☐ **Talk** ☒ **Poster**

Computational Investigation of Reductive Dehalogenation of Alkenyl Halides with Cobalamin-Dependent Enzymes

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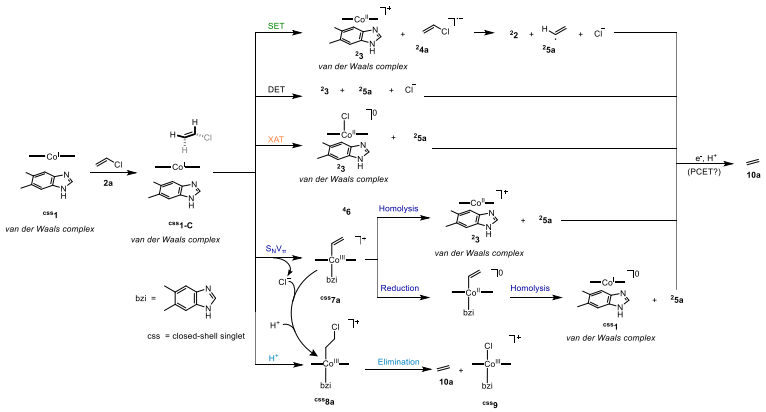
Halogenated alkenes such as vinyl chloride (VC) and perchloroethene (PCE), while useful synthetically and industrially, pose serious risks to environmental and human health.[1] Previous studies[2-4] have established the ability of some microbes to process VC and PCE enzymatically with a vitamin B12 (cobalamin) cofactor, to varying overall yields, though the mechanism by which this process occurs is still poorly understood. Recent[5] X-ray absorption spectroscopy experiments suggest that VC and PCE are reductively dehalogenated *via* different mechanisms, evidenced by the observation of different Co(III)–C bond types in XANES data for each alkene. In this work, we leverage computational techniques including density functional theory (DFT) and time-dependent density functional theory (TDDFT) to investigate the processes by which cobalamin catalyzes the reductive dehalogenation of VC and PCE. Specifically, we present calculations for each of the multiple proposed mechanisms in the literature[2-4] and computationally derived XANES spectra as additional confirmation for experimentally derived spectra.



References

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[5] Yang, Dali; Cao, Rui; Giles, Logan J.; Sarangi, Ritmukta Unpublished Work (Manuscript in Preparation)