMR (600 MHz, DMSO-d$_6$):
$^{13}$C-NMR (150 MHz, DMSO-$d_6$):

COSY:
NOESY:

UV/VIS (IPyr-HCl in DMSO; $c = 10^{-5}$ molL$^{-1}$):

- $\lambda_{max} = 279$ nm
- $\lambda_{max} = 332$ nm
- $\lambda_{max} = 348$ nm
The lowest energy conformation of the title compound in the gas phase was calculated using DFT methods (B3LYP, 6-31G*) in the program package SPARTAN’06. The HOMO (highest occupied molecular orbital) of the pyrene residues is shown in red and blue.