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Gaseous wavelength shifting in CF_4 -based mixtures: from microscopic modelling to scintillation observables

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Gaseous wavelength shifting (GWS) plays a key role in the optical readout of modern micropattern gaseous detectors (MPGDs). It is closely analogous to Penning transfer, but involves excitation transfer rather than ionization transfer. In principle, GWS enables trace additive concentrations to tailor both the spectrum and intensity of gas scintillation.

Indirect, mostly qualitative, evidence suggests that GWS is present in CF_4 -based mixtures under conditions relevant to gaseous detectors. Here we show that a joint description of primary X-ray-induced and secondary avalanche-induced scintillation in Ar-CF_4 and He-CF_4 mixtures provides a stringent test of this hypothesis. We develop a simple kinetic model based on the atomic and molecular states populated during electron transport, as estimated using state-of-the-art Degrad/Garfield++ cross sections. The model reproduces scintillation yields and emission spectra for both primary and secondary processes using the same input parameters.

We argue that the combination of Degrad/Garfield++ electron transport with the proposed kinetic model provides a practical and internally consistent framework for predicting primary and secondary scintillation in the technologically relevant wavelength range, from 400 to 800 nm, over pressures from 50 mbar to 10 bar and arbitrary CF_4 concentrations. The data indicate a strong wavelength-shifting capability in Ar-based mixtures, driven by transfer from Ar excited p-states to CF_3 Rydberg-like p-states, followed by $p \rightarrow s$ and $p \rightarrow p$ radiative branches contributing to the visible and UV regions, respectively. Unquenched Ar excited p-states emit intensely in the red/near-infrared region. No comparable enhancement of either the visible component or the red/near-infrared emission is observed in He-based mixtures, resulting in lower scintillation yields per electron.

We conclude by presenting state-of-the-art theoretical predictions, including DFT and coupled-cluster calculations, to describe the main spectral observations qualitatively. Finally, we place this work in the broader context of Ar/N_2 and Ar/Xe systems, whose study is also at an advanced stage.

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