

Raman 光谱

张梦真

2013-6-26

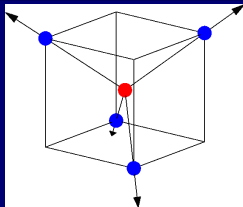
振动模式 (CCl₄) 1 A₁+1 E+2 F₂

E	8 C ₃	3 C ₂	6 σ _d	6 S ₄
9	0	-1	3	-1

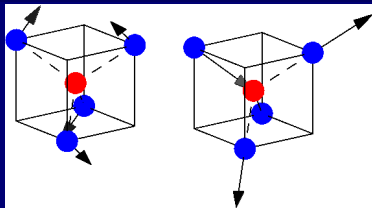
T _d	E	8 C ₃	3 C ₂	6 σ _d	6 S ₄
A ₁	1	1	1	1	1
A ₂	1	1	1	-1	-1
E	2	-1	2	0	0
F ₂	3	0	-1	1	-1
F ₁	3	0	-1	-1	1

简正振动

A₁

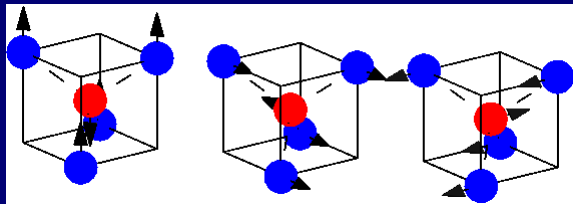


E

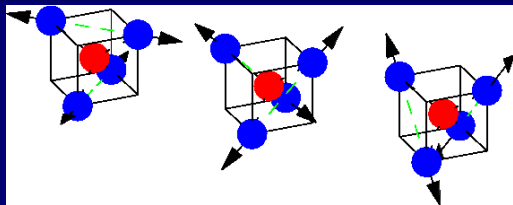


简正振动

F₂



F₂



经典解释

$$\vec{\mu}_i = \alpha \vec{E}$$

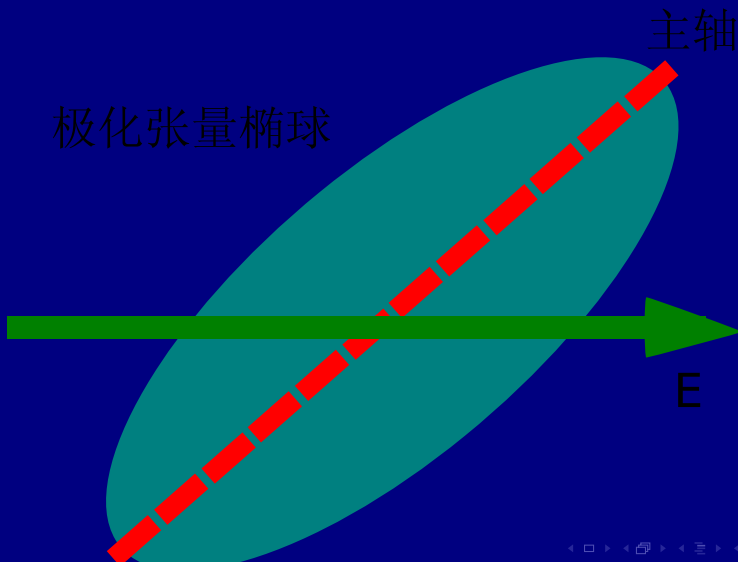
$$\alpha = \alpha_0 + \left(\frac{\partial \alpha}{\partial r}\right)_{r=r_0} + \cdots$$

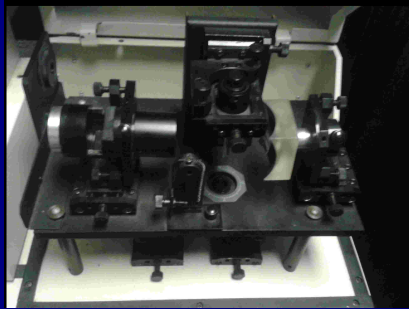
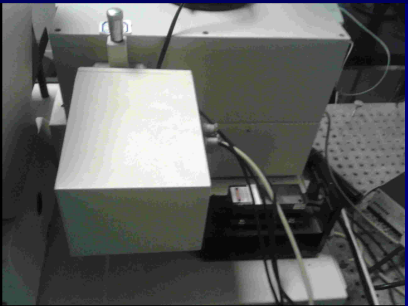
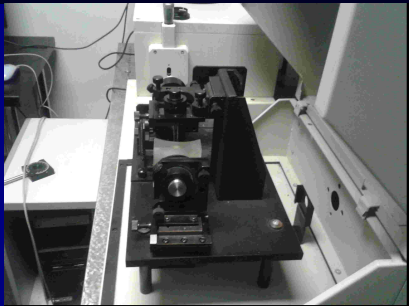
$$r = r_0 \cos 2\pi\nu_v t$$

■ 偶极振子

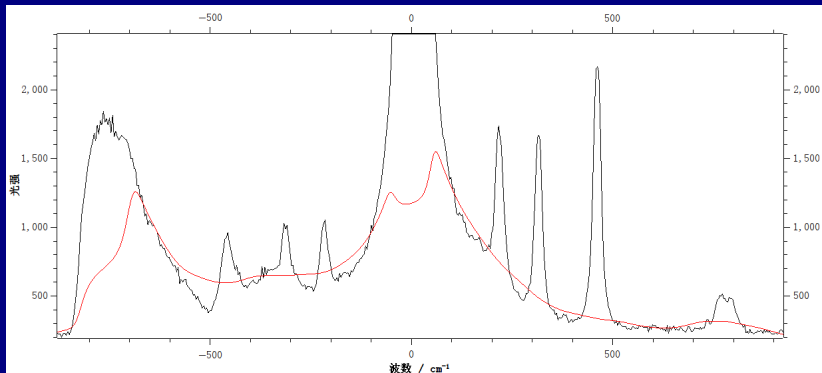
$$\begin{aligned} \mu_i = & \alpha_0 E_0 \cos 2\pi\nu_0 t + \frac{1}{2} \left(\frac{\partial \alpha}{\partial r}\right)_{r=r_0} E_0 (r - r_0) \cos[2\pi(\nu - \nu_v)t] \\ & + \frac{1}{2} \left(\frac{\partial \alpha}{\partial r}\right)_{r=r_0} E_0 (r + r_0) \cos[2\pi(\nu + \nu_v)t] \end{aligned}$$

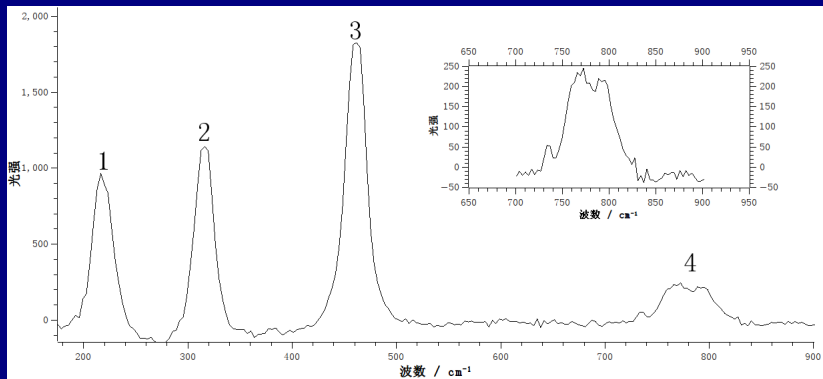
偏振



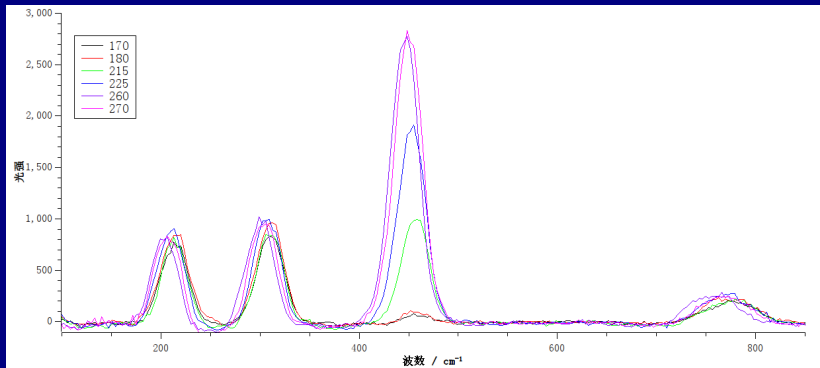


CCl₄ 光谱

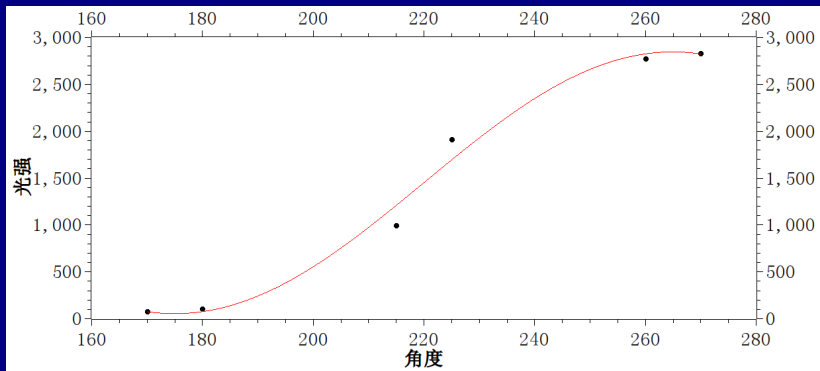


扣除本底的 CCl_4 光谱

不同偏振角 CCl_4 光谱



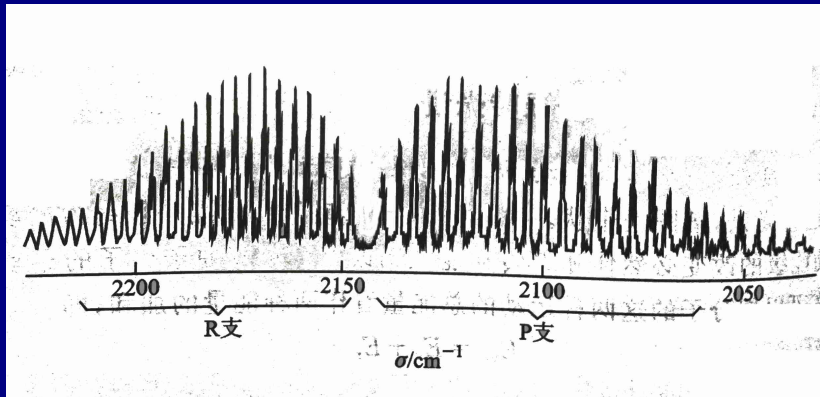
峰3的偏振性



总结

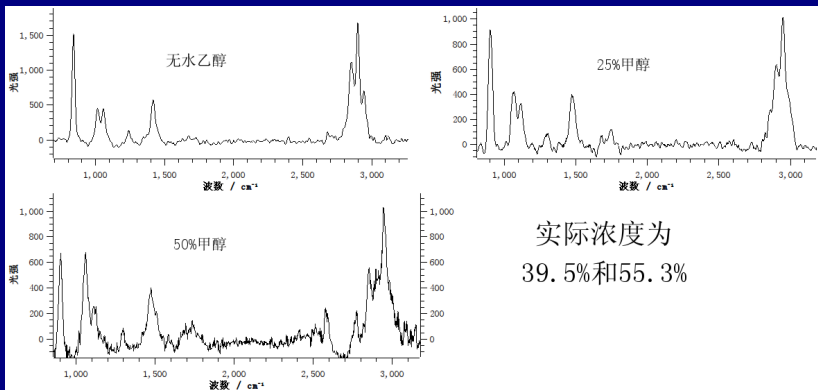
峰	1	2	3	4 (1)	4 (2)
波数 / cm^{-1}	216.5	316.1	461.8	769.2	792
相对光强	964.3	1142.8	1825.9	226.9	221.4
振动模式	F_2	E	A_1	F_2	F_2

振动转动光谱

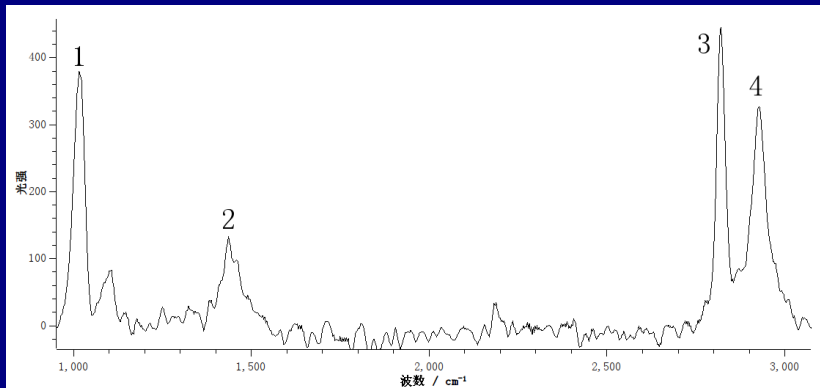


引自《谱学基础与结构分析》（浙江大学 陆维敏等编）

不同浓度乙醇 (C_2H_5OH) 甲醇 (CH_3OH) 溶液的 Raman 光谱



无水甲醇溶液的raman光谱



CH₃OH官能团

