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Theory of Positron Annihilation on Molecules

GLEB GRIBAKIN, Queen's University Belfast, UK

Recently there has been a rapid progress in understanding enhanced positron annihilation on polyatomic molecules. Building on the hypothesis about the role of vibrational Feshbach resonances [1] and their first observations in alkanes [2], positron binding energies have been determined for many molecules [3]. Also, first calculations of resonant annihilation have been performed and showed excellent agreement with the measured annihilation rates in methyl halides [4]. I will review the current theoretical understanding of the two annihilation mechanisms, direct and resonant. While the complete problem of positron-molecule annihilation is very complex, its various aspects can be modeled by relatively simple means. Thus, by using zero-range potentials we can study the scaling of the positron binding energy with the size of the molecule. For small polyatomics with infrared active modes (e.g., methyl halides), a complete calculation of resonant annihilation can be done, in good agreement with experiment. Applying this theory to other molecules highlights the role of overtones and combination vibrations, and ultimately, intramolecular vibrational redistribution.

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