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Fourier Transform Infrared Spectroscopy of Metal Organic Framework Compounds ADDIE WILSON, BRANDON YOST, University of North Carolina at Chapel Hill, BRADLEY GIBBONS, Department of Chemistry, Virginia Polytechnic Institute and State University, LAURIE MCNEIL, University of North Carolina at Chapel Hill — Metal organic framework compounds (MOFs) have crystalline structures that are highly porous at the molecular level and have large surface areas that are advantageous to catalysis, such as for the decontamination of chemical warfare agents. UiO-66 is a MOF with a zirconium metal center and benzene-1,4-dicarboxylate (BDC) linkers. We have used Fourier Transform Infrared (FTIR) spectroscopy to characterize the vibrational modes of UiO-66 as a function of defect density, where the defects may be missing linkers or missing metal clusters. We have found that as the defect density increases, there is a characteristic broadening in some of the infrared bands. We have also determined from our FTIR spectra that the modulator used to synthesize the UiO-66 is not completely removed after synthesis. This was determined by identifying the presence of Trifluoroacetic Acid (TFA) in a sample that was created using a TFA modulator. We will also report on changes in the spectrum after exposing the UiO-66 samples to formic acid, which can also be used as a modulator.

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