Naval Research Laboratory

Washington, DC 20375-5320

NRL/MR/6394--19-9918

IR Absorption Spectra for Nitrosamines Calculated Using Density Functional Theory

Samuel G. Lambrakos

Center for Computational Materials Science

Materials Science and Technology Division

L. Massa

Hunter College

New York City, NY

S. Wallace

Lehman College
The Bronx, NY

September 27, 2019

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	**2. REPORT TYPE**	**3. DATES COVERED** *(From - To)*
27-09-2019	NRL Memorandum Report	

4. TITLE AND SUBTITLE

IR Absorption Spectra for Nitrosamines Calculated Using Density Functional Theory

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

Samuel G. Lambrakos, L. Massa*, and S. Wallace**

5d. PROJECT NUMBER
63-1G69-09

5e. TASK NUMBER

5f. WORK UNIT NUMBER
1G69

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Naval Research Laboratory
4555 Overlook Avenue, SW
Washington, DC 20375-5320

8. PERFORMING ORGANIZATION REPORT NUMBER

NRL/MR/6394--19-9918

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Office of Naval Research
One Liberty Center
875 North Randolph Street, Suite 1425
Arlington, VA 22203-1995

10. SPONSOR / MONITOR'S ACRONYM(S)

ONR

11. SPONSOR / MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT

DISTRIBUTION STATEMENT A: Approved for public release distribution is unlimited.

13. SUPPLEMENTARY NOTES

*Hunter College, 695 Park Ave, New York, NY 10065-5024
**Lehman College, 250 Bedford Park Blvd W, The Bronx, NY 10468-1527

14. ABSTRACT

Vibration absorption spectra for nitrosamines are calculated using density function theory (DFT). Absorption spectra within the IR range of frequencies for electromagnetic-wave excitation, calculated using DFT, can be interpreted with respect to molecular structure. DFT calculated absorption spectra corresponding to vibration excitation states of these molecules in continuous solvent backgrounds can be correlated with additional information obtained from laboratory measurements. The DFT software GAUSSIAN was used for the calculations of excitation states presented here. This study provides proof of concept for using DFT-calculated spectra to construct templates, which are for spectral-feature comparison and thus detection of spectral-signature features associated with target materials.

15. SUBJECT TERMS

Density functional theory Absorption spectra
Spectral signature features

16. SECURITY CLASSIFICATION OF:			**17. LIMITATION OF ABSTRACT**	**18. NUMBER OF PAGES**	**19a. NAME OF RESPONSIBLE PERSON**
					Samuel G. Lambrakos
a. REPORT	**b. ABSTRACT**	**c. THIS PAGE**	Unclassified Unlimited	44	**19b. TELEPHONE NUMBER** *(include area code)*
Unclassified Unlimited	Unclassified Unlimited	Unclassified Unlimited			(202) 767-2601

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std. Z39.18

This page intentionally left blank.

Contents

This page intentionally left blank.

Introduction

Identification of unknown materials using infrared (IR) spectroscopy is by comparison of measured spectra with reference spectra of known materials. Such comparison entails correlation of measured spectra with spectra within a database of known molecular structures [1] using signal processing algorithms [2]. Specifically, signature structure within a measured spectrum is filtered using spectral templates having patterns associated with known materials. References [3-7] describes algorithms for signal processing of measured spectra for correlation with reference spectra within a database. For detection in practice, measured spectra can be correlated with different databases, providing complementary information, which includes different types of information concerning interpretation of spectral features. Typically, databases of spectra consist of spectroscopic measurements, which are obtained using different types of spectroscopies, based on transmission and reflection [8,9]. Presented in this report are calculations of IR absorption spectra of molecular structures using density functional theory (DFT) and associated software technology (see reference [10] for the case of pure water), which provides complementary information to that obtained from laboratory measurement.

This report presents DFT calculated IR spectra for *N*-nitrosodimethylamine ($C_2H_6N_2O$), *N*-nitrosodiethylamine ($C_4H_{10}N_2O$), *N*-nitrosodipropylamine ($C_6H_{14}N_2O$), *N*-nitrsopyrrolidine ($C_4H_8N_2O$), *N*-nitrosomethylethylamine ($C_3H_8N_2O$) and *N*-nitrosodibutylamine ($C_8H_{18}N_2O$) of isolated molecules and molecules within different solvent backgrounds. The properties of these molecules are of major importance for monitoring and detection of nitrosamines, which are among toxic and carcinogenic contaminants commonly found in the environment [11-16]. The detection of these nitrosamines, especially in the presence of water, is of particular interest. Specifically, IR spectral signatures, i.e., fingerprint spectra, can be correlated with the presence of target molecules (see references [17-19]). A previous study [17] introduced and demonstrated the concept of using DFT calculated IR spectra. The concept of database enhancement using DFT calculated spectra is independent of specific types of detection technology. Methodologies for comparison of detected spectral features with database spectra represent a separate problem.

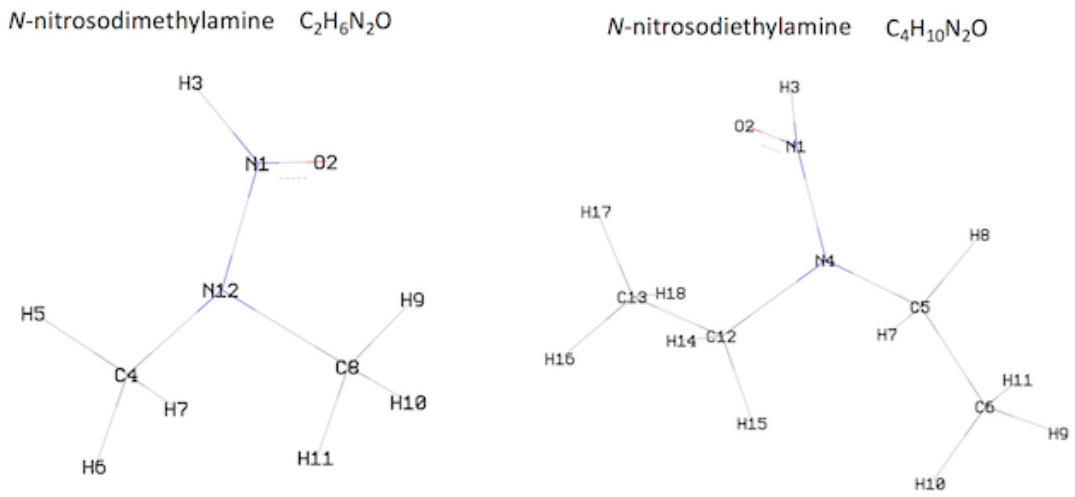
Given in reference [17] is a description of the formalism underlying DFT calculation of IR spectra, and implementation of this formalism in terms of the DFT software GAUSSIAN16. The commercial computer program GAUSSIAN16 (G16) is designed to compute the IR spectrum of a molecule, including the effect of a continuous solvent background [20, 22]. Second derivatives of the energy with respect to the Cartesian nuclear coordinates are calculated and subsequently changed to mass-weighted coordinates at the equilibrium geometry of the molecule. The IR spectrum is obtained from the ground state energy surface calculated in the Born-Oppenheimer approximation by solving the DFT Kohn-Sham equations [23-29]. The electronic density, the

Manuscript approved August 28, 2019.

potential energy *V,* and the equilibrium geometry are calculated. The details followed by Gaussian for IR analysis are given in references [22] and [28].

DFT Calculation of IR Spectra

Results of a computational investigation using DFT concerning $C_2H_6N_2O$, $C_4H_{10}N_2O$, $C_6H_{14}N_2O$, $C_4H_8N_2O$, $C_3H_8N_2O$ and $C_8H_{18}N_2O$ molecules in different solvent backgrounds are presented. These results include the ground-state energies for energy-minimized configuration of these molecules within different backgrounds, and their ground-state oscillation frequencies and IR intensities. For example, graphical representations of molecular geometries for stable molecules of $C_2H_6N_2O$, $C_4H_{10}N_2O$, $C_6H_{14}N_2O$, $C_4H_8N_2O$, $C_3H_8N_2O$ and $C_8H_{18}N_2O$ within a water background, are shown in Fig. (1). For these calculations, geometry-energy optimization and vibration analysis was effected using the computer program Gaussian 16 with the DFT chemical model B3LYP [29,30] and basis functions 6-311++g(3df,3pd) [31,32]. These basis functions designate the 6-311G basis set supplemented by diffuse functions, indicated by the sign ++, and polarization functions (df), having a set of d and f functions on heavy atoms [33]. Graphical representations of molecular geometries for stable molecules of $C_2H_6N_2O$, $C_4H_{10}N_2O$, $C_6H_{14}N_2O$, $C_4H_8N_2O$, $C_3H_8N_2O$ and $C_8H_{18}N_2O$ within a water background are shown in Fig. (1). Shown in Figs. (2) through (7) are IR spectra of these molecules. Values of the IR intensities as a function of frequency for these molecules within different backgrounds are given in Tables 1 through 6.



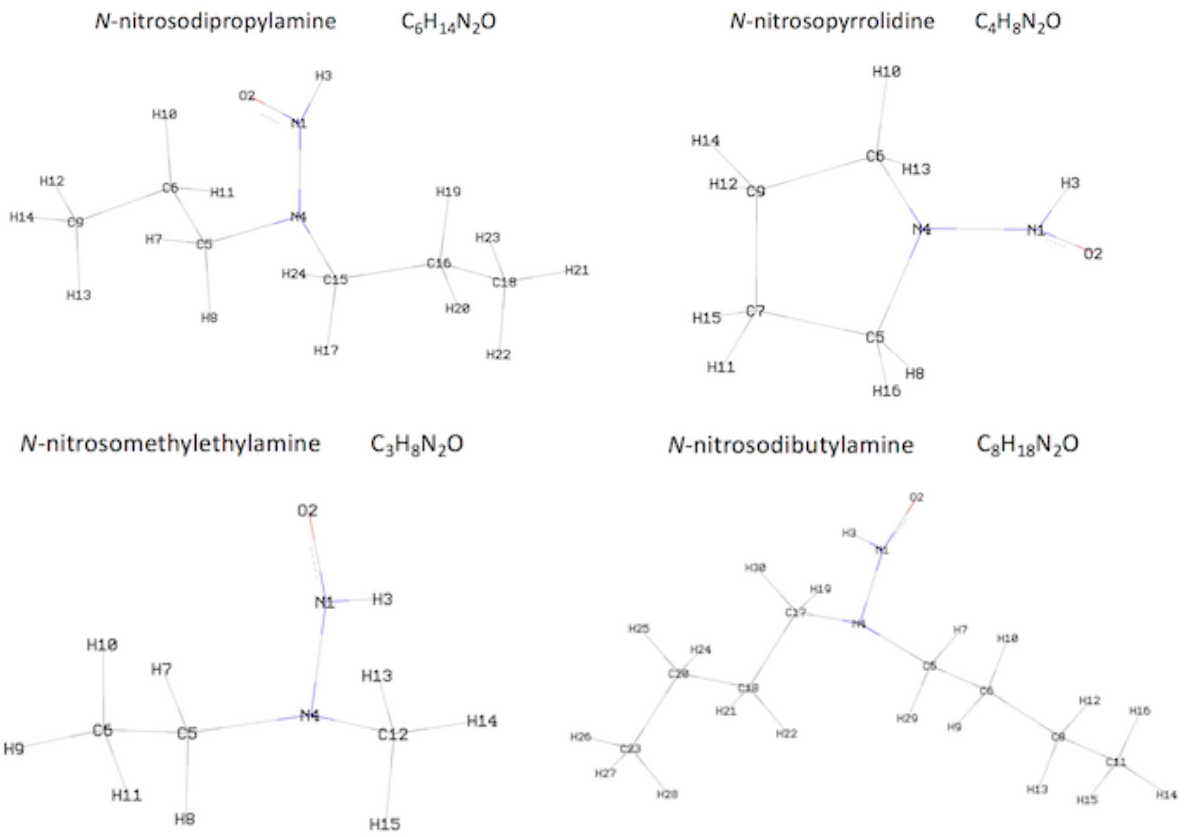


Figure 1. Molecular geometries for $C_2H_6N_2O$, $C_4H_{10}N_2O$, $C_6H_{14}N_2O$, $C_4H_8N_2O$, $C_3H_8N_2O$ and $C_8H_{18}N_2O$ in water background.

Discussion

The DFT calculated IR spectra calculated here should provide reasonable templates for filtering of IR spectral measurements associated with different types of detector schemes and complex spectral-signature backgrounds. In principle, these templates can be linear combinations of spectra given in the tables below, having adjustable weight coefficients of the component spectra, as well as correlation-lag parameters for adjustment of absorption-maxima frequencies. The DFT calculated IR spectra given here are to be adopted as complementary database information concerning spectral features to that obtained from laboratory measurement.

Conclusion

The DFT calculated absorption spectra given here provide information concerning molecular level dielectric response structure. The calculations of IR spectra associated with $C_2H_6N_2O$, $C_4H_{10}N_2O$, $C_6H_{14}N_2O$ and $C_4H_8N_2O$ molecules within different backgrounds using DFT are meant to serve as reasonable estimates of molecular level response characteristics, providing interpretation of dielectric response features for comparison with experimental

measurements. Specifically, the DFT calculated IR spectra calculated here should provide reasonable templates for filtering of IR spectral measurements associated with different types of detector schemes.

Figure 2. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosodimethylamine ($C_2H_6N_2O$)

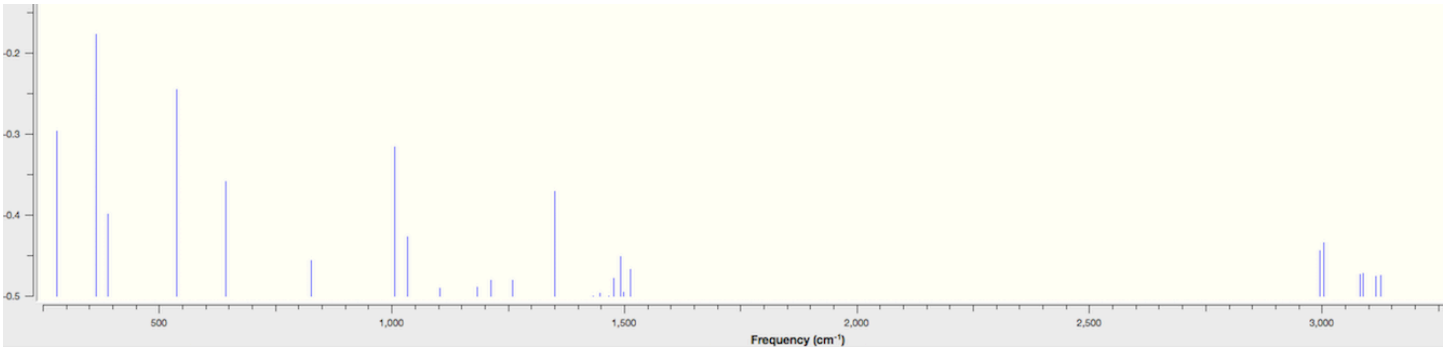


Figure 2A. *N*-nitrosodimethylamine ($C_2H_6N_2O$), Isolated Molecule (Energy: -265.141096 au)

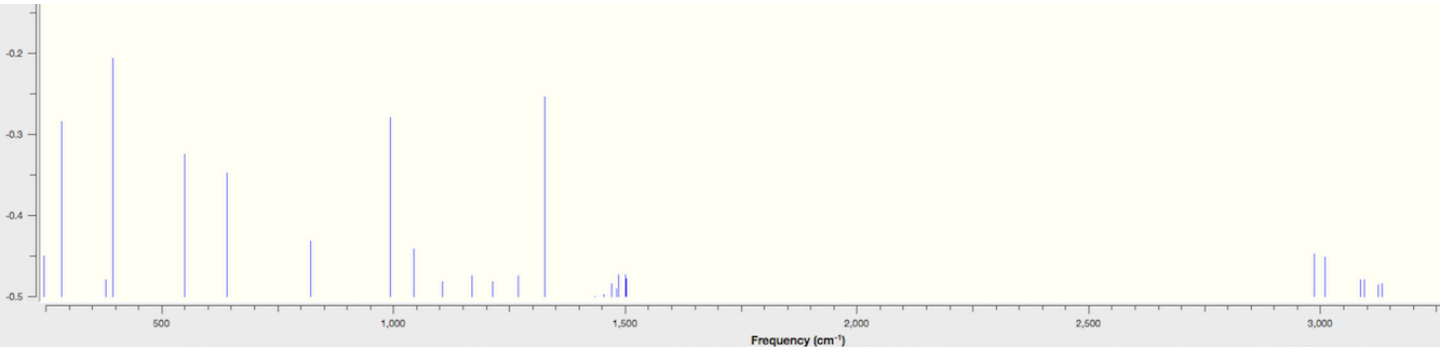


Figure 2B. *N*-nitrosodimethylamine ($C_2H_6N_2O$), DMSO Background (Energy: -265.1486773 au)

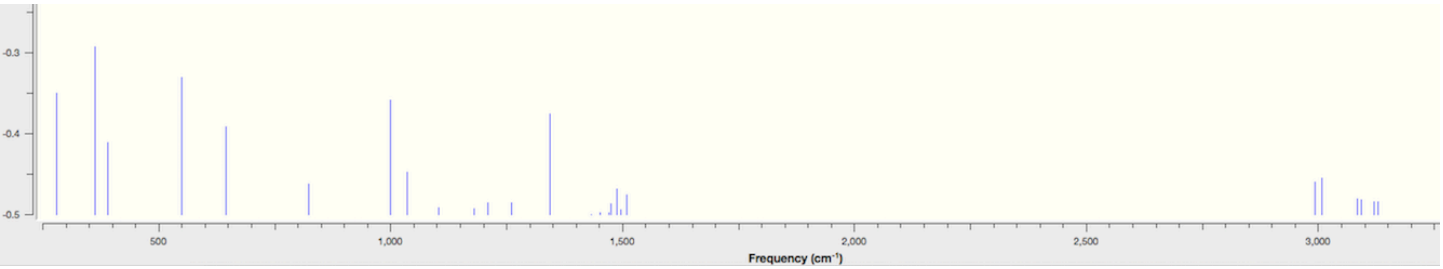


Figure 2C. *N*-nitrosodimethylamine ($C_2H_6N_2O$), Toluene Background (Energy: -265.1445304 au)

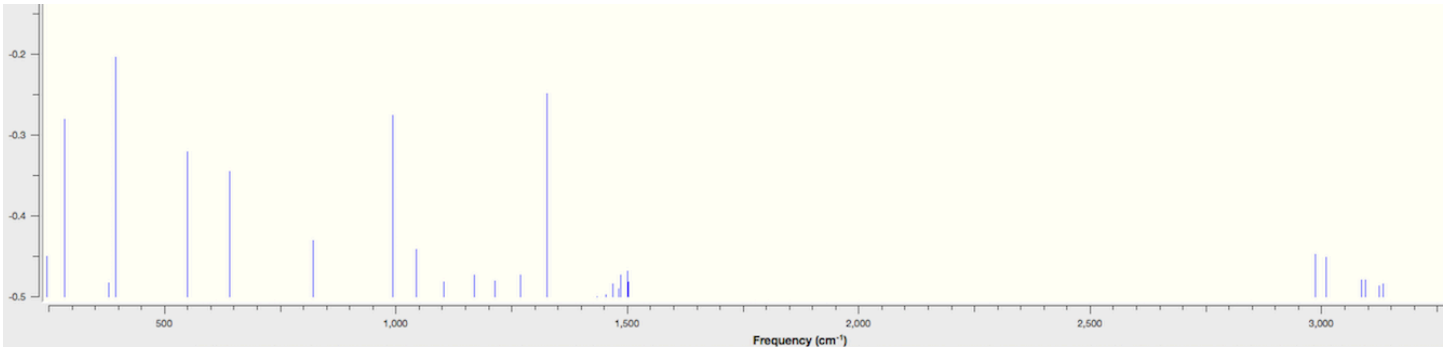


Figure 2D. *N*-nitrosodimethylamine ($C_2H_6N_2O$), Water Background (Energy: -265.1488006 au)

Figure 3. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosodiethylamine ($C_4H_{10}N_2O$)

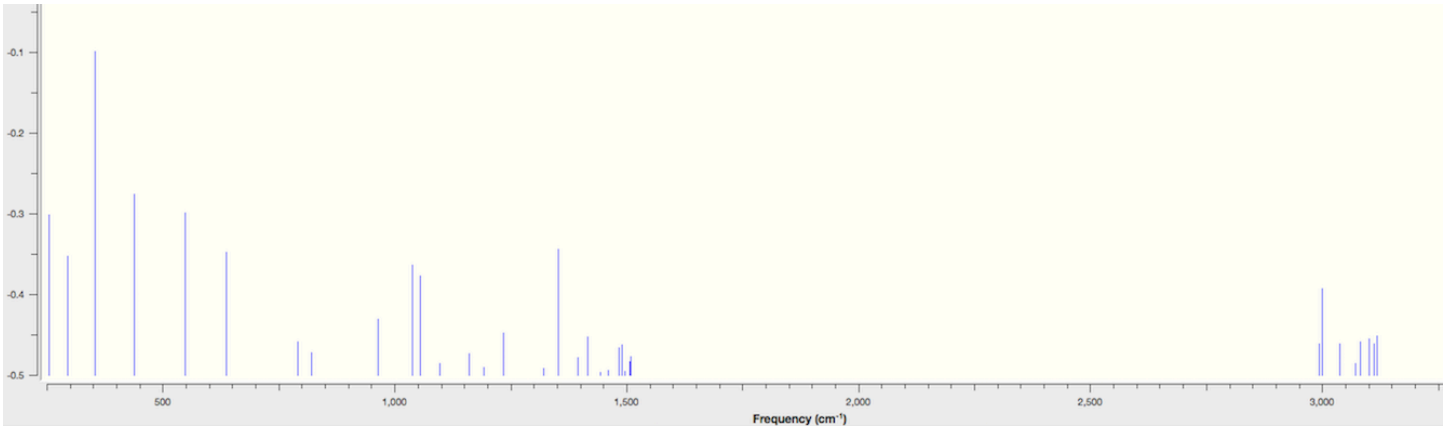


Figure 3A. *N*-nitrosodiethylamine ($C_4H_{10}N_2O$), Isolated Molecule (Energy: -343.7956752 au)

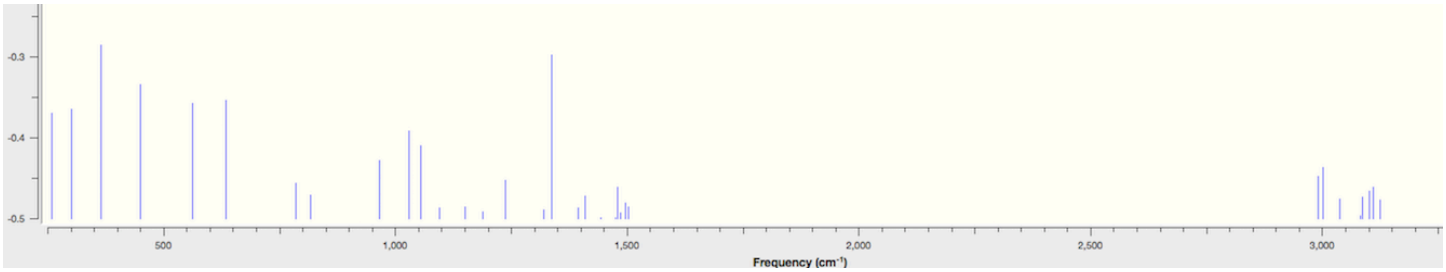


Figure 3B. *N*-nitrosodiethylamine ($C_4H_{10}N_2O$), DMSO Background (Energy: -343.8050967 au)

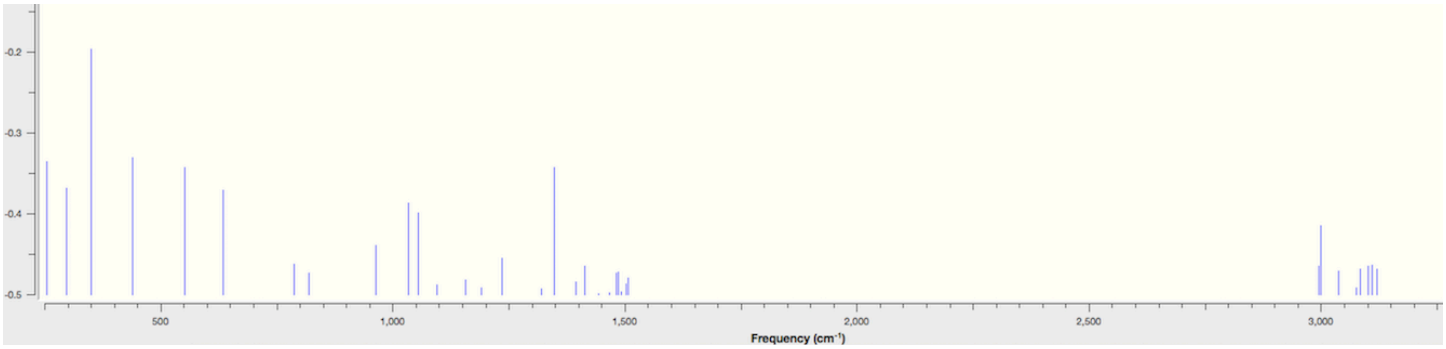


Figure 3C. *N*-nitrosodiethylamine ($C_4H_{10}N_2O$), Toluene Background (Energy: -343.8013687 au)

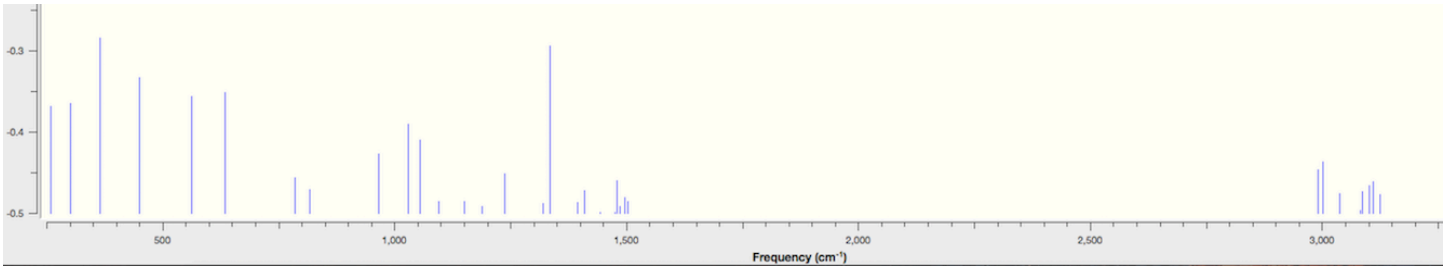


Figure 3D. *N*-nitrosodiethylamine ($C_4H_{10}N_2O$), Water Background (Energy: -343.8052031 au)

Figure 4. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosodipropylamine ($C_6H_{14}N_2O$)

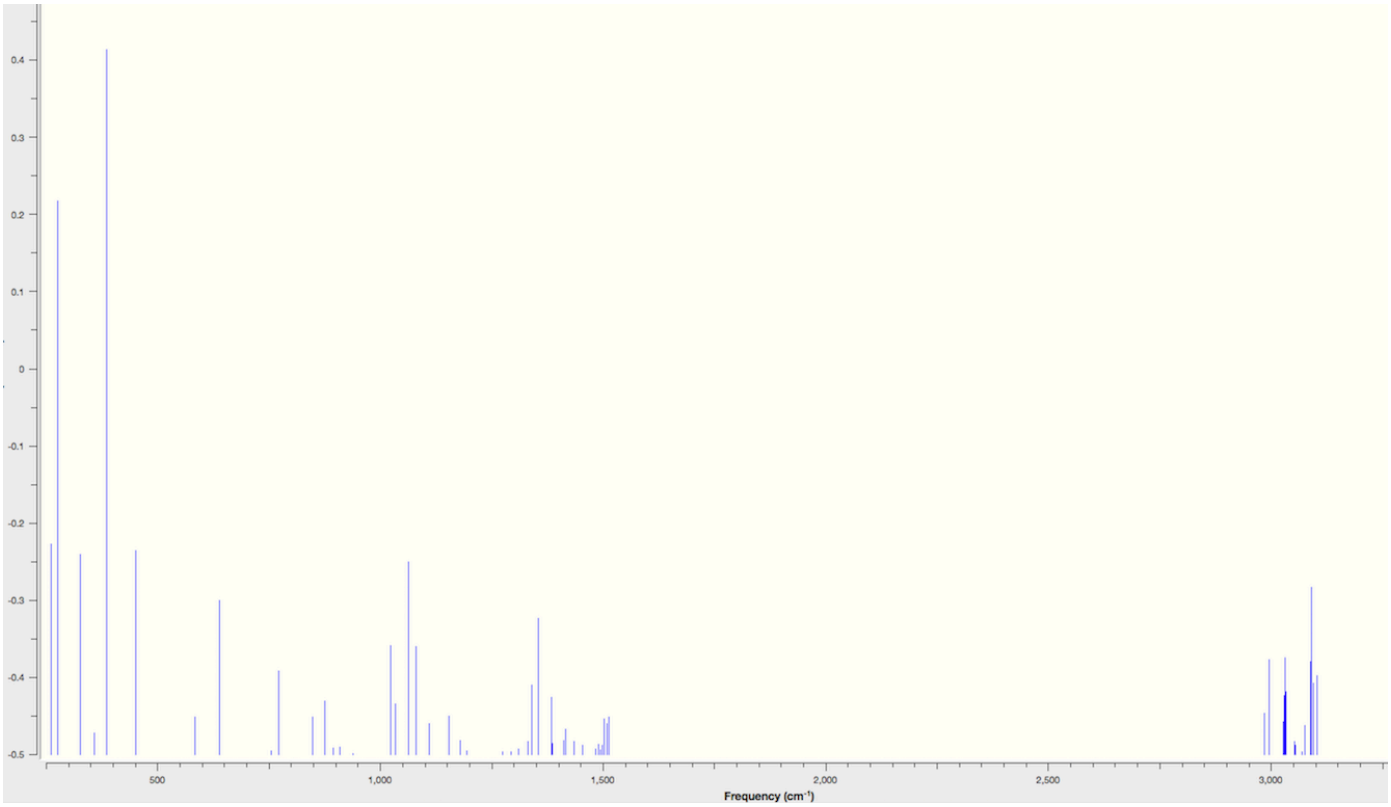


Figure 4A. *N*-nitrosodipropylamine ($C_6H_{14}N_2O$), Isolated Molecule (Energy: -304.4705191 au)

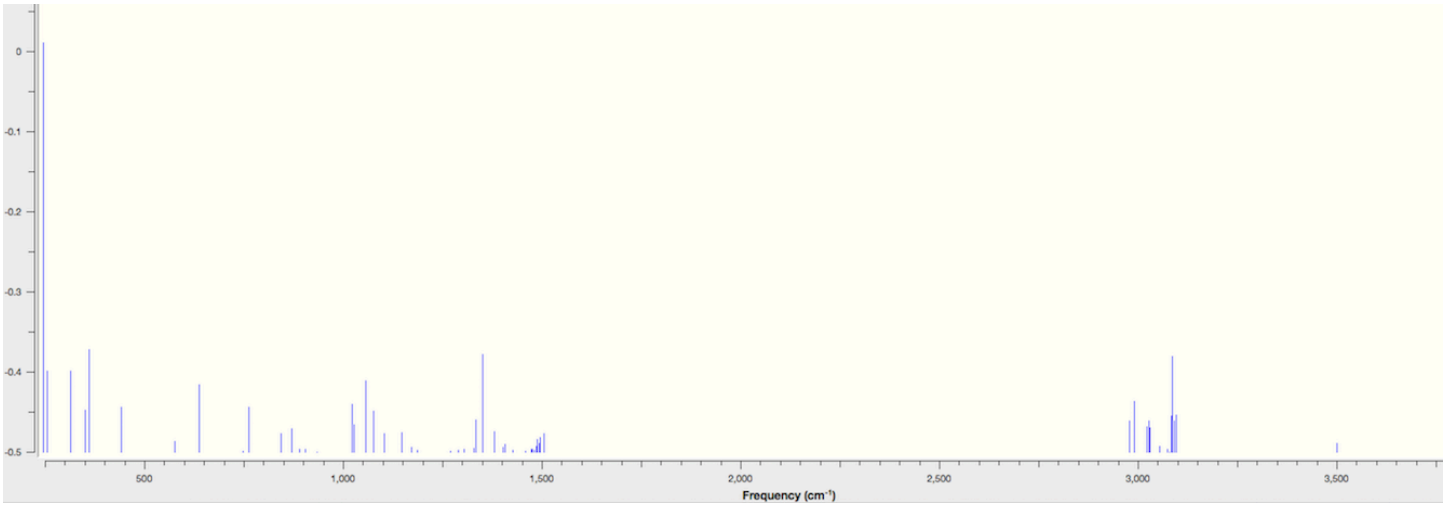


Figure 4B. *N*-nitrosodipropylamine ($C_6H_{14}N_2O$), DMSO Background (Energy: -304.4776376 au)

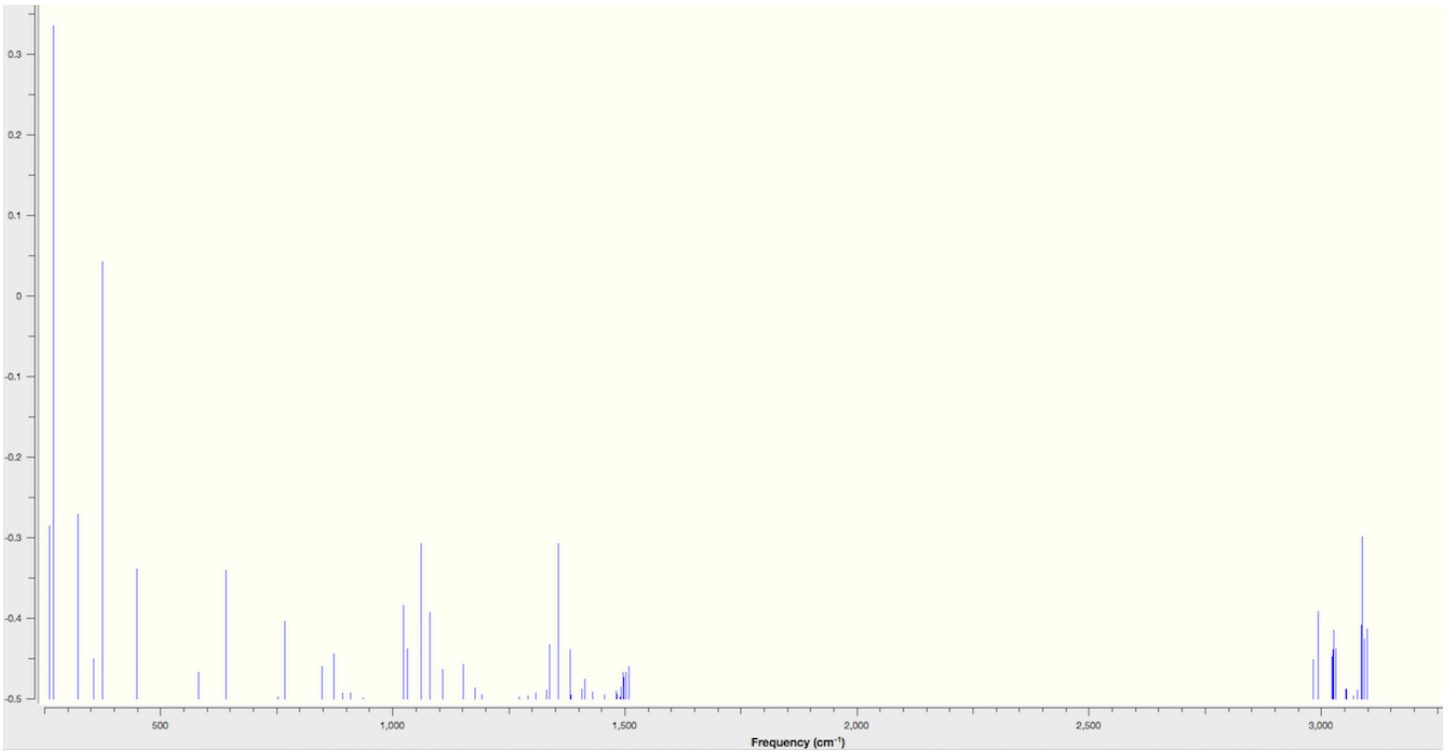


Figure 4C. *N*-nitrosodipropylamine ($C_6H_{14}N_2O$), Toluene Background (Energy: -304.4737994 au)

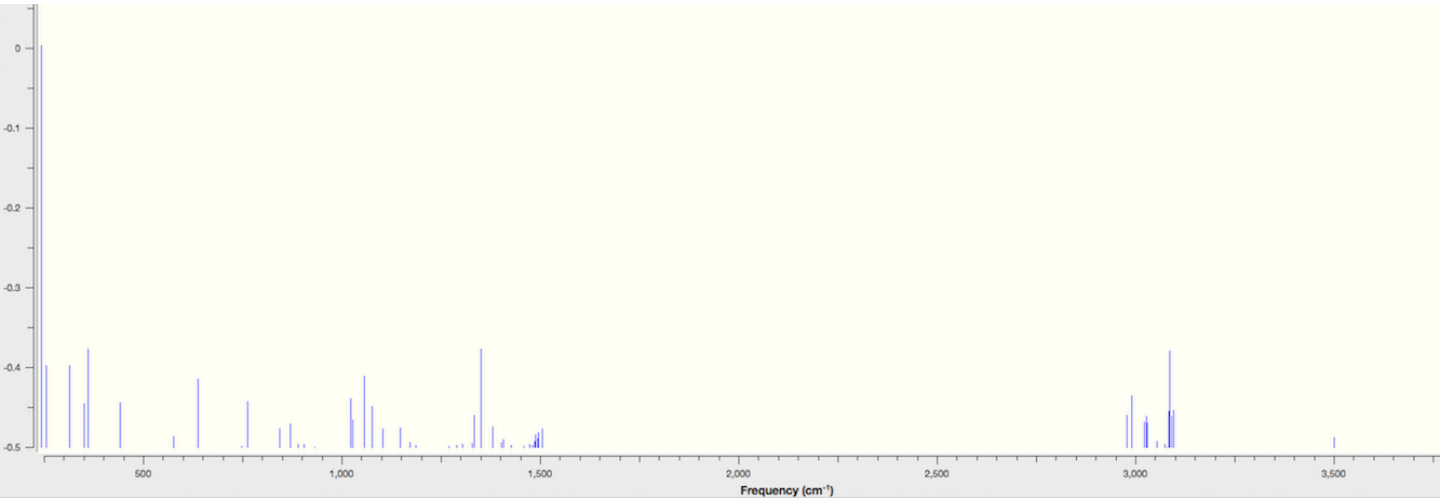


Figure 4D. *N*-nitrosodipropylamine ($C_6H_{14}N_2O$), Water Background (Energy: -304.4777479 au)

Figure 5. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosopyrrolidine ($C_4H_8N_2O$)

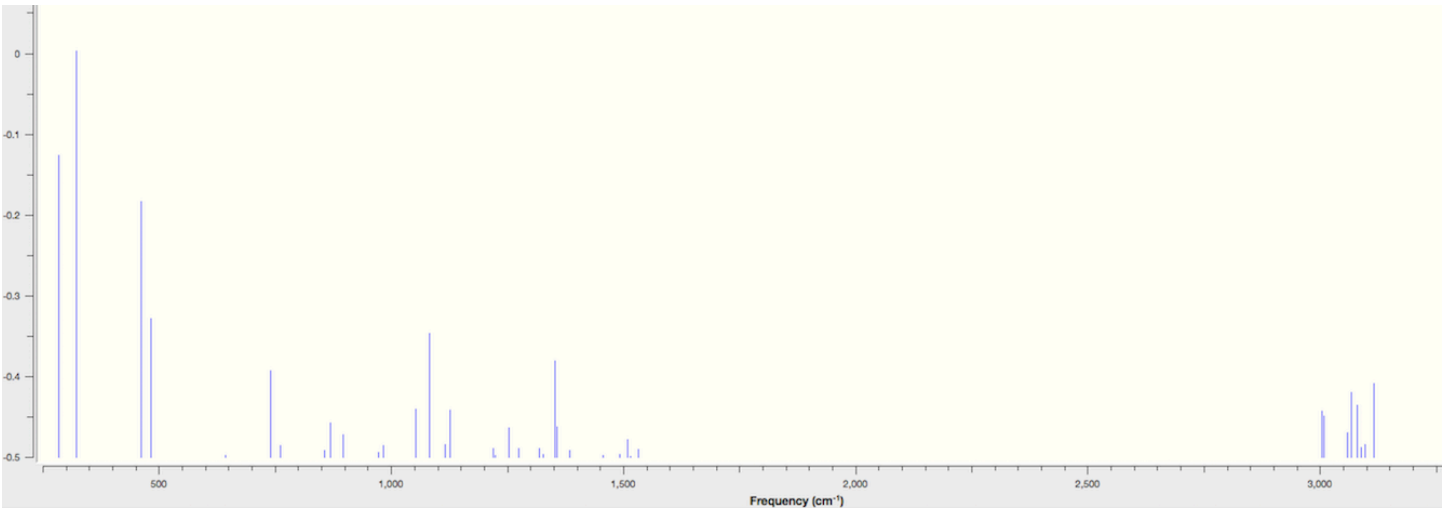


Figure 5A. *N*-nitrosopyrrolidine ($C_4H_8N_2O$), Isolated Molecule (Energy: -422.4501449 au)

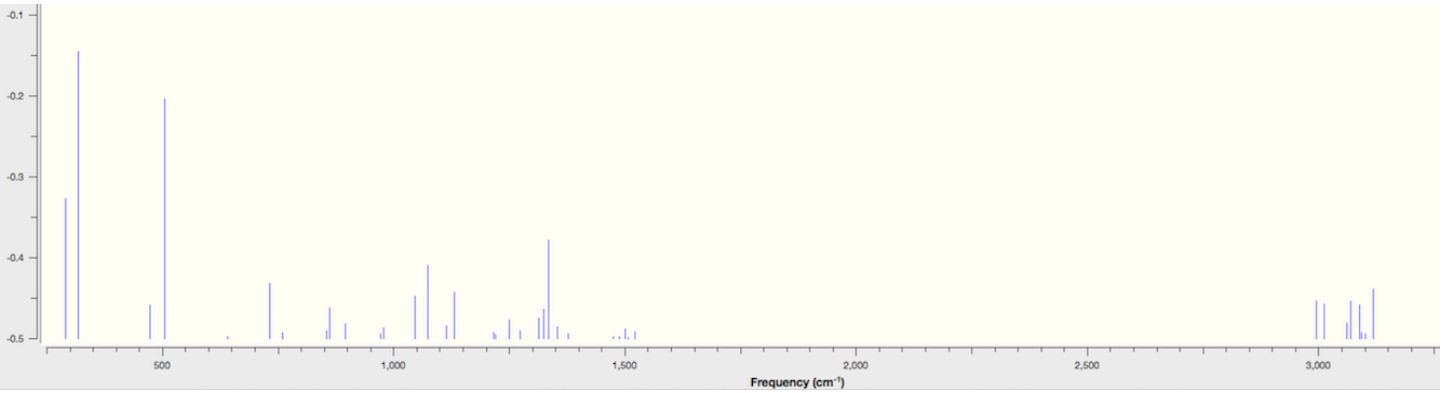


Figure 5B. *N*-nitrosopyrrolidine ($C_4H_8N_2O$), DMSO Background (Energy: -422.4596433 au)

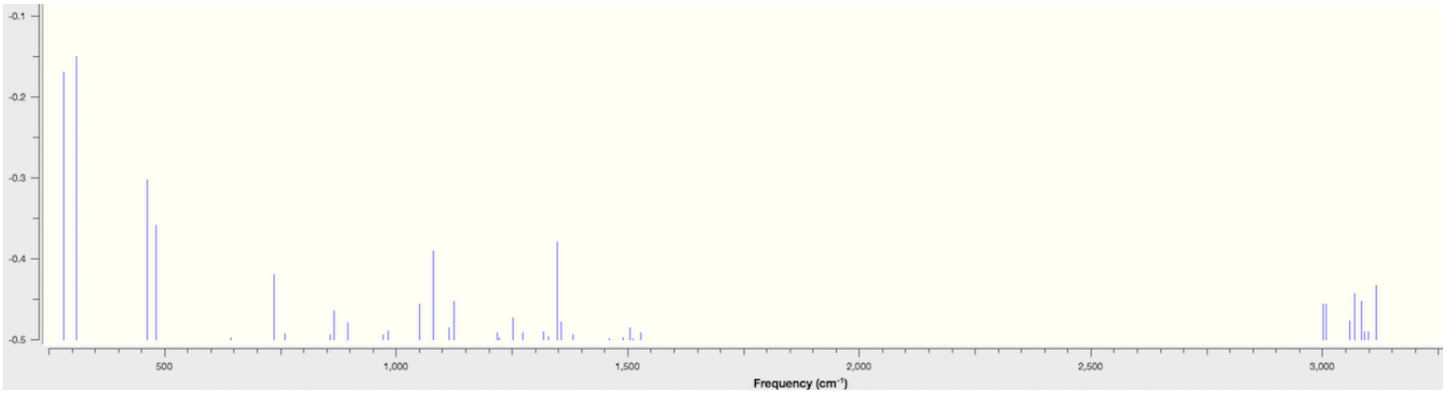


Figure 5C. *N*-nitrosopyrrolidine ($C_4H_8N_2O$), Toluene Background (Energy: -422.4560395 au)

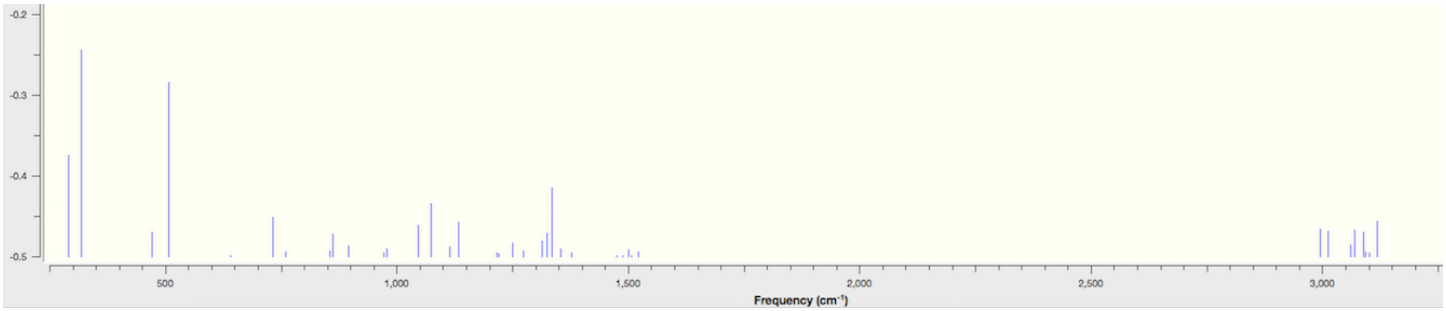


Figure 5D. *N*-nitrosopyrrolidine ($C_4H_8N_2O$), Water Background (Energy: -422.4597461 au)

Figure 6. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosomethylethylamine ($C_3H_8N_2O$)

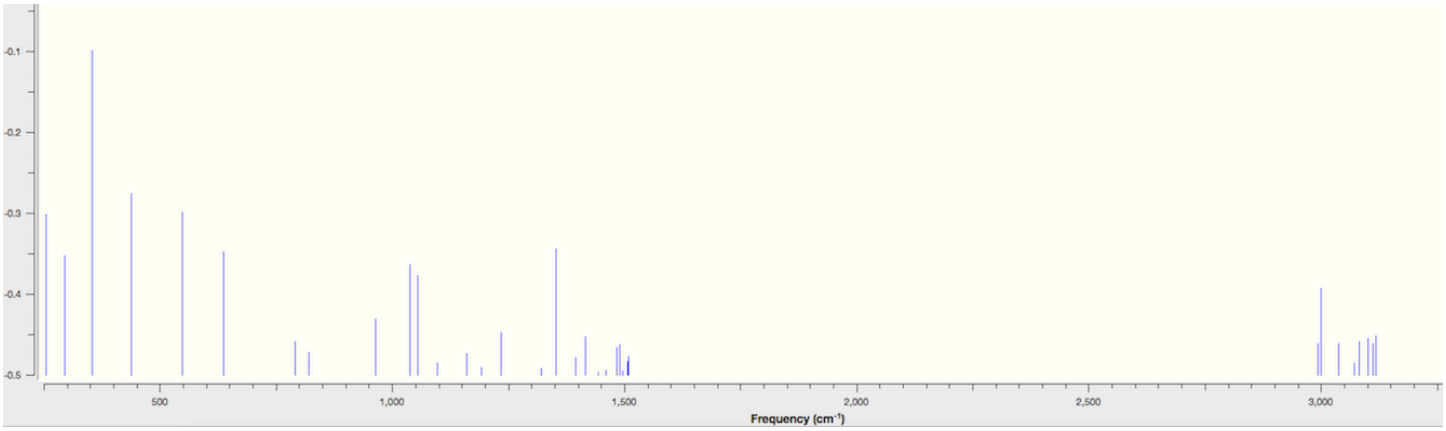


Figure 6A. *N*-nitrosomethylethylamine ($C_3H_8N_2O$), Isolated Molecule (Energy: -342.5843252 au)

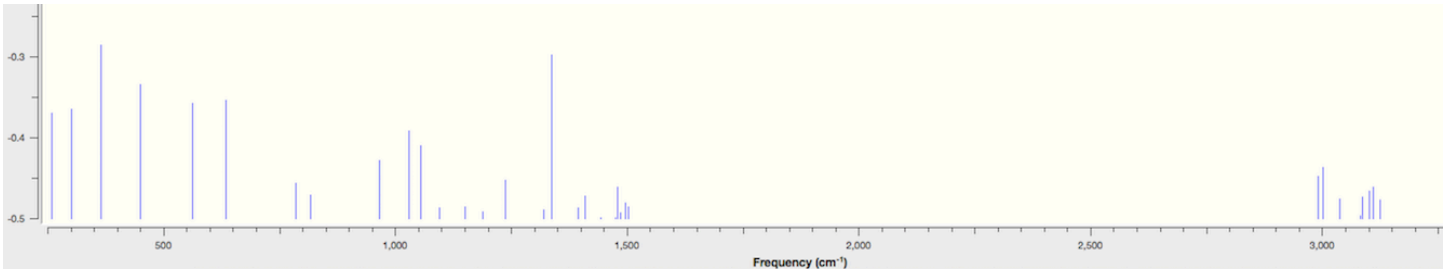


Figure 6B. *N*-nitrosomethylethylamine ($C_3H_8N_2O$), DMSO Background (Energy: -342.5913857 au)

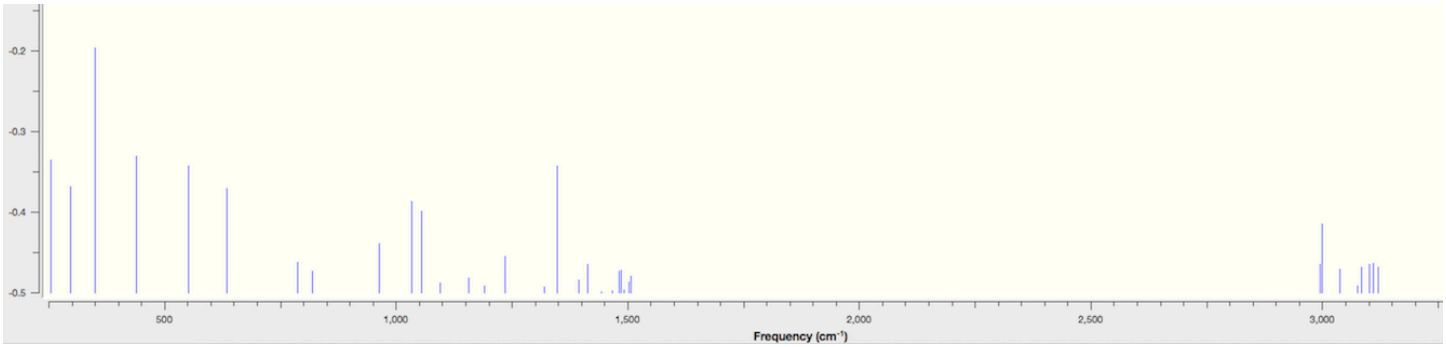


Figure 6C. *N*-nitrosomethylethylamine ($C_3H_8N_2O$), Toluene Background (Energy: -342.5876242 au)

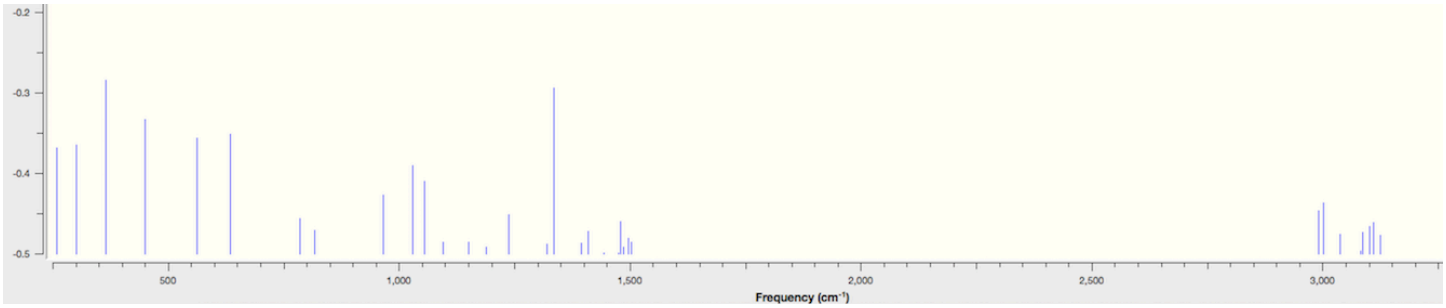


Figure 6D. *N*-nitrosomethylethylamine ($C_3H_8N_2O$), Water Background (Energy: -342.5914929 au)

Figure 7. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosodibutylamine ($C_8H_{18}N_2O$)

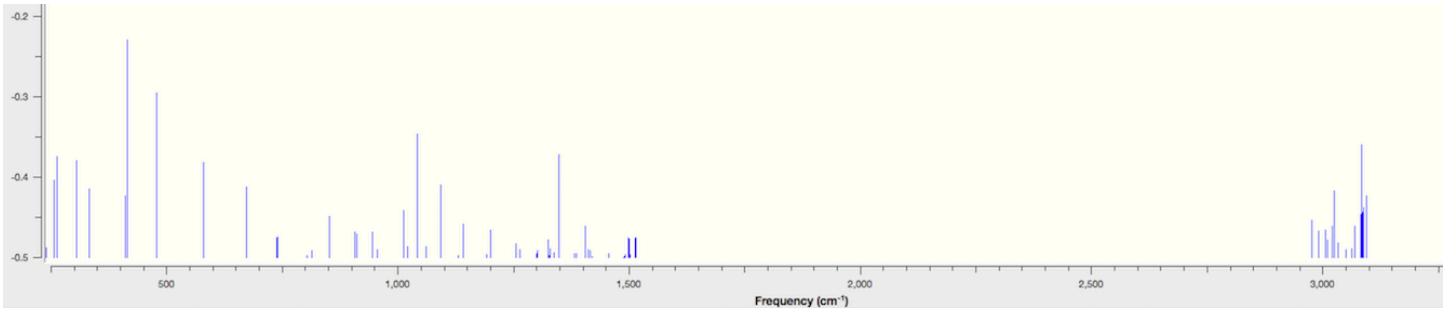


Figure 7A. *N*-nitrosodibutylamine ($C_8H_{18}N_2O$), Isolated Molecule (Energy: -501.106478 au)

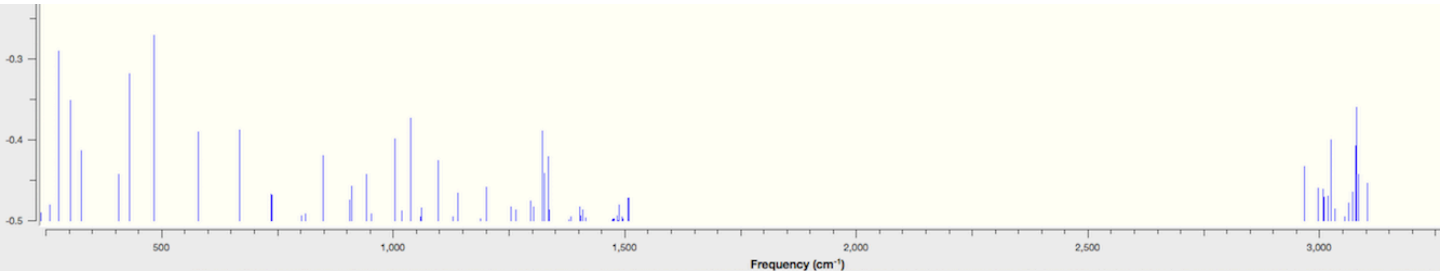


Figure 7B. *N*-nitrosodibutylamine ($C_8H_{18}N_2O$), DMSO Background (Energy: -501.11395 au)

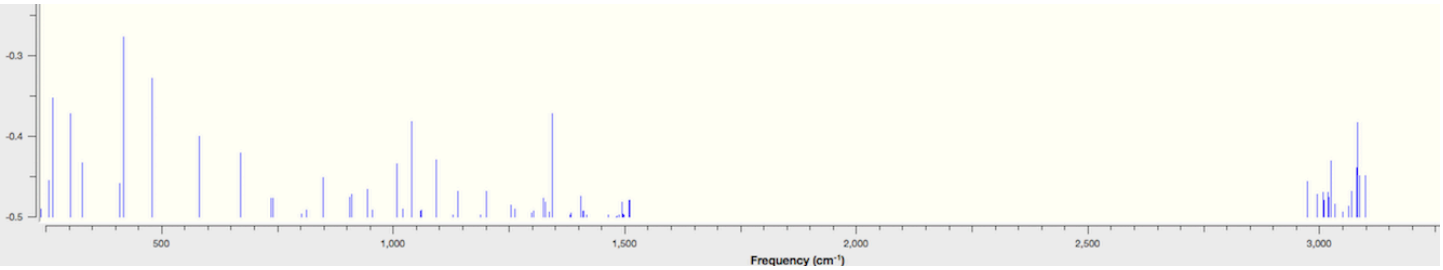


Figure 7C. *N*-nitrosodibutylamine ($C_8H_{18}N_2O$), Toluene Background (Energy: -501.109886 au)

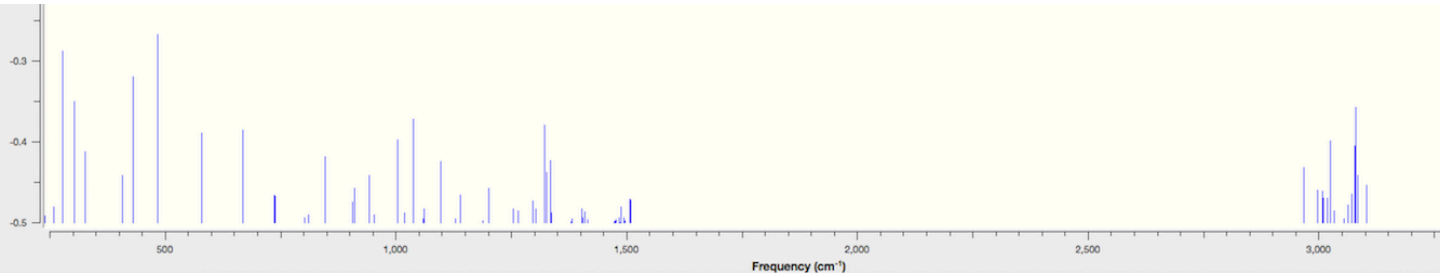


Figure 7D. *N*-nitrosodibutylamine ($C_8H_{18}N_2O$), Water Background (Energy: -501.11408 au)

Table 1. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosodimethylamine ($C_2H_6N_2O$)

	N-nitrosodimethylamine (DMSO)	
	Frequency (1/cm)	Intensity
1	69.0535000000	1772.1039169997
2	233.9261000000	5.3686283836
3	247.1314000000	89.6297724995
4	286.7431000000	389.2423837064
5	381.7068000000	37.1476619309
6	396.3352000000	528.8929591754
7	550.9504000000	316.8359081334
8	641.7004000000	274.6757766265
9	821.8648000000	123.7887452803
10	993.8067000000	398.0856256907
11	1046.2209000000	105.0431354358

12	1106.0241000000	32.5604923343
13	1170.6862000000	46.2311418441
14	1214.1965000000	33.8620054485
15	1270.5607000000	46.2619254690
16	1328.3584000000	442.7066375197
17	1436.7232000000	0.9499205199
18	1455.1927000000	4.2161386974
19	1470.9692000000	28.0516649444
20	1482.9166000000	16.9654428278
21	1486.0046000000	48.2817607167
22	1501.6123000000	48.4656272387
23	1503.0581000000	39.8242192650
24	2987.2454000000	93.5844825716
25	3009.2202000000	87.9044266317
26	3086.9551000000	36.7723885694
27	3094.2287000000	36.9173775895
28	3124.9618000000	25.2540240139
29	3132.9398000000	28.8431461107
30	3470.2016000000	12.4258485817

N-nitrosodimethylamine		
	Frequency (1/cm)	Intensity
1	77.7663000000	892.1090452918
2	221.7691000000	11.5021465783
3	233.0244000000	57.7546047280
4	282.3006000000	182.5721297536
5	366.5726000000	290.6938349828
6	391.5476000000	90.7750123266
7	539.6638000000	229.0867564770
8	645.5613000000	127.3519672386
9	829.2653000000	39.6594349111
10	1007.5937000000	165.4608559988
11	1034.6960000000	65.7780801200
12	1105.4880000000	8.3928016613
13	1185.7932000000	10.3644856089
14	1213.4588000000	17.3622759881
15	1260.1123000000	17.3725939097
16	1350.6272000000	115.8532408409
17	1433.9282000000	0.2286923891
18	1448.8021000000	3.3001696909
19	1467.6688000000	0.5189017868
20	1478.3648000000	19.7067539084
21	1491.9737000000	43.4605982055
22	1499.4309000000	4.8476272263
23	1514.3930000000	29.7799460233
24	2996.1469000000	50.5692577180
25	3004.5181000000	59.2684516654
26	3082.3758000000	23.5880279342
27	3088.9717000000	25.5658270175

28	3116.3539000000	21.7513960682
29	3125.9940000000	23.4681920845
30	3457.5543000000	1.8519974537

N-nitrosodimethylamine (Toluene)		
	Frequency (1/cm)	Intensity
1	66.8752000000	1428.4594928404
2	226.7888000000	7.8965120450
3	236.6478000000	78.9626499841
4	282.5264000000	239.9472438800
5	364.2840000000	330.7961308509
6	391.8402000000	143.3775497333
7	551.5970000000	270.7980939437
8	646.2829000000	173.4443043766
9	825.2885000000	60.4358863579
10	1001.2463000000	226.0471641039
11	1037.3481000000	83.9438281053
12	1104.5208000000	13.5564719513
13	1181.3264000000	12.4393607953
14	1211.8664000000	23.2506775213
15	1262.2358000000	23.8165516098
16	1344.0983000000	198.6117520148
17	1433.9639000000	0.2359200947
18	1453.5662000000	2.9358541730
19	1471.2029000000	3.2515477077
20	1475.3033000000	22.1462032860
21	1488.6113000000	51.4043057340
22	1496.6315000000	9.5166689875
23	1510.1691000000	39.8760342445
24	2993.2303000000	65.2356899714
25	3007.9620000000	71.2555429674
26	3084.3603000000	30.7128314345
27	3091.7608000000	29.3150490265
28	3120.1338000000	24.5383448162
29	3128.8999000000	25.6155811939
30	3464.3231000000	5.6900037619

N-nitrosodimethylamine (Water)		
	Frequency (1/cm)	Intensity
1	69.6035000000	1761.5169627579
2	234.1908000000	5.1104450673
3	247.5004000000	90.3730029438
4	286.7813000000	394.6422329304
5	381.9521000000	30.4140919141
6	397.3553000000	532.8241785157
7	550.8179000000	322.2760517253
8	641.5006000000	278.7034567708
9	821.7755000000	126.0726969154
10	993.7633000000	404.7509140982

11	1046.4333000000	105.5673653178
12	1105.9717000000	33.4129599114
13	1170.3095000000	48.5377856338
14	1214.3176000000	34.2745474568
15	1270.8154000000	47.4367757149
16	1327.8409000000	451.7229969785
17	1436.7336000000	1.0187761353
18	1455.1541000000	4.2200887253
19	1470.8314000000	28.2696529971
20	1482.9319000000	17.5867061691
21	1485.9504000000	48.0123625823
22	1501.6294000000	57.2061903555
23	1503.3711000000	32.4640335697
24	2987.2182000000	94.5492907460
25	3009.1132000000	88.5498888269
26	3087.0770000000	37.0363728079
27	3094.2775000000	37.1654979308
28	3125.1601000000	25.2092744649
29	3133.0540000000	28.9276622466
30	3470.4705000000	12.7402008849

Table 2. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosodiethylamine ($C_4H_{10}N_2O$)

N-nitrosodiethylamine (DMSO)		
	Frequency (1/cm)	Intensity
1	50.4476000000	2044.7563526914
2	87.1865000000	439.3821118070
3	95.2491000000	37.1216411672
4	195.1960000000	189.8987986487
5	220.4983000000	11.5069220198
6	271.8330000000	133.7474634238
7	272.4002000000	101.8218246270
8	320.5443000000	643.1139947279
9	371.0471000000	433.9064009763
10	438.8745000000	111.8577854291
11	526.1247000000	181.2258493734
12	677.6047000000	155.5736442498
13	754.6346000000	63.2052072908
14	811.2092000000	47.6715779281
15	818.4619000000	26.0748623334
16	928.2468000000	24.5364365071
17	999.5335000000	47.1543340872
18	1043.7071000000	184.6772260021
19	1066.6865000000	107.1776562698
20	1099.1682000000	13.7139502937
21	1137.6449000000	138.0643121771
22	1184.9857000000	46.9657055164
23	1203.3105000000	64.2893090824

24	1310.6493000000	44.8417455621
25	1319.5255000000	35.4908920570
26	1340.5865000000	295.0939892196
27	1387.3115000000	32.8362671114
28	1403.8192000000	5.8319770347
29	1410.6726000000	16.7613374102
30	1414.5766000000	36.0154405497
31	1466.3342000000	2.1691825394
32	1481.1825000000	7.7461804401
33	1482.1065000000	15.1809619426
34	1486.0482000000	7.3339712299
35	1490.1114000000	31.9122577519
36	1502.0039000000	27.8327475104
37	1508.3194000000	24.8959211593
38	2986.1360000000	78.1768712201
39	2992.6448000000	108.4802306714
40	3034.6359000000	42.2118369039
41	3035.5948000000	36.1246361768
42	3083.3246000000	3.0364359977
43	3089.5461000000	12.0882296136
44	3099.3538000000	51.7041023531
45	3102.0949000000	35.1681243082
46	3105.7402000000	79.6791436024
47	3111.7600000000	92.7560278843
48	3492.7614000000	16.1493112116

N-nitrosodiethylamine		
	Frequency (1/cm)	Intensity
1	52.8251000000	759.0073780229
2	78.9556000000	249.7857652249
3	97.2489000000	128.5400431194
4	199.2401000000	80.5527889336
5	223.1463000000	3.1643963580
6	266.4936000000	86.2613759300
7	280.1693000000	71.6134006174
8	305.5157000000	381.7076036611
9	375.5543000000	302.8072514126
10	438.2759000000	80.9119402854
11	511.6275000000	90.5402619265
12	672.6152000000	89.5452975788
13	760.8656000000	24.2536336677
14	811.0499000000	21.4504225972
15	822.5558000000	23.3644003403
16	932.4647000000	7.6064537667
17	995.8998000000	34.4232307702
18	1049.1654000000	103.9167346579
19	1069.4769000000	63.1233658883
20	1102.4322000000	9.5382316076

21	1140.4608000000	79.4541772621
22	1191.0291000000	16.1226668802
23	1206.4622000000	35.7840152769
24	1313.3478000000	28.5122331294
25	1325.3437000000	7.8192982051
26	1353.2454000000	115.0253381251
27	1388.2079000000	20.6483619831
28	1406.5587000000	3.2892364603
29	1417.0769000000	20.9864135285
30	1419.3569000000	26.3374556150
31	1451.3658000000	3.6470009590
32	1491.8174000000	5.4630948395
33	1494.3231000000	12.4344041189
34	1496.5545000000	8.7886169688
35	1502.7017000000	16.2849104145
36	1510.2153000000	14.0216572933
37	1516.5013000000	14.0077316465
38	2985.8379000000	45.6609048452
39	2997.3894000000	47.7012445490
40	3038.3917000000	30.5032700078
41	3039.1145000000	24.1725533147
42	3080.2181000000	3.0473988618
43	3088.1536000000	6.9670171503
44	3101.0299000000	28.7691828053
45	3102.6066000000	27.2488660753
46	3108.3095000000	45.9819544330
47	3112.8257000000	51.0909837241
48	3470.0754000000	3.3860855442

N-nitrosodiethylamine (Toluene)		
	Frequency (1/cm)	Intensity
1	52.7051000000	919.8039520200
2	80.0352000000	443.8296318368
3	97.1104000000	162.9479928985
4	197.4599000000	115.1179931737
5	222.8465000000	3.2742752686
6	266.5740000000	134.7787591610
7	276.8944000000	94.5818950573
8	305.4915000000	519.9472098699
9	371.4534000000	330.4140221500
10	438.3410000000	86.8165667738
11	516.0398000000	115.5057933271
12	676.1964000000	113.7798477964
13	758.4796000000	35.9118539217
14	810.3387000000	31.1372784094
15	821.4664000000	25.0417165335
16	930.6215000000	11.6262569439
17	997.6869000000	37.2969769048

18	1047.5468000000	132.9904749373
19	1067.4940000000	82.5722079146
20	1100.8182000000	12.2231259765
21	1139.0212000000	102.9518564235
22	1188.4069000000	24.6042742357
23	1204.4700000000	43.5002538003
24	1310.9482000000	33.8071424079
25	1322.4449000000	11.9705008544
26	1351.7066000000	175.5913607515
27	1387.6064000000	24.6455416277
28	1405.1547000000	4.0062767928
29	1414.1029000000	17.7159800924
30	1416.8975000000	33.0211978321
31	1455.5589000000	2.0736900922
32	1487.0423000000	9.8294131362
33	1489.3034000000	11.5960933987
34	1491.5756000000	8.4384249669
35	1496.8954000000	20.0299333315
36	1505.3419000000	20.0002300241
37	1512.1364000000	16.7204518547
38	2989.1154000000	40.6611872709
39	2992.7962000000	81.2560821420
40	3034.6244000000	35.8484162456
41	3035.6230000000	29.3593557885
42	3080.4547000000	3.0485893752
43	3088.2539000000	8.2977294162
44	3099.2581000000	37.3863837465
45	3101.0472000000	27.7235099209
46	3105.7506000000	59.6333067861
47	3111.5229000000	67.0313836476
48	3485.5168000000	8.6555370855

N-nitrosodiethylamine (Water)		
	Frequency (1/cm)	Intensity
1	50.7191000000	2039.1358044940
2	87.2794000000	446.8859707657
3	95.1677000000	34.4956862131
4	195.0909000000	192.7780643144
5	220.6985000000	12.0875766642
6	272.1999000000	134.7675214854
7	272.3646000000	95.7623759937
8	321.6118000000	638.5294919982
9	371.3636000000	444.0739794073
10	438.9645000000	114.5731262701
11	526.6341000000	185.1434744668
12	677.6155000000	157.1766602292
13	754.5062000000	64.4209682946
14	811.1526000000	48.4947655221

15	818.3166000000	25.9444511572
16	928.1946000000	25.1369601461
17	999.6015000000	47.8208140677
18	1043.5636000000	186.6874497294
19	1066.6795000000	107.7191657926
20	1099.1277000000	13.7503886886
21	1137.6353000000	139.2581213633
22	1184.8599000000	48.0791012084
23	1203.2591000000	65.3483714911
24	1310.5960000000	46.0441057080
25	1319.4109000000	37.1953657511
26	1340.1700000000	298.8715536344
27	1387.2992000000	33.1183726808
28	1403.7413000000	5.8928347408
29	1410.5367000000	16.6359623828
30	1414.4999000000	36.0729545254
31	1466.8286000000	2.2584749147
32	1480.9601000000	7.7872118169
33	1481.8787000000	15.1507209482
34	1485.8836000000	7.3487449565
35	1489.9613000000	32.4954229024
36	1501.9224000000	27.8063677828
37	1508.2148000000	25.2589701080
38	2985.9074000000	80.1447495168
39	2992.6563000000	109.1736727556
40	3034.6597000000	42.4432717890
41	3035.6086000000	36.3612908268
42	3083.4169000000	3.0561406043
43	3089.6168000000	12.2542630669
44	3099.3599000000	52.2384328139
45	3102.1211000000	35.8598359676
46	3105.7721000000	79.9388239657
47	3111.7967000000	93.6537608139
48	3492.9305000000	16.3926035917

Table 3. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosodipropylamine ($C_6H_{14}N_2O$)

N-nitrosodipropylamine (DMSO)		
	Frequency (1/cm)	Intensity
1	45.1772000000	67.9069662839
2	55.6745000000	1639.0820175386
3	72.4464000000	313.1818807820
4	84.8317000000	223.6613673117
5	132.5788000000	165.5924839236
6	155.1423000000	178.6922163822
7	205.9105000000	46.9306679908
8	236.7454000000	199.1754827603
9	249.5253000000	919.5899677498

10	259.8264000000	183.1681275279
11	317.6261000000	183.1731515063
12	355.1354000000	95.0911932564
13	364.9985000000	230.1443631146
14	446.6086000000	100.9719726410
15	581.5795000000	23.2457813491
16	642.1784000000	151.9718312354
17	752.2853000000	1.5787143583
18	766.6110000000	100.9324915064
19	846.5328000000	41.5300677641
20	874.0924000000	52.5828234340
21	893.5468000000	6.3130525646
22	908.4726000000	6.7859127456
23	936.6286000000	0.9557905616
24	1025.7390000000	108.0942851309
25	1031.3895000000	61.8885069208
26	1059.5943000000	159.1690022080
27	1080.4242000000	92.3448746756
28	1107.3677000000	40.6369119150
29	1150.9534000000	43.0459889305
30	1175.9214000000	10.8066971686
31	1190.2807000000	5.2785044387
32	1272.8497000000	1.9849047147
33	1292.1058000000	4.7557009716
34	1307.6420000000	6.5223759194
35	1332.3039000000	8.2847950187
36	1337.8422000000	71.9852094730
37	1354.6082000000	219.6587901858
38	1383.4333000000	4.6741785372
39	1383.7526000000	45.9727633899
40	1404.7414000000	10.4887927423
41	1409.9707000000	17.7333813935
42	1430.9369000000	3.8128165387
43	1461.2032000000	2.6300151212
44	1477.1584000000	6.8501167878
45	1477.6967000000	5.4958614161
46	1483.8745000000	4.3836001316
47	1488.0885000000	13.8068371115
48	1491.3976000000	27.5042563437
49	1495.0336000000	18.7825680894
50	1498.2744000000	32.3409515016
51	1507.1506000000	41.3045336807
52	2979.1844000000	70.8733709995
53	2991.3410000000	113.7368770022
54	3022.6207000000	56.1825946723
55	3023.8810000000	55.8937361888
56	3027.6128000000	70.6544380210
57	3030.1743000000	55.0095723668
58	3054.1481000000	13.4687228905

59	3055.1484000000	12.5454251185
60	3073.9882000000	6.3668379348
61	3079.7070000000	0.4691874054
62	3084.5224000000	81.0478769858
63	3087.9478000000	214.6025894473
64	3091.3748000000	70.2826981763
65	3096.8299000000	83.3292665417
66	3500.2597000000	20.7590557591

N-nitrosodipropylamine		
	Frequency (1/cm)	Intensity
1	42.5650000000	57.4720658515
2	60.4133000000	385.7373450307
3	76.0291000000	188.6839919816
4	87.7779000000	190.8939145379
5	137.8962000000	69.7686430749
6	154.5599000000	85.3425988807
7	205.7921000000	3.9410866137
8	237.7848000000	14.4788479011
9	263.2244000000	122.7323155050
10	278.2028000000	322.6475125360
11	327.0358000000	116.9607187617
12	359.7428000000	12.7008986341
13	386.8558000000	411.1621583021
14	451.6097000000	118.7571100161
15	584.5917000000	21.9065111249
16	639.4761000000	89.8643008927
17	756.3003000000	2.0714474888
18	773.2223000000	48.8754159423
19	849.0221000000	21.7724270925
20	876.0465000000	31.1356850042
21	896.3448000000	3.9865275586
22	910.9064000000	4.5157961944
23	940.2428000000	0.5498855216
24	1024.4387000000	63.4494281070
25	1034.4167000000	29.5135050598
26	1064.0582000000	112.5975820341
27	1080.9486000000	62.8516819826
28	1110.5065000000	17.9189533867
29	1154.3494000000	22.6338415588
30	1180.7259000000	8.3553522621
31	1194.5423000000	2.1520943057
32	1276.6519000000	1.8527475781
33	1294.8471000000	1.6566426875
34	1312.3262000000	3.4840791528
35	1332.7529000000	7.5450408514
36	1341.9283000000	40.5551939334
37	1356.8416000000	79.6079130561

38	1385.3251000000	33.4382794759
39	1386.7702000000	6.5739593542
40	1412.2387000000	8.1415714169
41	1417.5148000000	14.9732411709
42	1435.3511000000	7.4212434755
43	1454.7366000000	5.5782148070
44	1485.3069000000	3.0721413474
45	1490.2727000000	6.1516494364
46	1495.6093000000	2.8546580265
47	1498.7844000000	5.7025446624
48	1503.1316000000	20.9288342435
49	1503.7541000000	19.0569976246
50	1509.6832000000	18.0805190919
51	1515.0947000000	21.7130776072
52	2984.9564000000	24.2339718381
53	2995.5370000000	55.2730141702
54	3027.3794000000	18.9905516327
55	3029.0405000000	34.7539168444
56	3030.6659000000	56.6747750214
57	3032.8631000000	36.9749515206
58	3052.8624000000	7.9196962549
59	3055.4085000000	5.6093481939
60	3069.0746000000	1.8166980366
61	3076.5614000000	16.8741723303
62	3088.3181000000	54.2367817647
63	3091.4648000000	97.6110776094
64	3095.7890000000	41.8688473734
65	3103.6521000000	46.1827081153
66	3475.7023000000	3.6924599157

N-nitrosodipropylamine (Toluene)		
	Frequency (1/cm)	Intensity
1	46.7580000000	75.0304989451
2	58.9419000000	678.1824638156
3	75.6147000000	284.8962833469
4	87.3399000000	167.3091418730
5	136.5078000000	103.2975700613
6	156.3042000000	116.8149928159
7	207.8850000000	12.2108548611
8	237.7090000000	27.3205474772
9	262.8558000000	150.3006642736
10	270.5545000000	584.9062656486
11	322.8859000000	160.3649636495
12	358.0169000000	34.6504037695
13	375.8681000000	380.2402004763
14	449.7001000000	112.6620832520
15	583.6075000000	22.8259502891
16	642.3746000000	112.0317263133

17	754.1566000000	1.5737390950
18	769.4636000000	67.1541444797
19	848.4056000000	28.0567896301
20	875.1840000000	39.1320908767
21	894.6566000000	5.2113947812
22	909.6145000000	5.2147294303
23	938.4433000000	0.7188576013
24	1025.1229000000	80.9376983906
25	1032.9051000000	43.1342531989
26	1061.6079000000	134.9560706811
27	1080.8770000000	74.9202554164
28	1109.0003000000	25.2799662881
29	1152.8080000000	30.0192457440
30	1178.0618000000	9.6099473976
31	1192.5335000000	3.4041901462
32	1273.9746000000	1.9436957090
33	1292.8403000000	2.5161302880
34	1309.1900000000	5.0129909757
35	1331.9293000000	7.6212916654
36	1339.6576000000	47.3317063142
37	1357.8853000000	134.5283786516
38	1383.9348000000	42.6998055122
39	1384.4969000000	3.3488537628
40	1408.9475000000	8.1379377547
41	1413.9150000000	16.7355970565
42	1432.6212000000	6.1034704859
43	1457.7475000000	3.7777215635
44	1482.8935000000	7.0953421072
45	1483.8441000000	4.0457384983
46	1490.0612000000	1.3919479992
47	1493.1109000000	10.1416148622
48	1497.1613000000	23.1687871005
49	1499.5285000000	18.8928097498
50	1503.7636000000	22.6407363853
51	1510.8270000000	28.3704775580
52	2983.1965000000	34.5058138539
53	2993.6461000000	75.6638545905
54	3023.4804000000	36.5248291558
55	3024.6837000000	42.8510042572
56	3027.5576000000	59.8443026081
57	3030.8313000000	43.5568776648
58	3053.0288000000	8.4565802737
59	3055.2154000000	8.1543801447
60	3070.0444000000	2.7755148744
61	3077.3090000000	7.5077924047
62	3085.5302000000	64.2255017202
63	3088.9186000000	141.0031484609
64	3092.7523000000	52.0977311282
65	3099.5144000000	60.6335389859

66	3490.7324000000	9.9109439481

N-nitrosodipropylamine (Water)		
	Frequency (1/cm)	Intensity
1	44.9422000000	69.9752563723
2	55.4291000000	1684.4411828205
3	72.1736000000	313.4757100909
4	84.6635000000	226.4287597959
5	132.4076000000	168.9762325851
6	154.9842000000	181.5849937437
7	205.8277000000	49.6785635005
8	236.5604000000	227.5180382822
9	248.6596000000	907.0815872381
10	259.6872000000	185.2096442984
11	317.4300000000	184.0114732930
12	354.9984000000	98.6340810015
13	364.6463000000	222.3440144878
14	446.4585000000	100.2821318250
15	581.5096000000	23.2732730892
16	642.1164000000	153.3881325571
17	752.2047000000	1.5709281112
18	766.5273000000	102.1561630478
19	846.4629000000	41.9939594211
20	874.0397000000	53.0652475634
21	893.5066000000	6.3146760601
22	908.4307000000	6.8380457471
23	936.5571000000	0.9669385975
24	1025.7531000000	108.8842590930
25	1031.3518000000	62.4396560894
26	1059.5710000000	159.9281591641
27	1080.3962000000	92.8775154999
28	1107.3106000000	41.2846257371
29	1150.8859000000	43.5012216379
30	1175.8627000000	10.8588063082
31	1190.2083000000	5.3304439888
32	1272.8226000000	1.9990512888
33	1292.0794000000	4.8524393678
34	1307.5821000000	6.5461671982
35	1332.3213000000	8.2981612636
36	1337.7897000000	72.8728179145
37	1354.5331000000	222.6945312404
38	1383.3792000000	4.2841823636
39	1383.7482000000	46.4434212271
40	1404.5981000000	10.5767742114
41	1409.8525000000	17.7331703411
42	1430.8780000000	3.7438291893
43	1461.2411000000	2.6116549477
44	1476.9411000000	6.7989929892

45	1477.4418000000	5.5292120792
46	1483.7000000000	4.5812059598
47	1487.9270000000	13.8858217585
48	1491.2303000000	27.6277277786
49	1494.8848000000	18.7945787516
50	1498.1118000000	32.7007644409
51	1507.0174000000	41.8079784267
52	2979.0224000000	72.3766862314
53	2991.1595000000	115.4605549173
54	3022.5857000000	56.8470040689
55	3023.8541000000	56.3913489804
56	3027.6175000000	71.1085288057
57	3030.1123000000	55.3522198251
58	3054.1600000000	13.8807820493
59	3055.1230000000	12.6038989401
60	3074.1065000000	6.6055072404
61	3079.7610000000	0.4978066217
62	3084.4848000000	81.6284265716
63	3087.9111000000	217.1032361528
64	3091.3278000000	70.9652864322
65	3096.7485000000	84.0948759863
66	3500.5088000000	21.1427843299

Table 4. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosopyrrolidine ($C_4H_8N_2O$)

N-nitrosopyrrolidine (DMSO)		
	Frequency (1/cm)	Intensity
1	57.0741000000	1779.4076384784
2	61.2377000000	532.8625339806
3	149.6314000000	140.1275055349
4	292.5099000000	310.7683124415
5	319.1943000000	637.9612788849
6	473.8175000000	75.1945849625
7	506.1980000000	532.5693181423
8	643.3596000000	4.1638927143
9	733.2300000000	122.4534929069
10	760.6384000000	13.3973208653
11	857.2564000000	17.3535745993
12	863.8851000000	68.3723113406
13	896.2131000000	32.2605859533
14	972.8452000000	11.6403960744
15	980.5291000000	24.8922058569
16	1048.3654000000	93.6443388430
17	1076.0354000000	163.3856598266
18	1115.1549000000	28.9132107932
19	1133.3397000000	104.1592954823
20	1218.2011000000	13.0262778620
21	1221.6111000000	9.4329319512

22	1250.6438000000	41.4655041546
23	1274.3909000000	17.7937034361
24	1314.8313000000	45.7722996787
25	1326.2354000000	65.0938451506
26	1336.3784000000	218.5809564284
27	1355.2087000000	25.5511726822
28	1378.6323000000	10.9302181899
29	1475.9326000000	3.5000722171
30	1489.0171000000	3.9288013152
31	1501.4687000000	21.5089197642
32	1507.5021000000	1.5161012167
33	1522.6629000000	14.7897143605
34	2994.8432000000	82.7754716515
35	3011.2726000000	77.0554355588
36	3060.0271000000	36.1867732119
37	3070.1080000000	82.8913040268
38	3088.0400000000	74.4667963292
39	3093.5555000000	13.8258800780
40	3100.5607000000	11.1891367363
41	3117.2777000000	109.4826299804
42	3482.3053000000	13.2741803778

N-nitrosopyrrolidine		
	Frequency (1/cm)	Intensity
1	53.4376000000	30.6534457129
2	92.4676000000	660.0991066317
3	142.2180000000	70.1113772554
4	286.7634000000	261.7423226235
5	324.7229000000	351.8014595872
6	462.5108000000	221.4758207740
7	484.1436000000	119.8169937802
8	644.9998000000	1.9507850058
9	740.9009000000	75.1043935201
10	762.1853000000	10.4824458883
11	858.3406000000	5.7140081200
12	869.6958000000	29.5098485301
13	898.5105000000	19.5236207344
14	974.6715000000	4.5740042564
15	984.0035000000	10.4117225717
16	1053.0080000000	41.9281344272
17	1083.2919000000	107.7285291925
18	1116.8335000000	10.7822661467
19	1127.0824000000	40.7437419667
20	1220.4043000000	7.8656622344
21	1225.9574000000	1.5704323683
22	1254.3478000000	25.3654050246
23	1276.1889000000	7.7178411675
24	1320.6643000000	7.4700140070

25	1329.3065000000	2.2286256074
26	1352.8226000000	83.8632344658
27	1357.5554000000	26.5469970894
28	1384.6176000000	6.0960997532
29	1457.2084000000	1.5120309364
30	1493.7908000000	2.5969433119
31	1510.2572000000	15.7197753476
32	1515.4904000000	1.1408880130
33	1533.2541000000	7.0126822818
34	3003.4080000000	40.4400606204
35	3007.3229000000	36.0807357744
36	3057.9149000000	21.4615461849
37	3067.7796000000	56.6502618648
38	3081.0185000000	45.5631507095
39	3089.4904000000	8.9060878056
40	3096.6360000000	10.8436244617
41	3115.0729000000	63.6885025198
42	3472.5490000000	2.6214193024

N-nitrosopyrrolidine (Toluene)		
	Frequency (1/cm)	Intensity
1	57.4899000000	66.4507495405
2	82.0226000000	1154.6025960430
3	146.7235000000	86.5699248436
4	284.1318000000	397.0304909000
5	312.5636000000	419.3656376090
6	463.3005000000	236.9611665193
7	483.5783000000	170.0511573314
8	644.7205000000	2.7145850604
9	738.3345000000	96.5331783764
10	761.2699000000	9.4537730989
11	857.8614000000	8.0437943415
12	867.2957000000	43.0372234663
13	897.6132000000	25.4707011153
14	974.0605000000	6.8536375325
15	983.3156000000	13.6922644880
16	1051.8602000000	52.8775397619
17	1081.4163000000	130.9992260485
18	1115.6232000000	18.1739805909
19	1126.9973000000	56.7964823628
20	1219.8411000000	9.9316230703
21	1224.0941000000	2.5919312483
22	1252.8689000000	32.4760738951
23	1275.1498000000	10.4519318586
24	1319.3917000000	11.5809360972
25	1329.0657000000	5.0349769702
26	1348.9921000000	144.2789247453
27	1357.1812000000	25.9637764771

28	1383.3166000000	7.7938387073
29	1462.0777000000	1.3738405207
30	1491.4574000000	3.2501878869
31	1506.4404000000	18.0132457180
32	1512.7033000000	1.0696741282
33	1529.0780000000	9.6225931407
34	3002.1983000000	52.4689371931
35	3008.2654000000	52.7592369496
36	3058.8293000000	27.1468927769
37	3068.7574000000	68.0823880259
38	3084.0872000000	56.9789881422
39	3091.5137000000	11.1492291165
40	3098.2392000000	11.6816710124
41	3116.0524000000	79.8174607621
42	3479.4071000000	6.9554612971

N-nitrosopyrrolidine (Water)		
	Frequency (1/cm)	Intensity
1	56.1429000000	2098.2833728497
2	61.0140000000	286.7457022702
3	150.0432000000	141.4578665591
4	292.4324000000	314.1179591306
5	319.8697000000	639.4067019090
6	473.6794000000	75.5736067687
7	507.8510000000	538.9175481501
8	643.2876000000	4.2400179941
9	732.9254000000	123.2713188780
10	760.6220000000	13.9310175388
11	857.2547000000	18.1456670052
12	863.7427000000	69.1489076182
13	896.1583000000	32.2394100222
14	972.7949000000	11.8230807866
15	980.4111000000	25.7318101666
16	1048.1856000000	96.1244083326
17	1075.8690000000	165.1470482804
18	1115.2020000000	29.5047460812
19	1133.7746000000	106.8181739974
20	1218.1680000000	12.8966176618
21	1221.5688000000	10.1716556024
22	1250.6214000000	41.8617984323
23	1274.4165000000	18.2625887265
24	1314.6488000000	50.1539007646
25	1325.9985000000	74.4748528224
26	1335.8313000000	214.6602688524
27	1355.1453000000	25.2382551244
28	1378.4900000000	11.0120900623
29	1476.4861000000	3.7489610545
30	1488.9695000000	3.9139228275

31	1501.3196000000	21.6255838027
32	1507.3005000000	1.5589161325
33	1522.4604000000	15.0055030566
34	2994.4961000000	84.2218907861
35	3011.3816000000	77.8944072995
36	3060.0657000000	36.4636130250
37	3070.1569000000	83.3161907682
38	3088.0898000000	75.1248345263
39	3093.5595000000	14.1294297085
40	3100.6267000000	11.0360454617
41	3117.3248000000	110.5444483074
42	3482.0683000000	13.4660716531

Table 5. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosomethylethylamine ($C_3H_8N_2O$)

N-nitrosomethylethylamine (Toluene)		
	Frequency (1/cm)	Intensity
1	63.9549000000	1001.0655356116
2	116.0799000000	311.6942790222
3	218.5350000000	104.7573933445
4	228.9673000000	3.3365882432
5	256.5086000000	180.8201788955
6	298.0064000000	145.2912682872
7	352.4814000000	334.5894577894
8	441.0434000000	185.9871239179
9	554.2950000000	172.5698035041
10	636.8499000000	142.7782906753
11	789.2978000000	41.4341494804
12	819.9697000000	28.8658163198
13	965.2152000000	67.0685175682
14	1035.614400000	124.1468876505
15	1055.459800000	110.8803674747
16	1097.149400000	14.0326216548
17	1157.095700000	20.3825141889
18	1191.600900000	9.5292155344
19	1235.8524000000	49.8843985842
20	1321.7402000000	8.5487074113
21	1348.9890000000	173.5644518431
22	1395.0884000000	18.0775451331
23	1413.7396000000	38.8044590431
24	1444.9354000000	1.9784982593
25	1466.7346000000	2.6690552362
26	1481.8226000000	28.9276706103
27	1486.2814000000	31.4412898342
28	1492.4764000000	4.6868475732
29	1502.7235000000	15.0268403191
30	1507.6253000000	22.5703064850
31	2995.0964000000	38.6094639714
32	2999.1257000000	94.0250515492

33	3037.4330000000	32.7219233788
34	3075.2892000000	8.9282749652
35	3084.9330000000	35.0633618442
36	3101.5222000000	38.9220394525
37	3110.2354000000	40.5758989213
38	3120.6278000000	35.5010506781
39	3470.8182000000	6.8719848850

N-nitrosomethylethylamine (DMSO)		
	Frequency (1/cm)	Intensity
1	69.3689000000	1441.7152832147
2	113.7804000000	305.0942116361
3	214.1136000000	150.8869029753
4	230.8295000000	4.5972447509
5	260.3199000000	209.5200686267
6	302.5255000000	215.6704030742
7	366.3536000000	344.1857302933
8	451.6877000000	264.9236912139
9	564.1490000000	228.1318474727
10	635.3117000000	234.7252138545
11	786.6507000000	69.8626971053
12	818.1698000000	45.9860603232
13	966.3029000000	114.1931129491
14	1030.1421000000	174.0570217879
15	1057.0673000000	143.6891718450
16	1096.3315000000	22.0900665808
17	1151.5210000000	23.8649264403
18	1189.3771000000	14.2106989834
19	1239.0891000000	76.0780364857
20	1320.7364000000	17.6544168526
22	1337.5162000000	323.2741806672
23	1394.9675000000	21.4417231752
24	1410.5690000000	45.2424463161
25	1445.1208000000	1.3819552914
26	1475.4833000000	2.1438353080
27	1481.0884000000	62.2168783457
28	1481.1776000000	8.5404884611
29	1486.2419000000	12.4437666481
30	1496.9025000000	31.1848879972
31	1503.9841000000	24.1146237270
32	2991.4382000000	84.2265005885
33	3001.2157000000	100.7257756142
34	3037.0694000000	39.6480818942
35	3081.3863000000	6.2578172401
36	3086.9849000000	43.1554883437
37	3101.4644000000	54.0610391788
38	3109.3955000000	62.0043371375
39	3125.0681000000	37.0245031538

40	3475.9462000000	13.1093214251

N-nitrosomethylethylamine		
	Frequency (1/cm)	Intensity
1	68.0414000000	610.4637441807
2	116.2410000000	252.5887333384
3	220.9776000000	79.0919531665
4	225.6240000000	1.8990057808
5	255.9863000000	139.2872906196
6	295.8947000000	103.2664372561
7	356.0705000000	280.5895756470
8	439.3566000000	156.8240474788
9	550.6203000000	140.9851488963
10	637.6495000000	106.4415729495
11	791.6897000000	29.1793673188
12	821.5469000000	19.9385643184
13	964.5515000000	48.2714059372
14	1039.0996000000	95.3025210966
15	1056.3622000000	86.2879677569
16	1098.3315000000	10.5984965928
17	1160.8257000000	18.8509287779
18	1193.2805000000	6.9986935242
19	1235.2057000000	36.8090619867
20	1321.7199000000	6.0638410360
21	1353.0977000000	108.9890715242
22	1395.4283000000	15.4323709368
23	1416.1447000000	33.3545463987
24	1443.8134000000	2.4243418678
25	1461.5245000000	3.8462987587
26	1484.7495000000	23.8283784054
27	1490.3586000000	26.0996389903
28	1496.3276000000	3.4257048480
29	1506.9169000000	11.7962423245
30	1510.5070000000	16.1857065204
31	2993.9295000000	27.3723877531
32	2999.0230000000	75.1035879208
33	3037.3670000000	27.6355523852
34	3071.0580000000	9.9798002811
35	3082.8735000000	28.8299168606
36	3101.1691000000	31.4745133370
37	3110.7193000000	27.1399687219
38	3117.2165000000	34.2923570095
39	3463.8546000000	2.4314002215

N-nitrosomethylethylamine (Water)		
	Frequency (1/cm)	Intensity

1	69.5047000000	1453.7471626528
2	113.9149000000	302.4226085396
3	213.9797000000	152.6480788414
4	230.7603000000	5.0965194282
5	260.5621000000	210.4981160092
6	302.7589000000	217.1841841583
7	366.3889000000	344.8113190766
8	452.1165000000	266.3613104618
9	564.4908000000	230.2623004375
10	635.2806000000	238.7569947192
11	786.5459000000	71.1663919386
12	818.1511000000	46.7195036055
13	966.3668000000	116.1089106635
14	1029.9856000000	176.0278429494
15	1057.1188000000	144.4588280006
16	1096.3045000000	22.4868922877
17	1151.3822000000	24.0812397821
18	1189.3074000000	14.5057115574
19	1239.1938000000	77.1620021475
20	1320.6650000000	18.7180707914
21	1337.1088000000	328.8168525342
22	1394.9149000000	21.5065947572
23	1410.4603000000	45.2699747277
24	1445.2096000000	1.3763495215
25	1475.5867000000	2.2877870044
26	1480.9439000000	65.2147063434
27	1481.0876000000	5.6160713045
28	1486.0600000000	12.8595153657
29	1496.7497000000	31.9082555897
30	1503.8967000000	24.1420216943
31	2991.3050000000	85.5863212158
32	3001.2632000000	101.3975741576
33	3037.0290000000	39.8963515456
34	3081.6117000000	6.1417533962
35	3087.0733000000	43.4389442956
36	3101.4310000000	54.7196968586
37	3109.3447000000	62.8880780841
38	3125.2296000000	37.0259088028
39	3476.0965000000	13.3138424974

Table 6. DFT Calculated IR Spectra (Arbitrary Units) of *N*-nitrosodibutylamine ($C_8H_{18}N_2O$)

N-nitrosodibutylamine (DMSO)		
	Frequency (1/cm)	Intensity
1	38.9292000000	54.4672049708
2	44.8472000000	59.7601894957
3	53.3144000000	1394.6623328414
4	57.8914000000	488.9770691297
5	74.1901000000	93.0911910245

6	115.4764000000	41.9093250273
7	122.6898000000	10.5872516868
8	146.4217000000	72.9700864342
9	164.3268000000	176.8109719900
10	240.8469000000	4.2271427008
11	241.2554000000	12.9890218177
12	260.2226000000	27.8344383286
13	279.8992000000	294.3824517828
14	304.0994000000	207.5094200245
15	328.7954000000	121.3616418290
16	408.9893000000	80.4806385679
17	432.5144000000	254.9024766009
18	484.5101000000	320.3382276970
19	580.7074000000	152.8564814761
20	670.0772000000	156.6211764944
21	738.2204000000	46.7122720364
22	739.3571000000	44.6510371347
23	803.8519000000	7.7782767424
24	812.9742000000	12.7252566271
25	849.3138000000	112.4011949856
26	908.0328000000	36.4300543597
27	911.8078000000	59.3648581230
28	943.4436000000	79.8764429829
29	954.1426000000	12.6805410652
30	1005.4036000000	140.8799022518
31	1021.0778000000	17.1941257155
32	1039.2603000000	178.2683473149
33	1059.8181000000	6.4183858524
34	1061.6404000000	22.8310657322
35	1098.8610000000	104.8498331848
36	1129.6879000000	6.0906323668
37	1140.4852000000	47.9573415713
38	1188.8289000000	3.8980243622
39	1202.1037000000	58.6317816568
40	1255.0866000000	24.2986805775
41	1265.1060000000	19.4902786667
42	1297.9042000000	33.9443475091
43	1303.7249000000	23.3086273351
44	1323.9518000000	154.5881479265
45	1327.3536000000	82.2128914397
46	1328.0996000000	31.2176973574
47	1336.6822000000	110.2896385226
48	1338.8280000000	19.5142054124
49	1381.3753000000	2.5446075699
50	1383.9420000000	5.9854999358
51	1404.1998000000	23.5806887192
52	1406.2476000000	9.2210911468
53	1409.9403000000	17.9654981303
54	1416.9257000000	5.6755461984

55	1473.3890000000	2.1677313696
56	1476.1741000000	3.4146403255
57	1477.6148000000	4.0636044117
58	1483.7923000000	7.7357822834
59	1487.2741000000	0.7778830040
60	1489.5586000000	26.5727069346
61	1489.7365000000	25.8215902256
62	1494.6336000000	7.6420359366
63	1498.2791000000	3.9516433719
64	1507.4081000000	39.6381050046
65	1509.2311000000	38.6568659579
66	2968.2845000000	94.2492160249
67	2998.0803000000	55.6533974598
68	3008.1418000000	54.5099993332
69	3010.3012000000	41.2865292624
70	3017.8576000000	42.5920654197
71	3018.6759000000	42.4817981755
72	3024.0800000000	140.4098813256
73	3024.5622000000	105.9685880160
74	3032.4413000000	20.9248437143
75	3034.2496000000	9.3474909855
76	3053.7304000000	7.4709171727
77	3062.3384000000	30.3528067566
78	3071.1758000000	49.3154039909
79	3078.5516000000	130.3526870944
80	3080.3501000000	196.6690547825
81	3083.6352000000	80.0919697461
82	3084.9206000000	80.5730297987
83	3103.8669000000	64.1161183685
84	3472.4616000000	11.7351044853

N-nitrosodibutylamine		
	Frequency (1/cm)	Intensity
1	35.6606000000	163.0747823519
2	45.5951000000	7.1834369522
3	57.1729000000	8.9036432939
4	64.9028000000	742.5736956884
5	74.5322000000	56.6410266167
6	112.9720000000	16.6466198020
7	122.4613000000	5.0982693505
8	148.1543000000	23.8656786317
9	163.1804000000	117.9898425947
10	240.6634000000	9.3774213556
11	241.1934000000	7.6680565579
12	257.5695000000	76.8793390238
13	264.0455000000	100.1377719311
14	307.9643000000	96.9173230624
15	334.4379000000	68.0709220991

16	412.4133000000	61.7359651552
17	416.5676000000	215.8933683459
18	479.7011000000	163.3969263978
19	581.6699000000	94.3410652596
20	673.7509000000	70.3453425869
21	739.8052000000	19.0042382799
22	742.6002000000	20.4132886360
23	804.7272000000	2.3661923903
24	815.9883000000	7.2558205489
25	852.7169000000	41.2143789066
26	909.1924000000	24.9356972840
27	913.6317000000	23.7058745451
28	945.7145000000	25.6081891835
29	957.5386000000	7.9776398915
30	1013.4245000000	46.5670383450
31	1021.8971000000	10.7576227227
32	1044.2768000000	122.4321038378
33	1061.9491000000	10.3567766853
34	1063.2878000000	5.6316695167
35	1094.1818000000	72.3138614851
36	1131.6392000000	1.7950961347
37	1143.1569000000	33.3793097074
38	1193.0247000000	2.6871863986
39	1202.4367000000	26.9687507623
40	1255.7224000000	13.2057277581
41	1265.7430000000	7.8864905144
42	1299.9414000000	3.4666357253
43	1303.5206000000	6.8542487224
44	1326.5609000000	17.2629374723
45	1329.4572000000	2.2946900347
46	1330.4744000000	8.9750424995
47	1339.4864000000	4.6708738032
48	1349.7135000000	101.8502446301
49	1383.2988000000	3.8777910731
50	1387.0572000000	3.8175261721
51	1406.0790000000	31.0426340517
52	1412.7245000000	8.1319943698
53	1417.1125000000	7.2107489624
54	1421.0721000000	1.1285407356
55	1458.1488000000	3.6469986659
56	1488.8903000000	0.3874475261
57	1490.4357000000	1.3717909234
58	1492.3092000000	1.1463131121
59	1493.8733000000	3.1875157896
60	1500.3481000000	19.0712767791
61	1500.6302000000	18.7159745316
62	1501.8000000000	4.2786805068
63	1503.7004000000	3.1581947173
64	1514.2094000000	19.1627941400

65	1515.8098000000	19.5452363605
66	2975.6354000000	37.3532986123
67	2991.6715000000	26.7820371631
68	3006.8358000000	27.3295942043
69	3009.7975000000	17.6899926061
70	3020.3618000000	31.4926516760
71	3020.6440000000	20.8487419526
72	3025.1749000000	59.2580500416
73	3025.5892000000	66.0696197218
74	3032.6422000000	9.1293390910
75	3032.7462000000	14.4970759101
76	3050.4994000000	7.4694140982
77	3062.2001000000	9.0184193160
78	3070.1521000000	31.2590834074
79	3082.4766000000	42.5762852317
80	3083.9800000000	112.3664269059
81	3087.0898000000	45.2948199286
82	3088.6550000000	49.2097859341
83	3095.3055000000	61.0987762714
84	3460.1532000000	1.9106753319

N-nitrosodibutylamine (Toluene)		
	Frequency (1/cm)	Intensity
1	34.3419000000	158.9978485561
2	45.0426000000	26.9339635811
3	56.3793000000	64.1439098941
4	58.7789000000	1114.7377654945
5	72.2402000000	70.0351573926
6	112.8868000000	21.2498241952
7	121.2856000000	7.6080558417
8	146.0181000000	49.1891831972
9	163.0126000000	141.6713958508
10	240.5930000000	11.1643367282
11	240.8127000000	8.2914787986
12	258.0952000000	54.5387507035
13	266.1524000000	177.1657195531
14	304.2884000000	153.7844806791
15	331.3565000000	79.9332657990
16	411.7128000000	49.3625341556
17	419.7797000000	267.4983244137
18	480.3629000000	206.8243736565
19	582.1819000000	120.2496029452
20	671.6579000000	95.1456969393
21	738.9310000000	28.0752388741
22	741.2854000000	27.9758436918
23	804.2488000000	3.8512561510
24	814.5481000000	9.8414017867
25	851.0033000000	57.9421393658

26	908.6290000000	29.6323823722
27	912.8694000000	33.2915424920
28	945.0756000000	41.1174770266
29	956.1403000000	9.8143133951
30	1010.4058000000	78.9413666351
31	1021.4503000000	12.3546498361
32	1042.0125000000	142.3095162795
33	1060.9471000000	9.1373412221
34	1062.5072000000	10.4140401273
35	1094.8062000000	85.3353798219
36	1130.6999000000	2.7008790806
37	1141.9189000000	37.7625726210
38	1190.8298000000	2.8207831271
39	1201.5515000000	37.5621441242
40	1254.8132000000	16.9487199496
41	1265.0457000000	11.1194522196
42	1299.4285000000	5.6591464781
43	1303.5084000000	9.4630895721
44	1325.9433000000	28.0079106065
45	1329.0256000000	2.6946674631
46	1329.7813000000	22.6269034141
47	1339.0848000000	7.6172108451
48	1345.4695000000	153.5162626101
49	1382.5457000000	3.4632307302
50	1385.7630000000	5.1295266791
51	1405.2832000000	30.8739842443
52	1409.9415000000	8.7617592469
53	1413.5121000000	9.2041821124
54	1418.6677000000	2.3410509253
55	1465.8116000000	3.5266886585
56	1483.5695000000	0.6243981662
57	1485.0838000000	1.7482513950
58	1488.2336000000	2.9551218901
59	1489.4841000000	3.0678110474
60	1495.6454000000	22.5622435304
61	1495.7643000000	20.9943114696
62	1498.1484000000	5.0672044933
63	1500.4921000000	3.1024673978
64	1511.0860000000	24.6166923629
65	1512.7674000000	25.3646542292
66	2973.6284000000	52.6364404636
67	2994.7797000000	34.2354107270
68	3007.2342000000	37.0340335960
69	3009.9881000000	24.5890992864
70	3019.2901000000	36.1877174142
71	3019.7815000000	29.5755955569
72	3024.6417000000	84.0432807591
73	3024.9672000000	82.4789489420
74	3032.4823000000	19.6138733110

75	3033.2092000000	6.0647021415
76	3051.0784000000	7.8103097787
77	3062.1218000000	15.4207136153
78	3070.0687000000	38.4792808310
79	3080.9811000000	72.4574052989
80	3082.4856000000	139.7940557856
81	3085.5778000000	59.7123583132
82	3087.2197000000	61.1561982722
83	3098.6872000000	61.1571083145
84	3467.1997000000	5.7767565463

N-nitrosodibutylamine (Water)		
	Frequency (1/cm)	Intensity
1	39.0894000000	70.5018680478
2	44.8422000000	56.3416908765
3	53.4167000000	1319.9582095113
4	58.0936000000	556.2354538961
5	74.3202000000	97.5499512513
6	115.5856000000	44.1407954729
7	122.7864000000	11.1670012710
8	146.3643000000	73.8654640648
9	164.3174000000	177.4644697579
10	240.8204000000	4.3949230590
11	241.2619000000	12.7902453122
12	260.3037000000	27.8579507166
13	280.3115000000	297.2612451576
14	304.1686000000	209.4217026172
15	328.7179000000	122.6694136684
16	408.8710000000	81.6259914055
17	432.9828000000	252.7775229599
18	484.7291000000	325.4805532043
19	580.6296000000	154.7362050891
20	670.0406000000	159.6966183907
21	738.1991000000	47.5226330373
22	739.2837000000	45.2603956721
23	803.8226000000	7.9641776689
24	812.8869000000	12.8360647565
25	849.2753000000	115.0058391625
26	908.0095000000	36.6743925918
27	911.7835000000	60.5429793828
28	943.3698000000	81.7878020366
29	954.0599000000	12.9199854987
30	1005.2918000000	142.8194487899
31	1021.0665000000	17.4959432490
32	1039.1977000000	180.1087155117
33	1059.7975000000	6.3838790365
34	1061.6070000000	23.3041502260
35	1099.0002000000	105.6674653991

36	1129.6502000000	6.2617618464
37	1140.4292000000	48.5169524759
38	1188.7834000000	3.9381083583
39	1202.1500000000	59.3456670342
40	1255.0930000000	24.7292525236
41	1265.1189000000	19.8561870513
42	1297.8398000000	36.7380325775
43	1303.7174000000	23.9948172339
44	1323.7690000000	168.5600555609
45	1327.2173000000	86.6729773352
46	1328.0437000000	24.8262724907
47	1336.5146000000	106.8651324853
48	1338.7432000000	17.3305369047
49	1381.3132000000	2.5184400822
50	1383.8778000000	5.9941376360
51	1404.1294000000	23.2650783993
52	1406.1332000000	9.2377293417
53	1409.8309000000	18.2886290174
54	1416.8623000000	5.8193986368
55	1473.3565000000	1.9793237388
56	1475.8533000000	3.5024227716
57	1477.5585000000	4.3375385245
58	1483.6086000000	7.8881298342
59	1487.3217000000	0.8028032137
60	1489.3765000000	26.7197950148
61	1489.5512000000	25.9983533284
62	1494.5290000000	7.7883164402
63	1498.2731000000	4.1127503505
64	1507.2971000000	40.2741200853
65	1509.1351000000	39.1697847126
66	2968.1922000000	95.9452460535
67	2998.0985000000	56.8007388036
68	3008.1678000000	54.9949131690
69	3010.3070000000	42.0240816544
70	3017.8109000000	42.6881693676
71	3018.6385000000	42.9199024060
72	3024.0396000000	142.4036593458
73	3024.5538000000	107.4368014423
74	3032.4280000000	20.6764226908
75	3034.2831000000	9.5315876620
76	3053.8542000000	7.4433116291
77	3062.2933000000	31.2853701881
78	3071.2434000000	49.5724202668
79	3078.4634000000	132.6299582479
80	3080.2815000000	199.0726825588
81	3083.5815000000	80.6992297582
82	3084.8366000000	81.2528753275
83	3104.0335000000	64.1926184362
84	3472.5837000000	11.9313710225

Acknowledgments

Funding for this project was provided by the Office of Naval Research (ONR) through the Naval Research Laboratory's Basic Research Program.

References

[1] D. M. Haaland, Multivariate Calibration Methods Applied to Quantitative FT-IR Analyses, Chapter 8, Practical Fourier Transform Infrared Spectroscopy, Editors: J.R. Ferraro and K. Krishnan, Academic Press, Inc., San Diego, CA (1990).

[2] S.W. Smith, The Scientist and Engineer's Guide to Digital Signal Processing, Chapter 7: Properties of Convolution, Correlation, California Technical Publishing, San Diego, CA (1997).

[3] R.B. Lam, "On the Relationship of Least Squares to Cross-Correlation Quantitative Spectral Analysis," Appl. Spectros., 37 (1983) pp. 567-569.

[4] S.D. Brown, "The Kalman Filter in Analytical Chemistry," Anal. Chim. Acta 181 (1986) pp. 1-26.

[5] W.S. Cooper, "Use of Optimal Estimation Theory-in particular the Kalman Filter-in Data Analysis and Signal processing," Rev. Sci. Instrum. 57, No. 11 (1986) pp. 2862-2869.

[6] C.K. Mann, J.R. Goleniewski, C.A. Sismanidis, "Spectrophotometric Analysis by Cross-Correlation," Appl. Spectros., 36, (1982), pp. 223-227.

[7] C.K. Mann and T.J. Vickers, "Signal Enhancement by Data Domain Averaging," Appl. Spectros., 40, 4 (1986), pp. 525-531.

[8] N.J. Hanick, *Internal Reflection Spectroscopy*, Interscience Publishers, New York (1967).

[9] P.R. Griffiths and C.C. Christopher, *Handbook of Vibrational Spectroscopy*, John Wiley & Sons, New York (2002).

[10] L. Huang, S.G.Lambrakos, A.Shabaev, N. Bernstein, L. Massa, "Molecular Analysis of Water Clusters: Calculation of the Cluster Structures and Vibrational Spectrum Using Density Functional Theory,"Comptes Rendus Chimie (2015), Volume 18, Issue 5, May 2015, pp. 516-524.

[11] J. Choi and R.L. Valentine, "Formation of N-nitrosodimethylamine (NDMA) from reaction of monochloramine: a new disinfection by-product," Water Research, Vol. 36 (2001) pp. 817-824.

[12] W.A. Mitch and D.L. Sediak, "Formation of N-nitrosodimethylamine (NDMA) from dimethylamine during chlorination," Envirn. Sci. Technol., Vol. 36, No. 4 (2002) pp. 588-595.

[13] Agency for Toxic Substances and Disease Registry, Public Health Statesments, 2000; American Water Works Statistical Summary, 2000.

[14] A. Fristachi and G. Rice, "Estimation of the Total Daily Oral Intake of NDMA Attributable to Drinking Water," J. Water and Health, Vol. 05.3, U.S. Environmental Protection Agency (2007) pp. 341-355. Doi: 10.2166/wh.2007.030.

[15] W. Wang, J. Hu, J. Yu and M, Yang, "Determination of N-nitrosodimethylamine in Drinking Water by UPLC-MS/MS," J. Envirn. Sciences, 22(10) (2010) pp. 1508-1512.

[16] N.J. Farren, N. Ramirez, J.D. Lee, E. Finessi, A.C. Lewis and J.F. Hamilton, "Estimated Exposure Risks from Carcinogenic Nitrosamines in Urban Airborn Particulate Matter," Environ. Sci. Technol., ACS Publications, Vol. 49 (2015) pp. 9648-9656. DOI: 10.1021/acs.est.5b01620.

[17] L. Huang, S.G. Lambrakos, L. Massa, "IR Absorption Spectra for Chlorinated Ethanes in Water Using Density Functional Theory," Multiscale and Multidisciplinary Modeling, Experiments and Design, First Online 10 January 2019, DOI: https://doi.org/10.1007/s41939-018-00042-x.

[18] M. Lee, S. Lambrakos, C. Yapijakis, L. Huang, S. Ramsey, A. Shabaev, L. Massa, J. Peak, "Issues Concerning Spectral Analysis of Public Water Resources, Journal of Water Science and technology, IWA publishing, 69.11, (2014) pp. 2364-2371, doi: 10.2166/wst.2014.166

[19] R. Lu, B. Mizaikoff, W-W. Li, C. Qian, A. Katzir, Y. Raichlin, G-P. Sheng, H-Q. Yu, "Determination of Chlorinated Hydrocarbons in Water Using Highly Sensitive Mid-Infrared Sensor Technology," Scientific Reports, 3:2525, DOI: 10.1038/srep02525 (2013).

[20] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Revision A.1, Gaussian, Inc., Wallingford CT, 2009.

[21] W. Polkosnik and L. Massa, "Single determinant N-representability and the kernel energy method applied to water clusters", JCC, **39**, 17, 1038-1043 (2017)

[22] A. Frisch, M. J. Frisch, F. R. Clemente and G. W. Trucks, *Gaussian 09 User's Reference,* Gaussian Inc., 2009, p, 105-106, online: www.gaussian.com/g_tech/g_ur/g09help.htm

[23] P. Hohenberg and W. Kohn, "Inhomogeneous Electron Gas," Phys. Rev. **136**, B864, (1964).

[24] W. Kohn and L. J. Sham, "Self-Consistent Equations Including Exchange and Correlation Effects," Phys. Rev. **140**, A1133 (1965).

[25] R.O. Jones and O. Gunnarson, "The density functional formalism, its applications and prospects," Rev. Mod.Phys. **61**, 689 (1989).

[26] R. M. Martin, *Electronic Structures Basic Theory and Practical Methods*, Cambridge University Press, Cambridge 2004, p. 25.

[27] E. B. Wilson, J. C. Decius and P. C. Cross, *Molecular Vibrations* (McGraw-Hill, New York, 1955).

[28] J.W. Ochterski, "Vibrational Analysis in Gaussian," help@gaussian.com, 1999.

[29] A.D. Becke, "Density-functional Thermochemistry. III. The Role of Exact Exchange,"*J. Chem. Phys.*, **98**, 5648-5652 (1993).

[30] B. Miehlich, A. Savin, H. Stoll and H. Preuss, "Results Obtained with the Correlation Energy Density Functionals of Becke and Lee, Yang and Parr", *Chem. Phys. Lett.,***157**, 200-206 (1989).

[31] A. D. McLean and G. S. Chandler, "Contracted Gaussian-basis sets for molecular calculations. 1. 2nd row atoms, Z=11-18," *J. Chem. Phys.*, **72** 5639-48 (1980).

[32] T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. V. R. Schleyer, "Efficient diffuse function-augmented basis-sets for anion calculations, 3., the 3-21+G basis set for 1st-row elements, Li-F," *J. Comp. Chem.*, **4** 294-301, (1983).

[33] M. J. Frisch, J. A. Pople and J. S. Binkley, "Self-Consistent Molecular Orbital Methods. 25. Supplementary Functions for Gaussian Basis Sets," *J. Chem. Phys.*, **80** (1984) 3265-69.