

ENHANCING SPECTRAL RESOLUTION IN MAGIC ANGLE SPINNING NMR BY USING SINGLE CRYSTALS: PORPHINES Sneha Dugar^{1, 2}, Riqiang Fu², Ron Clark¹, Naresh S. Dalal^{1,2} 1. Florida State University, Department of Chemistry and Biochemistry, Tallahassee, FL32306, United States 2. National High Magnetic Field Laboratory, Tallahassee, FL32310, United States

Enhancement of spectral resolution in NMR of solids is always desirable. We find that using single crystals in magic angle spinning (MAS) measurements leads to significant improvement in resolution. This conclusion will be demonstrated for ^{13}C NMR on several octaethyl porphyrins (H_2OEP) and its metallated analogs NiOEP and ZnOEP . The use of single crystals leads to a significant enhancement in resolution and aids in the identification of all the observed resonance signals. The dipolar dephasing measurements were carried out to assign all the carbon atoms. The observed multiple peaks are attributed to the crystal packing and intermolecular ring current effect. For NiOEP , two CH_2 resonances are observed because of their slightly different proximity to the intermolecular π electron cloud in the unit cell. This ring current effect shields more on the CH_2 groups than on the CH_3 groups. Similarly, all the carbon atoms for H_2OEP and ZnOEP can be accounted for. With the significant enhancement in resolution, our results suggest that high resolution NMR can be correlated very well with the crystal structure and that unknown crystal structures can be predicted with good accuracy.