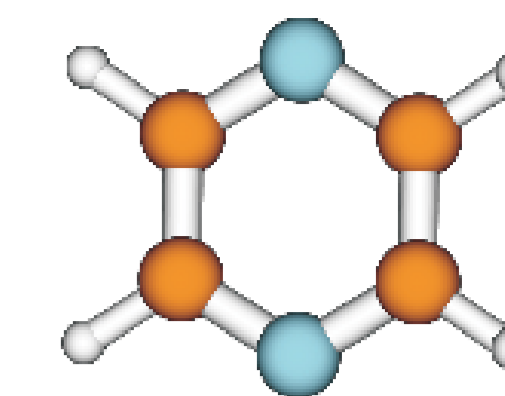


Theoretical and Experimental Study of Positron-Pyrazine Collisions

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Introduction

Reliable data for positron interactions with biomolecules, e.g. DNA nucleobases, can be used to improve, and develop future applications of Positron Emission Tomography. However, experimental measurements are challenging since biomolecules are difficult to get into the gas phase and calculations are costly due to their low symmetry. For this reason, more volatile model systems with higher symmetry, like pyrazine, are usually investigated. We have measured and calculated elastic and inelastic cross sections and compared them to previous calculation which used the SMC method [1]. Pyrazine belongs to the D_{2h} point group, is non-polar, but has a large polarizability of $\sim 60 a_0^3$.

Experimental details

Experiments were performed using the Australian Positron Beamline Facility which uses a Surko trap and beam system to generate pulses positrons with an energy resolution of 55 meV [2]. Using previously developed techniques for measuring scattering cross sections [3], measurements were made for a variety of processes, including grand total, (rovibrationally averaged) total elastic and inelastic scattering, as well as elastic DCS and discrete total electronic excitations.

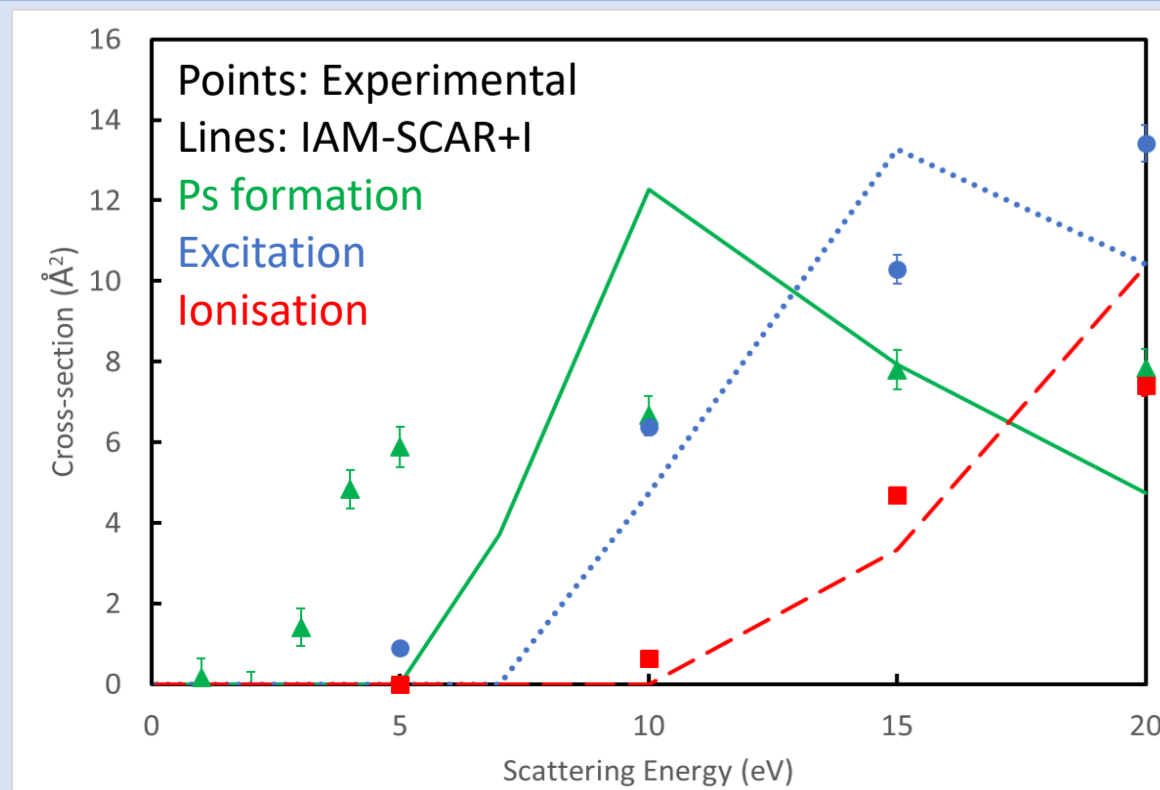
R-Matrix calculations [4,5]

The R-Matrix method solves the time independent Schrödinger equation by splitting the problem into two regions separated by a sphere of radius a . Calculations were carried out at Static plus Polarization (SP) and close-coupling (CC) levels, with the target states described at Hartree-Fock level (i.e. with a single configuration) and $a=18 a_0$. Details of SP calculation: 6-311+G(3df,3pd) basis set, partial waves with $l_{\max}=4$ for the continuum and 120 virtual orbitals (VO) to build the configurations describing correlation and polarization. CC calculation: 6-311+G**, $l_{\max}=5$, 80 VO and 80 states.

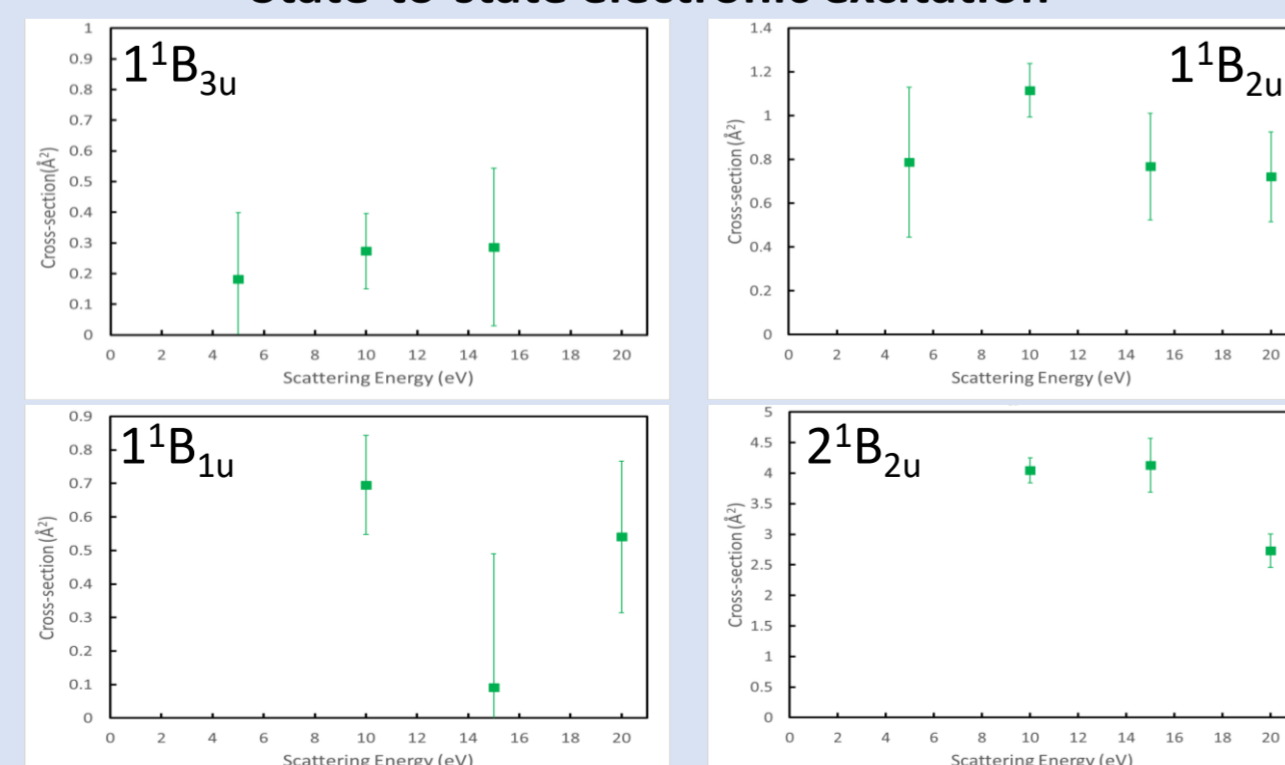
IAM-SCAR+I calculations [6,7]

IAM-SCAR+I treats the molecule as the sum of its constituent atoms, with atomic cross sections calculated using the optical potential method. It includes interference effects by means of an additional term added to cross sections, removing inconsistencies between integral differential cross sections.

Inelastic cross sections



State-to-state electronic excitation



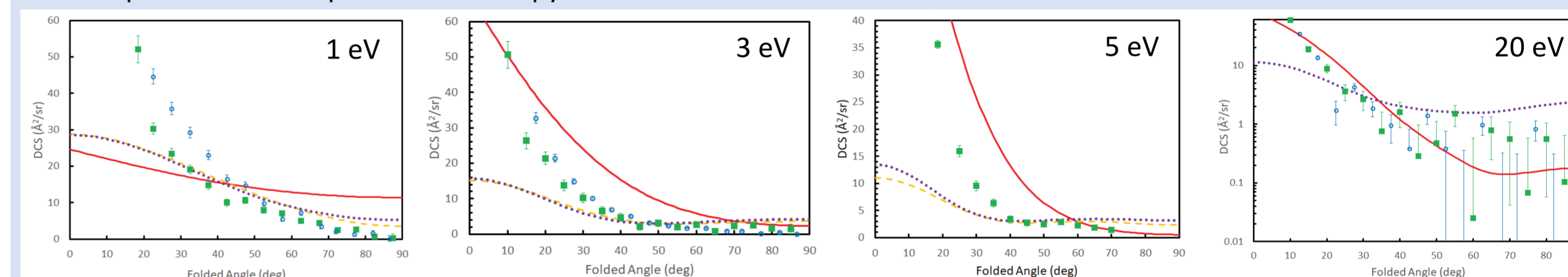
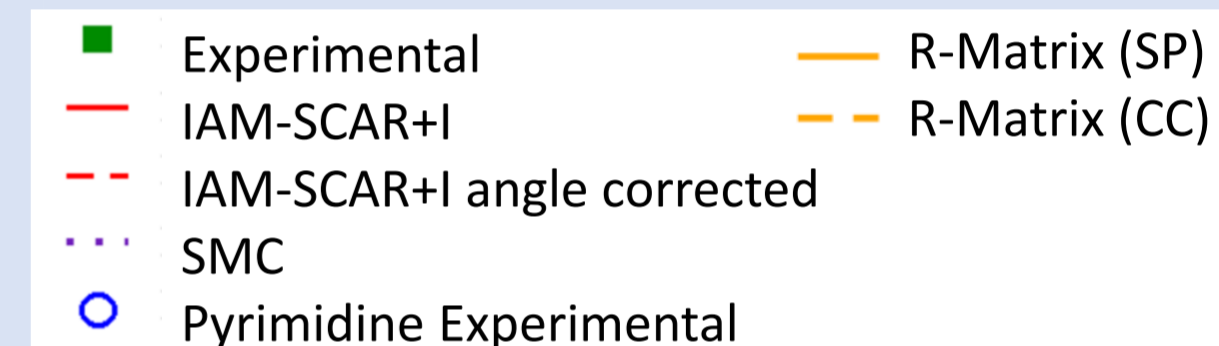
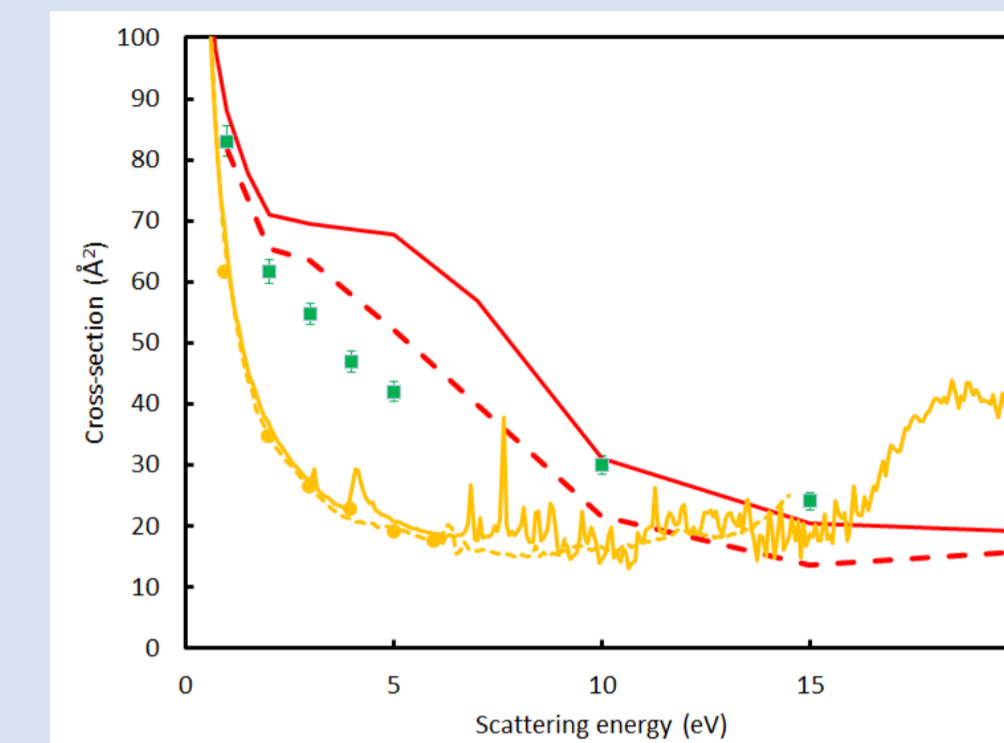
Elastic cross sections

Integral cross section

- R-Matrix CC method significantly reduces presence of pseudoresonances compared to SP.
- R-Matrix cross sections lower than the experiment.
- IAM-SCAR+I cross section larger than experimental results. Agreement is reasonable above 10 eV ("bump" due to the Ps formation threshold > 4 eV too high).

DCS (folded)

- R-Matrix DCS agree with the measurement for angles, $\sim 45^\circ$ to $\sim 90^\circ$ but have poor agreement at low angles, possibly due to issues with polarization description.
- R-matrix and SMC show fairly good agreement.
- IAM-SCAR+I cross sections agree better with the experimental results, particularly at higher energies, as expected.
- High similarity between experiment for pyrimidine and pyrazine. Unexpected due to dipole moment in pyrimidine.



Conclusions [8]

- R-Matrix elastic integral cross section underestimate experiment: polarizability possibly insufficiently described, including a virtual state (estimated scattering length indicates a bound state). DCS disagree most for forward angles.
- Elastic experimental and IAM-SCAR+I results agree much better, particularly at higher energies.
- Experimental and IAM-SCAR+I integral cross sections for Ps formation, ionization and electronic excitation also agree reasonably well.
- State-to-state experimental excitation cross section have been measured, no theoretical counterpart is available.

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