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Modeling the black intermediate formed in the cathode of Vanadium redox flow batteries LAURA JUDY, JUSTIN OELGOETZ, Austin Peay State Univ — There has been much research done into creating a battery that can hold charge indefinitely with little waste and scale to large industrial and even electric grid installations. One particular battery that has proven to be a viable candidate for low-waste, high-energy storage is the vanadium redox flow battery. As the battery discharges, VO^{2+} is reduced to VO_2^+ at the positive electrode and V^{2+} is oxidized to V^{3+} at the negative electrode. The process is reversed as the battery is charged. During this process, the reactions cause the solutions to change colors – turning from yellow to blue at the cathode and violet to green at the anode. In addition to the color change of the solutions, there is a black intermediate that forms during partial discharge at the cathode that has been hypothesized to be $V_2O_3^{3+}$. This poster presents results of semi-empirical methods (PM6 and PM7) models which aim to identify the black intermediate. We will present not only thermo-chemical results but also the predicted vibrational structure and the RAMAN lines.

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