Positron Attachment, Annihilation and Binding in Molecules

G. F. Gribakin[1]

[1]School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, UK
g.gribakin@qub.ac.uk

This talk will review the progress in our understanding of positron annihilation in polyatomic molecules. It has been known since the pioneering positronium experiments by Deutsch in the early 1950s, that positron annihilation rates in polyatomic molecules are strongly enhanced compared with the Dirac annihilation rate for an electron gas of the equivalent number density. Besides a strong dependence on the molecular size [1-3], experimental data for room-temperature positrons revealed a remarkable chemical sensitivity of the annihilation rates [4]. In spite of some remarkable insights and first estimates of positron binding energies based on thermal annihilation rates [3], the overall picture remained unclear for nearly half a century.

A concerted effort of theory and experiment over the past 20 years has changed the situation dramatically. Theoretical predictions of positron binding to neutral atoms made in mid-1990s indicated that most polyatomic molecules should be capable of binding the positron. Positron capture into such bound states, accompanied by a vibrational excitation of the molecule, gives rise to vibrational Feshbach resonances (VFR), which enhance the annihilation probability greatly. A theoretical understanding of the direct and resonant annihilation mechanisms and scaling of the positron annihilation rates with the binding energy [5,6] was quickly followed by observations of VFR in the annihilation rates with a trap-based positron beam [7]. In most cases, these resonances correspond to excitations of particular vibrational modes, allowing measurements of the positron binding energy. At present, these have been determined for over 70 molecules [8]. In turn, the strongly enhanced annihilation rates are due to the mode-based VFRs serving as doorways into dense spectra of multimode vibrational states [9]. Long-range dipole coupling between the positron and infrared-active modes allows to explain the resonant annihilation rates for small polyatomic molecules [10], and we have a good overall picture now [11]. However, the role of nondipole interactions [12] and the details of vibrational mode coupling [13] require more experimental and theoretical efforts, while calculations of positron binding are difficult [14], and for nonpolar molecules (e.g., alkanes), have just begun [15].

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