Poster

Exploring Novel Organometallic Compounds: Bridging Catalysis and Medicine through Crystallographic Insights

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The historical utilization of organic molecules (ligands) coordinated to transition metals, such as platinum (Pt), rhodium (Rh), rhenium (Re) and technetium (Tc), spans several decades particularly in the field of catalysis and medicine [1-2]. However, due to factors such as global warming, virus mutations and evolving catalytic technologies, the global demand for novel organometallic catalysts and smart drugs remains an ongoing project. This emphasizes the pressing need for intensive scientific efforts aimed at the design, synthesis, and evaluation of organometallic compounds that surpasses previous catalysts and medicine, offering fine-tuned efficiency and selectivity [3-4].

Using crystallographic programs such as Olex2, WinGX and Crystal Explorer, our research aims focuses on understanding how inorganic chemistry interacts with biological systems, with a specific focus on understanding how small metal-based compounds interact with more complex metal-containing biomolecules. By studying these interactions, we seek to uncover their reactivity and functions within biological contexts. Additionally, we are engaged in a parallel project dedicated to the development of environmentally sustainable organophosphorus catalysts.

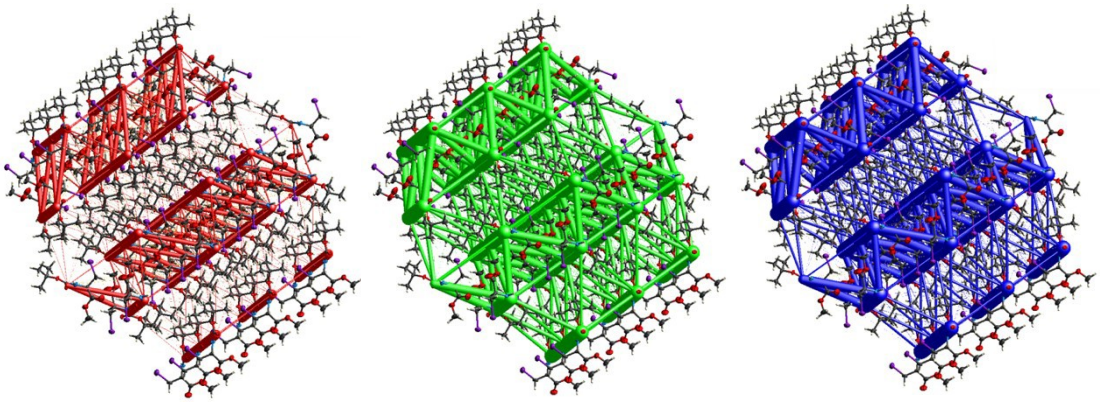

Figure 1. Energy frameworks for electrostatic (red), dispersion (green) and total interaction energy (blue) for a cluster of nearest-neighbour molecules in Boc-Ala(3-I)-OMe [5].

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