

## WETTING TRIACETONE TRIPEROXIDE ALLOWS ITS DETECTION BY MICROWAVE SPECTROSCOPY

SUSANA BLANCO, ALBERTO MACARIO, *Departamento de Química Física y Química Inorgánica, Universidad de Valladolid, Valladolid, Spain*; JOSÉ GARCÍA-CALVO, ANDREA REVILLA-CUESTA, TOMÁS TORROBA, *Departamento de Química, Universidad de Burgos, Burgos, Spain*; JUAN CARLOS LOPEZ, *Departamento de Química Física y Química Inorgánica, Universidad de Valladolid, Valladolid, Spain*.

Triacetone triperoxide (TATP) is a known peroxide-based explosive frequently used by terrorists in improvised devices due to its ease of synthesis and detection difficulty. Here we propose microwave spectroscopy as a highly selective detection method. The main conformer of TATP (95%) has  $D_3$  symmetry and thus it has no dipole moment. However, TATP-water adducts are polar species and their microwave observation could open a way to detect TATP in the gas-phase. In this work we have observed the spectrum of TATP- $H_2O$  and TATP- $(H_2O)_2$  which, on the other hand, have revealed the interesting properties of TATP. In TATP- $H_2O$  water lies close to the  $C_3$  axis and rotates around it. As a result, the ground state rotational constants average to those of a symmetric top. The complex exhibits a four center trifurcated  $O_w-H\cdots O$  hydrogen bond further stabilized by a weak four center  $C-H\cdots O_w$  chelated interaction. To our knowledge, those kinds of interactions have not been observed previously in the gas phase. The anomalous large  $O-H\cdots O$  distances associated to the main hydrogen bond interaction evidences that TATP oxygen atoms are to some extent encapsulated by their hydrocarbon environment. The dihydrated cluster can be envisaged as formed from the TATP- $H_2O$  adduct with the second water molecule acting as double hydrogen bond donor to the first water molecule and the closest TATP endocyclic oxygen atom.