

Modeling the Effects of O-sulfonation on the CID of Serine

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We present the results of direct dynamics simulations and DFT calculations aimed at elucidating the effect of O-sulfonation on the collision induced dissociation for serine. Towards this end, direct dynamics simulations of both serine and sulfoserine were performed at multiple collision energies and theoretical mass spectra obtained. Comparisons to experimental results are favorable for both systems. Peaks related to the sulfo group are identified and the reaction dynamics explored. In particular, three significant peaks (m/z 106, 88, and 81) seen in the theoretical mass spectrum directly related to the sulfo group are analyzed as well as major peaks shared by both systems. Our analysis shows that the m/z 106 peaks result from intramolecular rearrangements, intermolecular proton transfer among complexes composed of initial fragmentation products, and at high energy side-chain fragmentation. The m/z 88 peak was found to contain multiple constitutional isomers, including a previously unconsidered, low energy structure. It was also seen that the RM1 semi empirical method was not able to obtain all of the major peaks seen in experiment for sulfoserine. In contrast, PM6 did obtain all major experimental peaks.

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Supporting Information: Modeling the Effects of *O*-sulfonation on the CID of Serine

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S1 RM1 Results

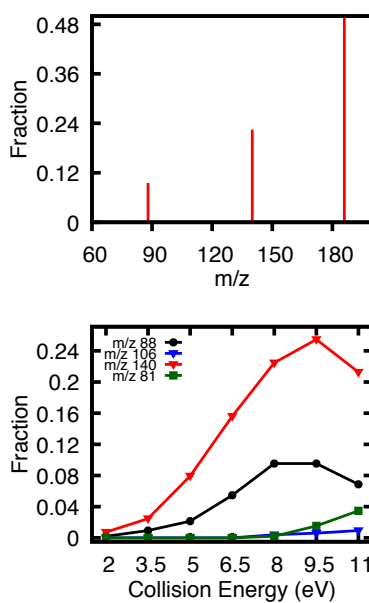


Figure S1: RM1 results analogous to the PM6 results shown in Figure 2 for sulfoserine.

S2 Energy Transfer Distributions

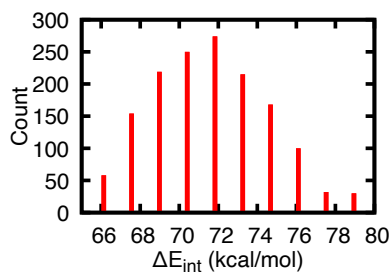


Figure S2: An example distribution for the change in internal energy, ΔE_{int} , for sulfoferine resulting from $E_i=3.5$ eV collisions with argonne.

Table S1: The average (standard deviation) for the change in internal energy, ΔE_{int} , change in vibrational energy, ΔE_{vib} , and change in rotational energy, ΔE_{rot} , for sulfoferine following collision with argonne for various collision energies, E_i . Collision energies are given in eV while all other values are in kcal/mol.

E_i	ΔE_{int}	ΔE_{vib}	ΔE_{rot}
2.0	40.2 (1.9)	34.7 (4.5)	5.5 (4.9)
3.5	71.5 (3.5)	63.9 (7.2)	7.6 (7.4)
5.0	103.5 (5.5)	95.4 (10.7)	8.1 (9.4)
6.5	136.1 (7.9)	128.7 (14.3)	7.4 (10.7)
8.0	168.8 (12.2)	162.9 (18.0)	5.9 (11.0)
9.5	197.0 (42.6)	193.2 (43.9)	3.7 (9.8)
11.0	219.1 (72.7)	216.3 (73.0)	2.7 (8.4)

S3 ACKNOWLEDGEMENTS

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