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Ammonia-Storage in Lithium Intercalated Fullerides

Electronic Supplementary Information

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Figure 1S: Laboratory powder diffraction profile of Li_6C_{60} before and after the ammoniation stages. The powder diffraction of the pristine Li_6C_{60} sample is displayed at the bottom, showing the typical fcc arrangement. The crystal structure deeply change after treatment with ammonia (1st amm., hyper-ammoniated phase), where the first peak is significantly shifted towards smaller angles, confirming the occurrence of ammonia co-intercalation in the sample. After the complete ammonia desorption, the sample recover again a fcc packing (1st des.). A second treatment in ammonia brings again to a hyper-ammoniated phase, with improved crystallinity (2nd amm.). Asterisk indicates the presence of peak arising from Li amide.

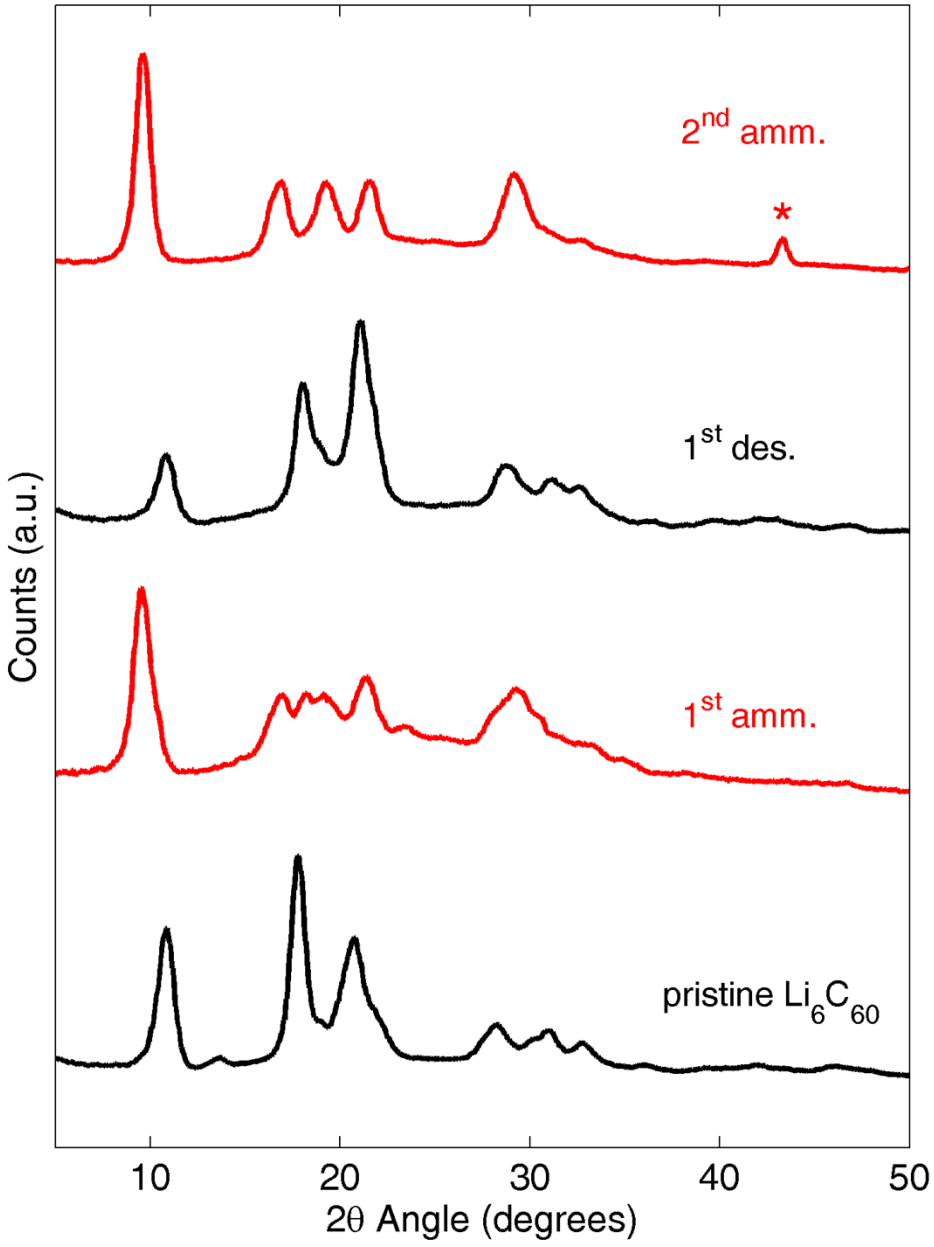

Figure 2S: Thermal evolution of the neutron powder diffraction profiles of $(ND_3)_yLi_3C_{60}$ (left) and $(ND_3)_yLi_{12}C_{60}$ (right) during in-situ measurements performed at WOMBAT in the temperature range 50-500K. Asterisks show peaks arising from Li amide.