Tunnel Junction Sensing of TATP Explosive at the Single-Molecule Level

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Abstract. Triacetone triperoxide (TATP) is a homemade, potent explosive and, unfortunately, is used in many terrorist attacks. It is hard to detect, and present techniques for its sensing do not offer portability. Fortunately, TATP is volatile, and gas-sensing-based devices for TATP detection would provide a higher level of safety. Here, we explore the possibility of single-molecule TATP detection in the air by tunneling current measurement in the N-terminated carbon-based nanogaps, at the DFT+NEGF level of theory. We found TATP averaged current amplitude of tens nano amperes, with a discrimination ratio with respect to prevalent indoor volatile organic compounds (VOC) of a few orders of magnitude. That high tunneling current is due to specific TATP HOMO contributions to electronic transport. The transport facilitates the strong, in-gap electrical field generated by N-C polar bonds from electrode ends and TATP-electrode hybridization, spurred by oxygen atoms from a probed molecule.