

## Didehydro Radical Anions from Ketones via $O^{\bullet-}$ Chemical Ionization

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### Abstract

Gas-phase ion-molecule reactions of the atomic oxygen radical anion,  $O^{\bullet-}$  with selected ketones are investigated to explore a strategy to 1,3-distonic radical anions. These  $O^{\bullet-}$  chemical ionization reactions, especially that of cyclopentanone, are examined in detail under the well-defined thermal energy conditions uniquely available by using the flowing afterglow technique. To further understanding of the reaction mechanism, a series of related ketones (acetone, 3-pentanone, 2-butanone, 2,4-dimethyl-3-pentanone, cyclohexanone) are also examined in detail. Rate constants for each ketone reaction are measured and products from each ketone examined are identified and their branching ratios reported. Based on these results, a detailed reaction scheme for each ketone reaction studied is proposed. The individual reaction schemes are summarized in a composite  $O^{\bullet-}$ /ketone reaction scheme and the specific reaction pathways are discussed. A strategy is developed to differentiate 1,1- and 1,3- $H_2^{\bullet+}$  abstraction products and to establish the absolute yields of 1,3-distonic radical anions from appropriate ketones.

*Keywords:* ion-molecule reaction;  $O^{\bullet-}$ ; ketone; radical anion

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