Mechanism of Ketene Elimination from Protonated 2-Methoxy- and 2-Hydroxy-Benzalacetophenone: Experiment and Theory

George Mathai1, V.S. Sebastian1, R. Srinivas2, P. Nagi Reddy2, Daryl Giblin3 and M.L. Gross3

INTRODUCTION

The gas-phase fragmentation of substituted benzalacetophenones (C6H5-C(=O)-CH(2)-CO-CH3) is of interest in the context of the structures of the 3'-C=O and 3'-CH2=CO moieties. We have previously reported that the gas-phase fragmentation pathways of the following substituted benzalacetophenones were studied: 1) 3'-substituted benzalacetophenones (C6H5-C(=O)-CH(2)-CO-R) and 2) 3'-methyl-2'-methoxychalcones (2-MeO-C6H4-C(=O)-CH(2)-CO-CH3) and 3'-methyl-2'-hydroxychalcones (2-HO-C6H4-C(=O)-CH(2)-CO-CH3). These compounds are of interest because of their potential as precursors to other compounds of biological interest, such as alkaloids and natural products.

In this study, we have used the CAD mass spectrometric technique to investigate the gas-phase fragmentation of 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

RESULTS AND DISCUSSION

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

Experimental Details:

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.

We have investigated fragmentation processes of the 3'-substituted benzalacetophenones and 3'-methyl-2'-methoxychalcones using the CAD mass spectrometric technique. We have observed that the gas-phase fragmentation pathways of these compounds are similar to those observed in previous studies, and that the fragmentation pathways are dependent on the substitution pattern of the phenyl ring.

We propose that the fragmentation routes to these products (Scheme 2) involve cyclization to a pyrrole form followed by elimination.