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# Nonlinear properties of perylene derivatives: The role of the Vibronic coupling.

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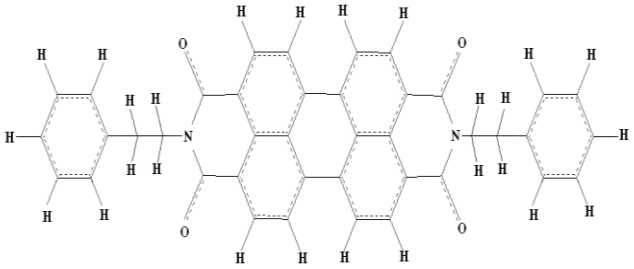
# Outline:

- Motivation
- Absorption Process
- WLC Z-Scan
- Results
- Conclusions

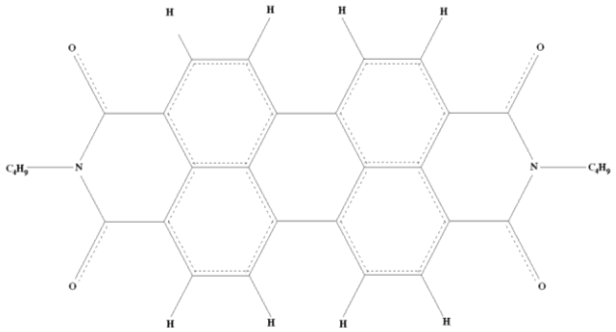
# Motivation

- π - conjugated organic molecules
  Easy manipulation
  Presents high nonlinearities due to its high deformable electronic cloud

- Applications:
  Microfabrication
  Optical limiting
  Photodynamic therapy
  Two photon pumping lasing

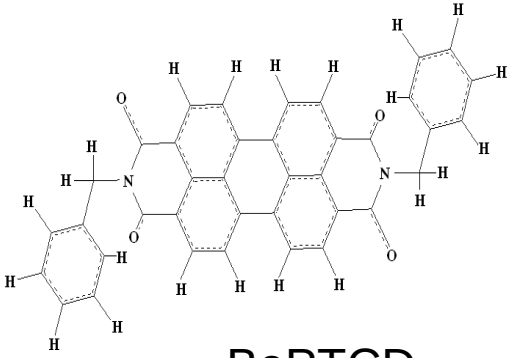


PhPTCD



BuPTCD

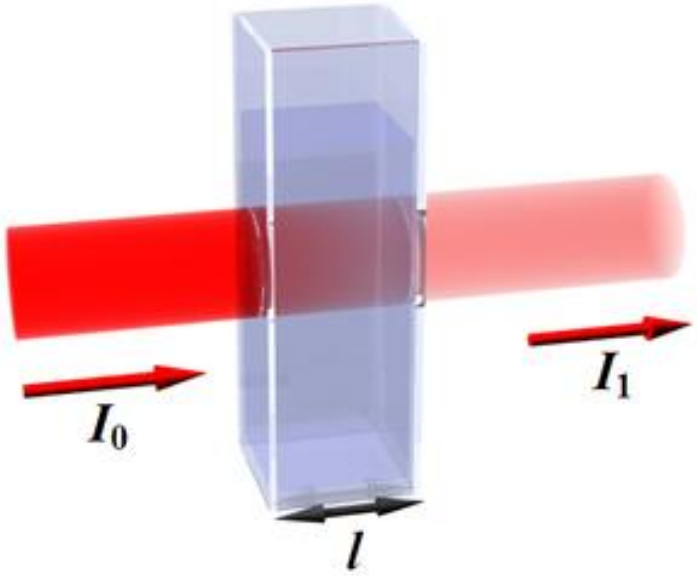
- Perylene Derivatives
  High 2PA cross section
  (3000 GM)



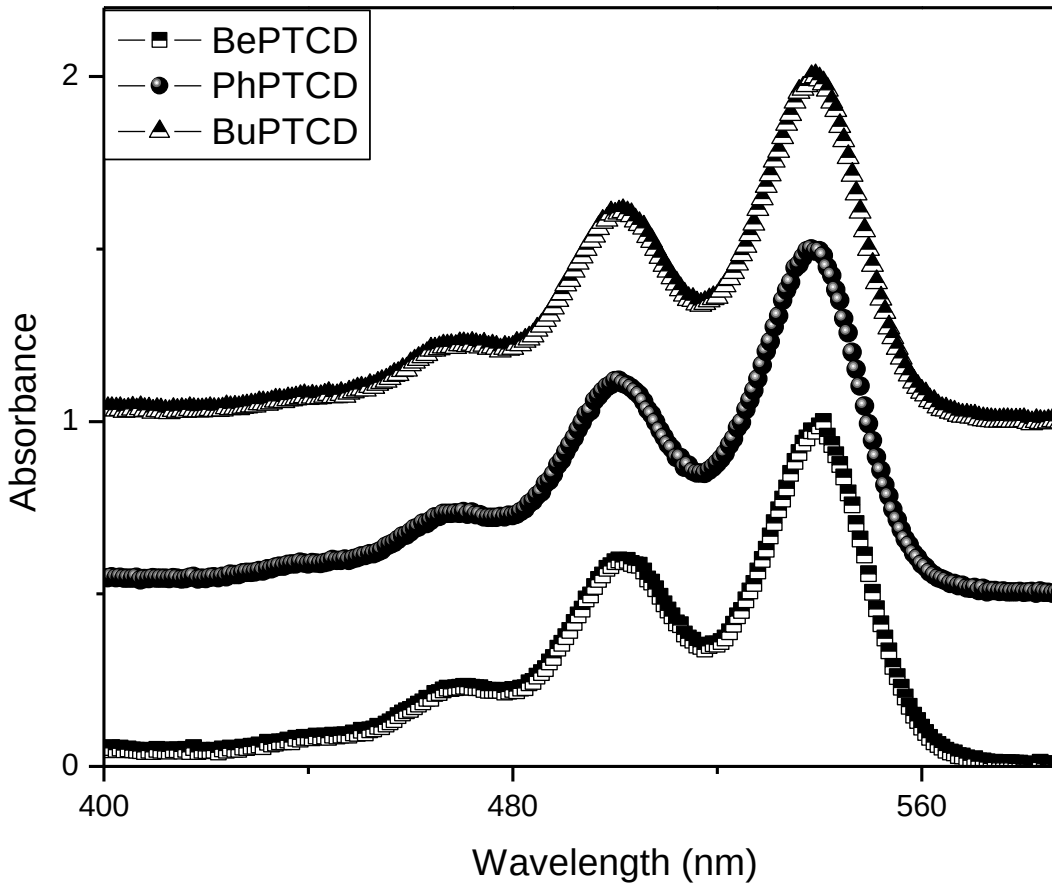
BePTCD

# Absorption Process

- Linear Absorption:

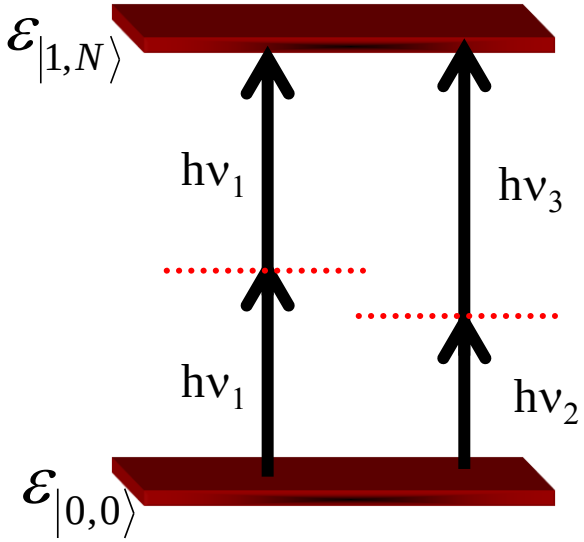



$$\alpha_\lambda = \ln\left(\frac{I_0}{I_\lambda}\right) \Big/ Lc_0$$

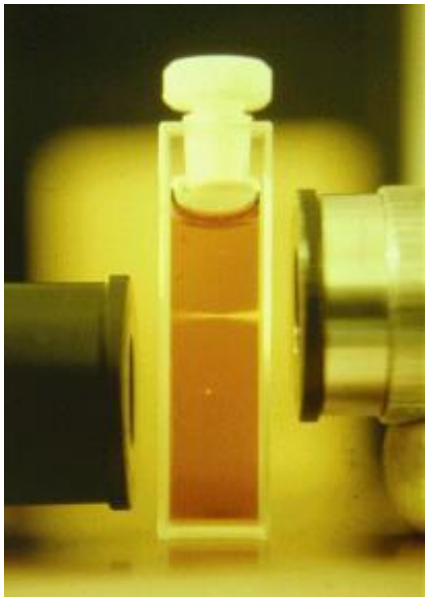


# Absorption Process

- Two Photon Absorption (2PA)
  Related to the $\chi^{(3)}$ tensor on the polarization expansion



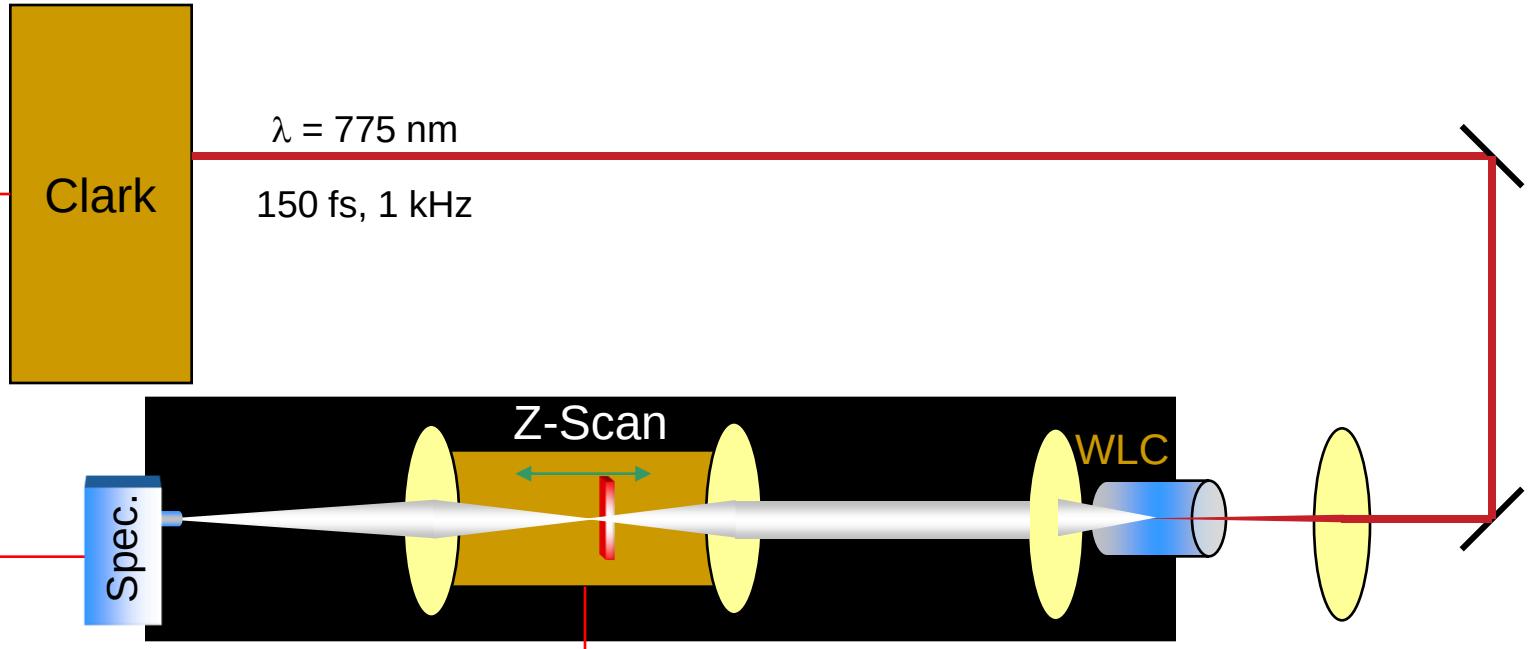

$$\mathcal{E}_{|1,N\rangle} - \mathcal{E}_{|0,0\rangle} = h\nu_0$$



$$\alpha_T(I) = \alpha_0 + \beta I$$

$$I_s(z,r,t) = \frac{I_0(z,r,t)}{1+\beta L I_0(z,r,t)} \quad \text{se} \quad \alpha_0 = 0$$

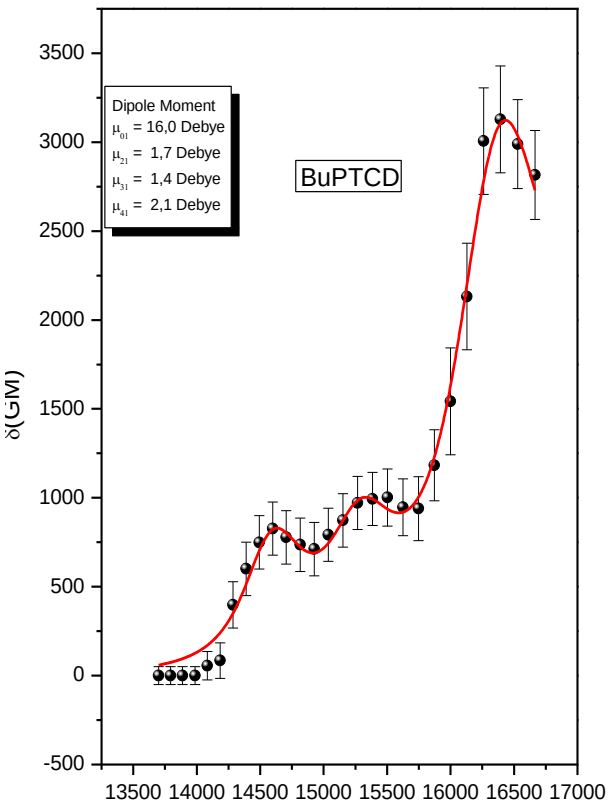
# WLC Z-Scan

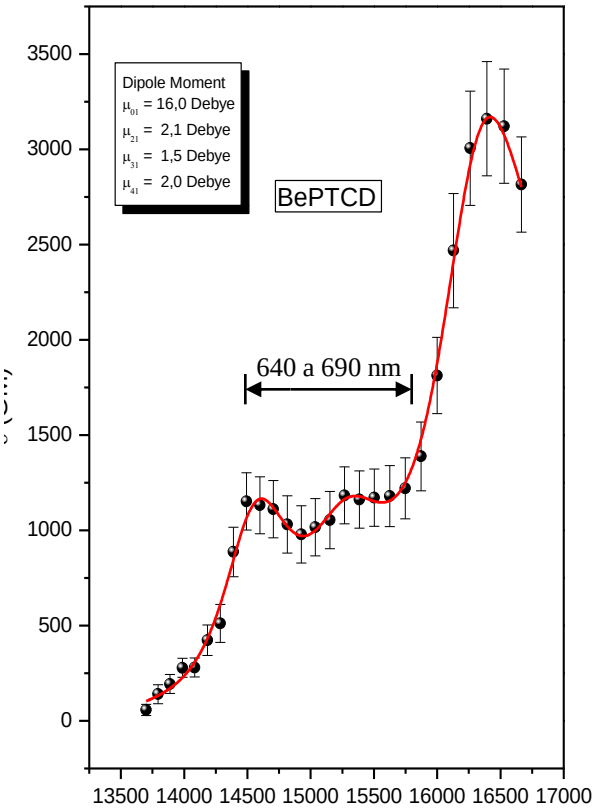


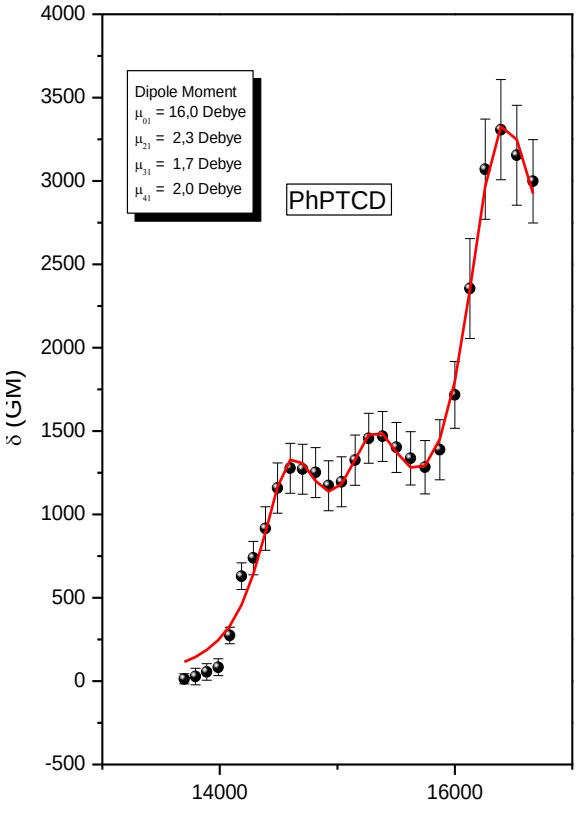

$$T = \frac{1}{\sqrt{\pi} q_o(z,0)} \int_{-\infty}^{+\infty} \ln\left[1 + q_o(z,0) e^{-r^2}\right] d\tau$$

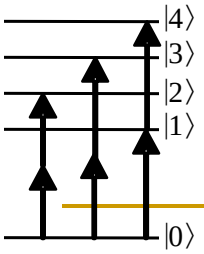
$$q_o = \beta I_o(\tau) L \left(1 + z^2 / z_o^2\right)^{-1} \Rightarrow \delta = h\upsilon\beta / N$$

# Results: 2PA



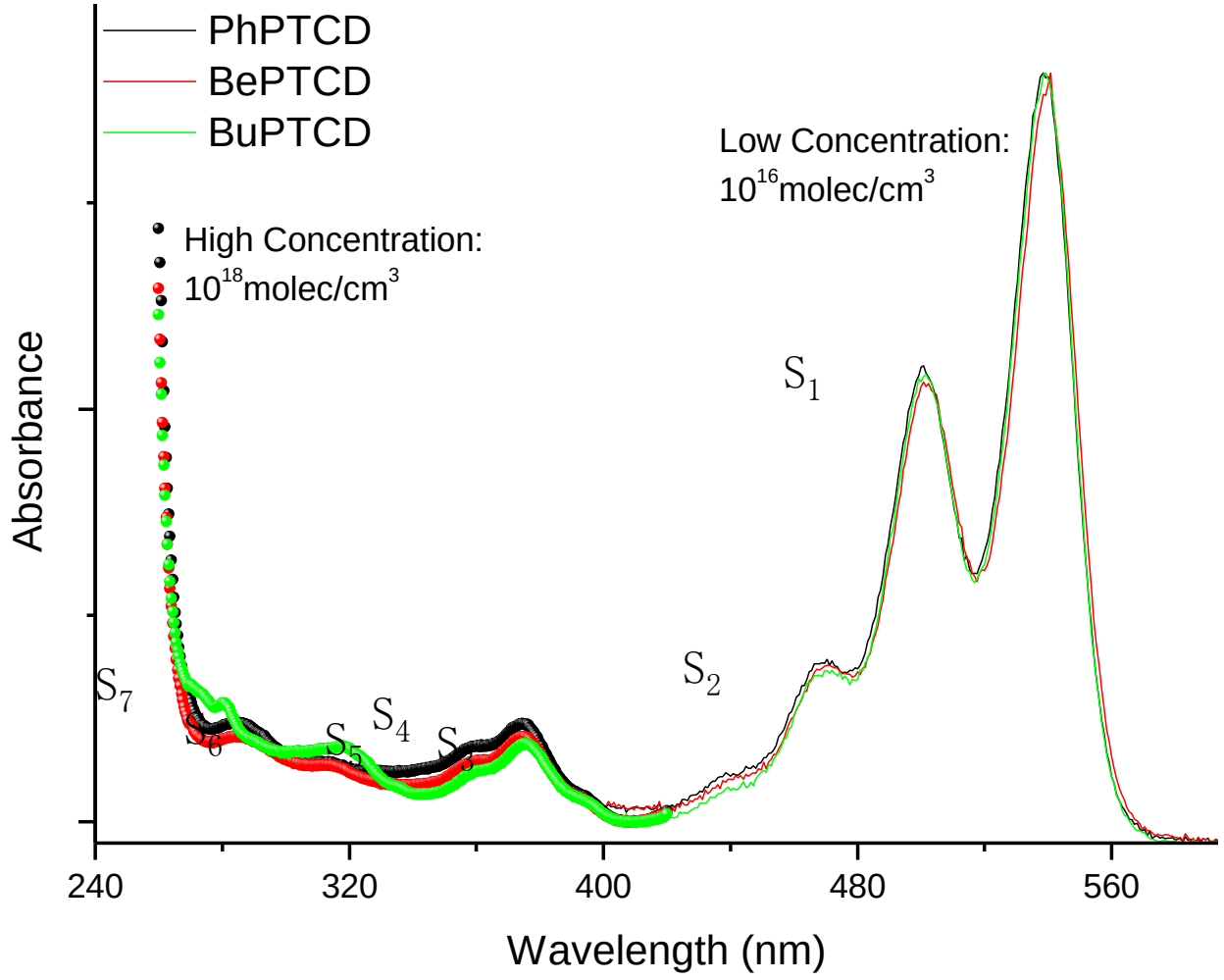




$$\delta(\upsilon) \propto \frac{\upsilon^2}{(\upsilon_{01}-\upsilon)^2+\Gamma_{01}^2}\left[\frac{A_2}{(\upsilon_{02}-\upsilon)^2+\Gamma_{02}^2}+\frac{A_3}{(\upsilon_{03}-\upsilon)^2+\Gamma_{03}^2}+\frac{A_4}{(\upsilon_{03}-\upsilon)^2+\Gamma_{03}^2}\right]$$

# Huang – Rhys Factor



# Huang – Rhys Factor

| Fator Huang - Rhys | PhPTCD | λ (nm) | BePTCD | λ (nm) | BuPTCD | λ (nm) |
|---|---|---|---|---|---|---|
| $S_1$ | 0,54 | 501,29 | 0,55 | 501,64 | 0,55 | 502,30 |
| $S_2$ | 0,13 | 468,00 | 0,14 | 468,27 | 0,14 | 468,87 |
| $S_3$ | 0,07 | 392,86 | 0,09 | 392,63 | 0,07 | 392,06 |
| $S_4$ | 0,22 | 376,94 | 0,24 | 377,54 | 0,21 | 376,57 |
| $S_5$ | 0,33 | 365,46 | 0,25 | 363,54 | 0,31 | 363,58 |
| $S_6$ | 0,28 | 314,92 | 0,35 | 316,63 | 0,24 | 317,47 |
| $S_7$ | 0,38 | 280,82 | 0,65 | 269,80 | 0,43 | 281,03 |

# Conclusions:

- Rigid conjugated structure: no significantly line shape changes due to radical alteration on the main perylene ring;
- Material with High Nonlinearities: Not affected by the temperature.
- High dependency between the 2PA and the electron – phonon coupling.