Matrix Isolation Spectrum, UV-Induced Photochemistry (λ > 215 nm) and Differential Scanning Calorimetry Analysis of 3-(*N*-Acetamide)-Coumarin

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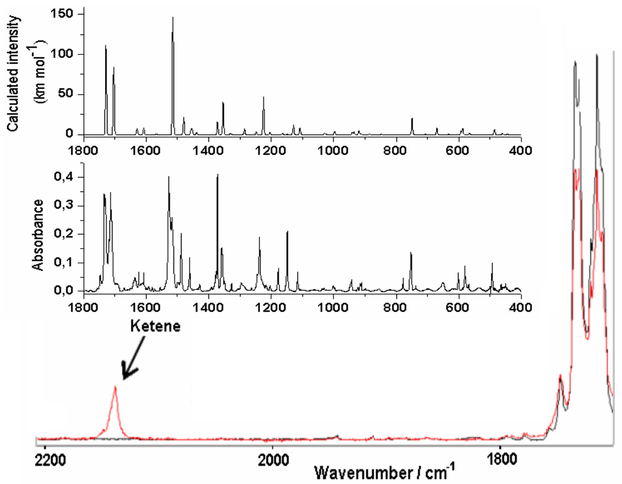
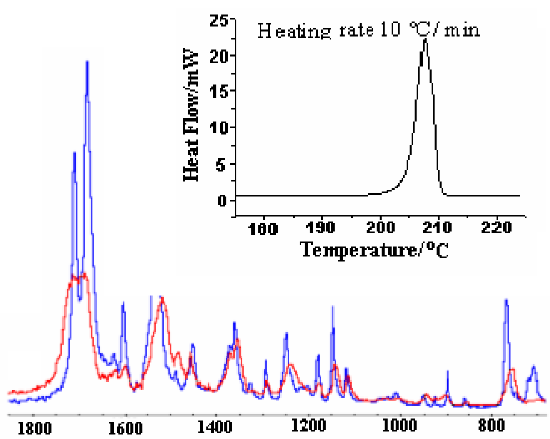
Coumarins are biologically relevant compounds and they also receive industrial application as dyes. From a structural point of view, these molecules can be considered substituted benzoderivatives of α-pyrones, a family of compounds that have been studied thoroughly in our laboratories [1-3]. As a general rule, matrix-isolated α-pyrones undergo easy photolysis upon *in situ* irradiation, with the two fundamental processes being ring-opening to ketenes and ring-contraction to their Dewar analogues.

Following the same lines of our previous studies on α-pyrones and related compounds, in the present study we considered 3-(*N*-acetamide)-coumarin (3NAC). Like for 3-methyl coumalate [4], UV (λ > 215 nm) irradiation of matrix-isolated 3NAC appears to lead exclusively to the ring-opening ketene photoproduct, as testified by observation of the characteristic ketene band around 2130 cm^{-1} in the IR spectra of the irradiated 3NAC matrices and absence of any bands ascribable to other possible photoproducts (Figure 1).

In addition to the matrix-isolation spectra of 3NAC, IR spectra of the pure compound in its neat condensed phases were recorded as a function of temperature (in the range 20-225 ºC). The observed spectra were correlated with results obtained by differential scanning calorimetry (DSC) (Figure 2). All spectroscopic data were rationalized with help of extensive theoretical DFT calculations on 3NAC and its possible photoproducts.





Figures: 1 (Left panel) - Calculated *vs.* experimental IR spectra of matrix-isolated 3NAC and results of *in situ* UV irradiation of the matrix-isolated compound (showing the characteristic band of the C=C=O asymmetric stretching of the photoproduced ketene). **2 (Right panel)** - DSC profile of the exothermic peak around 208 °C (melting) and IR spectra of crystal (room temperature; 20 °C - blue line) and melted phase (210 °C - red line).

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Acknowledgements:
This work was supported by the Portuguese FCT (Project POCI/QUI/58937/2004) and Eskişehir Osmangazi University (Project 200519010). SB also thanks to the Portuguese FCT for the Ph.D. grant ref. SFRH/BD/16119/2004.