Pergamon

TETRAHEDRO

Carbon-rich supramolecular metallacycles and metallacages

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SUPPORTING INFORMATION

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I. ^{1}H NMR spectroscopy:

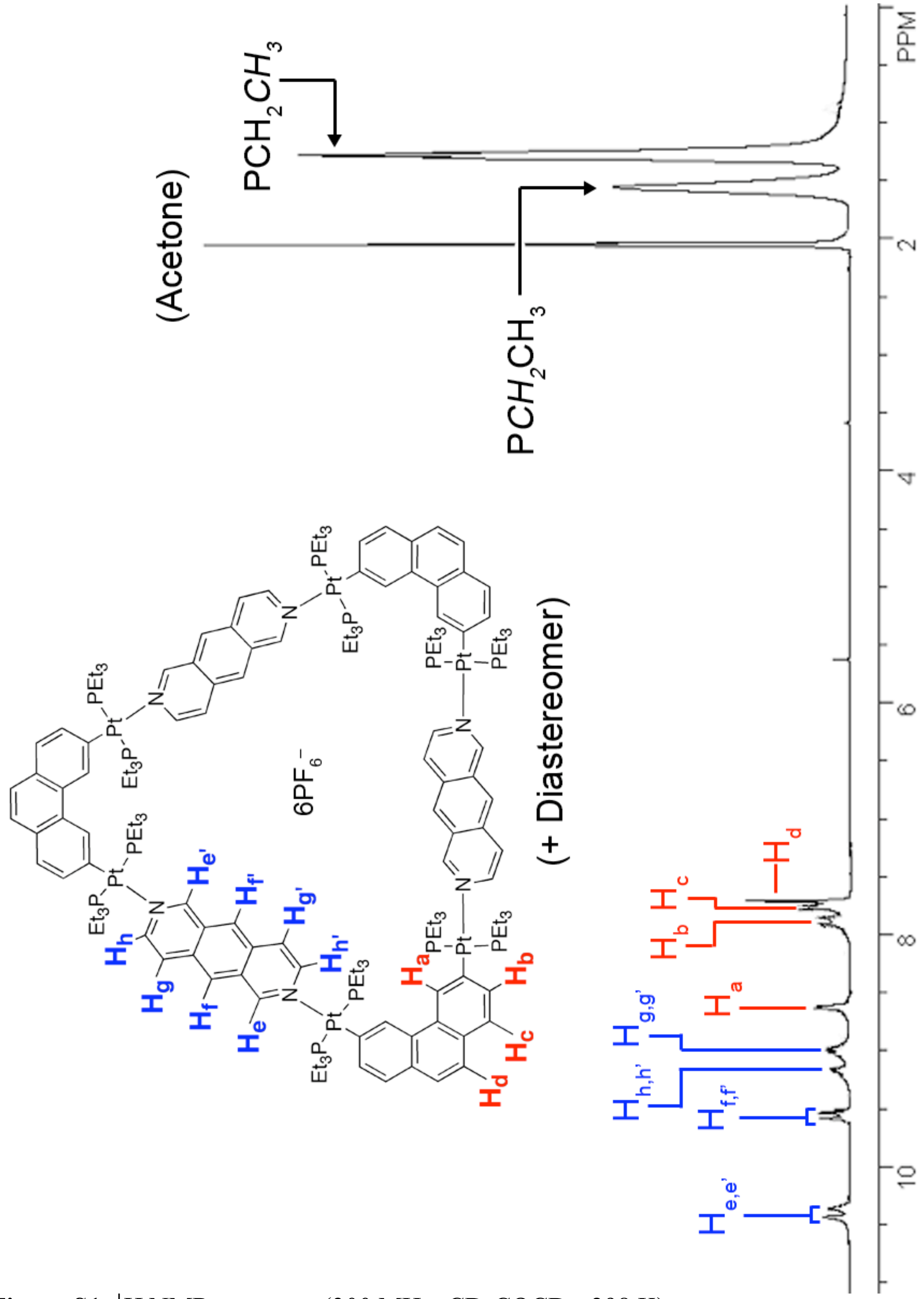

Figure S1. ^{1}H NMR spectrum (300 MHz, CD_3COCD_3, 298 K).

II. High-resolution Electrospray Ionization Mass Spectroscopy (ESI-MS).

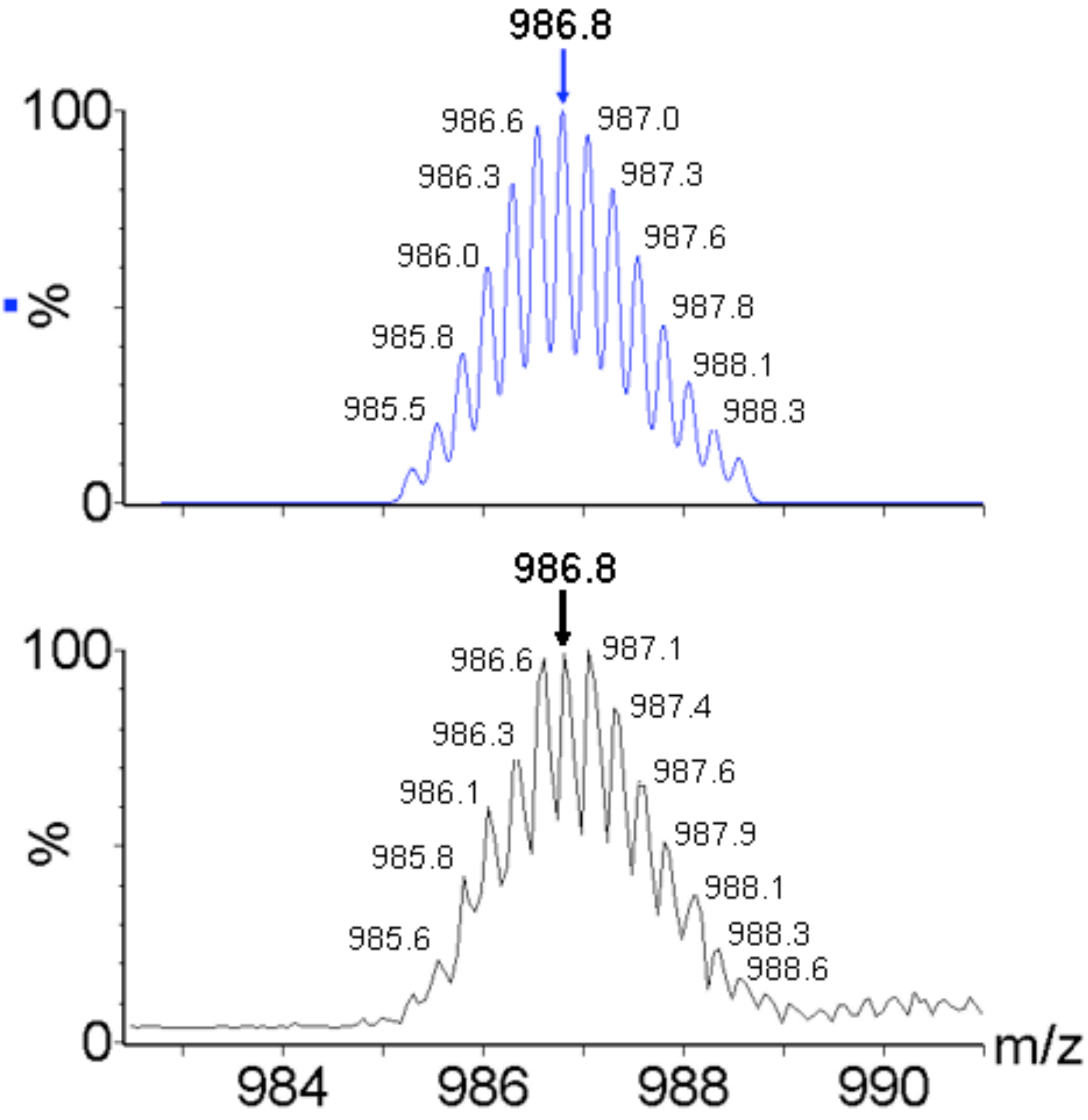

Figure S2. Calculated (top, blue) and experimental (bottom, black) ESI-MS spectra corresponding to the $[M - 4PF_6]^{4+}$ peak of the supramolecular triangle

III. Molecular modeling procedures.

Molecular models of both diastereomers of the supramolecular triangles were built within the input mode of the program Maestro v8.01.10. Each diastereomer was then subjected to a 1.0 ns molecular dynamics simulation (MMFF force field, 1.5 fs timestep) at 300 K in the gas phase. The SHAKE algorithm was applied to all bonds to hydrogen atoms. Following full equilibration, the output of each dynamics simulation was then energy minimized to full convergence (MMFF force field, gas phase) in order to determine the lowest energy structure of the stereoisomeric triangles. The results of molecular modeling indicated that the "symmetric" triangle is 6.9 kcal/mol more stable than the "asymmetric" triangle.

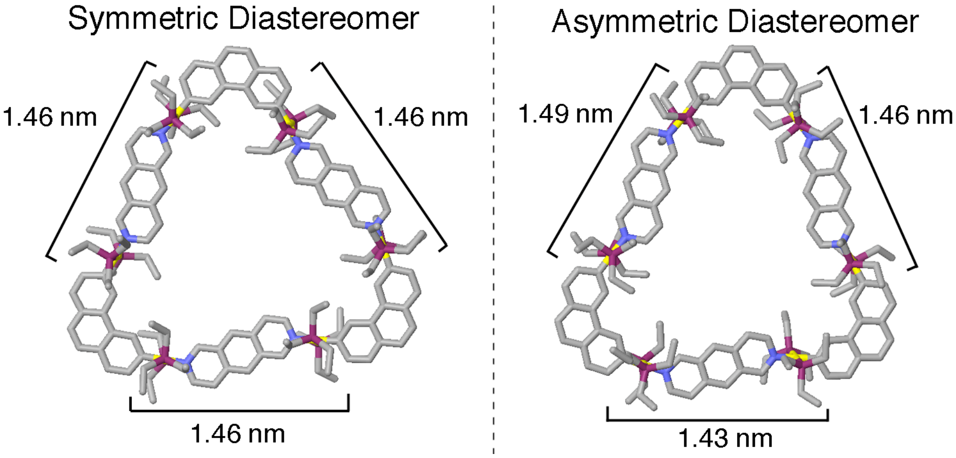

Figure S3. Lowest energy conformations of the symmetric and asymmetric diastereomers of the supramolecular triangles. Distances between neighboring phenanthrene units are given, which highlight the structural differences between the two diastereomers and indicate the sources of strain that give rise to the energetic difference between the two.