

Theoretical Efforts in Identification of Interstellar Organic Molecules

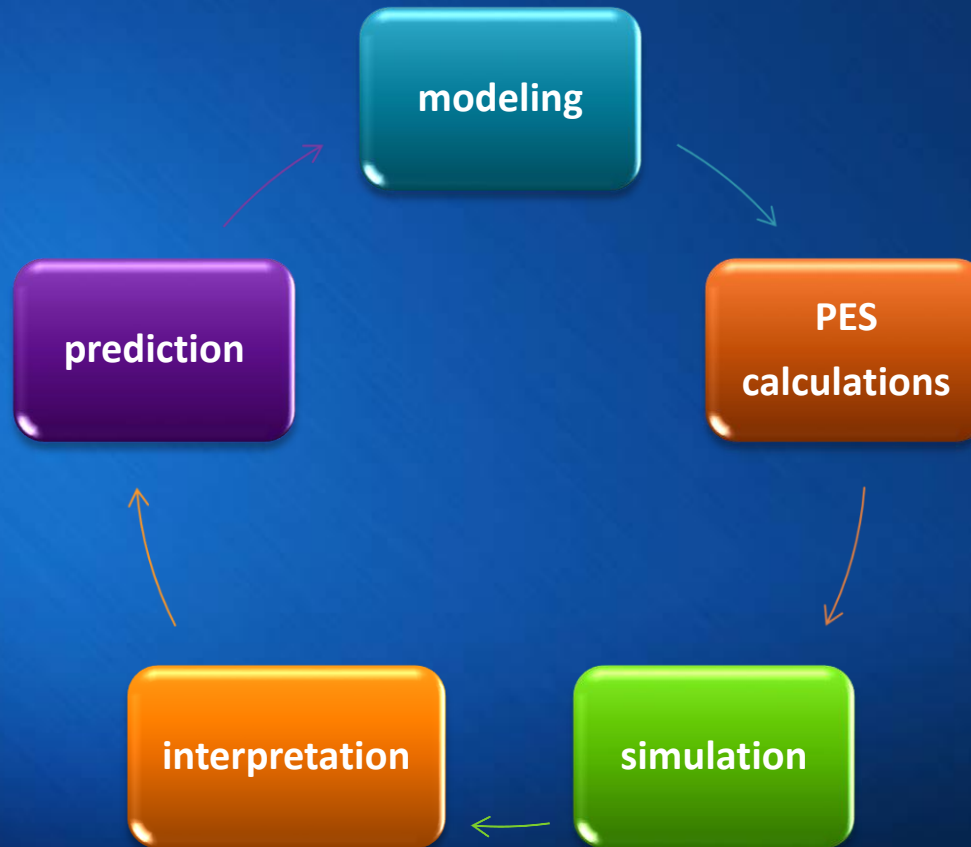
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December 17, 2015

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<http://www.scifac.hku.hk/kwok/sal/abdi.html>

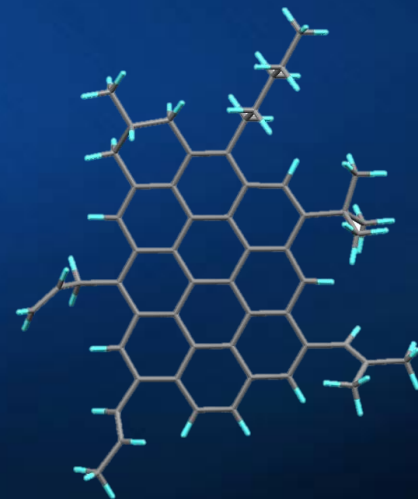
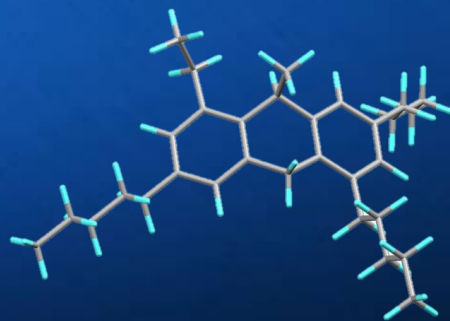
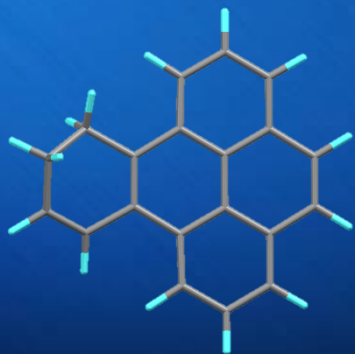
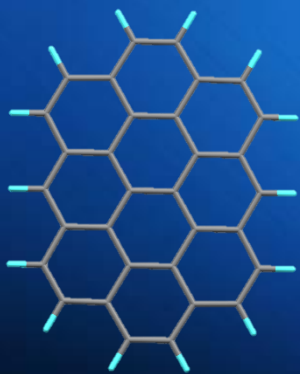
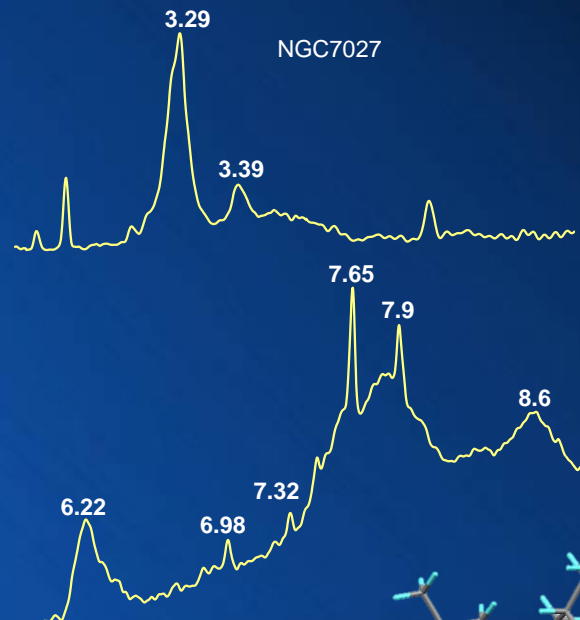
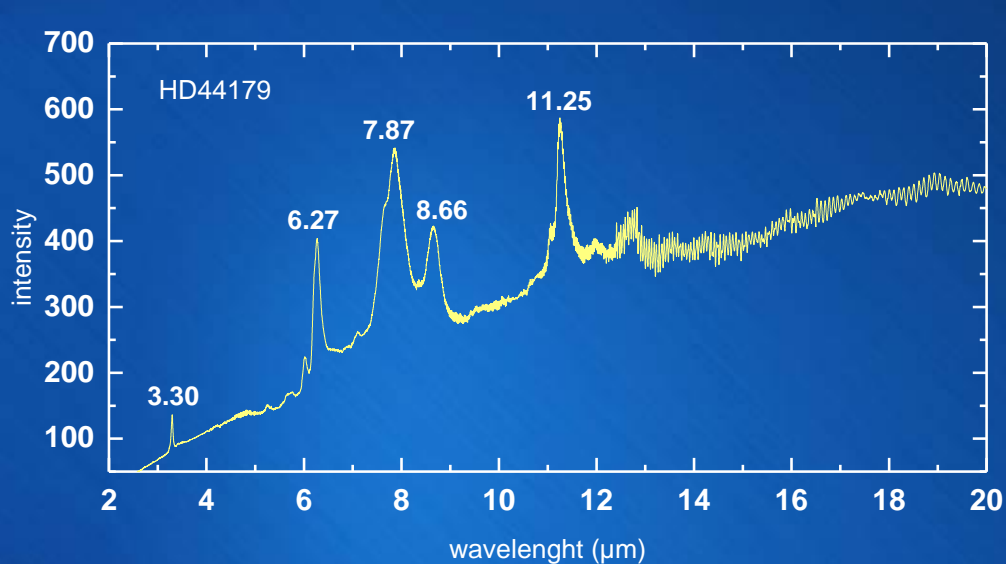


computational quantum chemistry & infrared spectroscopy

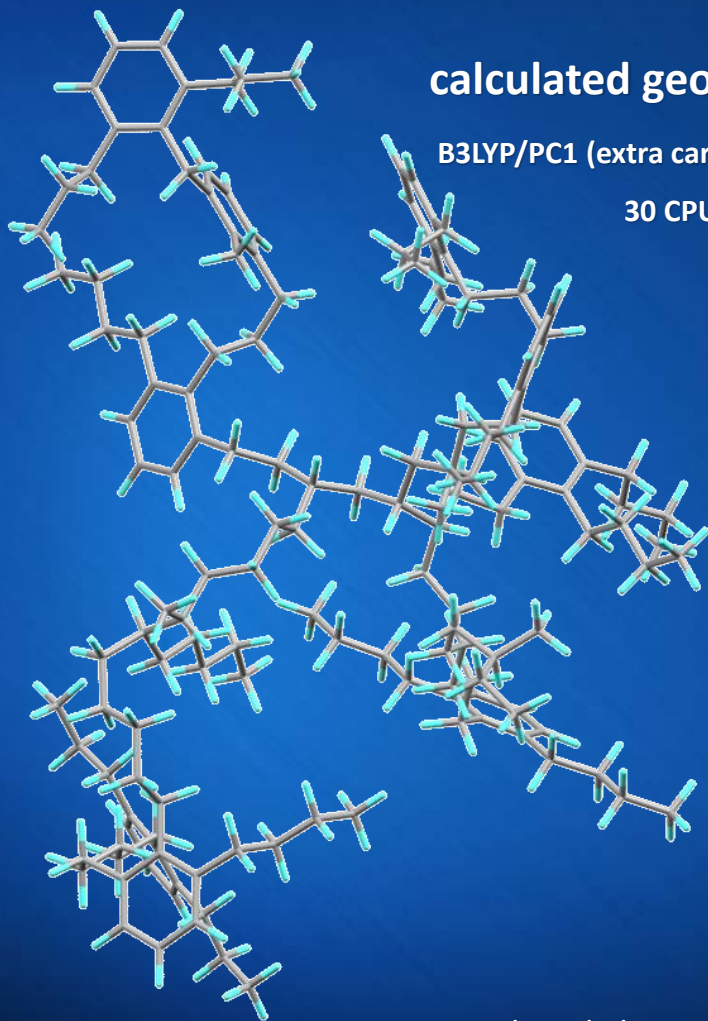


PAH model and its derivatives

observations and proposed models



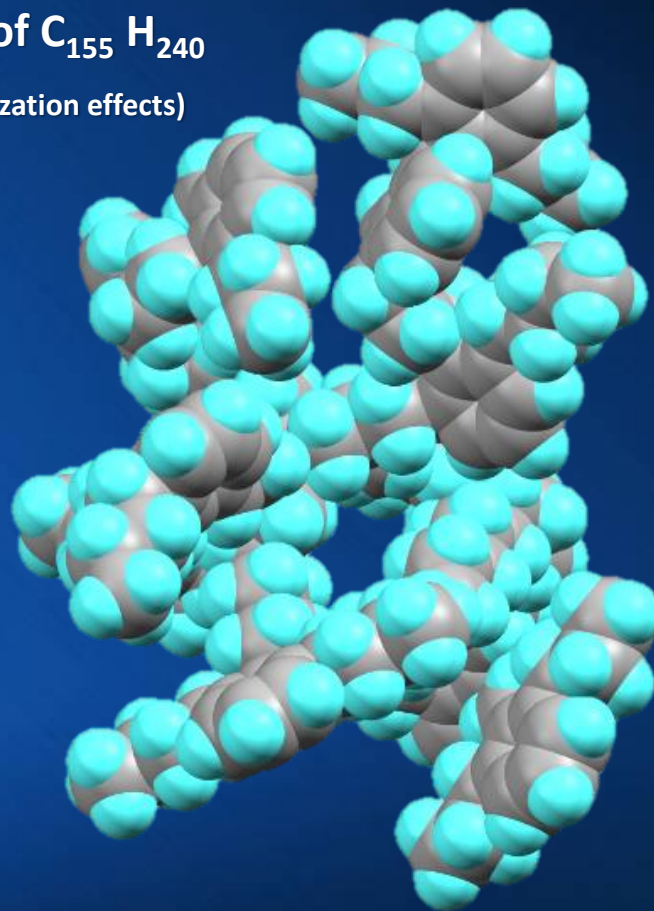
MAON model and PES calculations



calculated geometry of C₁₅₅ H₂₄₀

B3LYP/PC1 (extra care on polarization effects)

30 CPUs, 20 days

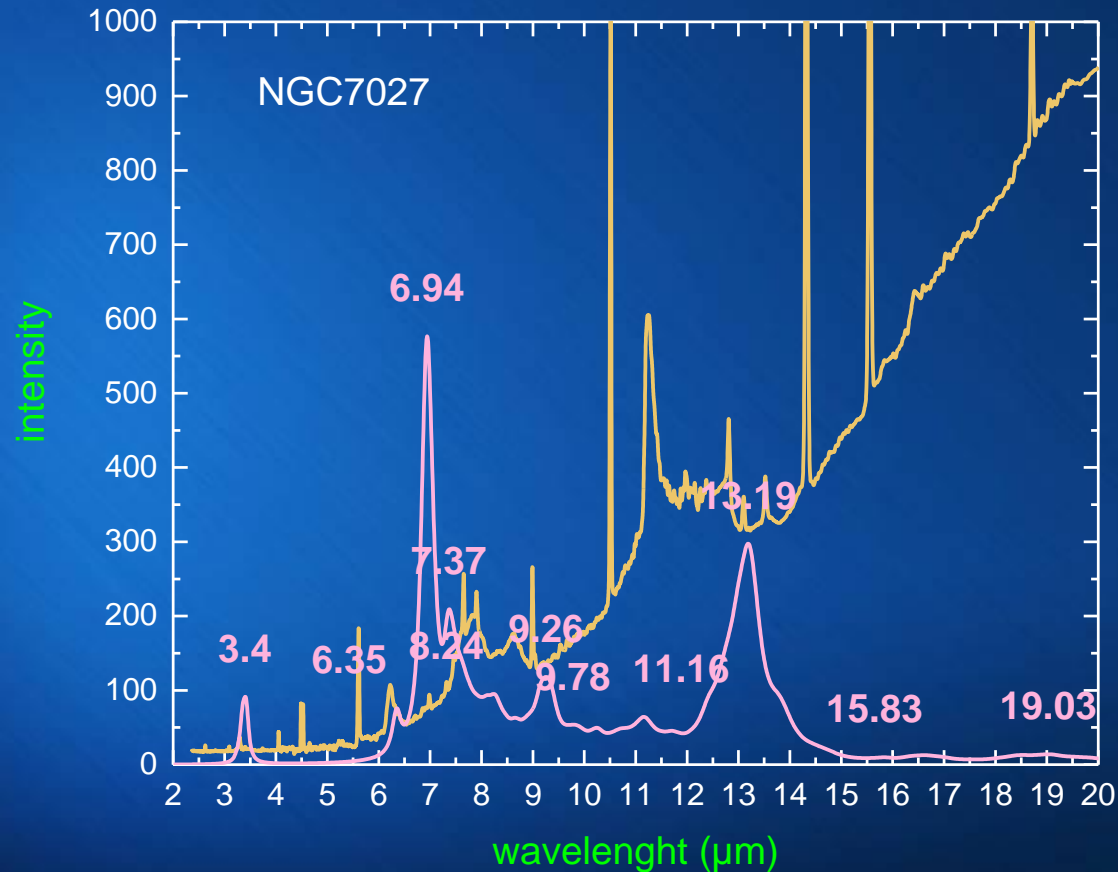


Kwok and Zhang, Nature, 479:80 (2011)

Sadjadi, Zhang and Kwok, ApJ, 807:95 (2015 July 1)

simulation

simulated IR spectra for $C_{155}H_{240}$, DFT/Drude, $T=500$ K

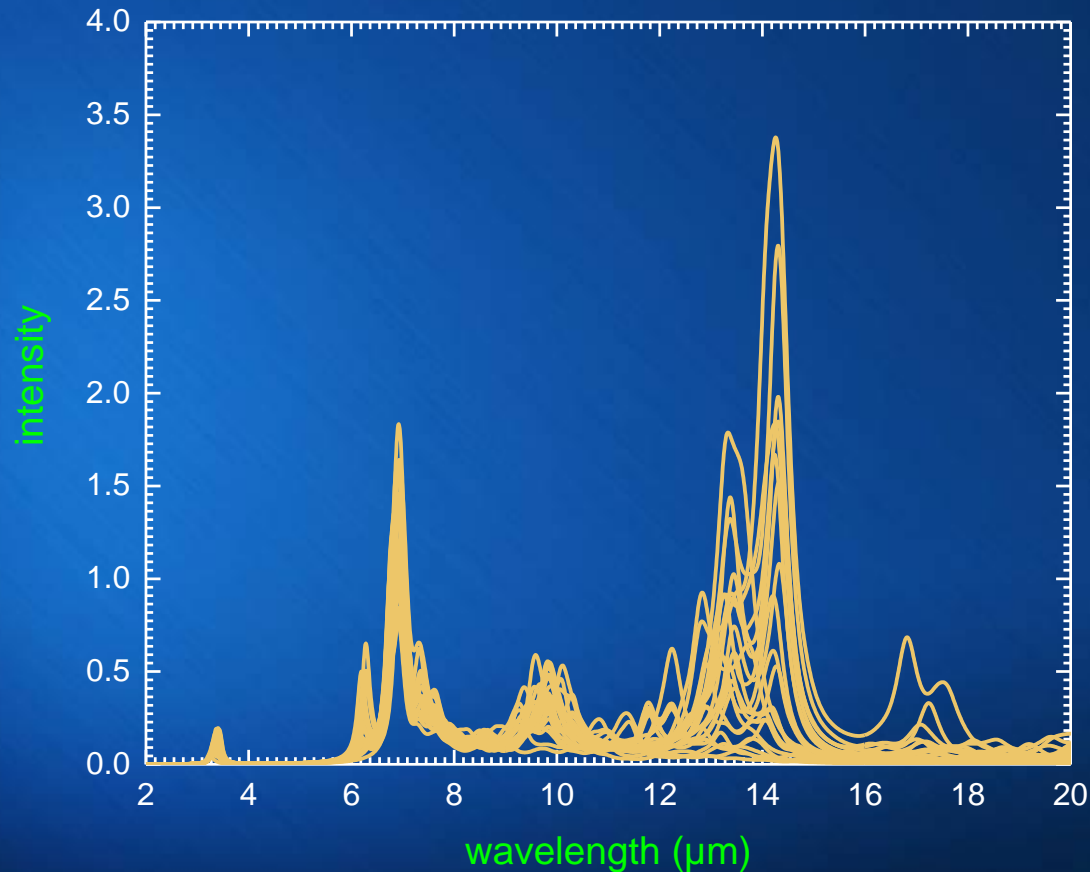


Sadjadi, Zhang and Kwok, ApJ, 807:95 (2015 July 1)



MAONs infrared fingerprint

simulated IR spectra for 40 MAONs, DFT/Drude, $T=500$ K

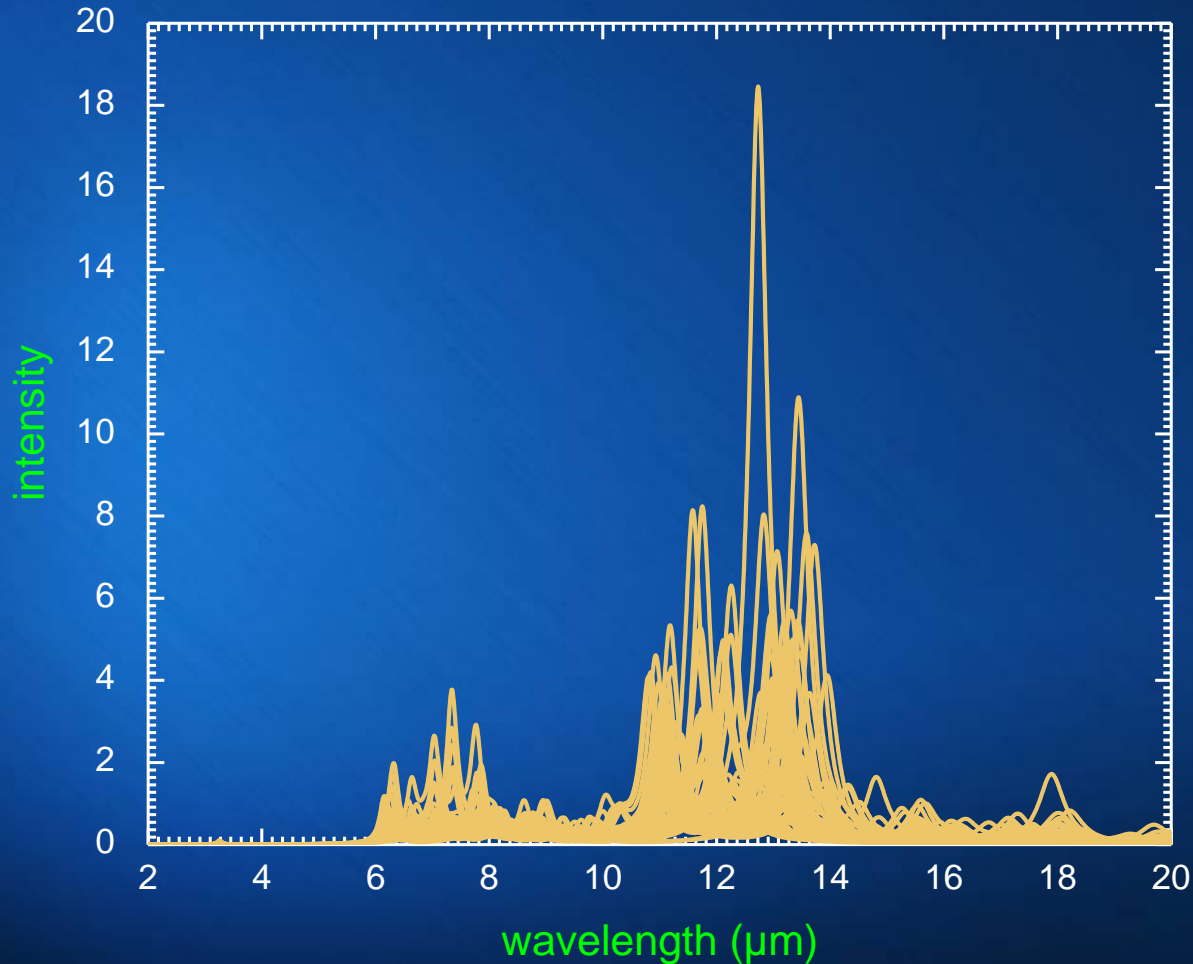


Sadjadi, Zhang and Kwok, ApJ, 807:95 (2015 July 1)



PAHs infrared fingerprint

simulated IR spectra for 60 PAHs, DFT/Drude, T=500 K



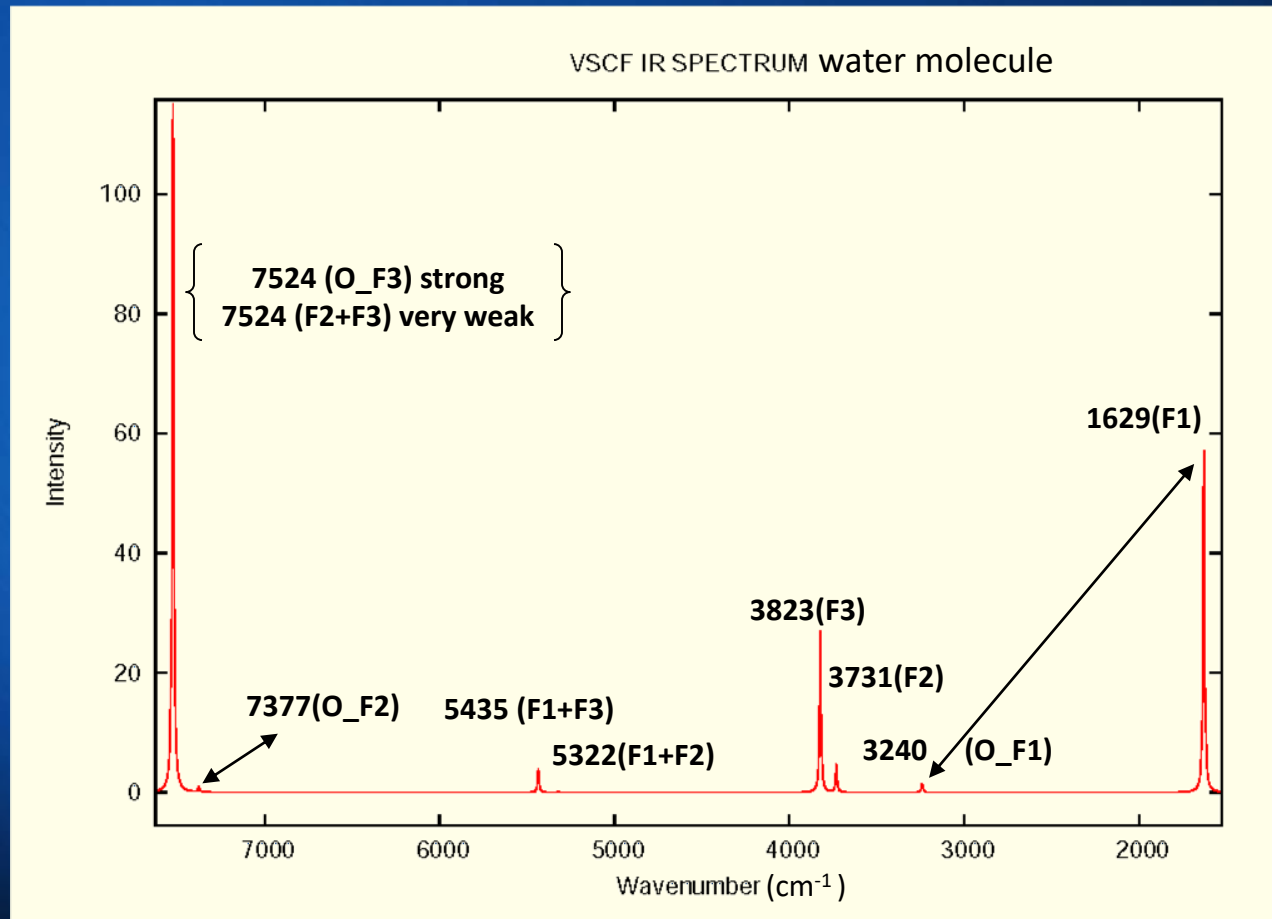
Sadjadi, Zhang and Kwok, ApJ, 807:95 (2015 July 1)



Annual meeting of the Hong Kong Astrophysical Society

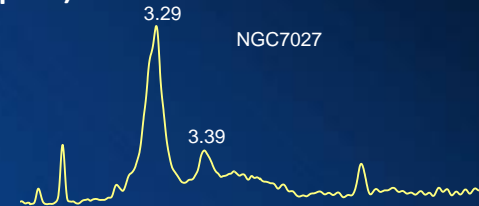
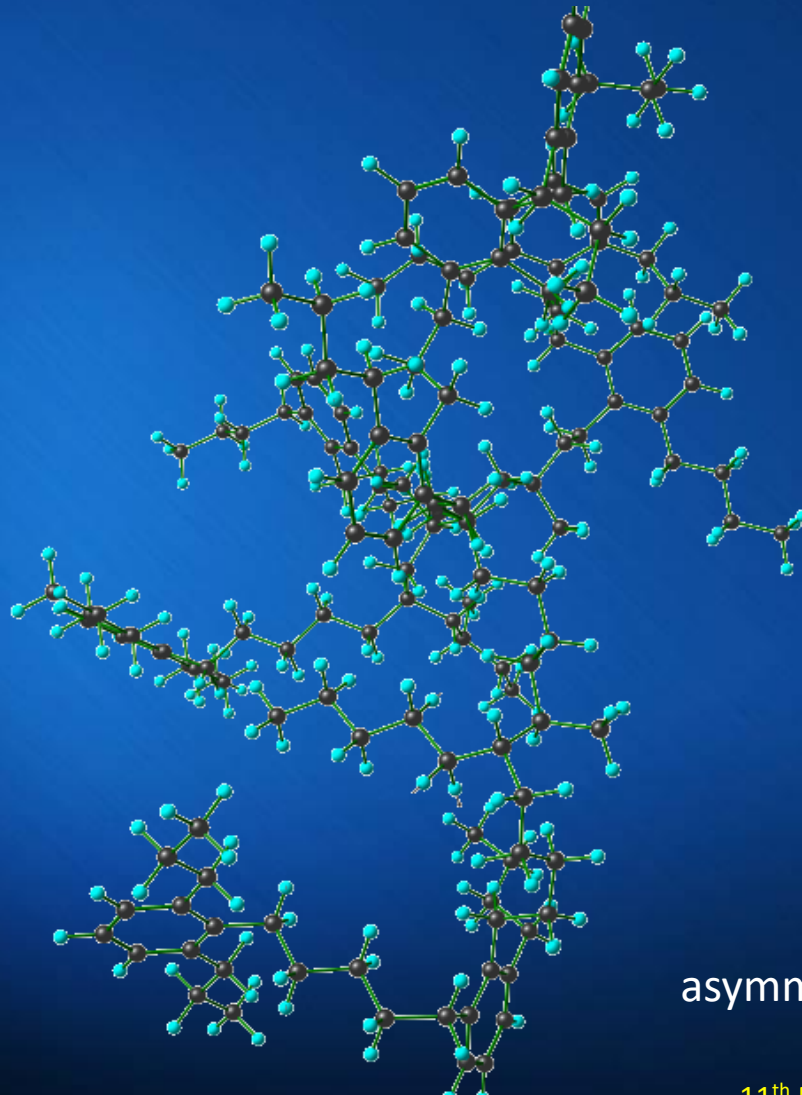
calculations of overtones and combination bands

Vibrational Self-Consistent Field (VSCF) calculations
perturbation theory, MP2/DZ or TZ



graphical interpretation

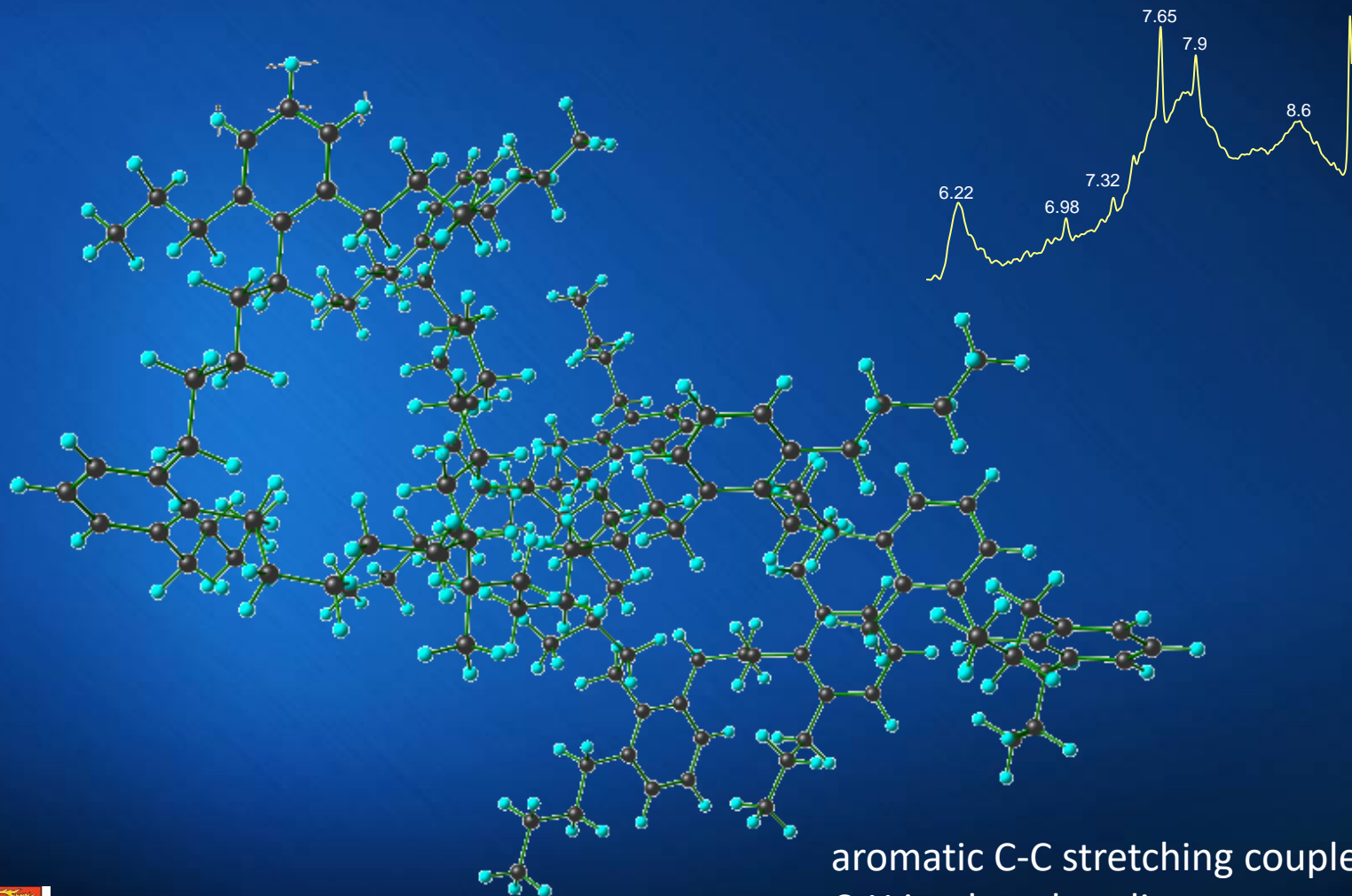
$C_{155}H_{240}$ (vibrational motion at $3.4\ \mu\text{m}$)



asymmetric methylene C-H stretching

graphical interpretation

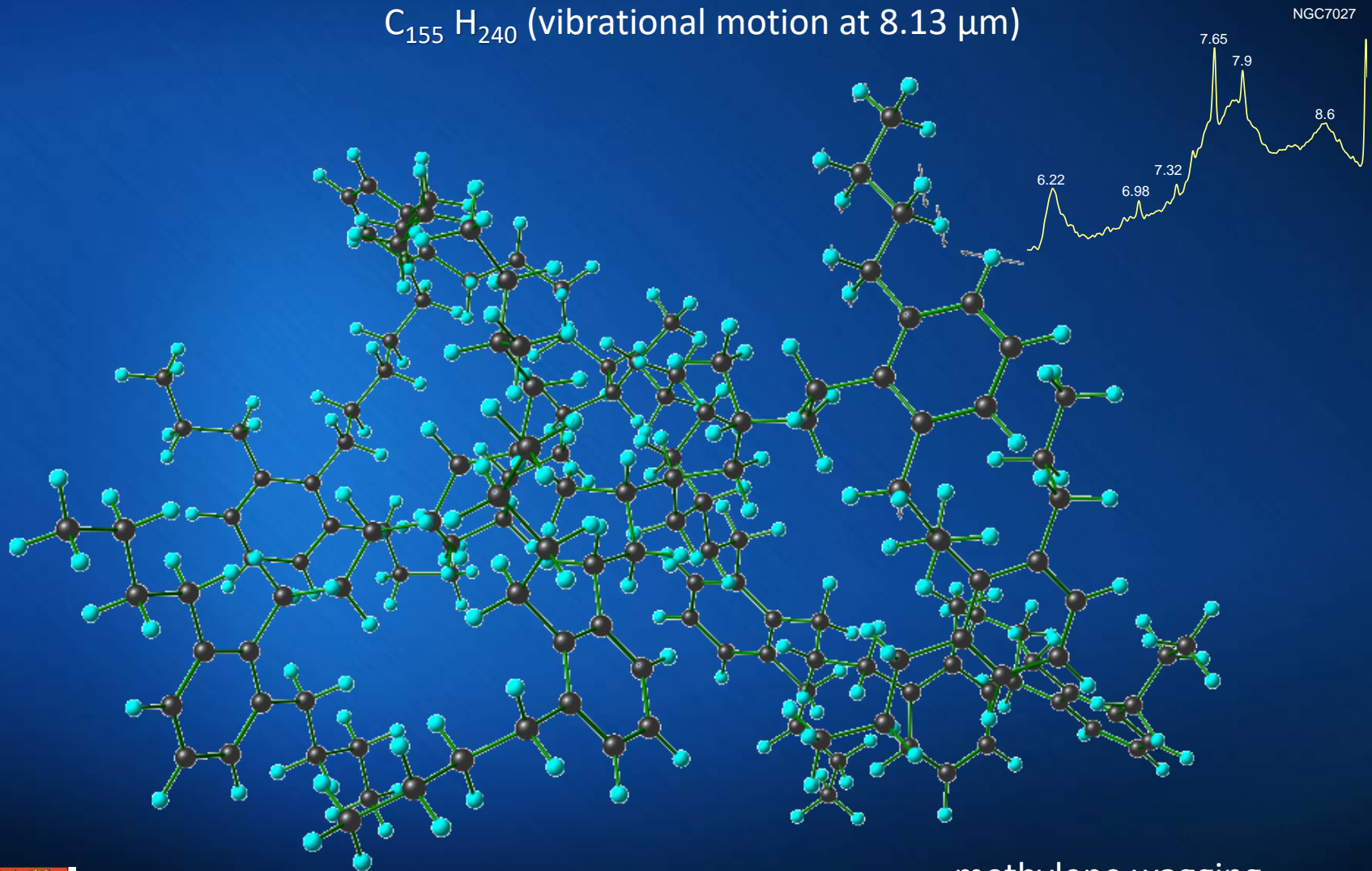
$C_{155}H_{240}$ (vibrational motion at $6.35\ \mu m$)



aromatic C-C stretching coupled with
C-H in plane bending

graphical interpretation

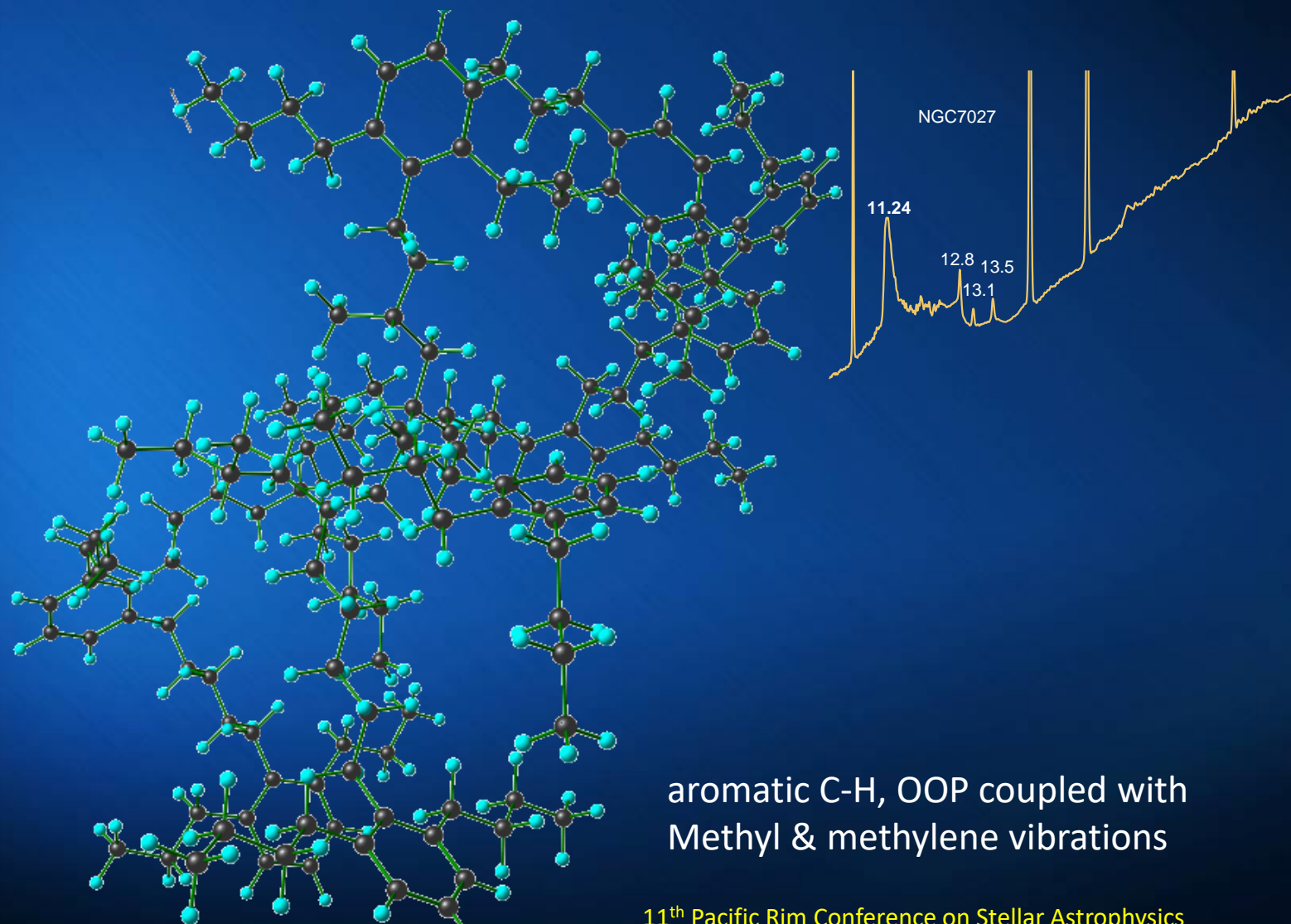
$C_{155}H_{240}$ (vibrational motion at $8.13\ \mu m$)



methylene wagging

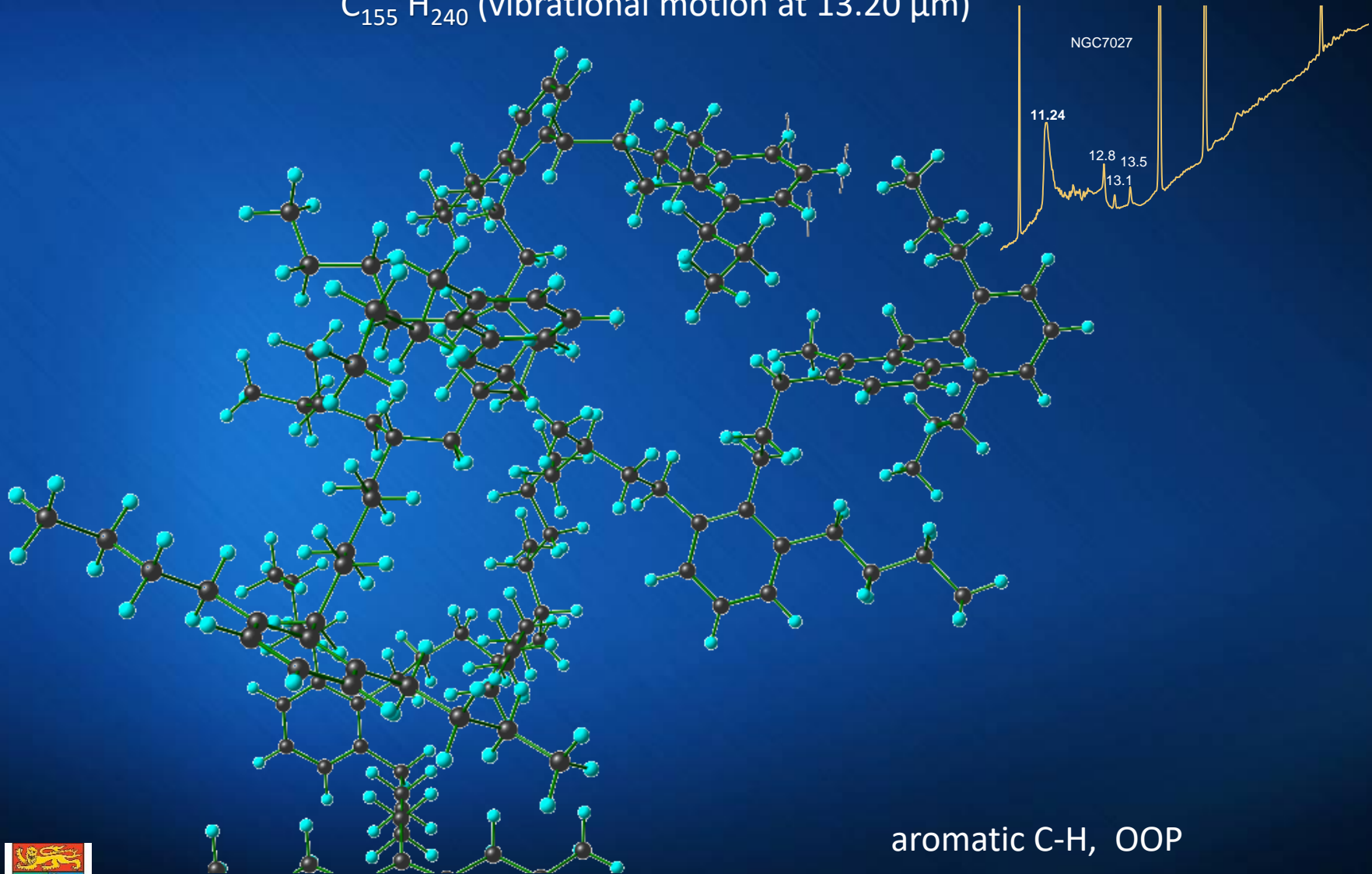
graphical interpretation

$C_{155}H_{240}$ (vibrational motion at 11.16 μm)



graphical interpretation

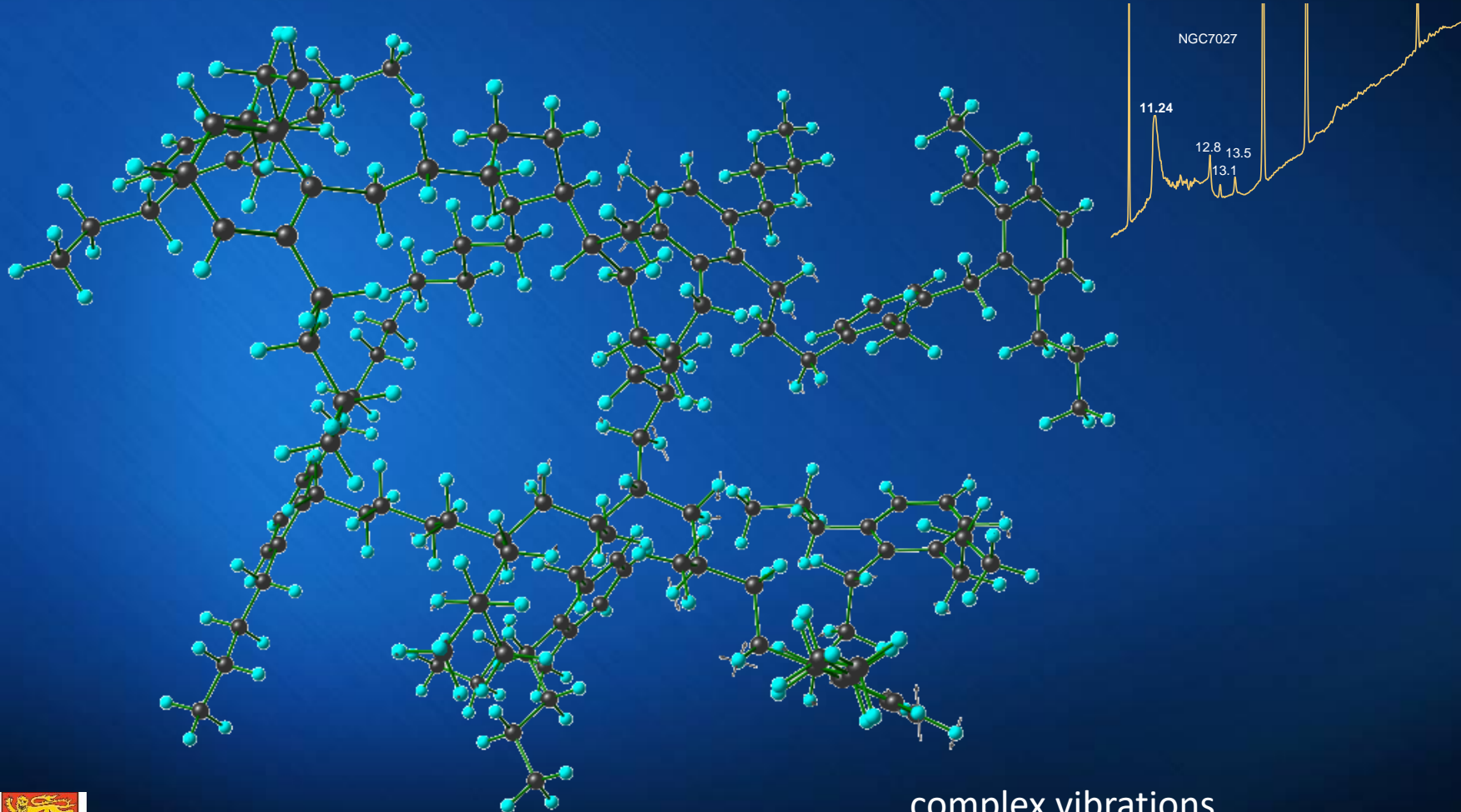
$C_{155}H_{240}$ (vibrational motion at $13.20\ \mu\text{m}$)



aromatic C-H, OOP

graphical and quantitative interpretations

$C_{155}H_{240}$ (vibrational motion at $19.06\ \mu m$: 32% aromatic, 68% aliphatic)



complex vibrations

interpretation of infrared spectra

1945

РАСЧЕТ ЧАСТОТ И ИНТЕРПРЕТАЦИЯ КОЛЕБАТЕЛЬНЫХ СПЕКТРОВ МНОГОАТОМНЫХ МОЛЕКУЛ

I. МЕТЕЛОВЫЙ СПИРТ

Б. И. Степанов

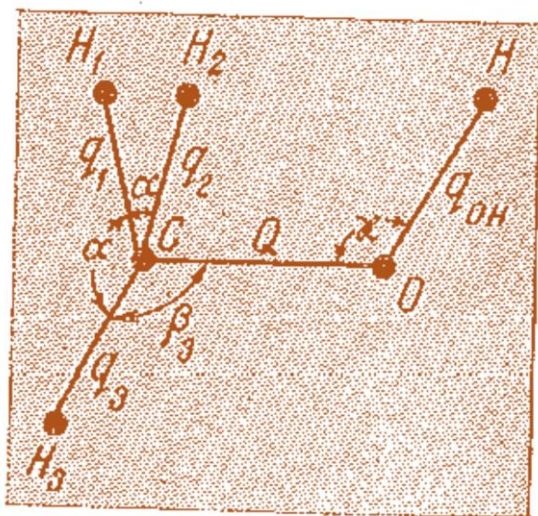
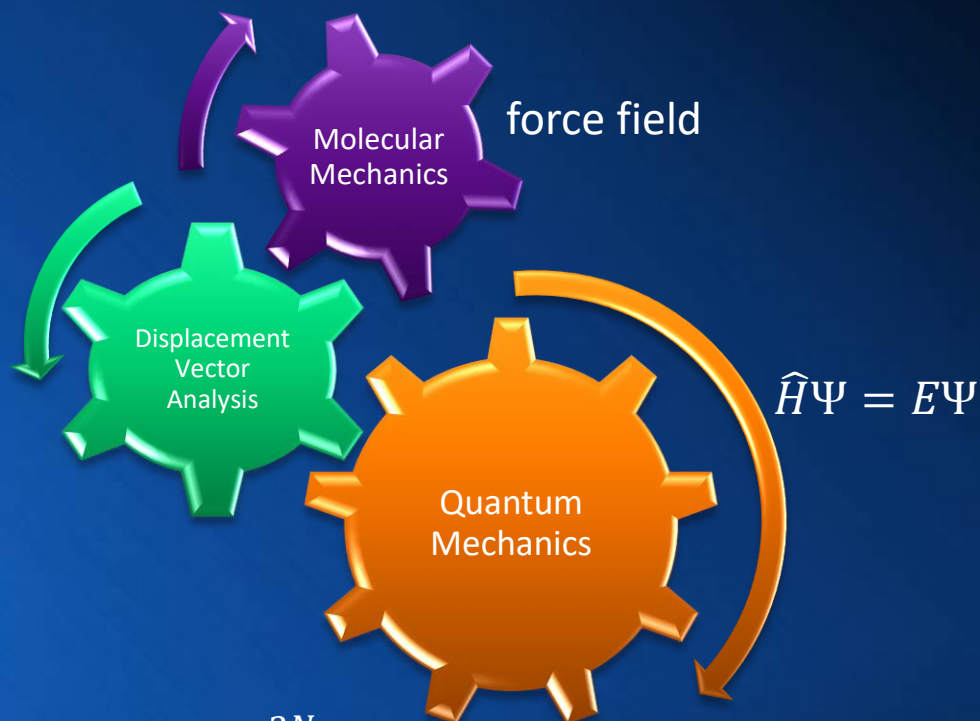


Рис. 1

$$U = \frac{1}{2} \sum h_q q_i^2 + \frac{1}{2} h_Q Q^2 + \frac{1}{2} h_q' q'^2 + \frac{1}{2} \sum k_{\alpha} \alpha_i^2 + \frac{1}{2} \sum k_{\beta} \beta_i^2 + \frac{1}{2} k_x x^2 +$$

$$+ \sum h_{\alpha} q_i q_j + \sum h_{\alpha Q} q_i Q + \sum a_{\alpha} q_i \alpha_{ih} + \sum a_{\beta} q_i \beta_{ih} + \sum A_{\beta} Q \beta_i + \sum A_x Q x +$$

$$+ a_x q' x + \sum l_{\alpha} \alpha_{ih} \alpha_{ij} + \sum l_{\alpha \beta} \alpha_{ih} \beta_i + m_{\beta} x + n x (\beta_1 + \beta_2).$$



$$I_{k,i}^{CART} = \sum_j \frac{D_{k,j} L_{j,i}}{\sqrt{m_k}}$$

$$N_i = \sqrt{\left(\sum_k (I_{k,i}^{CART})^2 \right)^{-1}}$$

displacement vector analysis

60 neutral honeycomb like PAH



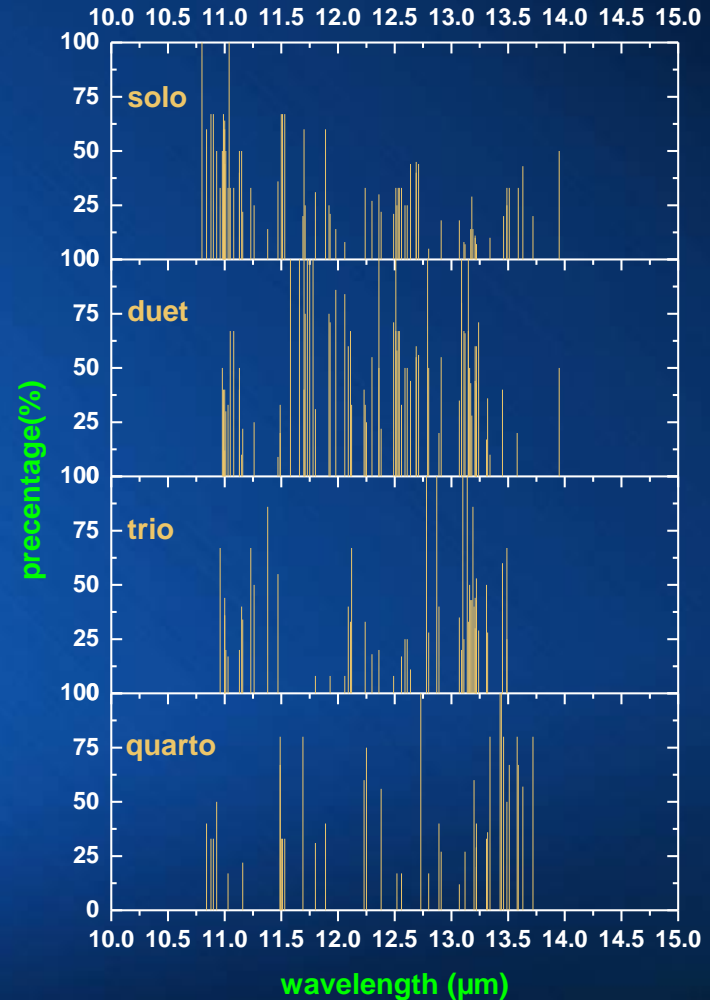
227 vibrations



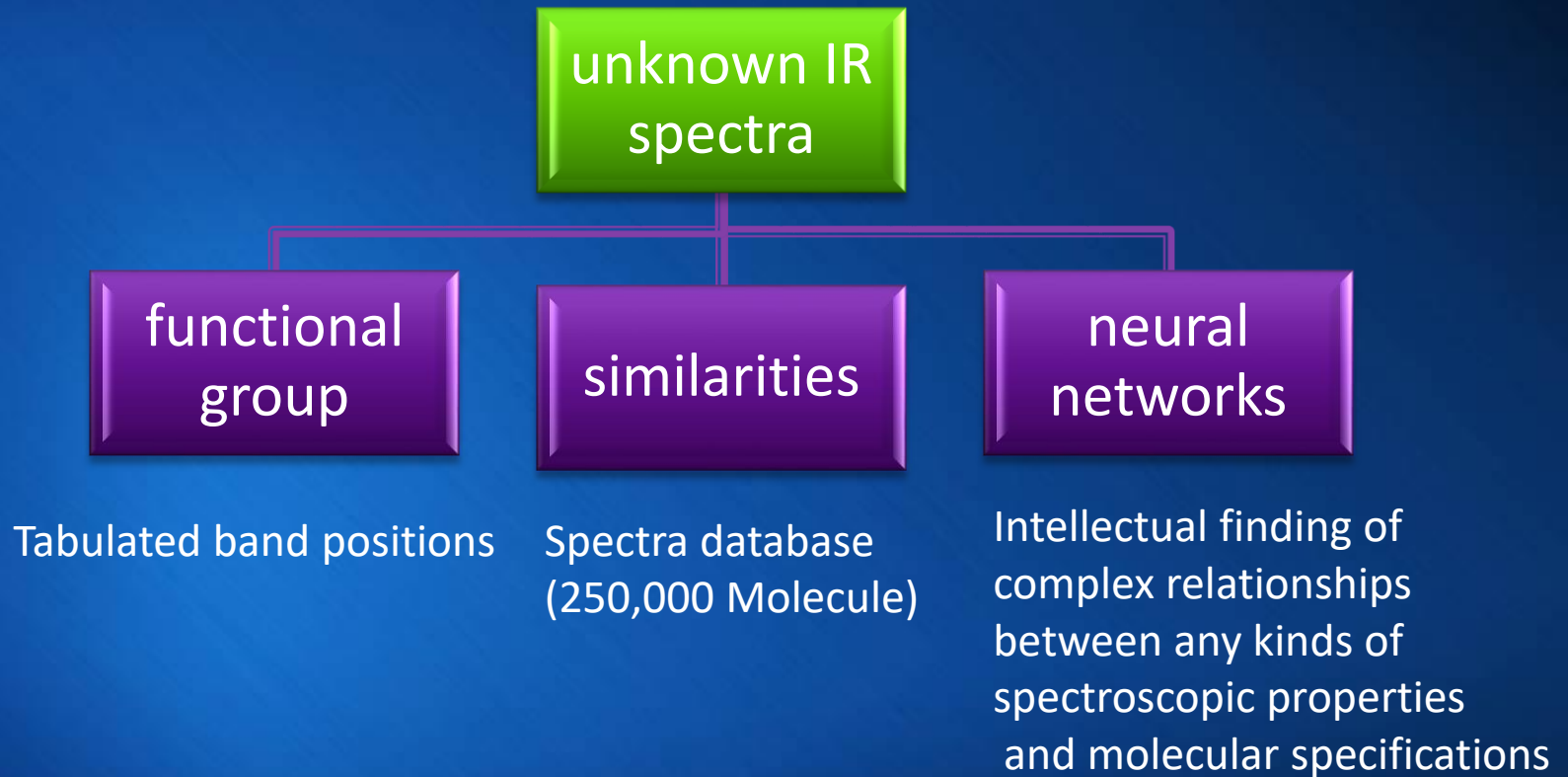
112
Pure OOP



%solo, %duet,
%trio, %quarto

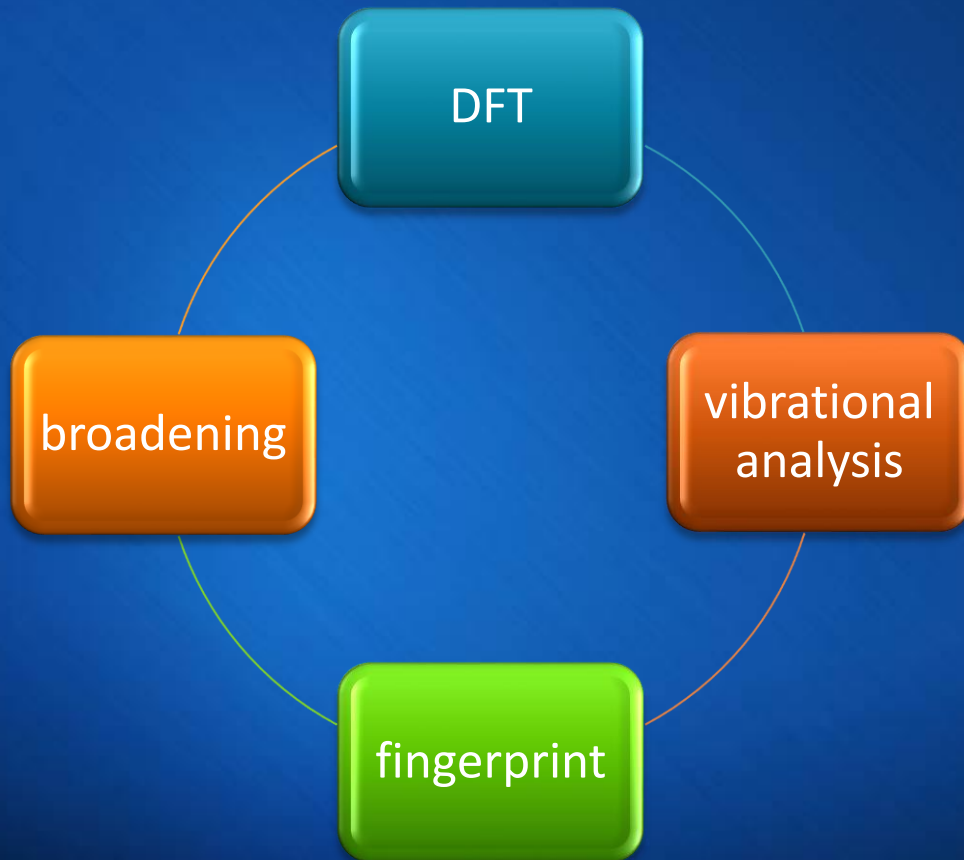


prediction



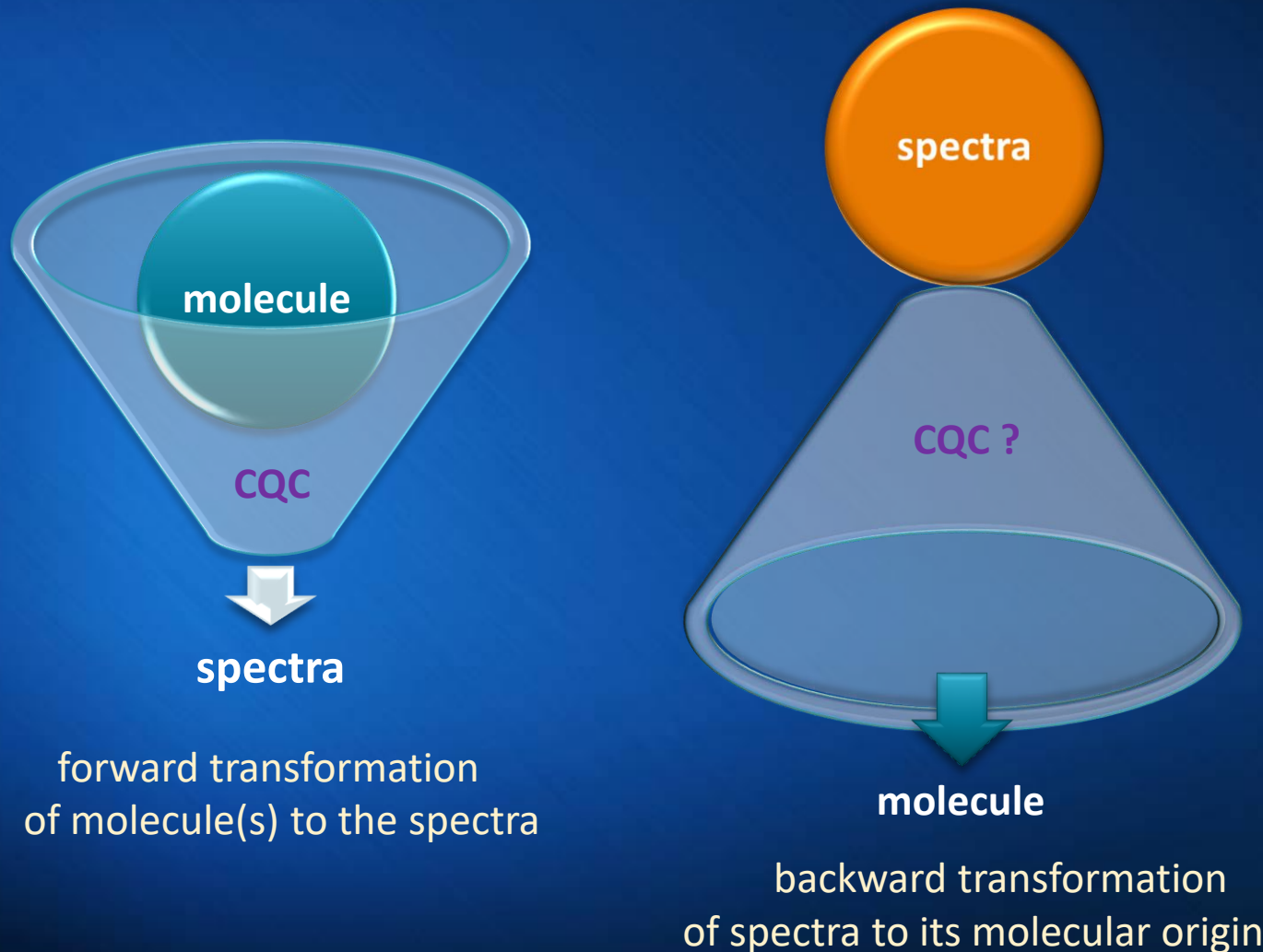
All these approaches are followed in our Lab

backbone of our theoretical approach



Sadjadi, Zhang and Kwok, ApJ, 801:34 (2015 March 1)

pictorial conclusion



Acknowledgments

- I am grateful to my supervisor:

Professor Sun Kwok



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Dr. Yong Zhang



Dr. Chih-Hao Hsia

- Professor Quentin Parker's group and all other colleagues in our LSR
- My colleagues in Chemistry Department (Professor G.H.Chen's group)