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Advancing Hydrocarbon Source Rock Assessment: An Integrated XRF, Gamma-Ray, and Multivariate Statistical Analysis of the Irati Formation, Paraná Basin

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This study employs an integrated geochemical and geophysical approach to refine the characterization and hydrocarbon potential assessment of the Irati Formation, a key organic-rich source rock interval in the Paraná Basin, Brazil. We combine X-ray fluorescence (XRF) and gamma-ray spectrometry data with statistical and multivariate methods using the Python programming language, enabling robust and reproducible analyses of geochemical data.

Methodologically, a reproducible computational pipeline enabled the objective analysis of geochemical partitioning. Key findings reveal a strong anti-correlation between SiO_2 and carbonate components, delineating clear depositional facies. Shale and marl intervals, characterized by elevated SiO_2, Al_2O_3, and U+Th contents, are identified as the primary source rock horizons. The enrichment of uranium in these layers serves as a key indirect proxy for anoxic conditions conducive to organic matter preservation. A critical revision of the K/U ratio confirmed a mineralogy poor in potassium feldspars and dominated by carbonate phases. Furthermore, the distinct geochemical behavior of U (associated with clays) and Th, along with the association of Cl with the carbonate fraction, provided novel insights into elemental fractionation. X-ray diffraction (XRD) analysis directly supported these interpretations, confirming the presence of montmorillonite (with high cation exchange capacity) and pyrite, which underscore the anoxic depositional setting critical for hydrocarbon generation.A distinct hybrid lithofacies, identified as "limestone-cucuruto," was statistically delineated, representing a significant transitional rock type. Furthermore, diagnostic K/U ratios consistently indicate a mineralogical assemblage poor in K-feldspars and dominated by carbonate phases, validating the geochemical classification.

The integration of these proxies provides critical insights into the depositional environment and diagenetic history governing the Irati formation's heterogeneity. More importantly, it demonstrates a practical application of modern, accessible computational tools to de-risk subsurface evaluation by quantifying mineral composition and lithofacies distribution—key parameters for modeling source rock quality and hydrocarbon generation potential. This case study highlights how the strategic fusion of conventional analytical techniques with data-driven statistics can build more predictive models, directly addressing the need for interdisciplinary advancements in exploration geochemistry within both mature and frontier basins.