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**Low Energy Positron Interactions with Biological Molecules** INDIKA WANNIARACHCHI, CAROLINE MORGAN, Physics Department, Wayne State University, BERNHARD SCHLEGEL, Chemistry Department, Wayne State University, GARY KEDZIORA, AFRL/DSRC, Wright-Patterson AFB, LARRY BURGGRAF, Engineering Physics, Air Force Institute of Technology, MICHAEL PAK, SHARON HAMMES-SCHIFFER, Chemistry Department, Penn State University — There is some experimental evidence that positrons can produce distinctive molecular fragmentation patterns. It is known that tuning the incident positron energy to near resonance with molecule vibrations can strongly enhance the positron annihilation probability for a molecule.[1] This suggests that fragmentation induced by slow positrons may provide valuable complementary information to existing techniques for identification and study of proteins. In order to study this concept, we are developing a general quantum method for reliably calculating the density distribution for positrons bound to large biological molecules using NEO/GAMESS. We developed transferrable atom-centered positron basis sets for first-principles calculations for molecules containing O, N, C, and H. The positron density in the bound state is concentrated near the most electronegative atomic sites so that $e^-e^+$ annihilation will be most likely to occur in these regions for low incident positron energies leading to positron trapping in the bound state. Using the basis sets and approximations we have tested to predict where annihilation occurs can ultimately help us understand the resulting fragmentation patterns of larger biological molecules.

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[1]Gribakin, Young, and Surko, Rev. Mod. Phys. 82 (2010) 2577

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