



Showcasing research from Professor Max Crossley's laboratory, School of Chemistry, The University of Sydney, NSW, Australia.

The Polytope Formalism: application to molecular constitution and the prospect of a complete description of Chemical Space

Chemical Space is vast, structured, and largely unexplored. This work extends the Polytope Formalism from stereoisomerism to molecular constitution, providing a mathematically complete and discretised framework for unifying isomerism, and organising chemical structure, reactivity, and transformation pathways. By treating atom connectivity as an abstract configuration space, the formalism systematically enumerates isomers and interconversion intermediates while encoding the topology of underlying potential-energy surfaces. The result is a unified, navigable representation of chemical possibility - offering a rigorous foundation for mechanism analysis, nomenclature, and the automated exploration of Chemical Space.

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As featured in:



See Peter J. Canfield and Maxwell J. Crossley, *Chem. Sci.*, 2026, **17**, 2102.