

Electronic Supplementary Information

Evaluation of polyketones with N-cyclic structure as electrode material for electrochemical energy storage: case of tetraketopiperazine unit

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General Methods:

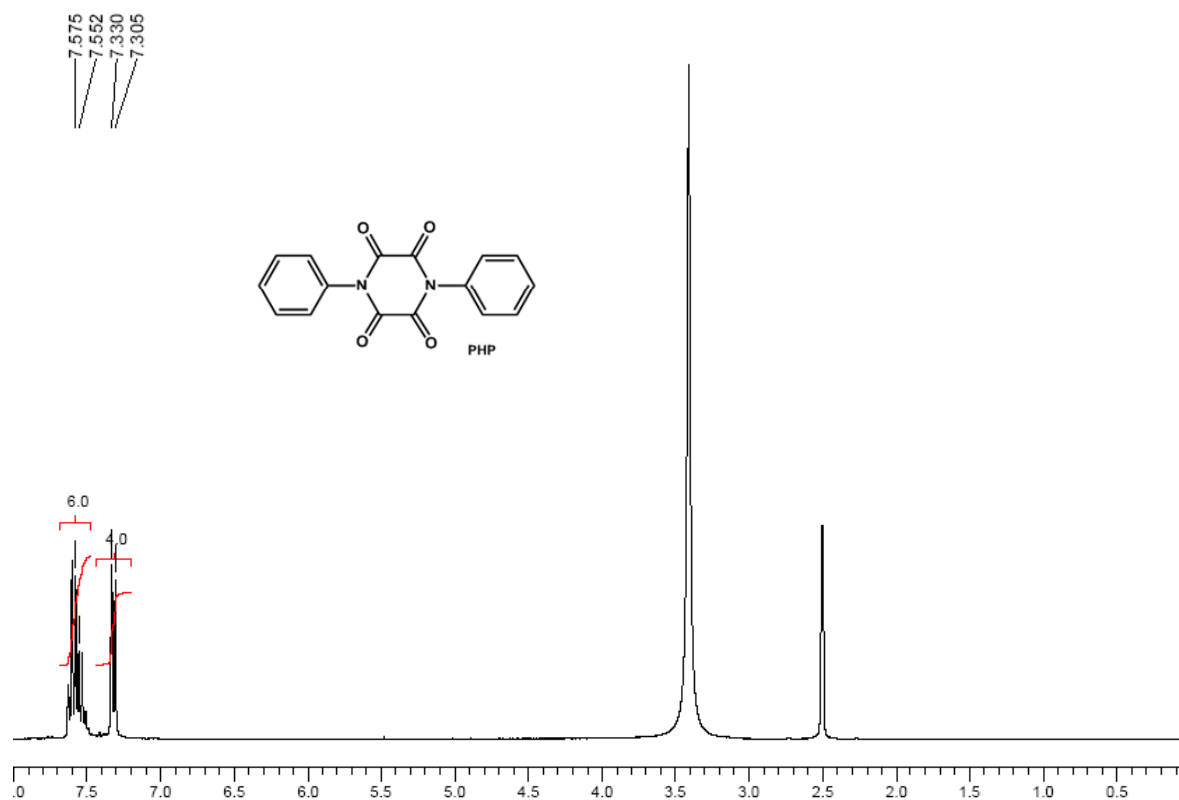
¹H and ¹³C NMR spectra were recorded at 300 MHz and 75 MHz respectively, on a BRUKER DMX 300, at room temperature. Chemical shifts (δ) were expressed in part per million (ppm) relative to residual solvent.

Infrared spectra were performed with a SHIMADZU 8400S FTIR spectrophotometer in the 400–4000 cm⁻¹ frequency range equipped with an attenuated total reflectance probe (ATR). ESI-HRMS experiments were performed in the positive ion mode on a Q-TOF Ultima Global instrument (Waters-Micromass, Manchester, UK) equipped with a pneumatically assisted electrospray ion source (Z-spray) and an additional sprayer for the reference compound (LockSpray). The prepared solutions were directly introduced (5 μ L/min) via an integrated syringe pump in the electrospray source. The source and desolvation temperatures were kept at 80 and 150 °C, respectively. Nitrogen was used as a drying and nebulizing gas at flow rates of 350 and 50 L/h, respectively. Calibration of the instrument was performed using the ions produced by a phosphoric acid solution (0.2% in H₂O/CH₃CN 50/50^{vol/vol}). The mass range was 50–1000 Da and spectra were recorded at 1 s per scan in the profile mode at a resolution of 10,000 full width at half-maximum (FWHM).

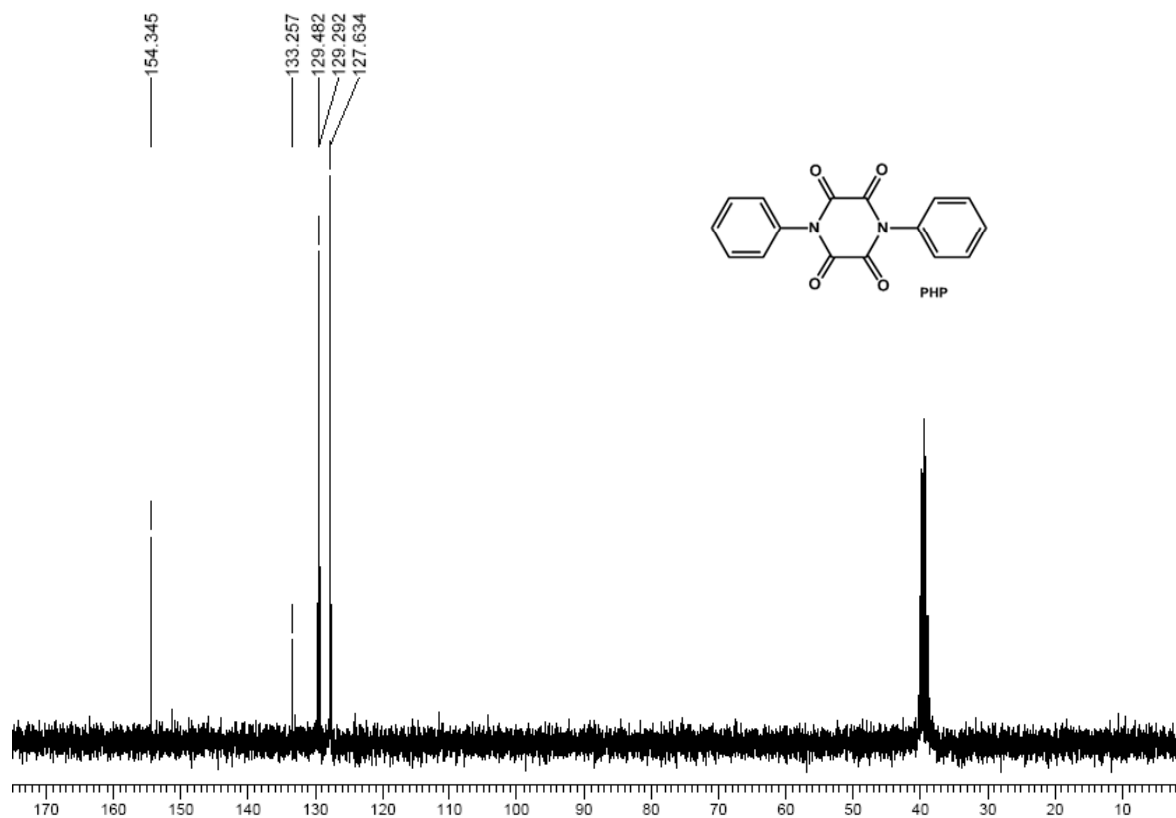
NMR Spectra:

¹H and ¹³C NMR spectra of 2,3,5,6-tetraketopiperazine derivatives PHP, AP, PRP and ¹H NMR spectrum of o-AP are presented herein.

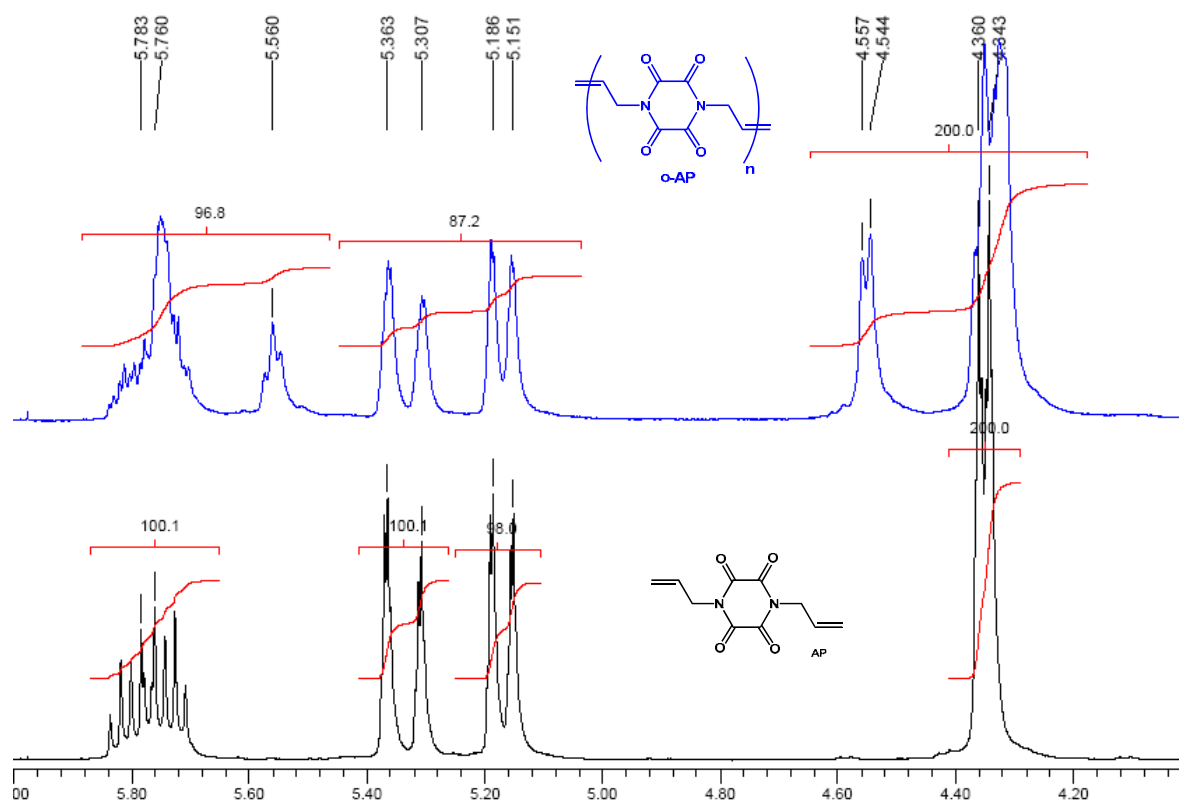
PHP: ^1H (300 MHz, DMSO- d_6)



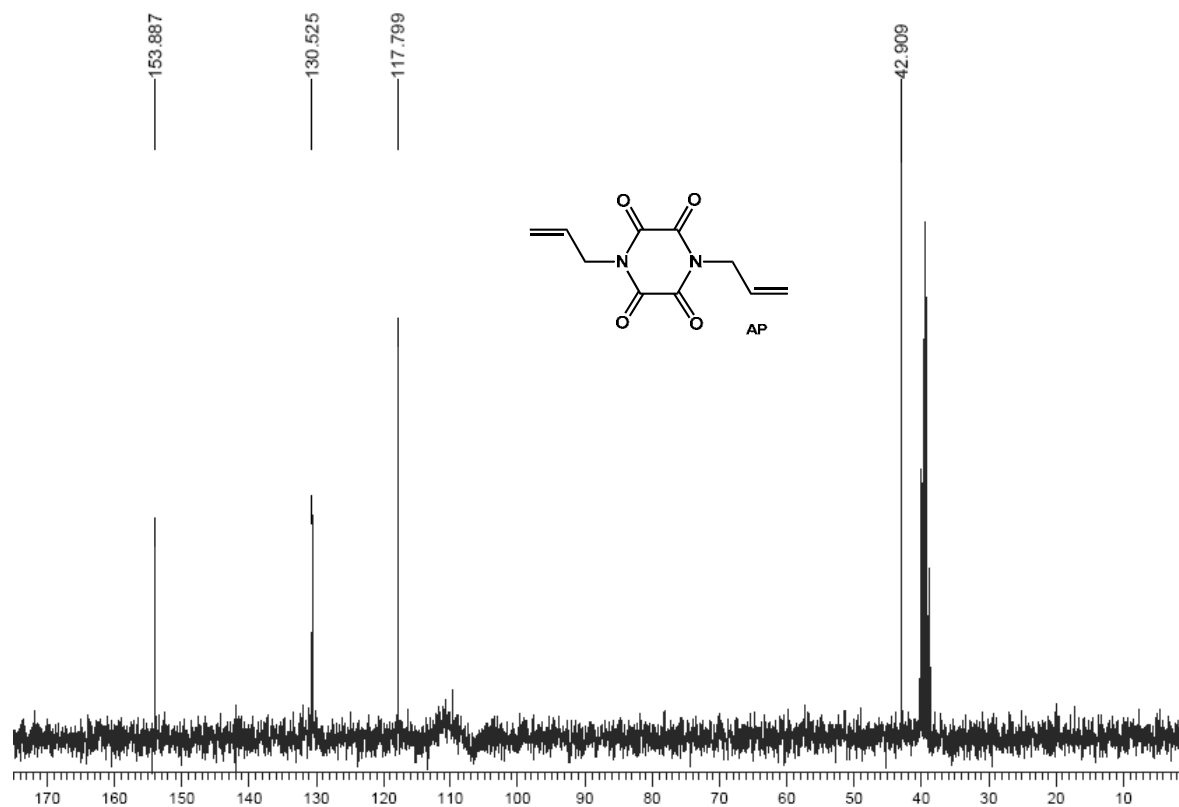
PHP: ^{13}C (75 MHz, DMSO- d_6)



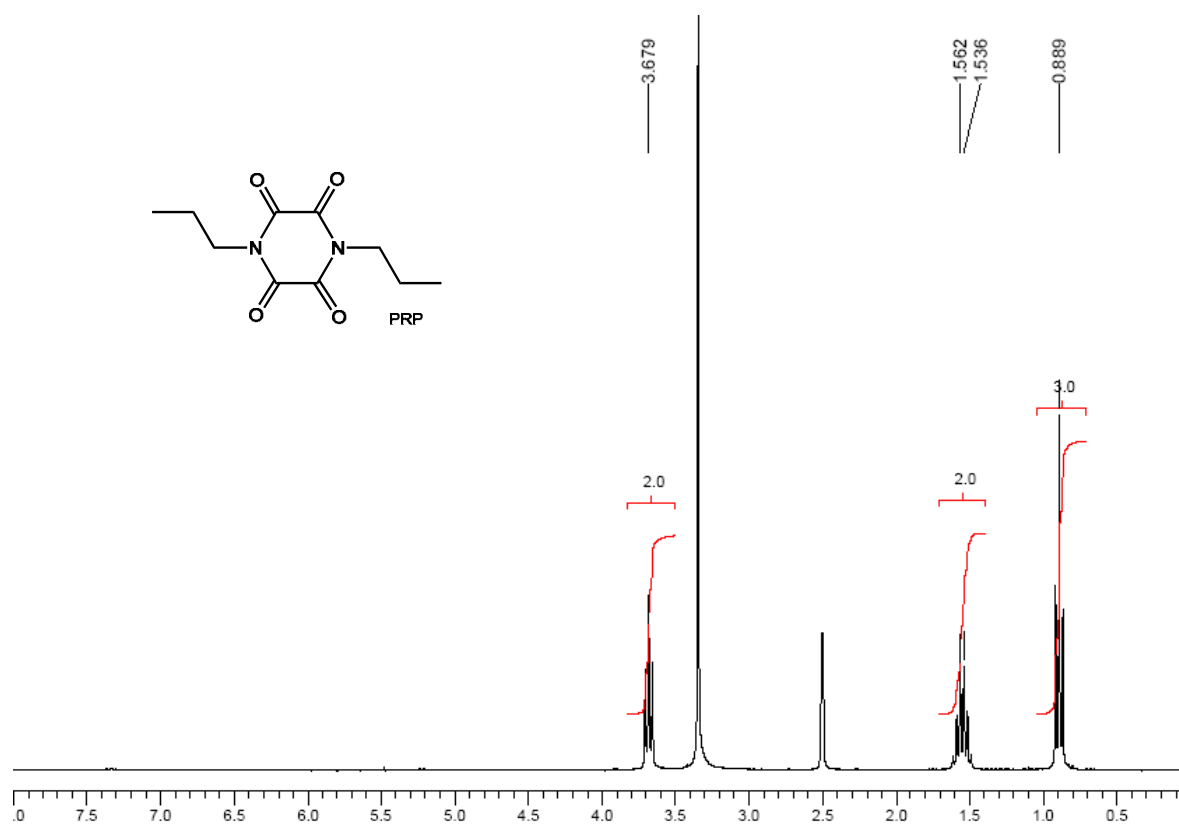
AP and o-AP: ^1H (300 MHz, DMSO-d_6)



AP: ^{13}C (75 MHz, DMSO-d_6)



PRP: ^1H (300 MHz, DMSO- d_6)



PRP: ^{13}C (75 MHz, DMSO- d_6)

