Chapter 7

Conclusions

In this thesis we have reported on cross section measurements for positron scattering from atomic and molecular compounds spanning the low energy range, typically from ~0.1 to ~50 eV. Investigated targets include a couple of the noble gases, molecular hydrogen, a series of isoelectronic molecules, some of the primary alcohols and a range of molecules of particular biological relevance, for a total of 14 species. Total cross sections were measured for all of these targets and, in addition, positronium formation and elastic differential cross sections, at selected positron impact energies, were also measured for tetrahydrofuran. The experiments were undertaken with the low-energy positron spectrometer at the University of Trento (Italy) and the buffer-gas trap and positron beam apparatus at The Australian National University in Canberra.

The total cross section results for all these species highlighted the important role played by the relevant physico-chemical properties of the target (especially its permanent dipole moment and its dipole polarisability), on the very low energy scattering process between the incoming positron and the target molecule or atom. In particular total cross sections were generally found to monotonically decrease in magnitude with increasing incident positron energy, up to typically the positronium formation threshold where a change in the slope was observed. A change in the cross section slope was also usually manifest near the first ionisation potential of the target, indicating the opening of the direct ionisation scattering channel. The effect of a significant permanent dipole moment and/or dipole polarisability of the target was typically reflected by the large values of the very low energy total cross section, namely below the positronium formation threshold. This is thought to be due to the long-range attractive polarisation potential being able to overcome the effects of the other main interaction (see e.g. Surko *et al.*, 2005) fundamentally driving the low energy positron-molecule dynamics. The presence of a significant target dipole polarisability and/or permanent polarity can, thus, lead to a nett positron-target attraction at very low energy, which is manifested by the enhanced scattering probabilities we observed at those low energies.

For quite a few of the investigated compounds, namely most of the molecules of biological interest and the primary alcohol ethanol, the present total cross section results appear to be original. The current measurements are, thus, the very first to have ever been undertaken on those species. In addition, even where earlier data had been reported in the literature, in many cases the present results extended the range of the available total cross section measurements to much lower energies. Namely, usually from below ~1 eV down to ~0.1 eV. The availability in the literature of experimental data in this energy range, in fact, proves to be very useful and especially so to theorists. This follows as they can use this low energy data to validate the results of their calculations, carried out with currently existing models and trying to reproduce the fundamental interactions driving the very low energy scattering process.

The present total cross sections were compared to the results of previous experiments on the same target species, when available. We often found a fairly good level of agreement, between the present results and the earlier data, but only above the positronium formation (Ps) threshold and sometimes only to within the overall uncertainties rather than merely the statistical component of the total error. Below Ps, however, the present total cross sections have regularly been somewhat larger in magnitude than those of the prior experimental investigations. This is possibly a consequence of the present measurements requiring a relatively smaller correction, to account for the forward angle scattering effect, compared to that needed by the previous experimental results. The angular discrimination of the positron spectrometer at the University of Trento and that of the buffer-gas trap and positron beam at The Australian National University, which are energy dependent, appear to be smaller than those of the earlier experiments and are also quite similar to each other. Indeed, we note that the present positron-atom results turned out to be in very good agreement with the corresponding results obtained by the ANU group, on the same targets, throughout almost the entire energy range of overlap. This led us to conclude that a case might well be made for considering the positron total cross sections for argon and krypton to have been, at least experimentally, benchmarked.

The results of the present measurements were also compared with relevant theoretical outcomes, when these were available in the literature. The agreement of theory with the present experimental results was usually found to be rather marginal, if not poor in places, as the calculations often seemed to fail in reproducing not only the magnitude but also the shape of the present total cross sections. This was the case, in particular, for the energy range above Ps where the positron-molecule models currently do not incorporate this scattering channel into the interaction process. In addition, above this threshold energy, fewer computations are usually available compared to at the lower energies. However, we note that the situation with respect to argon and krypton was a little better compared to that for the molecules we studied. In these two cases, in effect, the existing RPO and CCC calculations were found to successfully reproduce at least the very low energy dependence of the present measurements. Nevertheless, overall, the results in this thesis clearly indicated that some further development toward the improvement of positron scattering theory is needed, before the models can properly reproduce the observed data.

As we sometimes found no evidence for either previous measurements or calculations having been conducted on some of the studied target species, in those cases we compared our positron data with the corresponding cross sections for electron collisions, either theoretical or experimental, or even both. Electron TCSs are, in fact, usually more readily available in the literature, possibly reflecting the comparatively easier experimental task of finding an electron source and producing an electron beam as compared to its antimatter counterpart. This comparison of the electron cross section with the positron cross section actually turned out to be rather intriguing, as it enabled us to clearly uncover the major differences between the fundamental interactions driving the collision dynamics when employing either of the two particles as the scattering probe. Positronium formation is, in fact, an exclusive feature of positron scattering, whereas exchange can only occur with electrons. Moreover, the static interaction between the target nucleus and the incoming particle is repulsive for positrons and attractive for electrons, whereas the dipole interaction is attractive in both cases. As a consequence, at very low energy we expected the electron total cross sections to be larger in magnitude before tending to merge with the corresponding positron cross sections above about 100-300 eV. This expectation follows as the effects of positronium formation on one side, and of electron exchange on the other side, become negligible at those higher energies. Indeed, by comparing our positron measurements with the available electron cross sections, we often observed precisely that trend.

Finally, we investigated positron scattering from quite a few biological compounds. This work was undertaken in order to ultimately study the consequences of potential positron-induced radiation damage on biomolecular systems. It is still unclear whether low energy positrons can directly attach to and cause the fragmentation of the nucleic acids, the proteins, and their various components, just like secondary low energy electrons (Boudaiffa *et al.*, 2000). However, it was evident from the particularly large magnitude of the measured total cross sections at very low (epithermal) energies, for the biomolecules investigated in this thesis, that, if ever confirmed, positron binding might well turn out to possess a significant damaging potential on biological systems. In any case, our measured total cross sections remain an essential experimental data input for low-energy particle track simulation codes, as they define, for instance, the stopping power of those particles in the biological medium of interest (Sanz *et al.*, 2012). Finally, positron beams are also capable, through ionisation, of producing an abundance of secondary electrons so that cross sections for both the positrons and the electrons are useful in that respect.