

Spectroscopic identification of Quinacridone polymorphs for organic electronics

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Electronic Supplementary Information

TABLE OF CONTENT

Powder X-ray Diffraction	ESI-1
Raman spectra of QA powders in the intramolecular vibrations spectral region	ESI-2
Raman spectra of the films with and without background correction	ESI-3
References	ESI-4

Powder X-ray Diffraction

The program Mercury¹ has been used for the calculation of X-ray powder patterns on the basis of single-crystal data retrieved from the Cambridge Structural Database² (QNACRD06 for α' -QA, QNACRD07 for β -QA, and QNACRD08 for γ -QA). A comparison of calculated patterns with those measured on polycrystalline samples synthesized by us and provided by Prof. M. Schmidt is shown in Fig. S1.

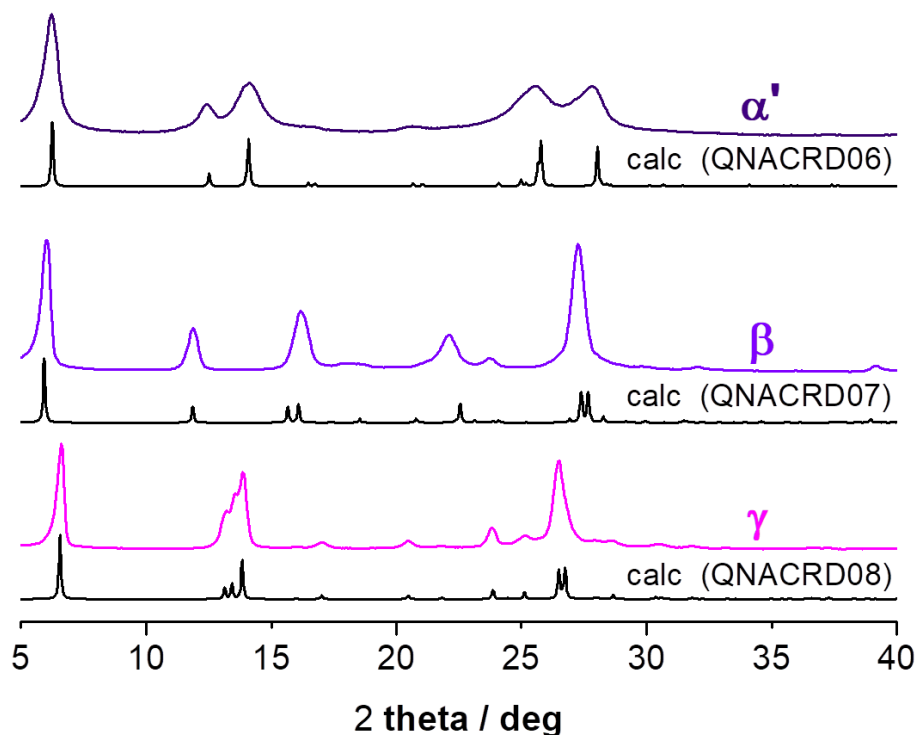


Fig. S1 - Comparison of calculated (on the basis of single crystal data) and measured X-ray powder patterns for α' -QA (top), β -QA (middle), and γ -QA (bottom).

Raman spectra of QA powders in the intramolecular vibrations spectral region

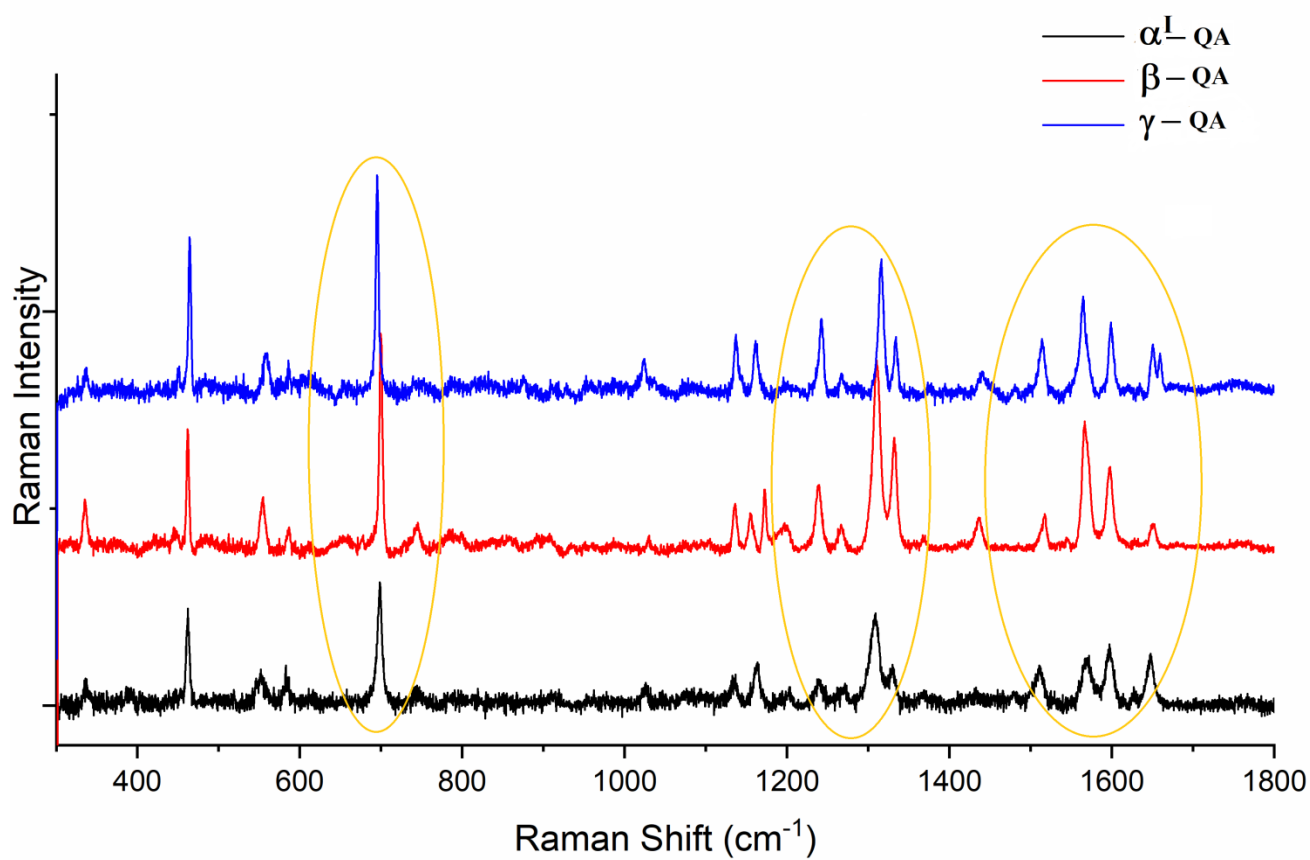


Fig. S2 – Raman spectra of QA powders in the intramolecular vibrations spectral region. Exciting line: 647.1 nm. The luminescence background has been subtracted. The orange ovals evidence the main spectral differences between the polymorphs.

Raman spectra of the films with and without background correction

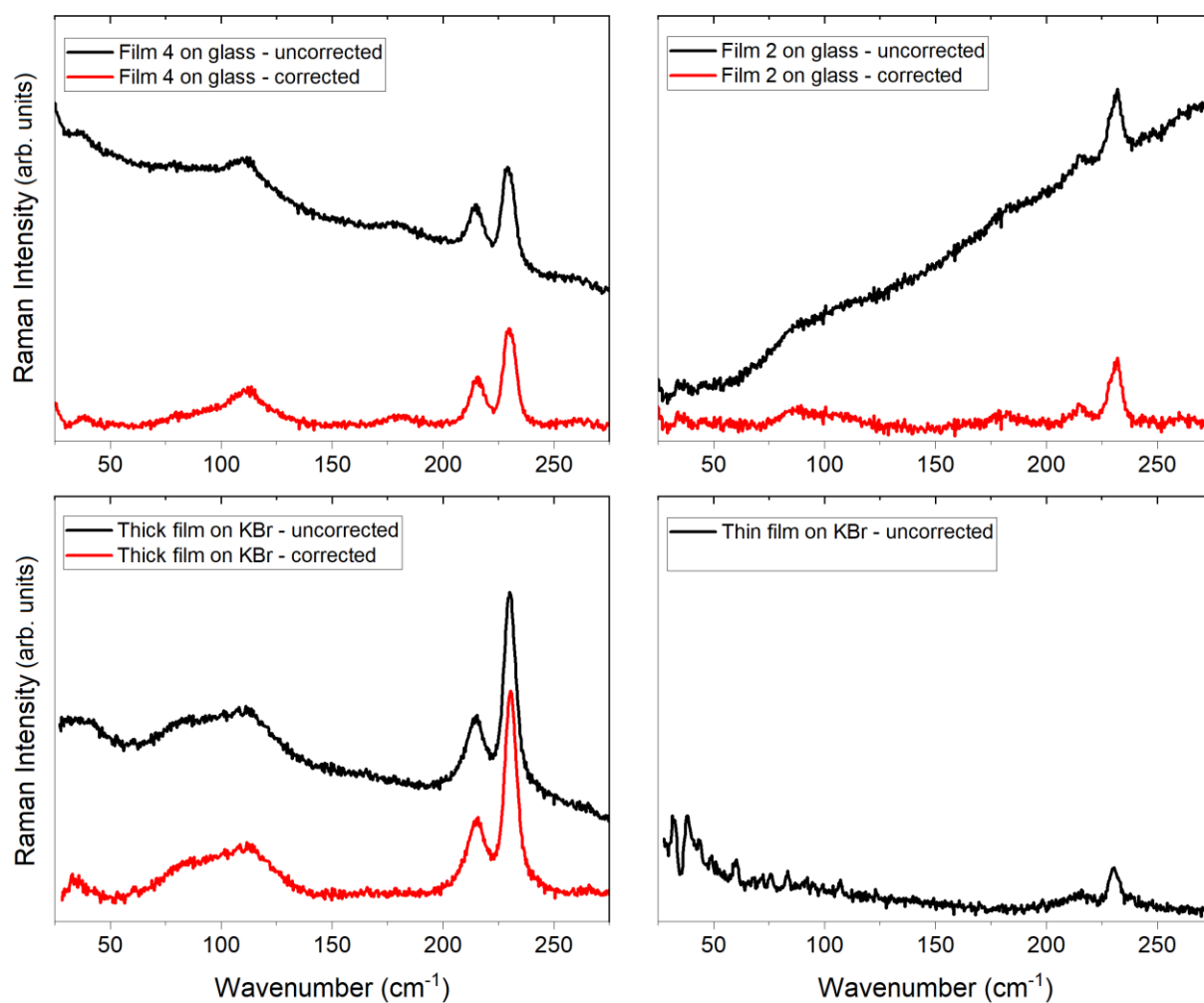


Fig. S3 - Uncorrected and background corrected Raman spectra of QA films. The background corrected spectra are reported in Figure 9 of the main text. No attempt of subtracting the background has been performed for the thin QA film on KBr, due to the low signal to noise ratio.

References

- [1] C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. Van De Streek and P. A. Wood, *J. Appl. Crystallogr.*, 2008, **41**, 466–470.
- [2] C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward, *Acta Cryst.*, 2016, **B72**, 171–179.