

# Synthesis, Structural Analysis and Safety Consideration of Halogen Bonded Functional Materials

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## Abstract

As always, scientists are always pushing the envelope for making novel “modern” materials. The supporting evidence for these scientific break-throughs is generally answered by spectroscopy. In the field of chemistry, a combination of various spectroscopic techniques such as multinuclear NMR, IR, Raman, mass spectroscopy etc. provide invaluable tools in determining the boundary between myths and realities. For example, the use of vibrational and NMR spectroscopy proved the existence of exotic species such as the  $N_5^+$  cation, which was further substantiated by x-ray crystallography. In the case of the attempted synthesis of  $N_3^+$ , structure elucidation based on IR spectroscopy was ultimately negated by elucidating the true chemical species using x-ray. Use of mass spectroscopy proved, beyond any doubt, the existence of the elusive pentazole ( $N_5^-$ ) anion. However, doubts still exist about its characterization in solution using  $^{15}N$  NMR spectroscopy. The use of spectroscopy and single crystal x-ray diffraction studies of some other “modern” materials will also be presented. The safety aspects in handling of these halogen-bonded materials will be discussed.

