

SUPPLEMENTAL INFORMATION

Py-GC/MS and MALDI-TOF/TOF CID Study of
Polyphenylsulfone Fragmentation Reactions

Sparkle T. Ellison¹, Anthony P. Gies^{2}, David M. Hercules², and Stephen L. Morgan¹*

¹Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC 29208

²Department of Chemistry, Vanderbilt University, Nashville, TN 37235

E-mail: A.Gies@Vanderbilt.edu

Macromolecules: April 14, 2009

TITLE RUNNING HEAD: Py-GC/MS and MALDI-TOF/TOF CID Study of PPSF.

CORRESPONDING AUTHOR FOOTNOTE: Address reprint requests to Anthony P. Gies,
Department of Chemistry, Vanderbilt University, 7330 Stevenson Center, Nashville, TN 37235.

Telephone: (615) 343-5980. E-mail: A.Gies@Vanderbilt.edu

DISSCUSSION

Figures S1-S3 display head-to-tail comparisons of the mass spectra for questionable species with the mass spectrum of their library match as well as the quality of the match. The peak intensity for the isotopes is in accordance with published values for C and S.¹ For instance, diphenyl disulfide, Figure S1, has 12 carbons and 2 sulfurs. Carbon is an “A + 1” isotopic pattern. For twelve carbons, A + 1 should be 13.2 % of the A. For diphenyl disulfide, A + 1 should be ~8% of the base peak (m/z = 109) in the mass spectrum. Sulfur, however, is an “A + 2” isotopic pattern. For two sulfurs, the A + 2 should be 8.8 % of the A. For diphenyl disulfide, A + 2 should be ~5 % of the base peak (m/z = 109) in the mass spectrum to fulfill this requirement. The same type of patterns can be fitted for the other two suspect species in Figures S2 and S3.

Reference:

- (1) McLafferty, F. W.; Tureček, F., Interpretation of Mass Spectra. In 4th ed.; University Science Books: Sausalito, CA, 1993; pp 19-34.

FIGURE CAPTIONS:

Figure S1. Head-to-head electron ionization fragmentation spectrum comparison of species 1-14 and diphenyl disulfide (94 % library match), obtain by Py-GC/MS and identified using NIST 98 software.

Figure S2. Head-to-head electron ionization fragmentation spectrum comparison of species 1-10 and diphenyl sulfide (98 % library match), obtain by Py-GC/MS and identified using NIST 98 software.

Figure S3. Head-to-head electron ionization fragmentation spectrum comparison of species 1-12 and dibenzothiophene (95 % library match), obtain by Py-GC/MS and identified using NIST 98 software.

Figure S4. MALDI-TOF/TOF mass spectrum PPSF (collision gas pressure: 5×10^{-6} Torr); for 1409.3 Da precursor ion.

Figure S5. MALDI-TOF/TOF mass spectrum PPSF (collision gas pressure: 5×10^{-6} Torr); for 1809.4 Da precursor ion.

Figure S6. Cropped MALDI-TOF/TOF mass spectrum PPSF (collision gas pressure: 5×10^{-6} Torr); for 1809.4 Da precursor ion.

Figure S1.

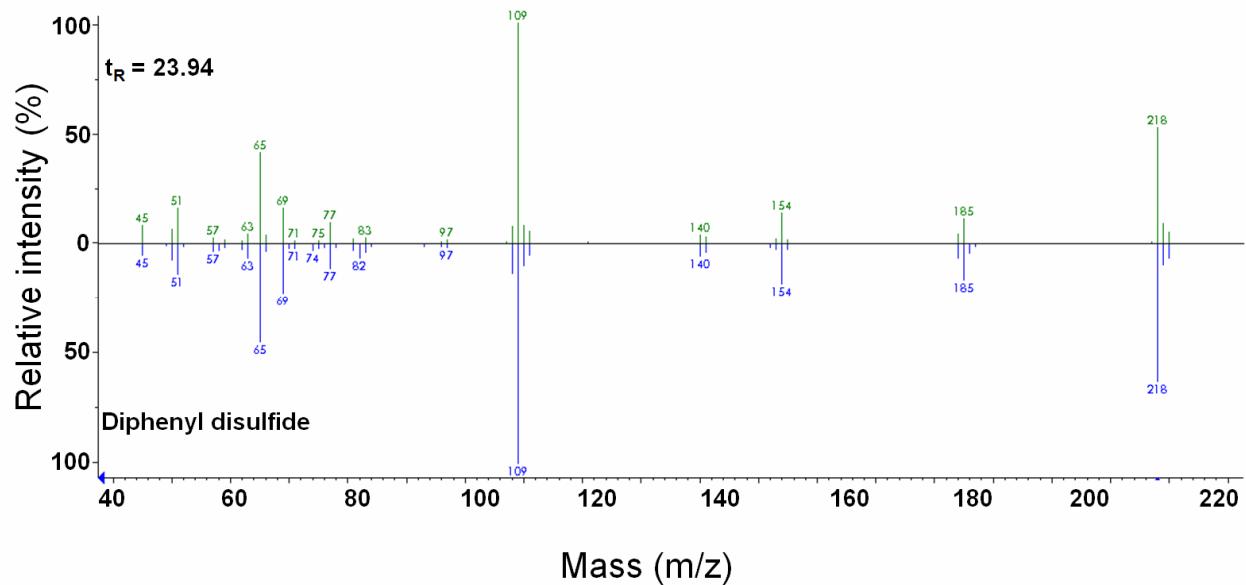


Figure S2.

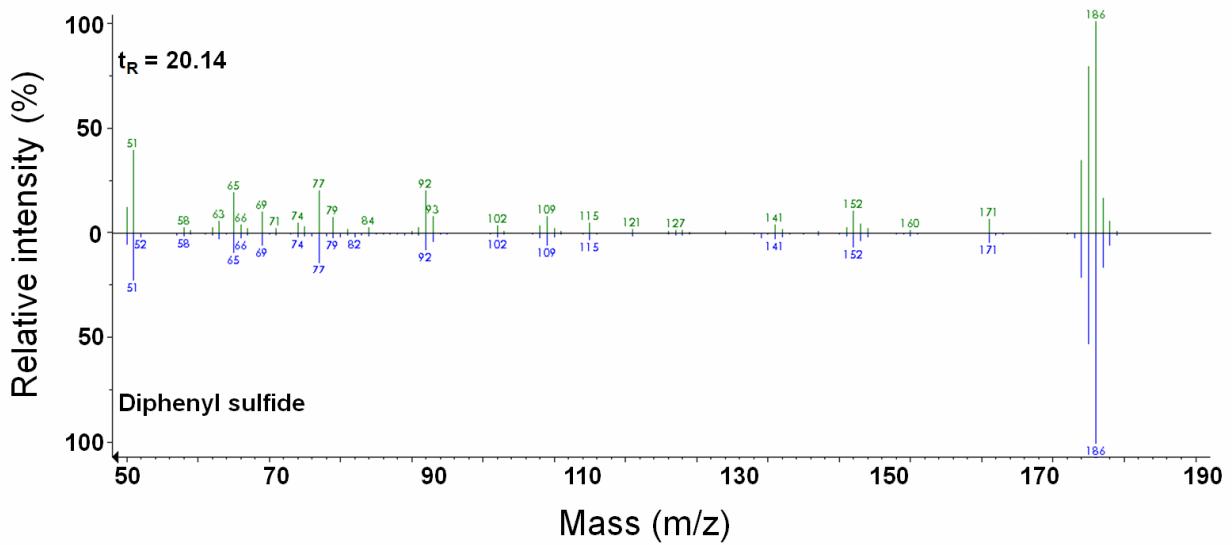


Figure S3.

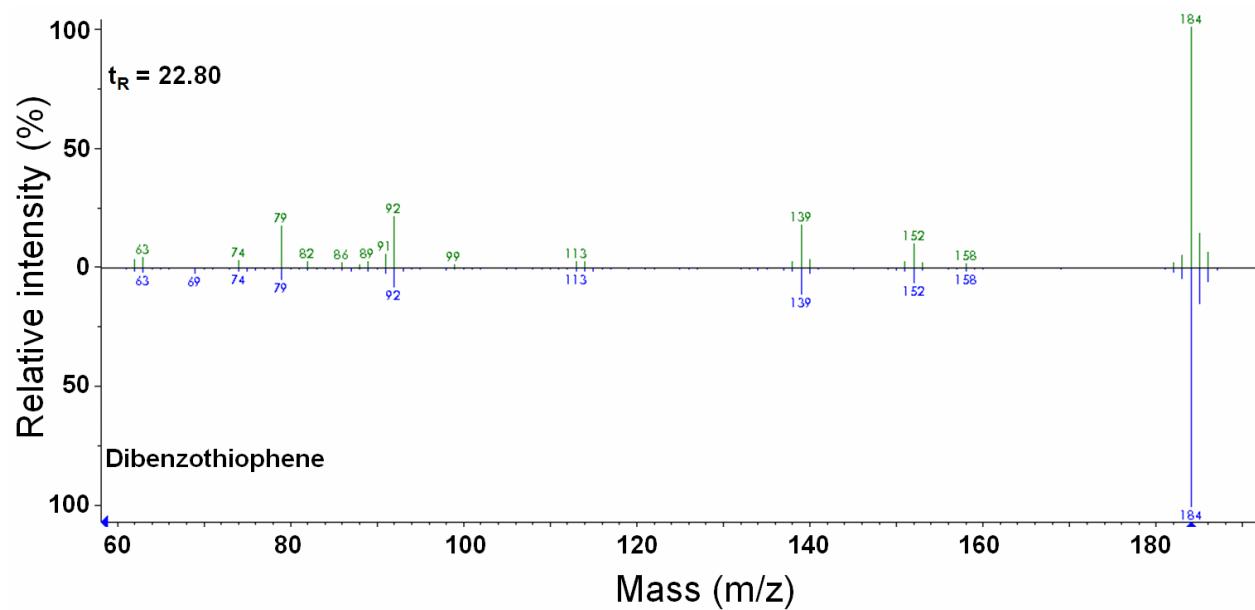


Figure S4.

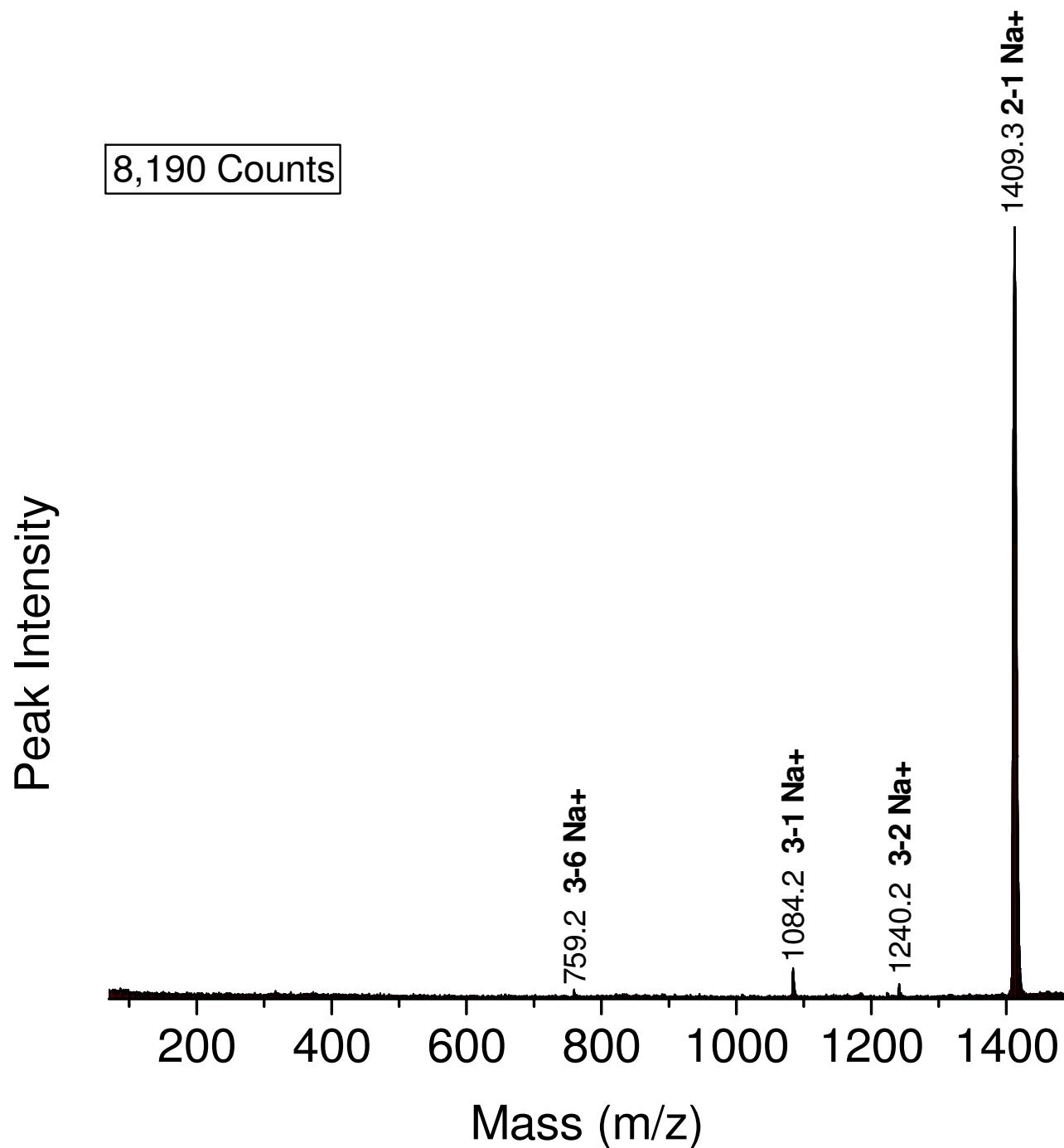


Figure S5.

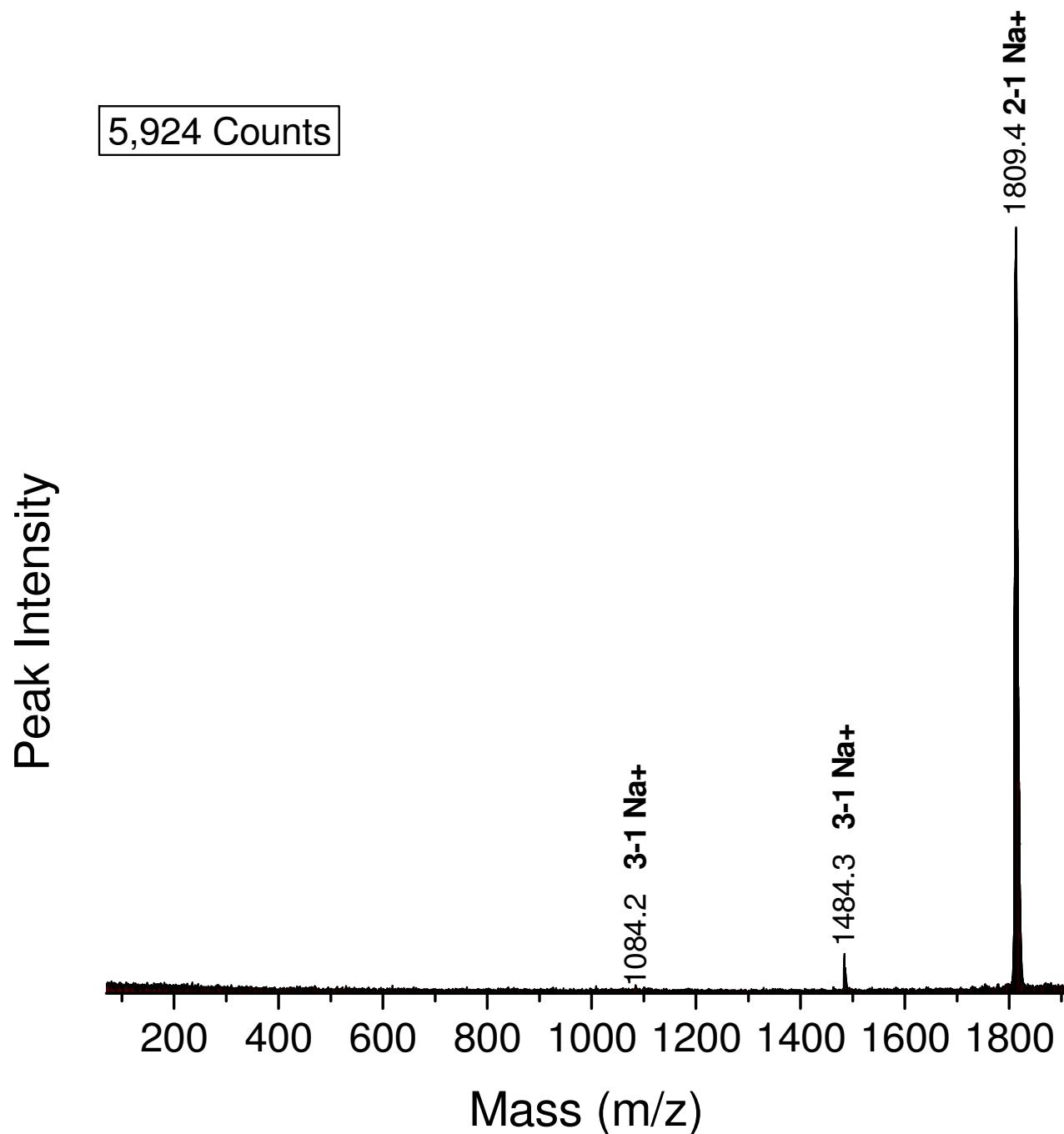


Figure S6.

