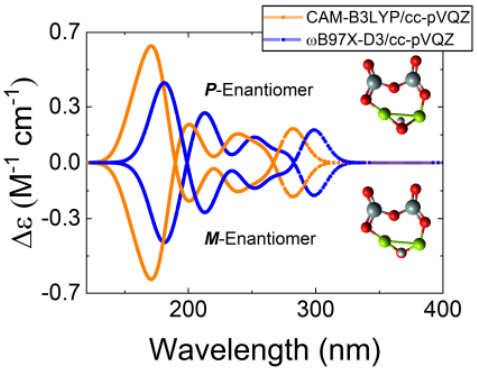
LIFE'S COSMIC HANDSHAKE: DFT AND TD-DFT PREDICTIONS FOR THE PROPERTIES OF ENSTATITE ($MgSiO_3$) MONOMERS AND DIMERS

KAMIL B. STELMACH, *Department of Chemistry, University of Virginia, Charlottesville, VA, USA*; CATHERINE A. DUKES, *Laboratory for Astrophysics and Surface Physics, University of Virginia, Charlottesville, VA, USA*; ROBIN T. GARROD, *Departments of Chemistry and Astronomy, The University of Virginia, Charlottesville, VA, USA*.

Silicates represent an understudied class of molecules in astrochemistry despite surfaces having been shown to have important chemical and physical effects. Clinoenstatite has been detected in interstellar space[a] and is a major component of meteorites.[b] Clinoenstatite is also interesting because it has chiral faces.[c] Structural and spectral studies utilizing density functional theory (DFT) and time-dependent (TD-) DFT were conducted on the monomer and a nanosilicate dimer of enstatite first described in Valencia et al.[d]; in addition, a 2D chiral conformer of the dimer was also studied. The HSE06/aug-cc-pVQZ level of theory was chosen for optimization, frequency, and energy calculations. CAM-B3LYP and ωB97X-D3 functionals were used with the cc-pVQZ basis set in the TD-DFT calculations to obtain the UV-Vis and ECD spectra. We modeled each structure in its bare silicate form but also with H, H^+, and H_2. Placing the neutral H on the 2D chiral enstatite conformer produces a 3D structure that makes it optically active. This provides a symmetry breaking mechanism for chiral silicates in the ISM.



[a] Jones, A. P. (2007). *EJM*, 19(6), 771-782.
[b] Mason, B. (1968). *Lithos*, 1(1), 1-11.
[c] Hazen, R.M. (2006). *Am Min*, 91(11/12), 1715.
[d] Valencia, E. M., et al. (2020). *MNRAS*, 492(1), 276-282.