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Machine Learning Models for Electron-Impact Ionization Cross Sections and Mass Spectra

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Electron-impact processes are fundamental to analytical chemistry, plasma physics, radiation science, and astrochemistry, yet experimental measurements remain costly and incomplete. We present machine learning approaches for predicting two key electron-impact observables directly from molecular structure: electron ionization mass spectra (EI-MS) and total electron-impact ionization cross-sections.

For EI-MS prediction, we developed a hybrid model combining a graph neural network encoder, a residual neural network decoder, cross-attention refinement, bidirectional prediction, and chemistry-informed masking. Trained on the NIST14 EI-MS database (molecules ≤500 Da), the model achieves strong library-matching performance (Recall@10 ≈ 80.8%). For ionization cross-sections, we introduce a stacked ensemble integrating LightGBM, CatBoost, a multilayer perceptron, and a graph neural network, combined through a residual LightGBM meta-model. Trained on 212 molecules from the Astrochemistry Low-energy Electron Cross-Section database, the ensemble achieves a test-set RMSE of 1.160 a_0^2 and a Spearman correlation of 0.990, outperforming all individual models.

The results demonstrate that graph-based molecular representations enable accurate prediction of complementary electron-impact properties. These approaches can augment reference databases, support molecular identification, and reduce the need for costly experimental measurements.

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