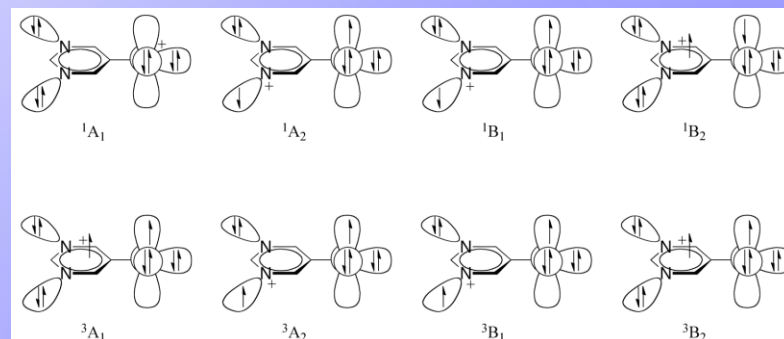
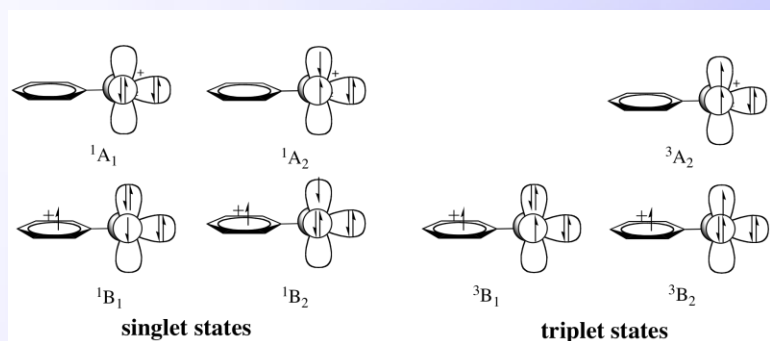


Theoretical and Experimental Investigation of Oxenium Ions

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Theoretical studies of Oxenium Ions. We have performed high-level multireference CASPT2/CASSCF computations on a variety of important oxenium ions, including the parent phenyloxenium ion as well as heteroaryl oxenium ions incorporating a ring nitrogen. Remarkably, we find that oxenium ions can adopt a variety of unusual low-energy electronic states including closed-shell and open-shell singlets and triplet states.



Experimental studies of oxenium ions. We have developed a novel photoprecursor to aryloxenium ions, protonated aryl hydroxylamines, which undergo heterolytic scission upon photolysis to yield aryloxenium ions, which can be studied by ultrafast laser flash photolysis experiments.

