Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information:

Optical and morphological properties of thin films of bis-pyrenyl π-conjugated molecules.

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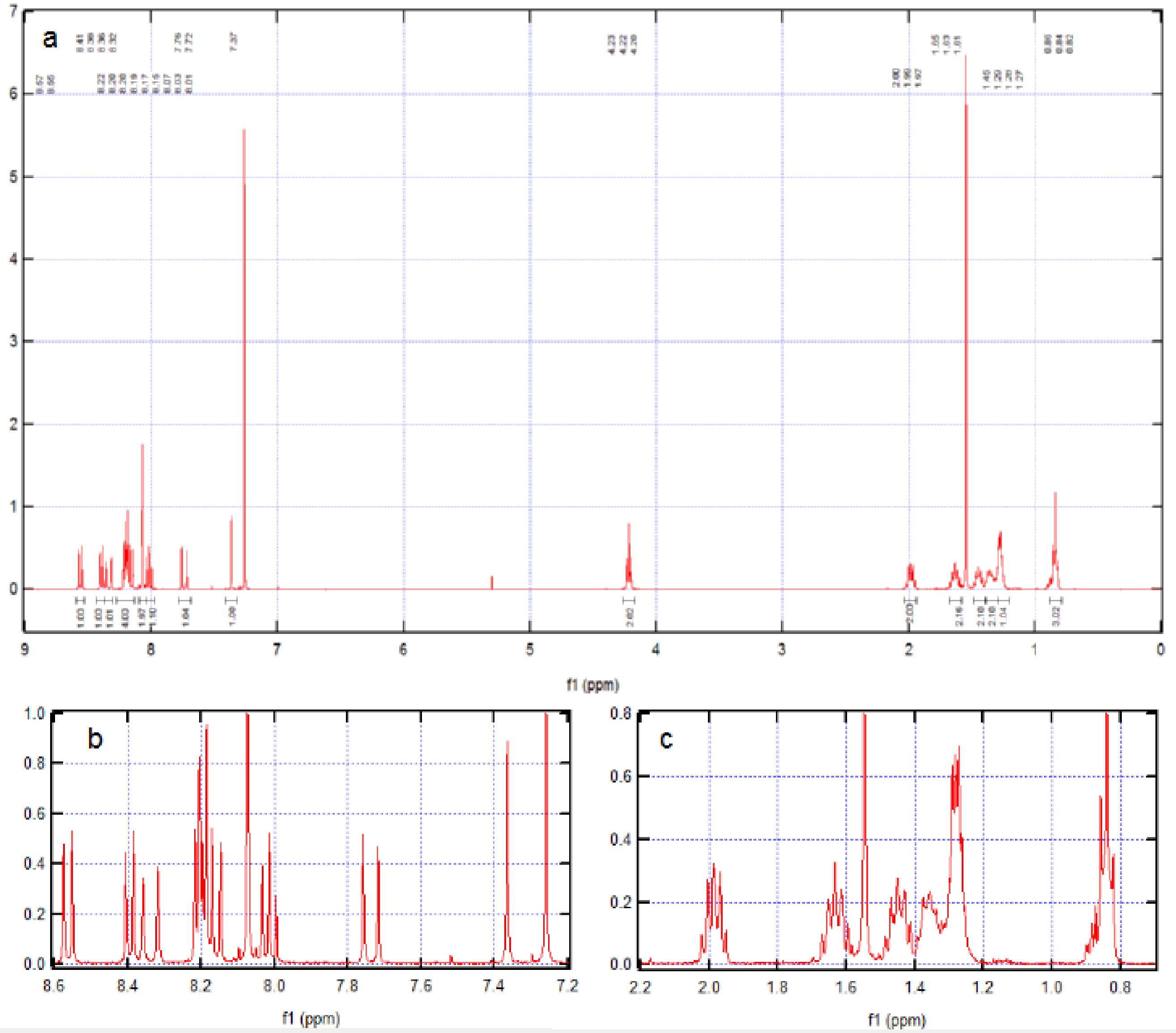

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Fig.S1: H NMR spectrum of bis-pyrene. a) full spectrum; b) & c) zoom. The all-*trans* configuration was confirmed by ^{1}H NMR, typical coupling constant values for *trans*-ethylenic configuration (ca. 16-17Hz) being found. F = 159-161°C; ^{1}H NMR($CDCl_3$, 250 Mhz) δ = 8.56 (d, ^{3}J=9.3Hz, 1H), 8.39 (d, ^{3}J=8.0Hz, 1H), 8.33 (d, ^{3}J=16.3Hz, 1H), 8.18 (m, 3H), 8.04 (m,4H), 7.73 (d, ^{3}J=16.1Hz, 1H), 7.37 (s,1H), 4.22 (d, ^{3}J=6.5Hz, 2H), 2.00 (m, 2H), 1.64 (m, 2H), 1.34 (m, 8H), 0.85 (t, ^{3}J=6.8Hz, 3H) ppm; EI-MS *m/z* 786(M^{+}); Anal. Calcd: C, 88.45; H, 7.49%.

Fig. S2 visualizes the data treatment process for obtaining the s-CRD spectra from the raw data.

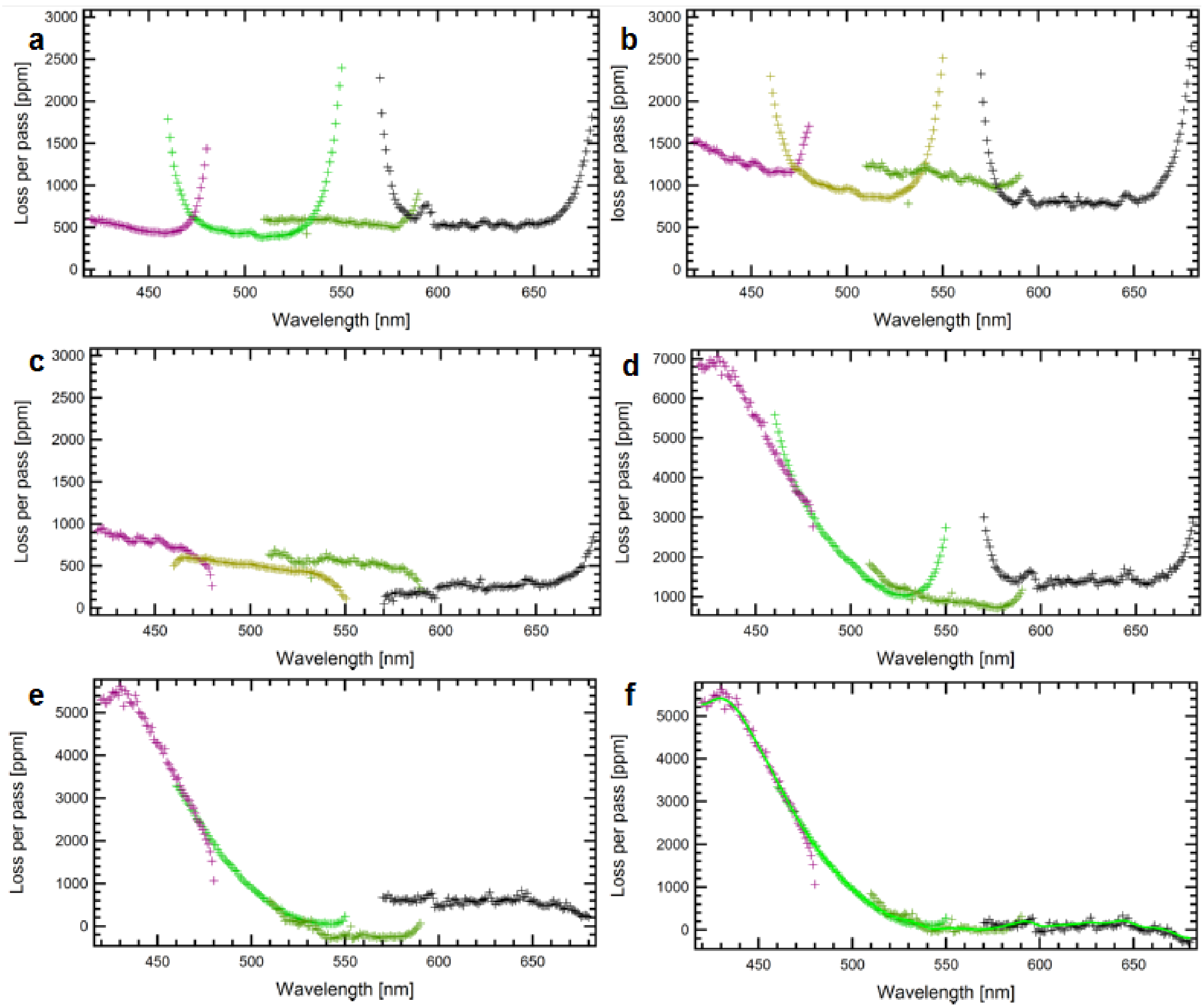

Fig.S2: s-CRD spectra: Acquisition and data treatment: a) s-CRD spectrum recorded for the empty cavity. Note the increasing loss at the edge of ranges covered by the different set of highly reflective mirror and the presence of peaks in the range 590-650nm, which are due to the lower quality of corresponding mirrors. b) s-CRD spectrum recorded after insertion of the glass substrate in Brewster angle configuration. c) s-CRD difference spectrum obtained by the subtraction of (b)-(a). d) s-CRD spectra recorded after deposition of bis-pyrene molecules on top of the glass substrate. e) s-CRD difference spectrum obtained by the subtraction of (d)-(b). f): s-CRD spectrum after adjustment of losses of adjacent cavities (coloured markers) and fit (green line).

The procedure for obtaining the final spectrum is as follows. In the overlapping regions losses recorded by both mirror are pondered to calculate the final loss: considering an overlapping region of n points between two sets of mirror a and b, points numbers i, ia and ib (ranging from 1 to n) and the loss per pass lpp(ia) and lpp(ib) recorded at the point i with mirrors sets a and b, (a stand for CRD data recorded on the overlapping region at the high energy side of a set of mirror, b stand for the losses recorded on the low energy side of the adjacent mirror set. To calculate the loss per pass (lpp) at the point i, losses recorded by both cavities are pondered using the following formula::

$$lpp(i)= (lpp(ia)*((n+1-i)/n)+lpp(ib)*((i-1)/n))$$

This procedure allows for a more reasonable estimation of the losses at the edges, less affected by the low reflectivity of mirror at the edges of the covered ranges. However, instead of these data treatment processes, some features remain in the final spectra such as the noise observed in the wavelength range 590-650nm.

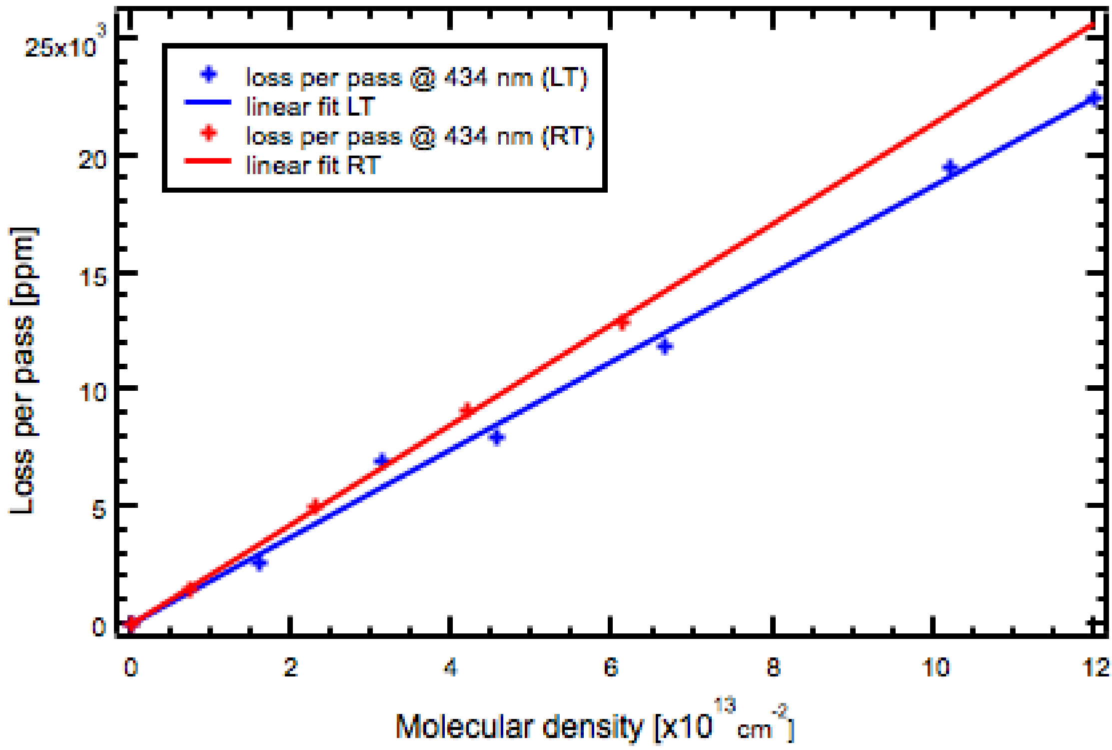

Fig.S3: loss per pass at 434nm measured as a function of the molecular density and at various temperature (120K: blue; RT: red). Loss per pass evolves linearly with the molecular density. Interestingly, for a given molecular density the absorption of bis-pyrene is more important at RT than at 120K.

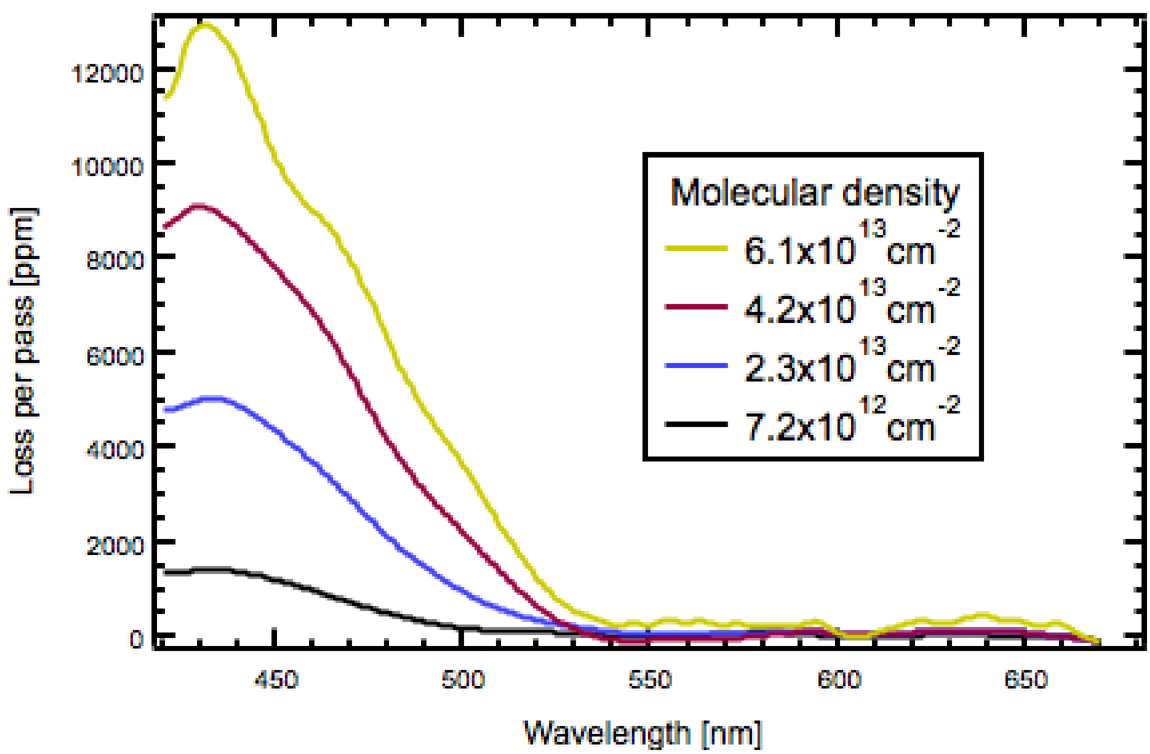

Fig.S4: Full s-CRD spectra recorded for various coverages of bis-pyrene deposited on BK7 substrate at RT: the compound strongly absorbs at 434nm independently of the coverage. A shoulder appears at 505nm between 2.3 and 4.2×10^{13} cm^{-2}. Independently of the coverage the film is transparent above 550nm. The spectrum recorded at molecular density of $6.1\times10^{13}cm^{-2}$ shows two particular artefacts: above 550nm the signal is noisy and in the range 440-470nm the shoulder is observed, which can attributed to the combination of the data from two mirror sets with different optical quality.