Destruction of TATP - theoretical considerations

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Abstract

This study is a theoretical-experimental collaboration intended to explore pathways of gentle decomposition procedures of peroxide based explosives such as TATP . We explore the role of metal ions on the decomposition mechanism based on TATP catalytic destruction in acidic solution.

Relevance

For law enforcement agencies the problems are detection and destruction. The problem is made acute by the extreme sensitivity of these explosives. Currently, the safest way to dispose such illegal explosives is to detonate them on the spot. This procedure safeguards the law enforcement sappers from handling and transporting these highly sensitive materials. However, in some instances, relatively large quantities, many kilograms, of peroxide explosives are discovered, located in apartments and other high-population density areas. Blow-in-place protocols are impractical in such situations. Hence, there is an urgent need for suitable safe protocols that will safely destroy large quantities of peroxide-based explosives.

To support the experimental effort to find a mode for gently destruction of peroxide explosives, a theoretical analysis of the interaction of various metallic ions with TATP is presented. First, we calculated and reported the binding of various metal ions to TATP . These quantum chemical calculations demonstrated that some metal ions bind to the TATP molecules to form complexes in which the TATP structure is not altered. However, a few ions bind to the TATP molecule and lead to destruction of the molecular ring.

Decomposition pathways catalyzed by metal ion in solution

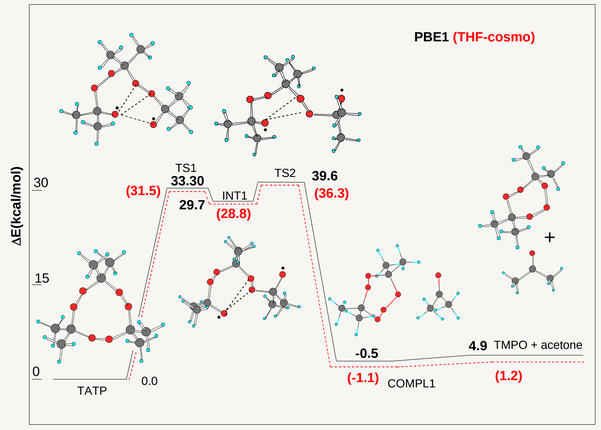

Fig. 1: TATP decomposition pathway, black line represents an isolated molecule while red line corresponds to a molecule dissolved in THF.

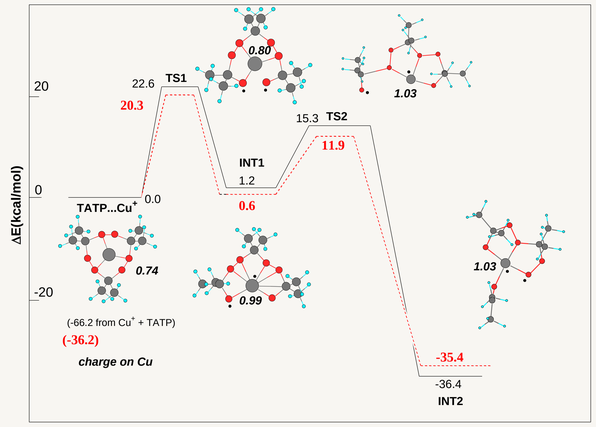

Fig. 2: Initial stages of Cu^+-TATP complex destruction pathway. The symbol • represents the location where localization of maximum spin density is found. The charge value on Cu is presented by bold italic font. Black line shows the decomposition of a gas phase complex while red line that of a complex in THF.

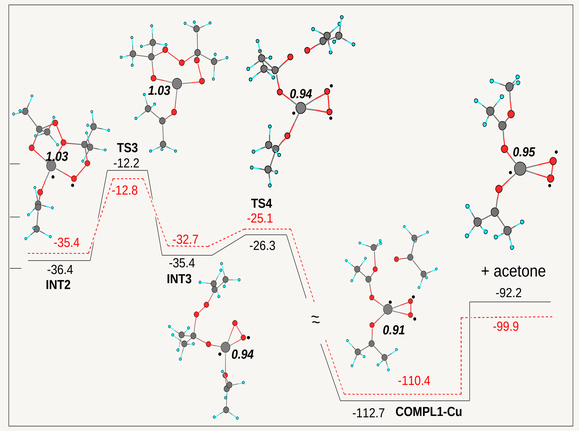

Fig. 3: The late stages of Cu^+-TATP complex destruction until the first acetone molecule is formed. . Black line shows the decomposition of a gas phase complex while red line that of a complex in THF

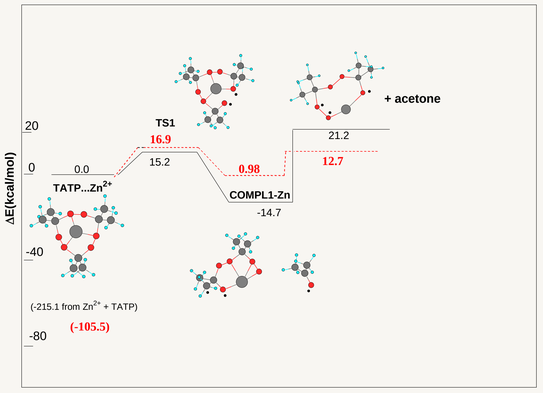

Fig.4: The stages in Zn^{2+}-TATP complex destruction. The symbol • represents the location of the localization of maximum spin density. The charge value on Zn is presented by bold italic font. Black line shows the decomposition of a gas phase complex while red line that of a complex in THF.

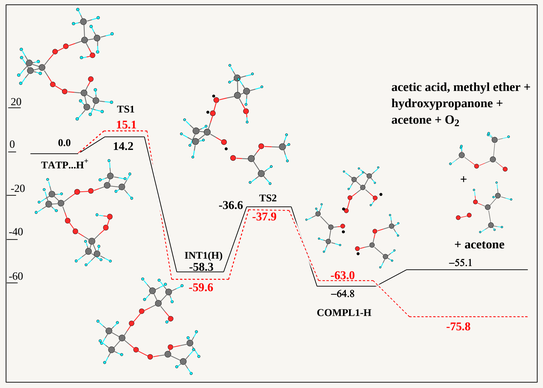

Fig.5: Initial stages of H^+-TATP complex destruction path way. The symbol • represents the location where localization of maximum spin density is found. The charge value on H is presented by bold italic font. Black line shows the decomposition of a gas phase complex while red line that of a complex in THF.

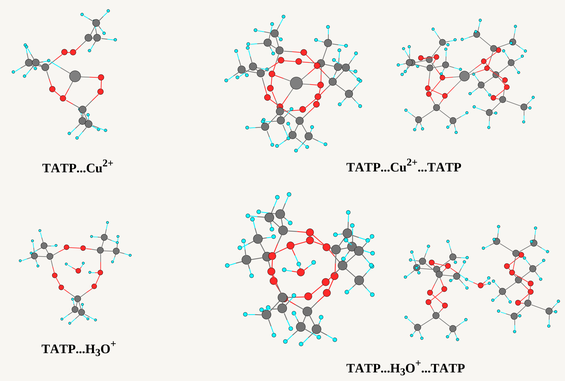

Fig.6: Optimized structures of ion-TATP (left column) and TATP-ion-TATP (right set of four pictures) complexes for Cu^{2+} and H_3O^+. In the case of sandwich type complexes the right column corresponds to side view while the left column to top view.

Accomplishments Through Current Year

This research may have an important impact on suggesting a route for destruction of peroxide based explosives. The electronic structure calculations allowed to understand and explain the behavior of selected metal ions in relation to the experimental findings.

Future Work

We intend to explore other metal ions as candidates for gentle decomposition of TATP. Other work on TATP will include calculation of spectra in the THz range.

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