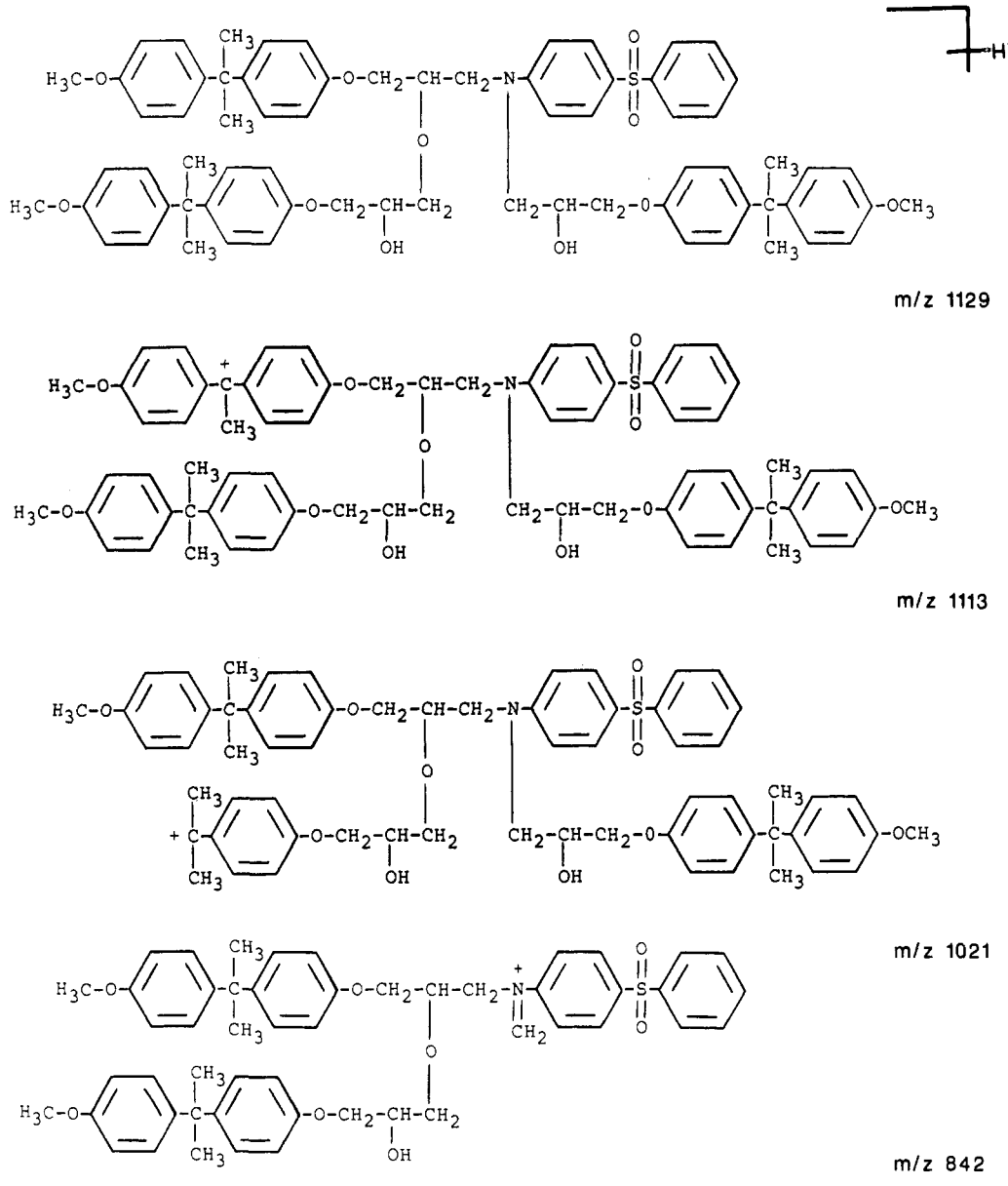
Scheme V
Structures of Pertinent Ions Derived from Product IV



rise to the peaks at m/z 1113 and 1021, respectively. Elimination of part of the lone MGEBA on the nitrogen yields the characteristic quaternary amine ion at m/z 842. This difference is 287 amu, clearly an anomaly to the proposed structure based on the previous examples, which eliminated 286 amu in forming the quaternary amine. The exact mass of the resulting ion, however, is 842.37 amu and is rounded down by the data system as nominal mass 842, effectively "losing" 1 amu by the transition. This mass defect artifact should be kept in mind when working with relatively high mass compounds at low resolution since it accounts for the "disappearance of a hydrogen atom". In addition to the above peak at m/z 842, the spectrum of IV also shows peaks at m/z 544, corresponding to the formation of the second possible quaternary amine, by eliminating the two ether linked MGEBAs, m/z 260, common to all the tertiary amines in this series, as well as peaks due to the nonspecific ions (i.e. m/z 246, 242, 227, and 149) discussed earlier.

The spectrum of the last example in this series, product V, is shown in Figure 8. The fragments associated with

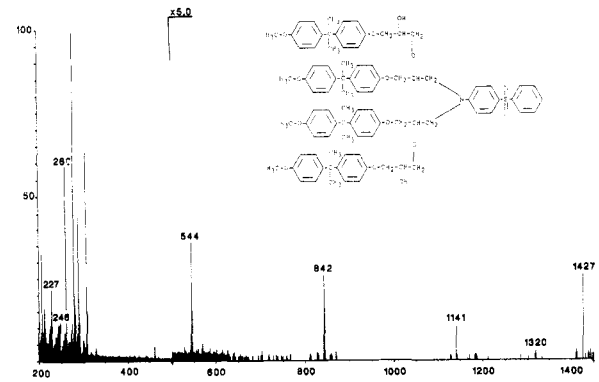
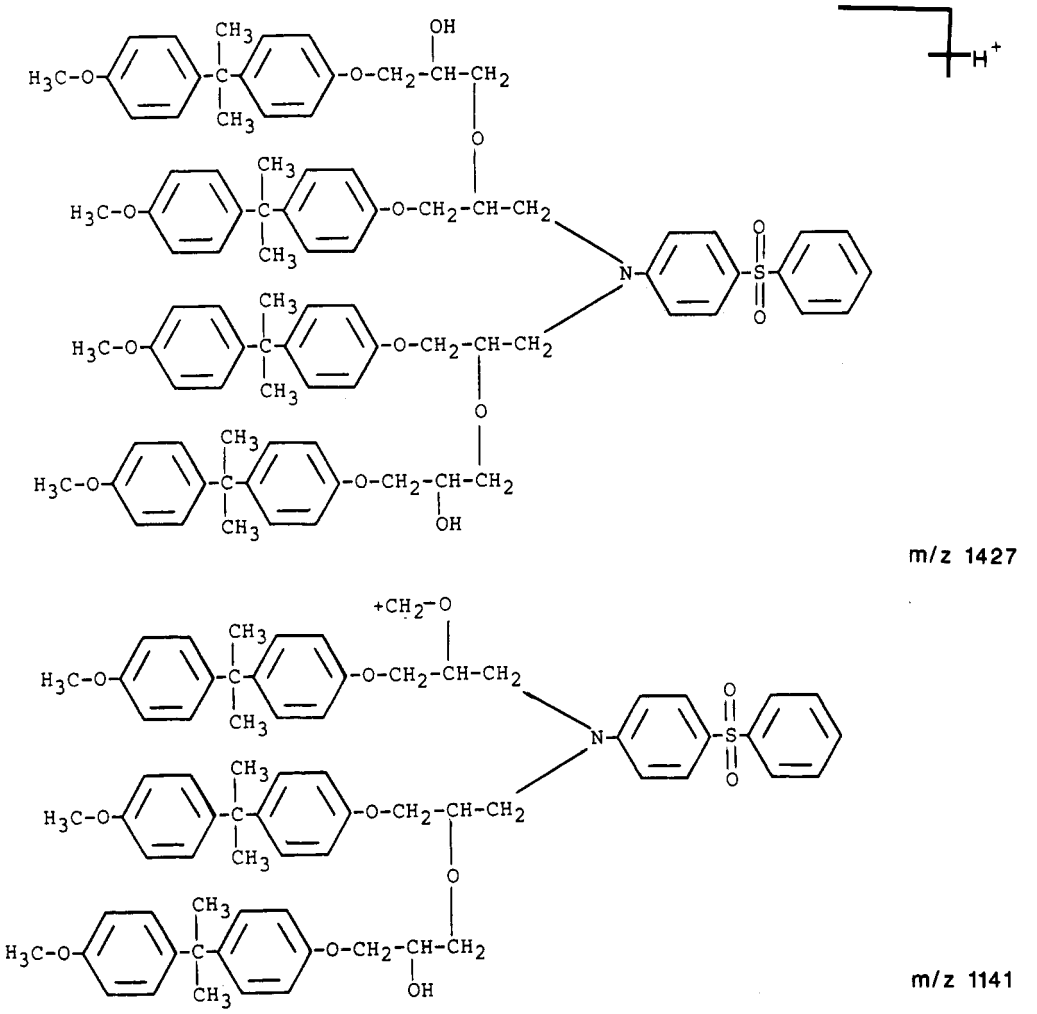


Figure 8. FAB mass spectrum of product V in 3-NBA.

symmetric substitution are summarized in Scheme VI, although similar peaks are expected for the asymmetric substituted. Once again, the protonated molecular ion of mass 1426.68 amu is seen at m/z 1427 due to the inherent mass defect of the compound. Elimination of a meth-

Scheme VI
Structures of Pertinent Ions Derived from Product V



oxybenzene or one of the MGEBA groups up to the terminal methylene gives the peaks at m/z 1320 and 1141, respectively, taking into account the mass defect. These are the only peaks which could be used to identify this homologue since the lower mass fragments (i.e. m/z 842, 544, 260, 246, 227, and 149) are common to one or more of the other homologues in the series.

Conclusion

The mass spectral characterization of the oligomers formed by the curing of the MGEBA with ADS are an excellent example of the utility of FAB mass spectrometry in identifying and/or confirming the structures of oligomer reaction products. We have showed that the fragmentation pattern, in addition to the molecular weight of the oligomers, provides insight as to the type of oligomer as well as the type of isomeric linkages which are present. Consideration of all the information provided by a mass spectrum would aid in structure identification and characterization.

Having obtained pure material with known structures, we have begun to establish a data base of particular reaction mixtures which links characteristic fragmentations with molecular structures. These characteristic fragmentation patterns may then be used in evaluating the formation of different products under different curing conditions (i.e. changes in temperature, pressure, stoichiometry), without the need of isolating large quantities which are required by other more conventional characterization techniques.

Acknowledgment. Gratitude is extended to D. Dunn for the HPLC measurements and Dr. M. Gilbert and Prof. J. Bornstein for their assistance in the model compound syntheses. This is publication no. 347 from the Barnett Institute.

Registry No. MGEBA, 117341-10-3; ADS, 7019-01-4; I, 117341-11-4; II, 117341-12-5; III, 117341-13-6; IV, 117341-14-7; V, 117341-15-8.

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