Dissociation of diatomic molecules

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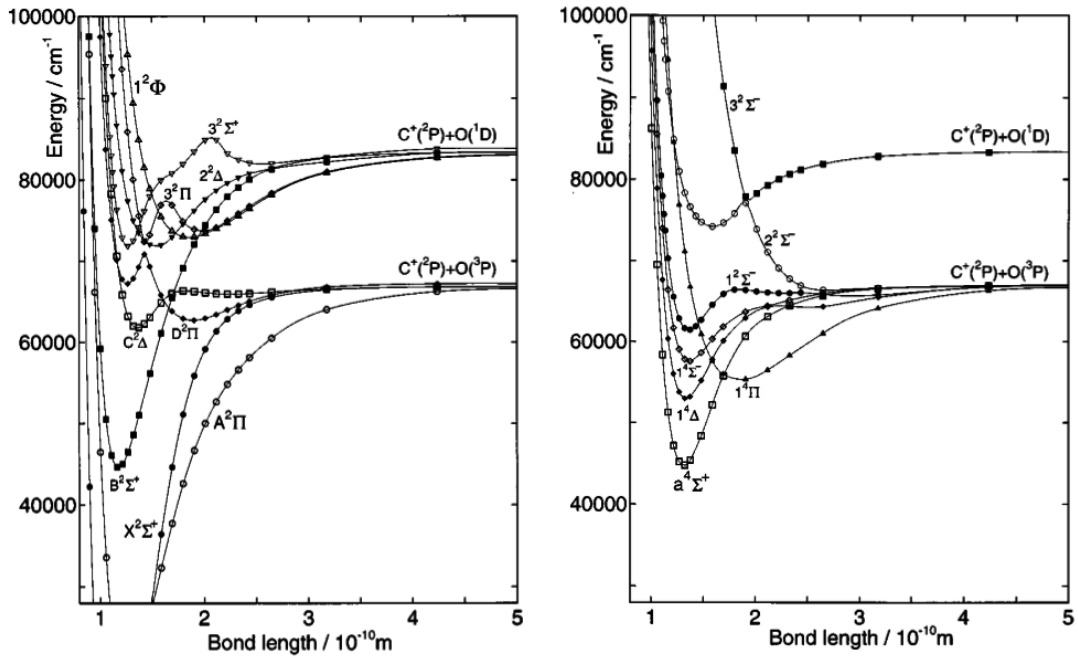
CO^+ molecule - molecular potentials, dipole couplings

- Potentials digitized from literature, interpolated and fit to 2nd order (Morse) approximation
- Dipole couplings calculated using Hartree-Fock SCF calculations with GAMESS quantum chemistry software
- Difficulties relating to "spaghetti" of low-lying CO^+ states

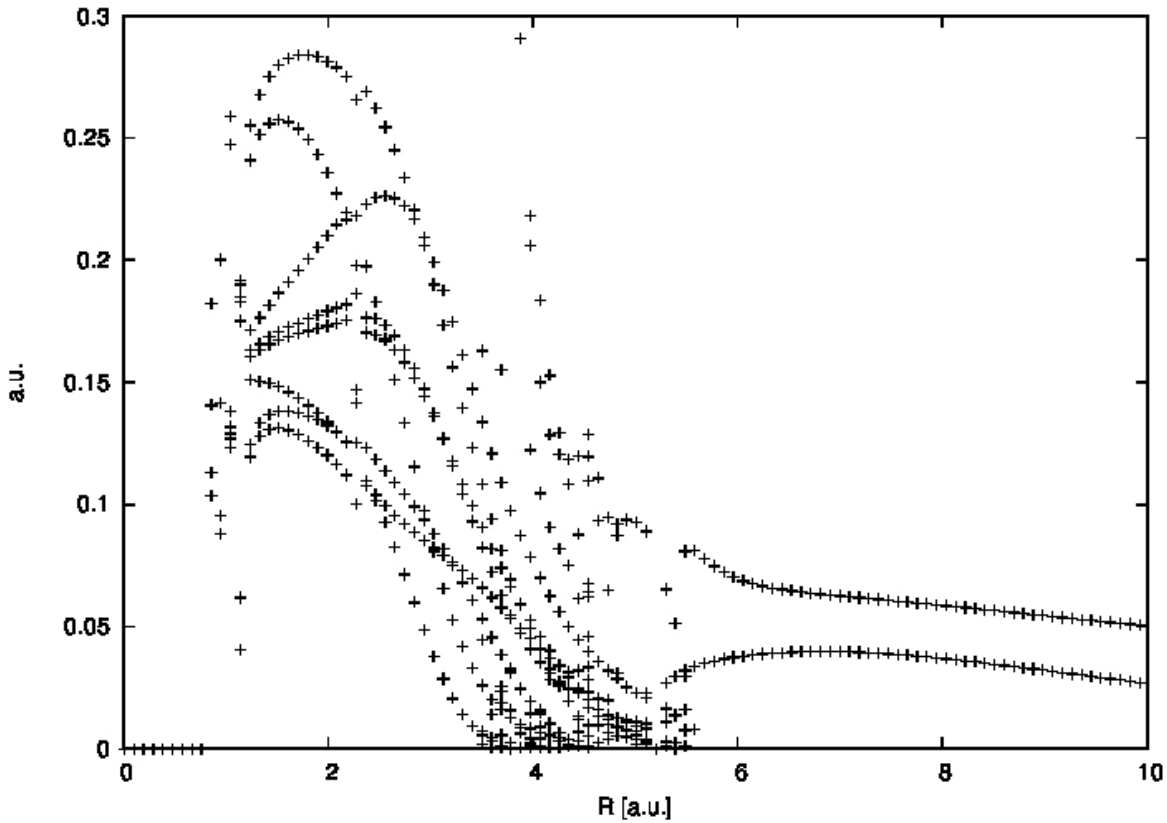
Figure: Low-lying CO^+ potential curves [1]



CO^+ molecule - dipole coupling issues

- Electron configuration degeneracy in GAMESS output
- Disagreement within literature and with calculated values

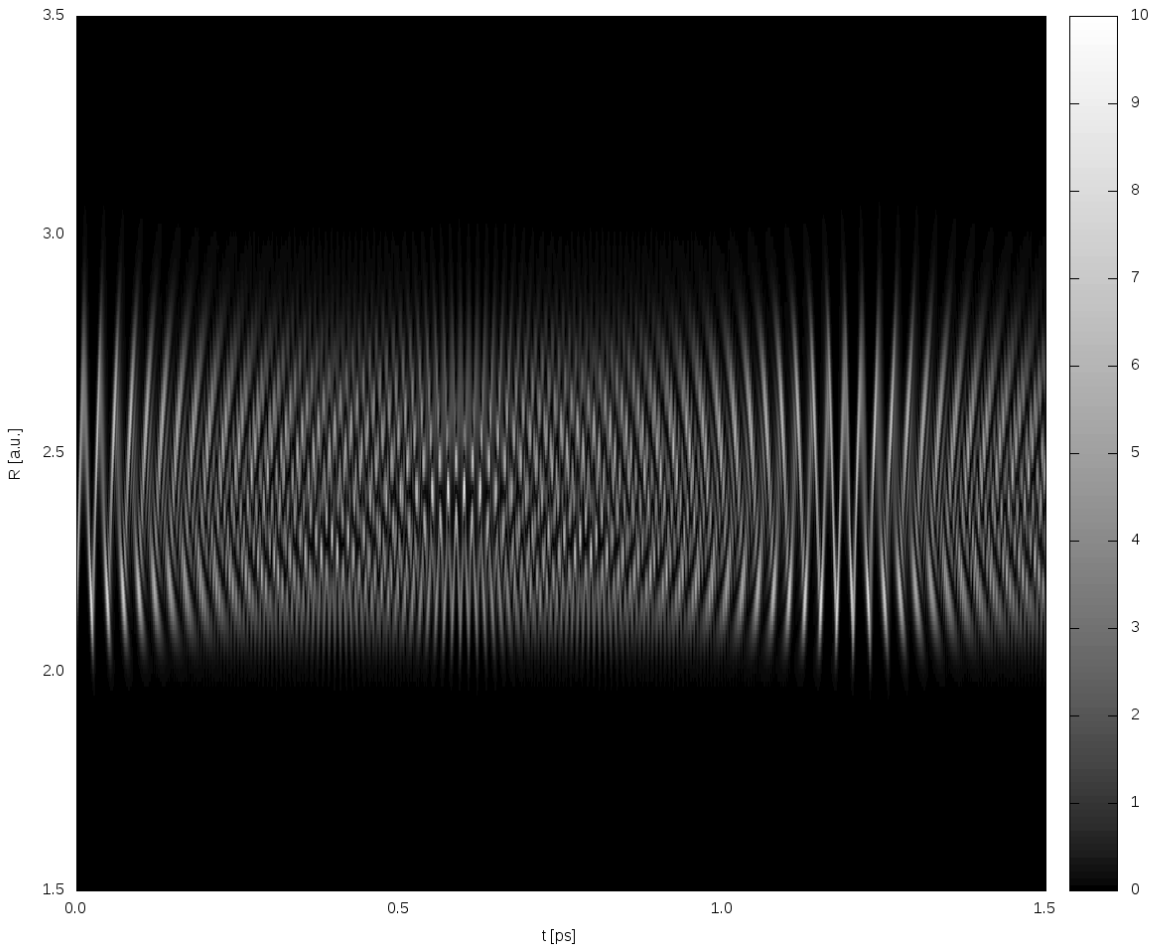
Figure: CO^+ $1^4\Pi - a^4\Sigma^+$ dipole coupling results



CO^+ - vibrational revivals

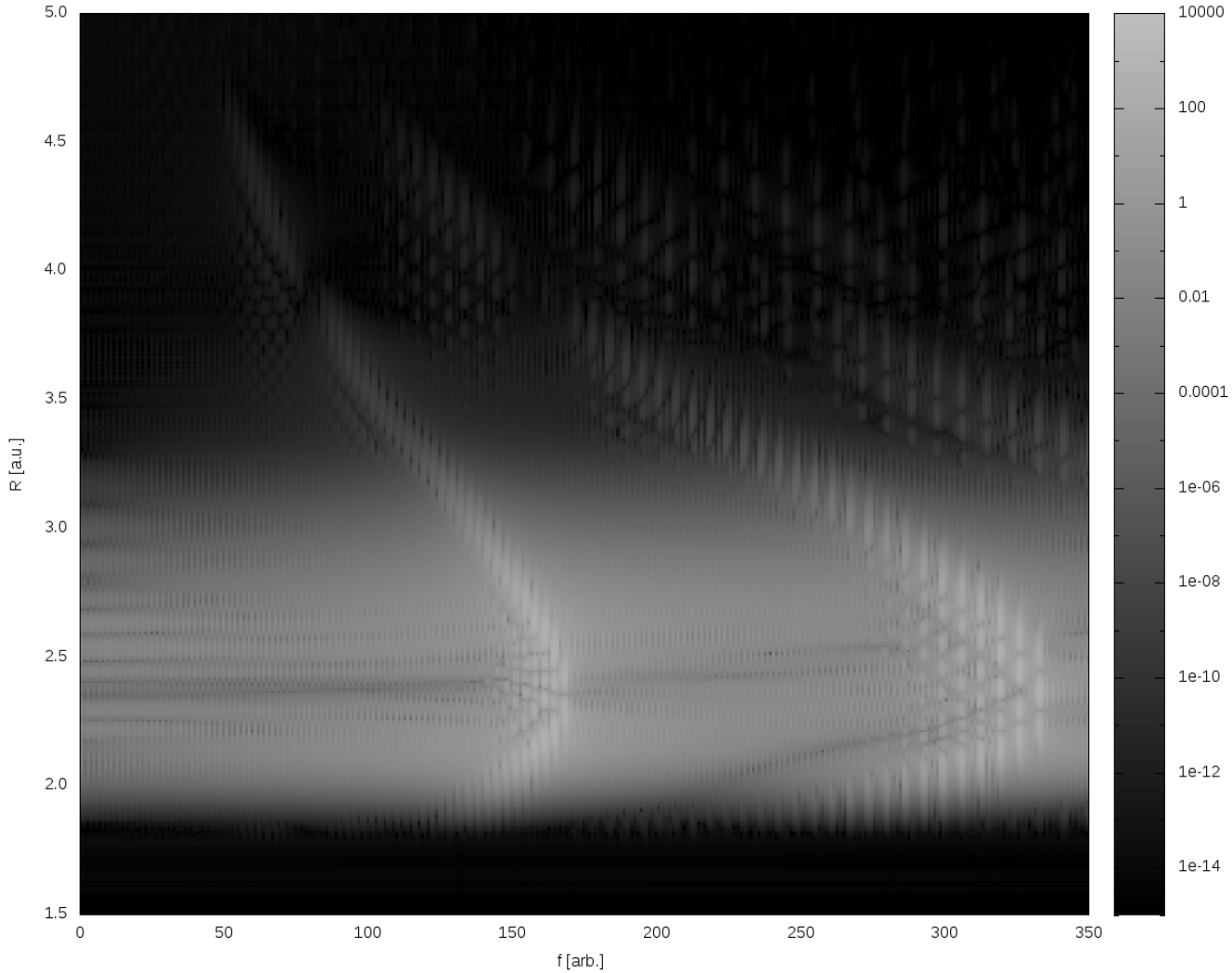
Calculated vibrational revival times and power spectra for available doublet and quartet states of CO^+

Figure: CO^+ $A^2\Pi$ vibrational revival



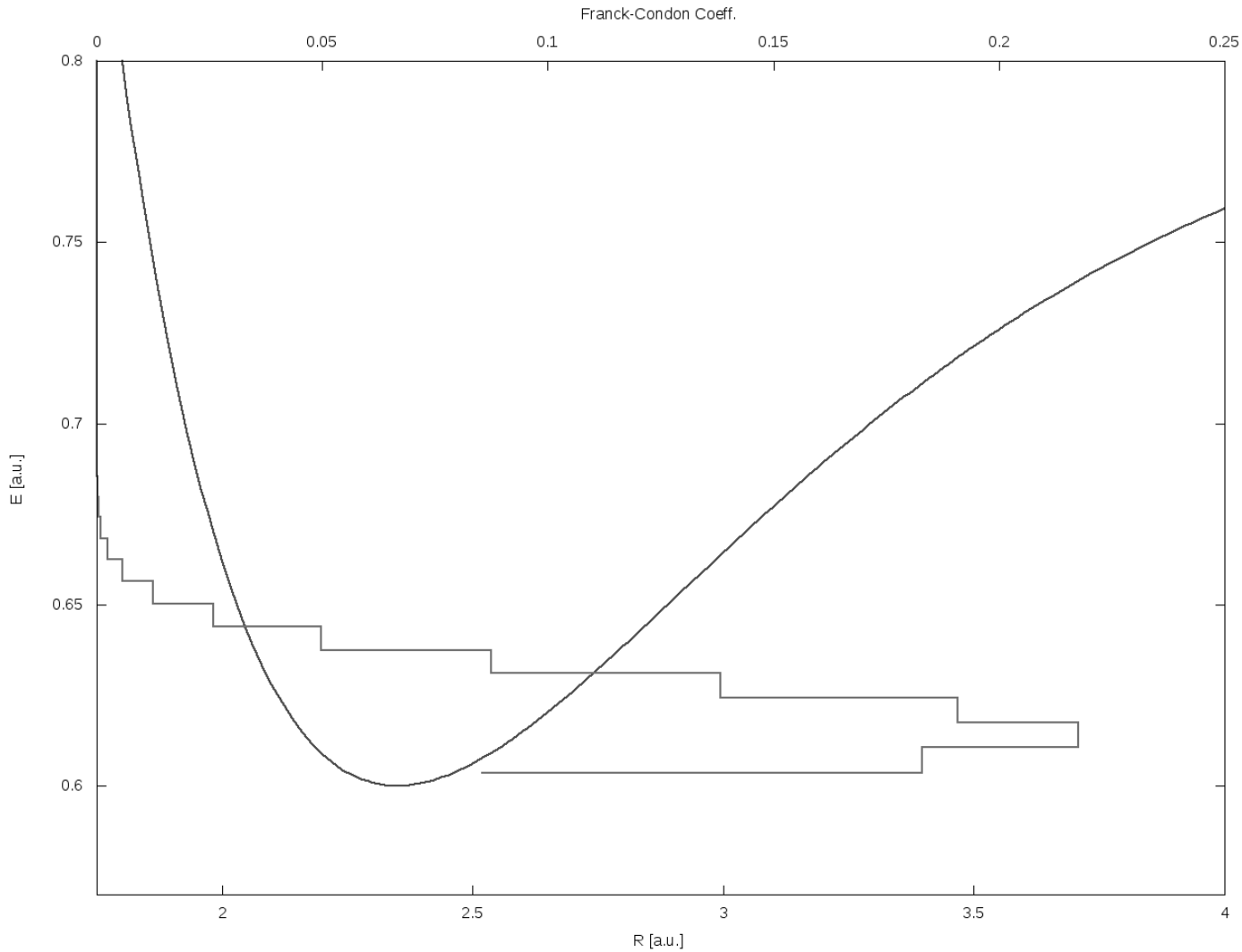
CO^+ - vibrational revivals

Figure: CO^+ $A^2\Pi$ vibrational revival power spectra



CO^+ - Franck-Condon factors

Figure: $\mathrm{CO}\left(X^1\Sigma^+\right) \rightarrow \mathrm{CO}^+\left(A^2\Pi\right)$ Franck-Condon coefficients



CO^+ - next steps

- Simulate 1- and 2-color IR pump-probe spectroscopic experiments and compre with experimental kinetic energy spectra
- Refine dipole coupling and potential curve calculations with GAMESS, including more realistic fittings
- Investigate C, O^+ vs. C^+, O dissociative channels

Other projects

- Continuing work with vibrational revival and 2-color IR pump-probe spectroscopy simulations of noble gas dimers to reproduce earlier results
- Isolating computational performance issues - looking into ways to parallelize existing code using OpenMP or MPI
- Investigating using split-operator Fourier transform propagation in place of split-operator Crank-Nicholson propagation

References

[1] Okada, K. and S. Iwata. "Accurate potential energy and transition dipole moment curves for several electronic states of CO^+." *J. Chem. Phys.* 112.4 (2000): p.1804-1808.