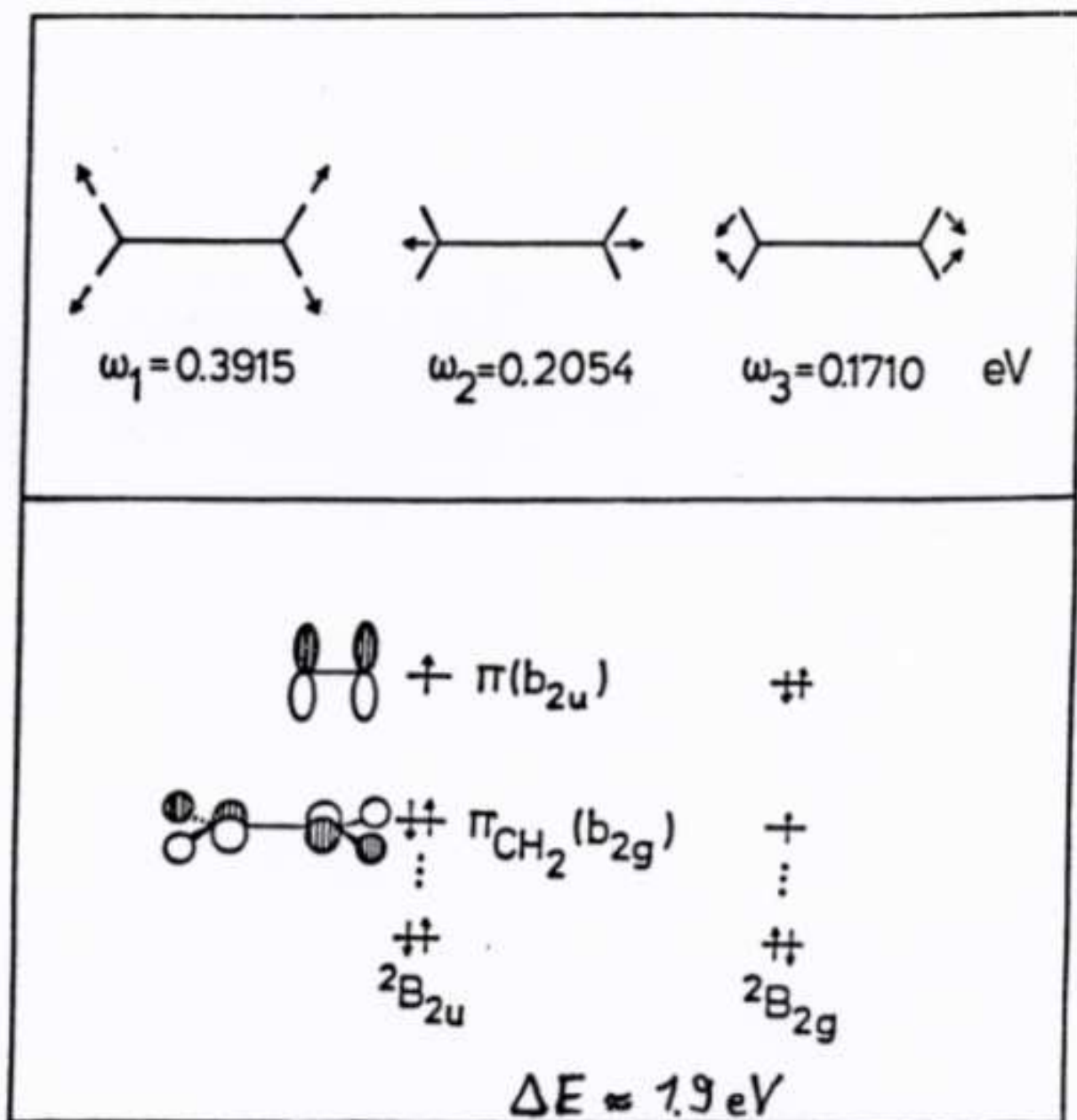


B.3) Conical intersection and vibronic dynamics in the ethene radical cation, $C_2H_4^+$

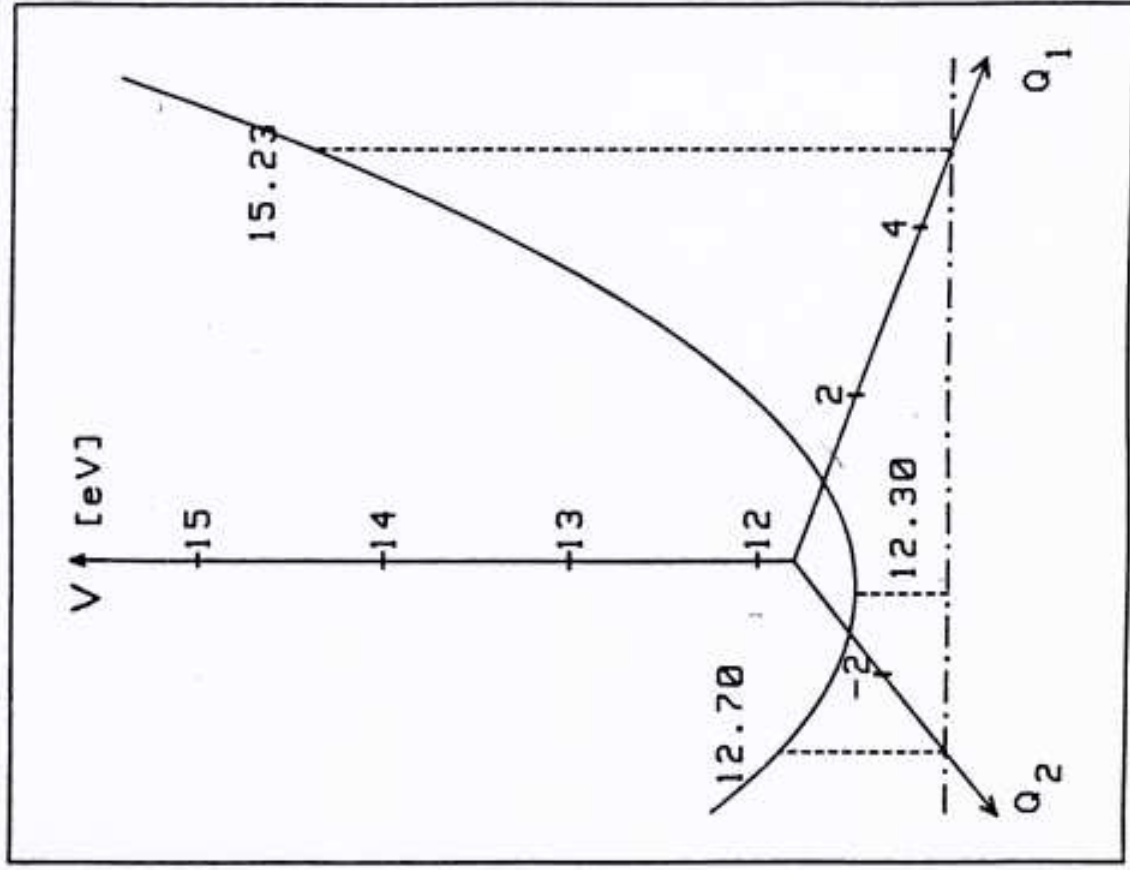
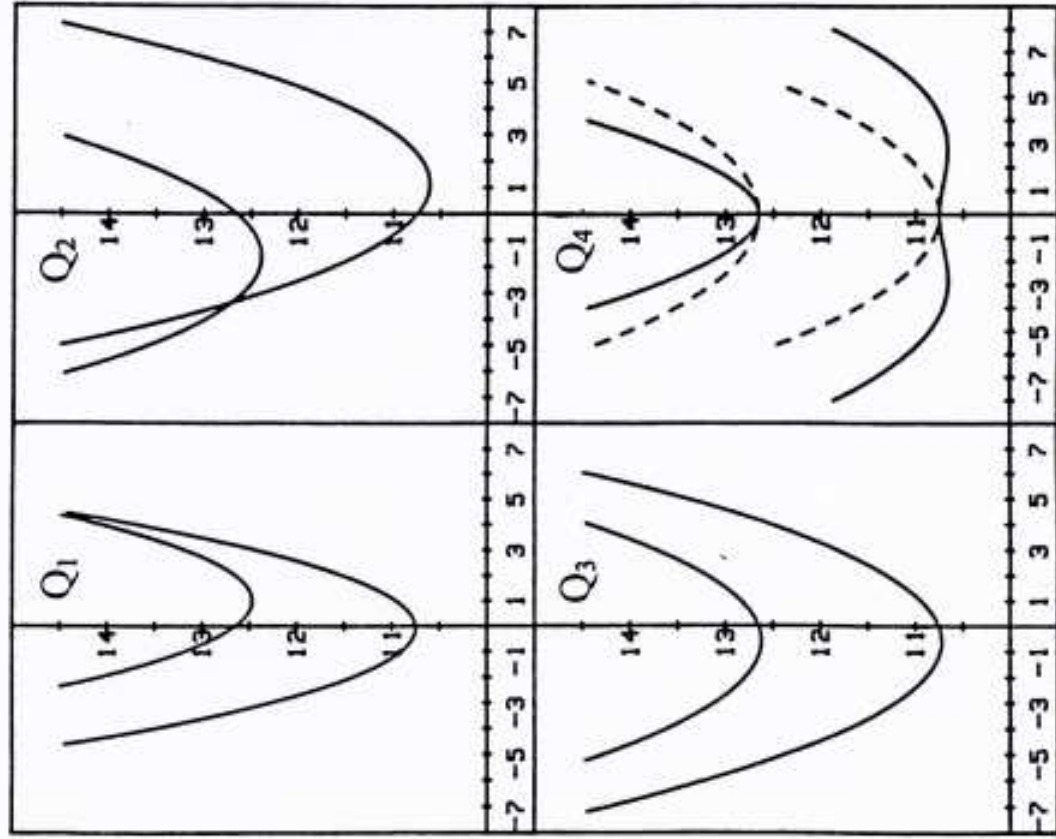
Schematic representation of the relevant vibrational normal modes and molecular orbitals of $C_2H_4^+$

(Mode 1-3: totally symmetric modes, Mode 4: Torsion)

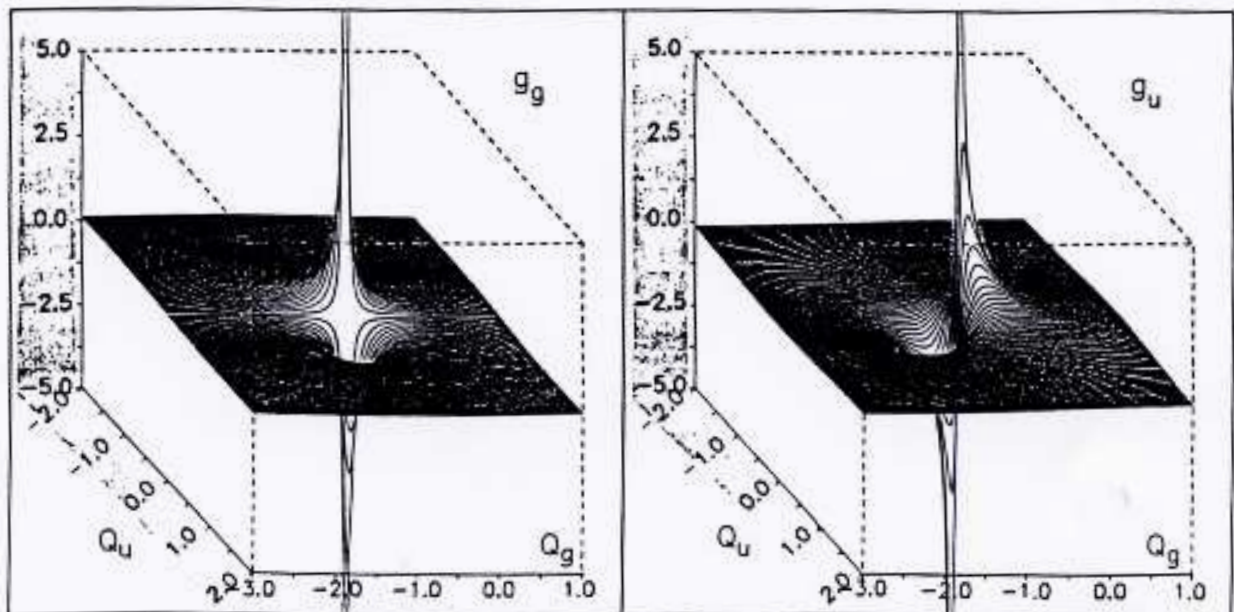
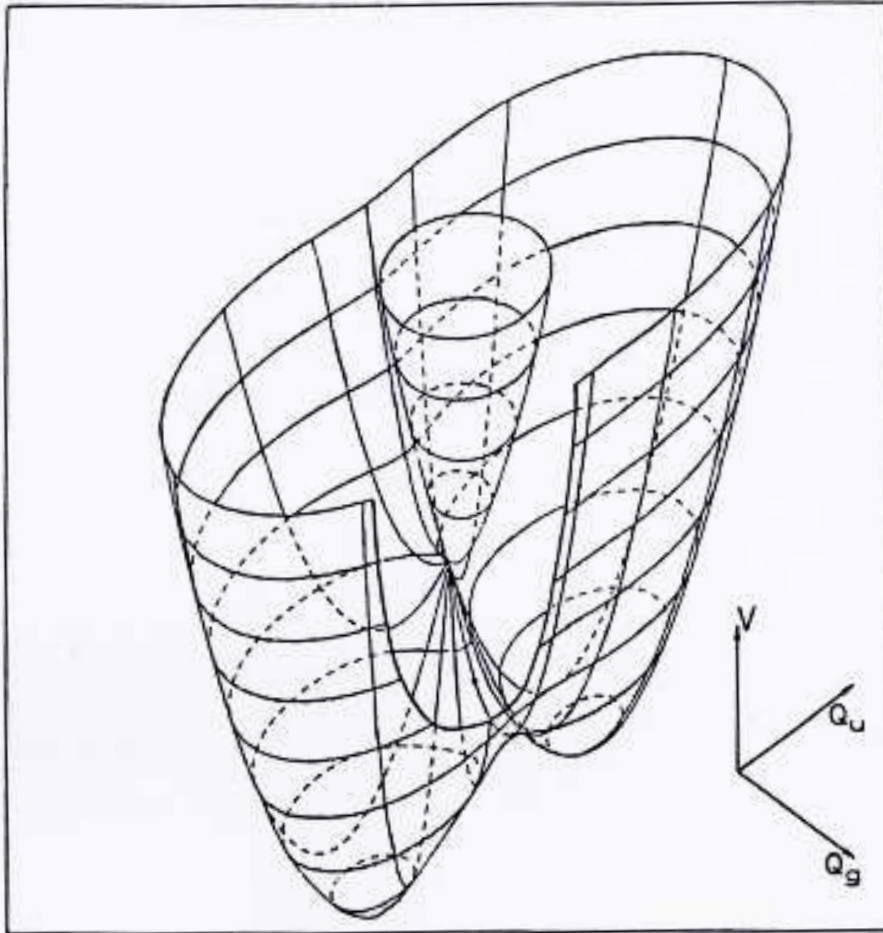


$$\underline{B_{2u} \times B_{2g} = A_u \text{ (Torsion)}}$$

Potentialkurven (links) und Durchschneidungssaum (rechts) von $C_2H_4^+$ (\tilde{X}, \tilde{A})



Perspektiv. Darstellung der konischen Durchschneidung und nichtadiabatischen Kopplungselemente des Prototyp g-u - Problems : $C_2H_4^+$ (\tilde{X}, \tilde{A})



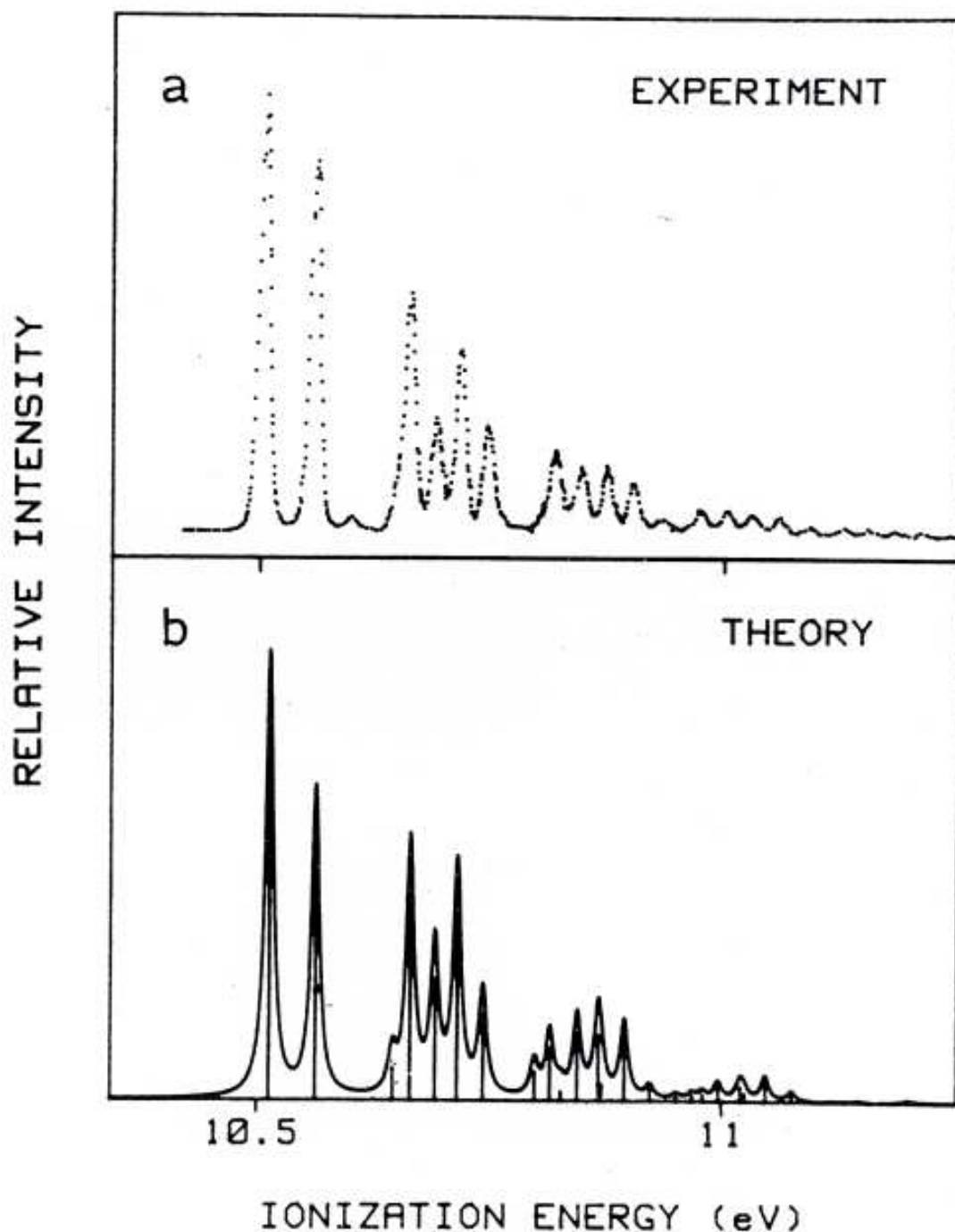
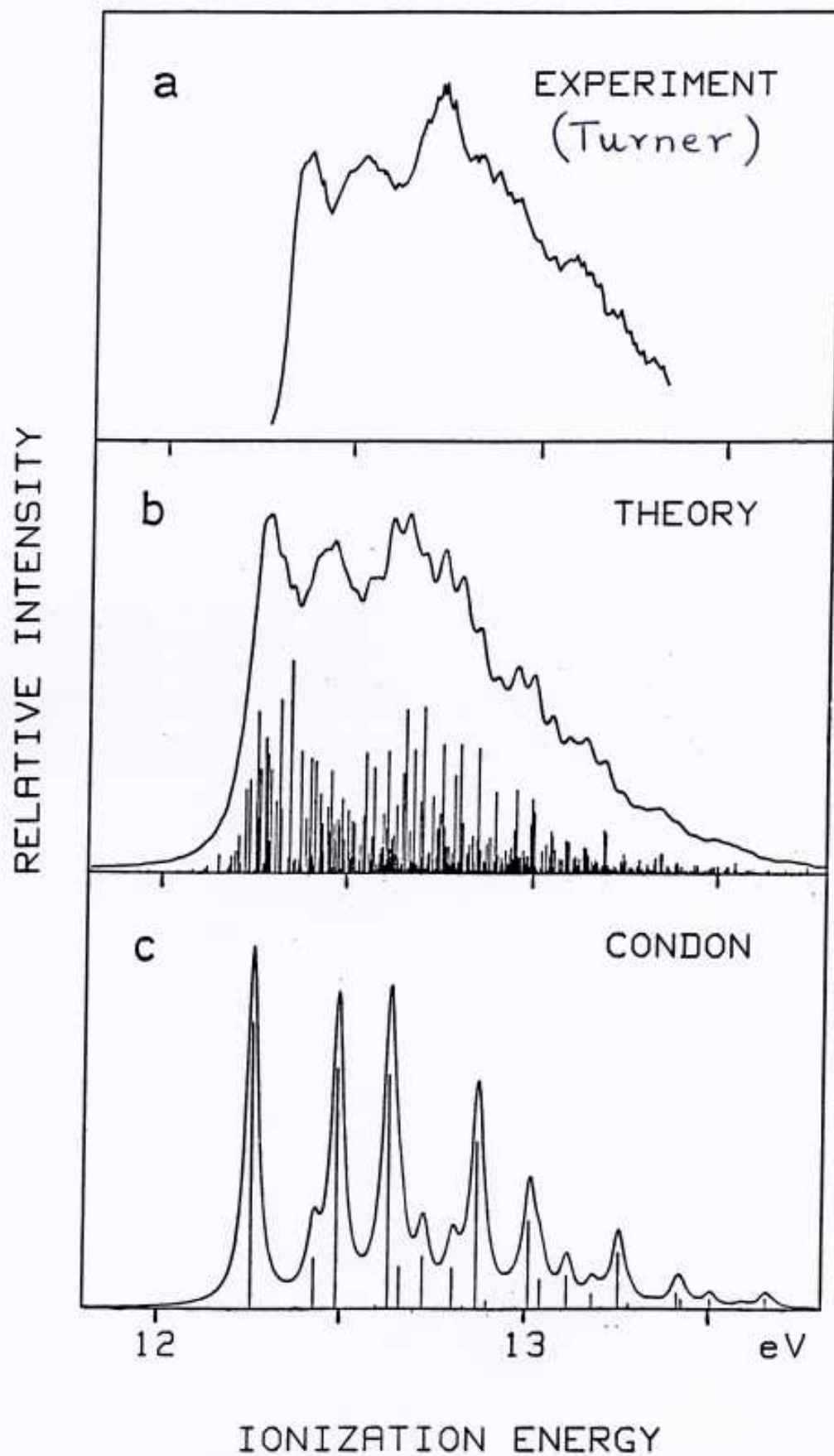
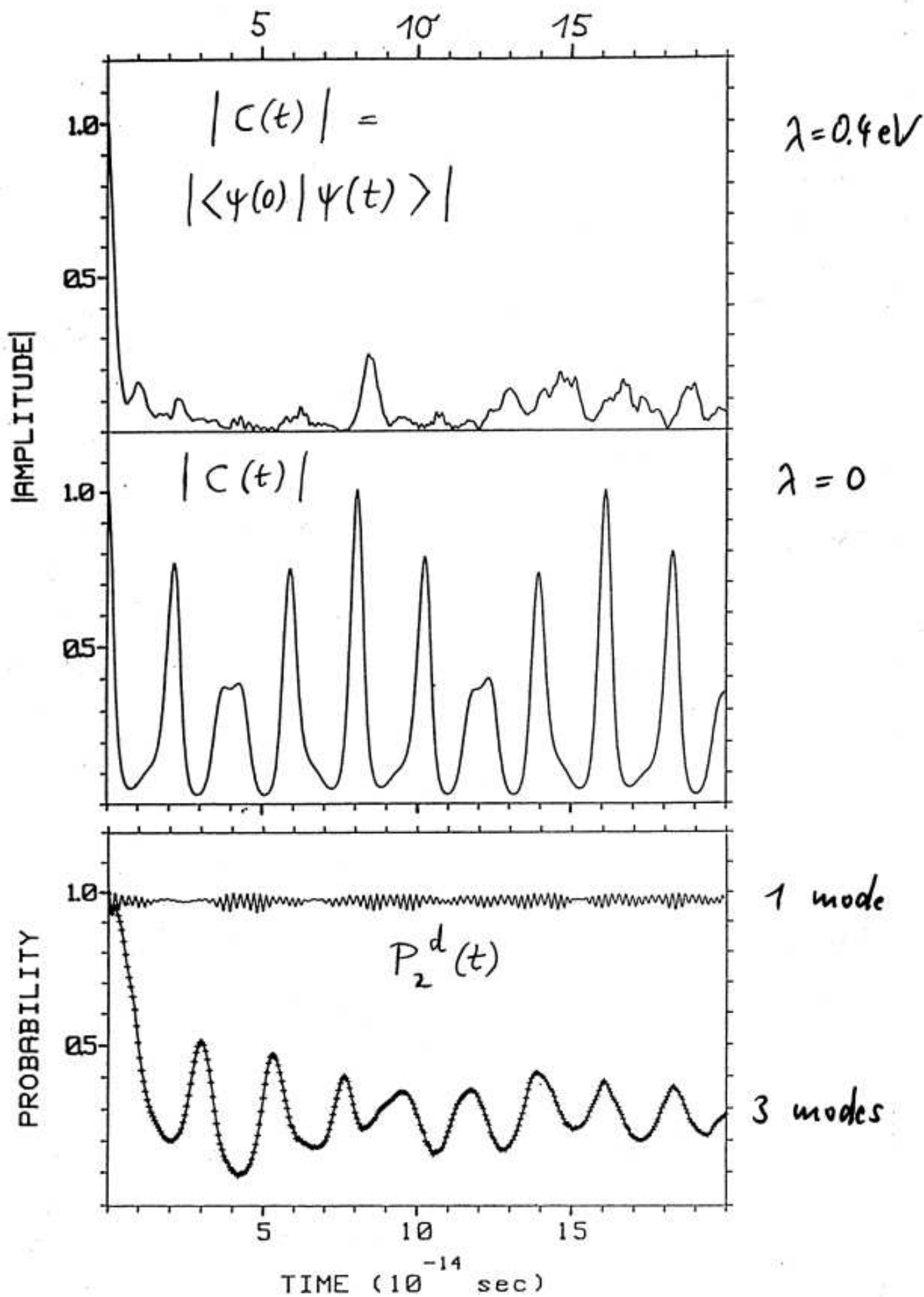


Fig. 26. The first band in the photoelectron spectrum of ethylene. (a) The experimental spectrum according to Pollard et al.²⁰⁹ (b) The result of the vibronic coupling calculation (fwhm = 0.01 eV). For the values of the parameters see Table V.

*Zweite Photoelektronenbande von Ethen:
Vergleich Theorie - Experiment*

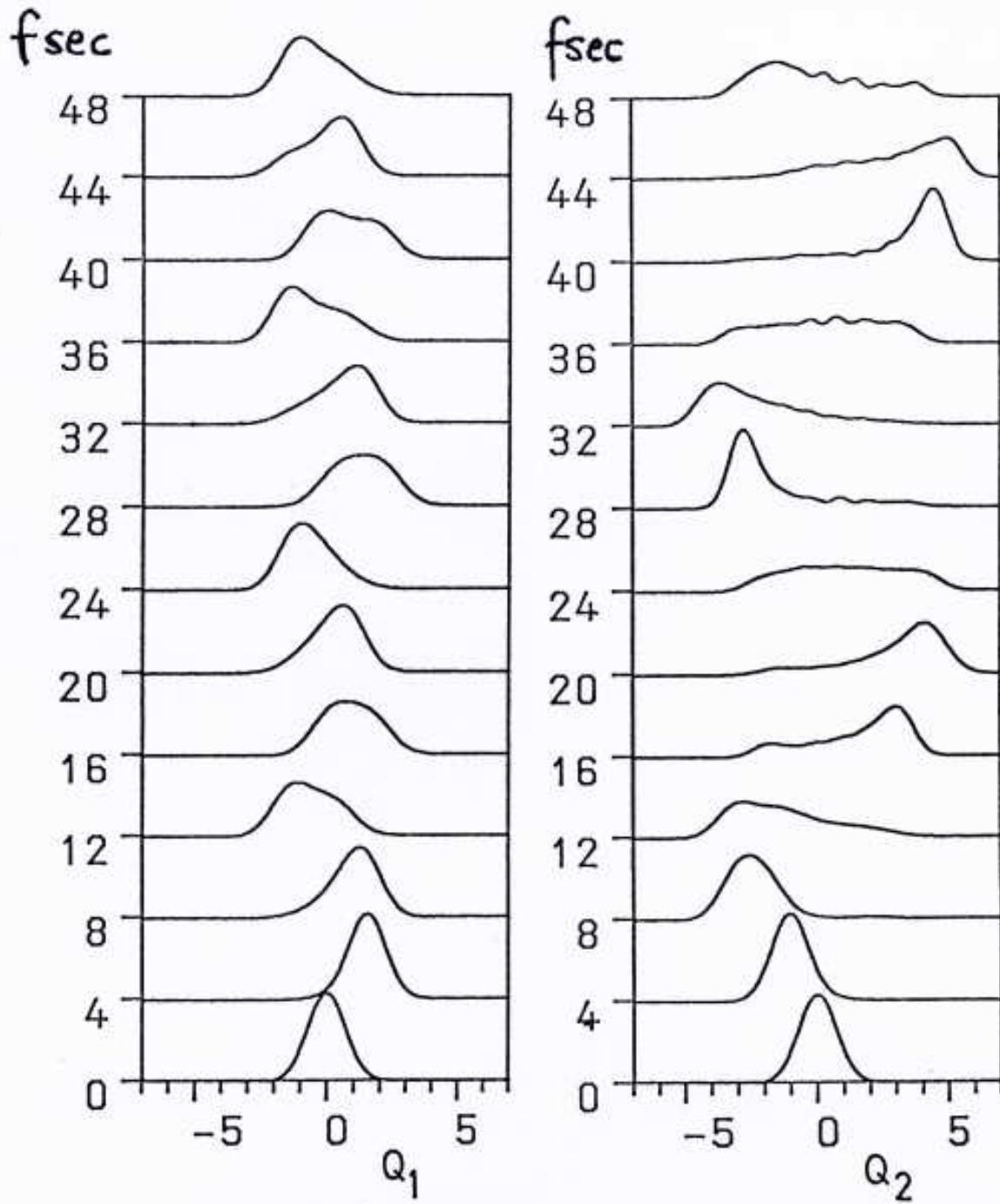


Wavepackets dynamics for $C_2H_4^+$ (\tilde{X}, \tilde{A})



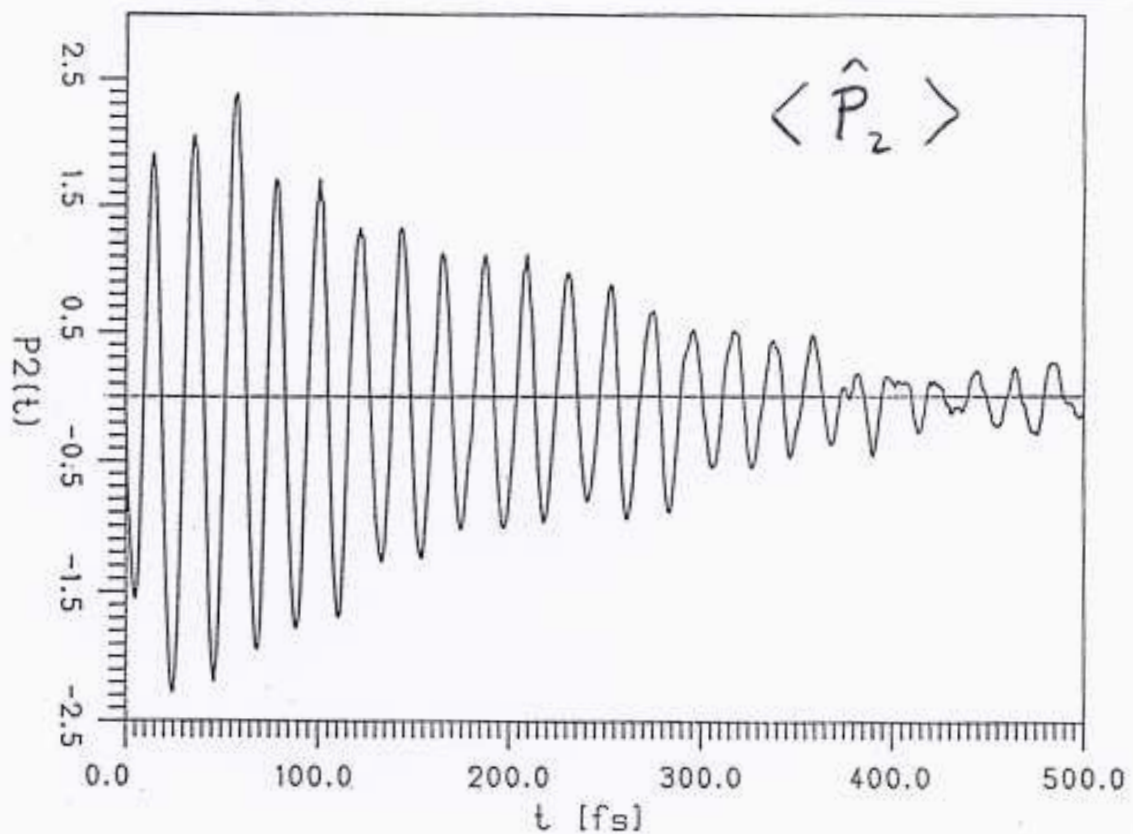
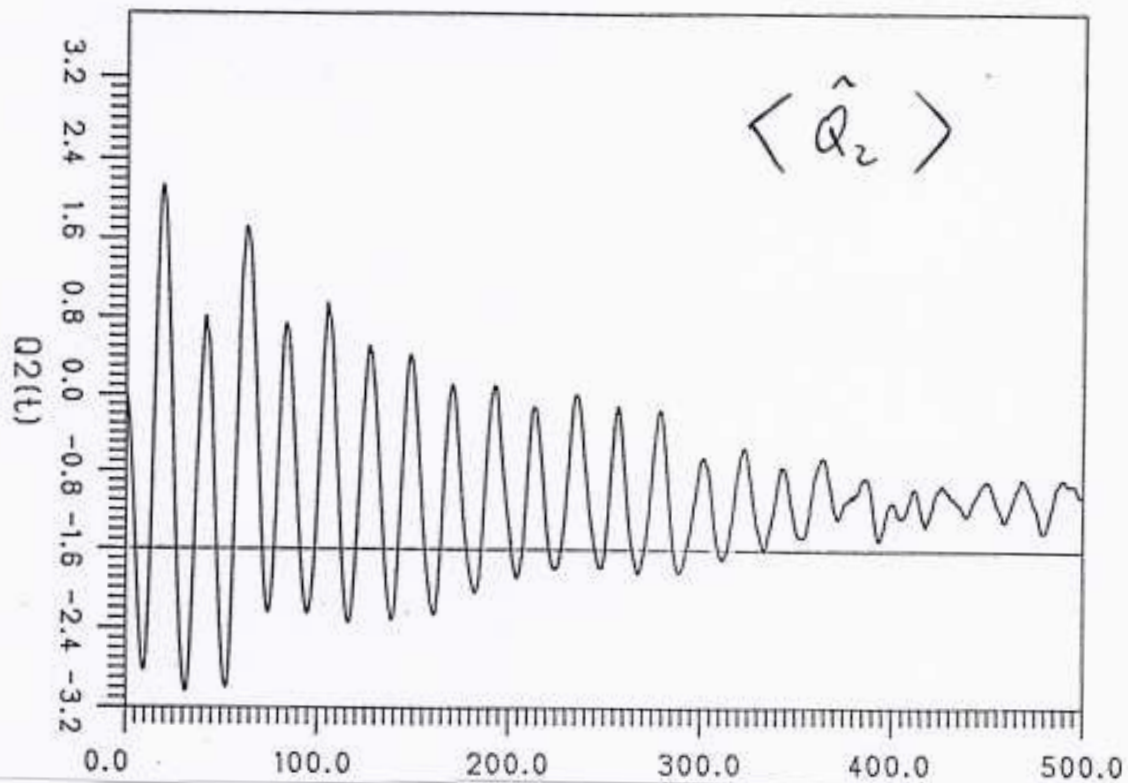
Short-time dynamics for $C_2H_4^+$ (\tilde{X}, \tilde{A})

Coherent motion for Q_1 and Q_2

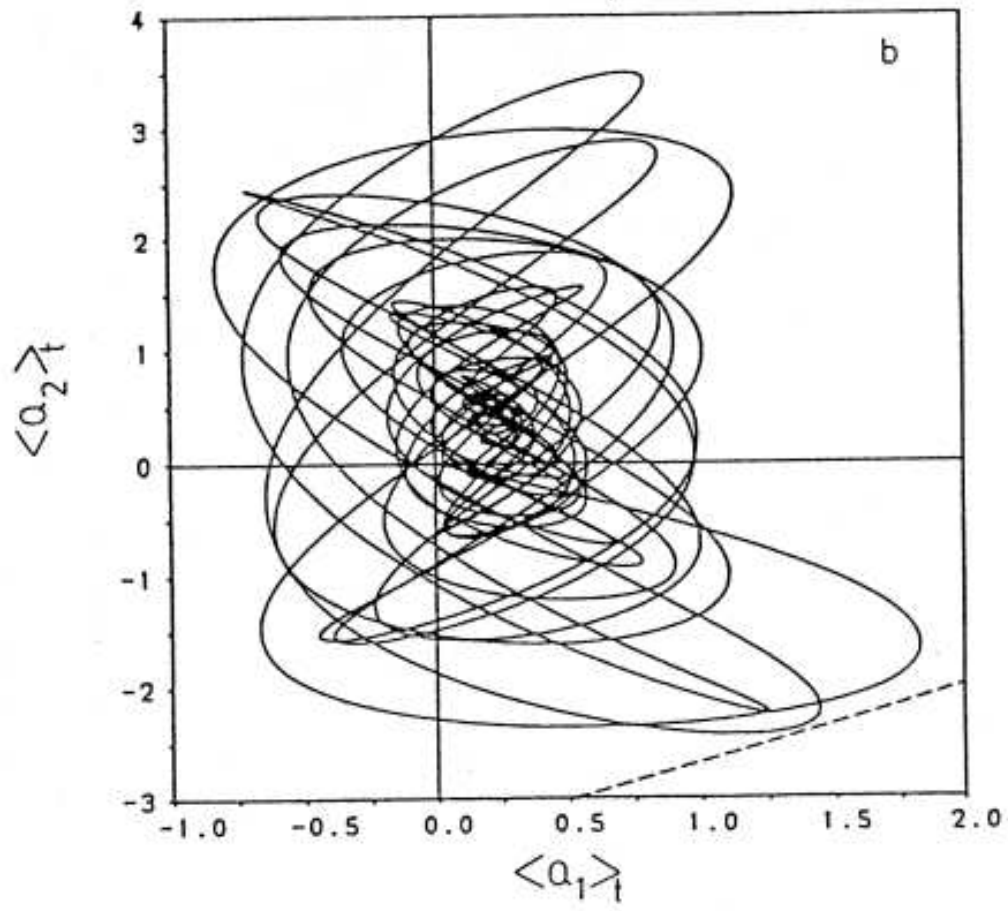
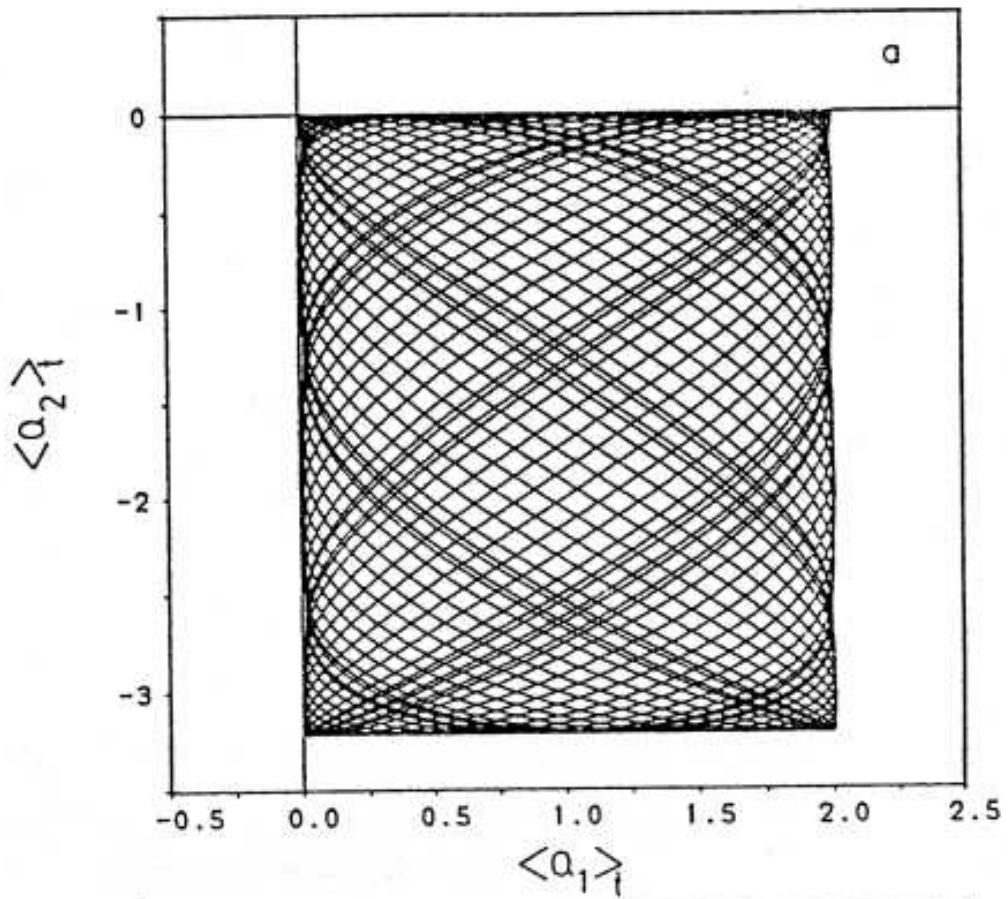


Long-time dynamics for $C_2H_4^+$ (\tilde{X}, \tilde{A})

Damping of the coherent motion in Q_2



Trajektorien im Raum $Q_1 - Q_2$ für $C_2H_4^+$ (\tilde{X}, \tilde{A}) [22]



$C_2H_4^+(\tilde{X}, \tilde{A})$: Wahrscheinlichkeitsdichte entlang der
Koordinate Q_4 der koppelnden Mode [23]

