Electronic Supplementary Information

Superelectrophilic Activation of 1-Nitronaphthalene in the Presence of Aluminum Chloride. Reactions with Benzene and Cyclohexane

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1. Experimental

All reagents were purchased from commercial suppliers (Sigma-Aldrich Chemical Co., Alfa-Aesar) and used as received.

The ^{1}H and ^{13}C NMR spectra were recorded on Bruker AV-600 and Bruker AVANCE III 500 spectrometers. The chemical shifts were measured relative to the residual proton and carbon signals of DMSO-d_6 (δ_H 2.5 ppm, δ_C 39.5 ppm) or $CDCl_3$ (δ_H 7.24 ppm, δ_C 76.9 ppm). IR spectra were acquired on a Bruker Vector-22 spectrometer. High-resolution mass spectra (HRMS) were acquired on a DFS Thermo Scientific instrument (EI, 70 eV). GC-MS data were obtained on an Agilent 6890N/5973N EI/PCI instrument using a HP-5MS column.

2,4,4-Triphenyl-3,4-dihydronaphthalen-1(2*H*)-one oxime (5): Compound **1** (0.2 g, 1.16 mmol) was added to a stirred suspension of $AlCl_3$ (0.75 g, 5.6 mmol) in 10 mL of benzene. The resulting mixture was stirred at 25 ^{o}C for 0.5 h, and then poured onto ice. The mixture was extracted with diethyl ether. The organic phase was dried over anhydrous $MgSO_4$ and concentrated in vacuo to obtain the crude product, which was recrystallized from ethanol to give **5** (0.27 g, 60%). M.p. 243–245 ^{o}C. ^{1}H NMR (600.3 MHz, $CDCl_3$-DMSO-d_6): δ = 2.63 (dd, *J* = 12.2, 13.5 Hz, 1H), 2.95 (dd, *J* = 13.5, 6.6 Hz, 1H), 3.92 (dd, 12.2, 6.6 Hz, 1H), 6.59 (d, *J* = 7.8 Hz, 1H), 6.93 (m, 4H), 7.07 (m, 1H), 7.11 (m, 1H), 7.12-7.29 (m, 6H), 7.28 (m, 1H), 7.84 (dd, *J* = 7.7, 1.4 Hz, 1H), 10.28 (br. s, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$-DMSO-d_6): δ = 39.4, 45.5, 52.5, 125.0, 125.3, 125.9, 126.0, 126.6, 126.8, 127.4, 127.7, 127.8, 127.8, 128.1, 128.3, 128.6, 133.2, 143.4, 144.1, 145.1, 146.6, 155.0 ppm. ^{15}N NMR (60.8 MHz, $CDCl_3$-DMSO-d_6): δ = 360.0 ppm. The NMR signal assignments are given below (p. S6-S7). IR ($CHCl_3$) cm^{-1}: 3577 (OH), 1600 (C=N), 925 (N-O). HRMS *m/z*: calcd. for $C_{28}H_{23}ON$ 389.1774 $[M]^+$; found 389.1777.

5-Phenyl-5*H*-5,10-methanodibenzo[a,d][7]annulen-11(10*H*)-one oxime (6). Method a: Compound **1** (0.2 g, 1.16 mmol) was added to a stirred suspension of $AlCl_3$ (0.75 g, 5.6 mmol) in 10 mL of benzene. The mixture was stirred at 25 ^{o}C for 170 h to provide, after usual workup, the crude product which was recrystallized from benzene to give **6** (0.21 g, 58%). M.p. 208–210 ^{o}C. ^{1}H NMR (600.3 MHz, $CDCl_3$): δ = 2.62 (dd, *J* = 11.1, 4.9 Hz, 1H), 2.72 (d, *J* = 11.1 Hz, 1H), 5.26 (d, *J* = 4.9 Hz, 1H), 7.16 (m, 1H), 7.18-7.25 (m, 4H), 7.37 (m, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.45 (m, 2H), 7.52 (d, *J* = 7.3 Hz, 1H), 7.68 (br. d, *J* = 7.1 Hz, 1H), 7.89 (m, 1H), 9.4 (br. s, 1H) ppm. ^{13}C NMR (151 MHz, $CDCl_3$): δ = 39.4, 53.2, 58.1, 124.2, 124.6, 125.3, 126.0, 126.7, 126.7, 126.8, 127.2, 127.4, 128.1, 128.4, 129.1, 142.5, 145.1, 148.7, 154.9 ppm. ^{15}N NMR (60.8 MHz, $CDCl_3$): δ = 337.1 ppm. The NMR signal assignments are given below (p. S10-S11). IR ($CHCl_3$) cm^{-1}: 3446 (OH), 1631 (C=N), 948 (N-O). HRMS *m/z*: calcd. for $C_{22}H_{17}ON$ $[M]^+$ 311.1305; found 311.1307. **Method b:** A mixture of compound **5** (0.1 g, 0.26 mmol), $AlCl_3$ (0.4 g, 3 mmol) and 5 mL of benzene was saturated with gaseous HCl and stirred at 25 ^{o}C for 240 h to give, after usual workup, a mixture of **5** and **6** (0.08 g) in a 2:8 molar ratio, according to ^{1}H NMR spectroscopic data.

5,6,7,8-Tetrahydro-1-naphthylamine (7). Method a: A mixture of **1** (0.2 g, 1.16 mmol), $AlCl_3$ (1 g, 7.5 mmol) and cyclohexane (5 mL) was stirred in a 15 mL pressure tube at 110 ^oC (oil bath temperature) for 1 h. After cooling, the upper transparent layer (mixture of alkanes) was removed by decantation. The residue was carefully treated with several grams of ice followed by workup with 2N HCl and diethyl ether until all solids were dissolved. The aqueous layer was separated, washed with diethyl ether, then made basic with aqueous NaOH and extracted with diethyl ether. The organic phase was dried ($MgSO_4$) and concentrated in vacuo to afford crude product, which was purified by flash column chromatography (benzene) to give **7** (0.156 g, 90%) as an oil. ^1H NMR (500 MHz, $CDCl_3$): δ = 1.7–1.9 (m, 4H), 2.48 (t, *J* = 6.5 Hz, 2H), 2.76 (t, *J* = 6.5 Hz, 2H), 3.35 (br. s, 2H), 6.53 (d, *J* = 7.5 Hz, 1H), 6.58 (d, *J* = 7.5 Hz, 1H), 6.97 (t, *J* = 7.6 Hz, 1H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ = 22.9, 23.3, 24.2, 30.1, 112.3, 119.8, 121.9, 126.1, 138.2, 144.4 ppm. GC-MS $[M]^+$: 147. The NMR data of **7** are comparable to those previously reported.[S1] **Method b:** A mixture of 1-naphthylamine (0.2 g, 1.4 mmol), $AlCl_3$ (1.3 g, 9.7 mmol) and cyclohexane (5 mL) was saturated with gaseous HCl and stirred in a 15 mL pressure tube at 110 ^oC for 3 h. The treatment of the mixture as described above gave **7** (0.181 g, 88%).

4-Chloroaniline (8): A mixture of **2** (0.2 g, 1.6 mmol), $AlCl_3$ (0.9 g, 6.7 mmol) and cyclohexane (5 mL) was stirred in a 15 mL pressure tube at 110 ^oC (oil bath temperature) for 1 h. The treatment of the mixture as described above afforded **8** (0.16 g, 77%). M.p. 63-65 °C (after sublimation in vacuo), ref.[S2] m.p. 63-65 ^oC. ^1H NMR (500 MHz, $CDCl_3$): δ = 3.6 (br. s, 2H), 6.61 (dm, *J* = 8.5 Hz, 2H), 7.1 (dm, *J* = 8.5 Hz, 2H) ppm. ^{13}C NMR (125 MHz, $CDCl_3$): δ = 116.4, 123.3, 129.2, 145.1 ppm. GC-MS $[M]^+$: 127.

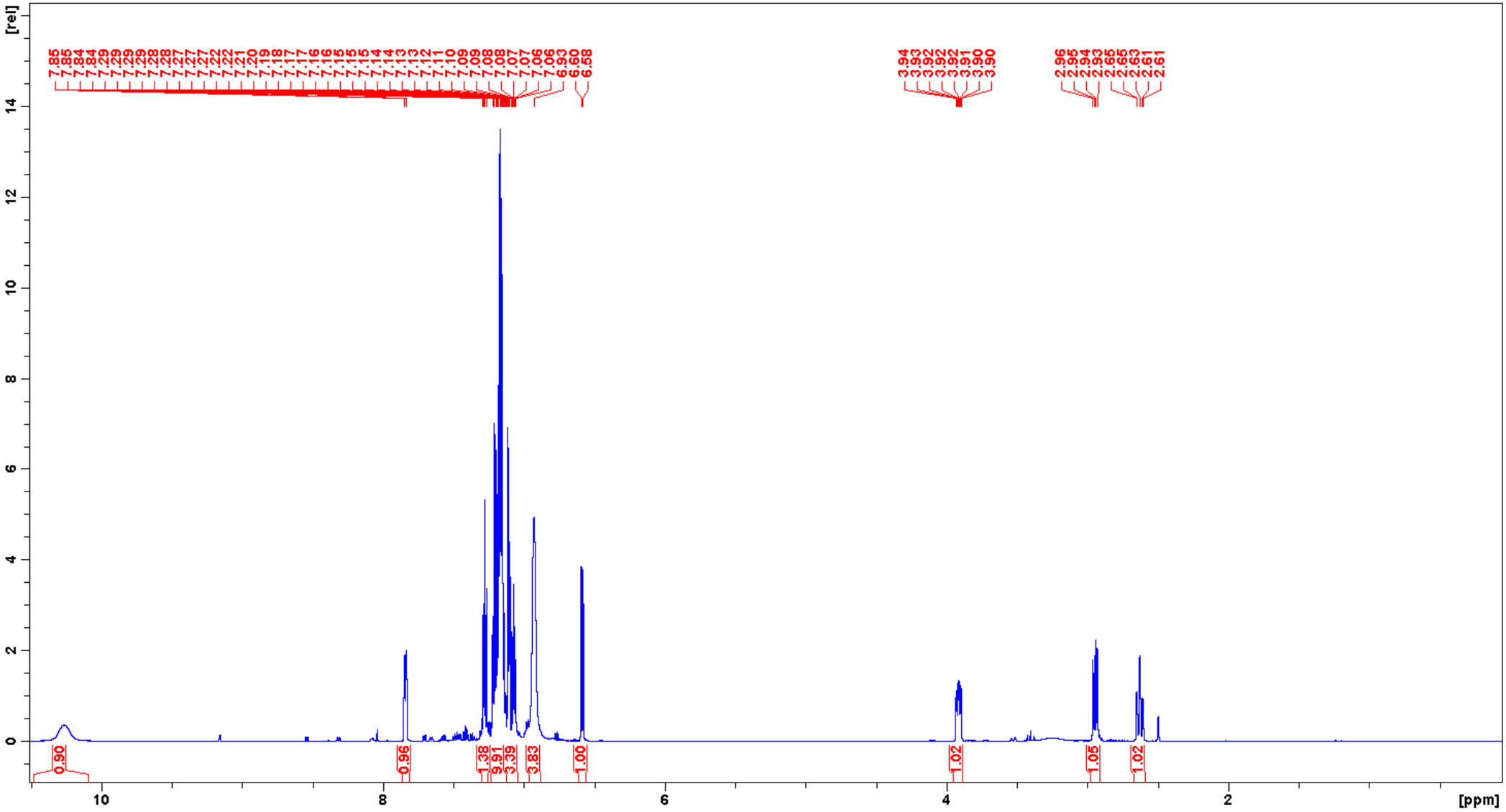
References

S1. Y. He, J. Tang, M. Luo and X. Zeng, *Org. Lett.* 2018, ***20***, 4159.

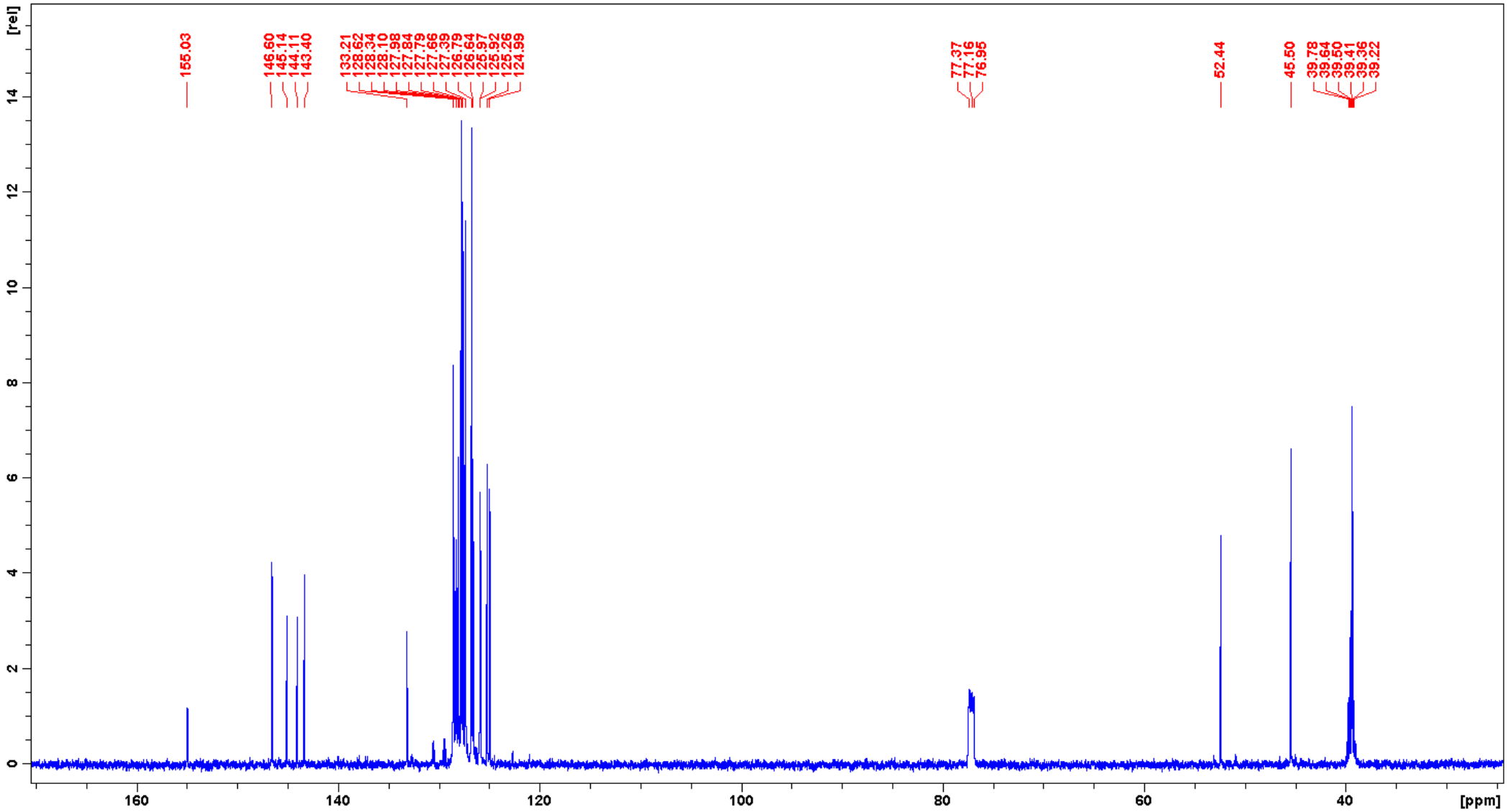
S2. M. Noshita, Y. Shimizu, H. Morimoto and T. Ohshima, *Org. Lett.* 2016, ***18***, 6062.

2. NMR data of compounds 5-8

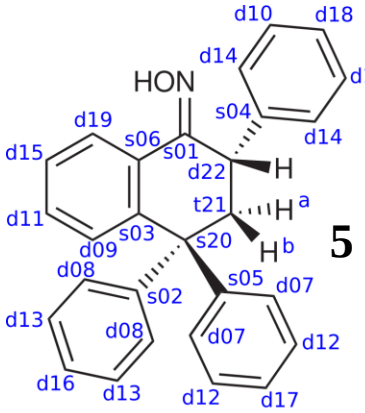
^{1}H NMR spectrum of oxime 5 at 25 ^{o}C (600.3 MHz, $CDCl_3$-DMSO-d_6 4:1 v/v)



^{13}C NMR spectrum of oxime 5 in $CDCl_3$ at 27 ^{o}C (151 MHz, $CDCl_3$-DMSO-d_6 4:1 v/v)



Signal assignment for ^{1}H NMR spectrum of oxime 5 at 25 ^{o}C (600.3 MHz, $CDCl_3$-DMSO-d_6 4:1 v/v)



Experiment Bruker_67,
2D 15N-1H via Jcoupling
N 360.0
d22-H - N

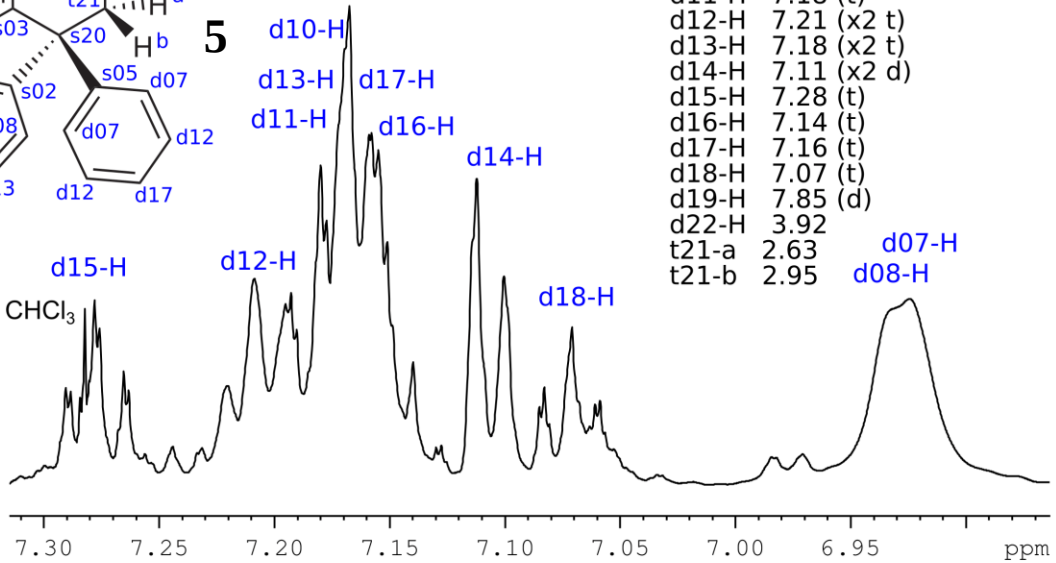
Experiment Bruker_90,
1D 1H

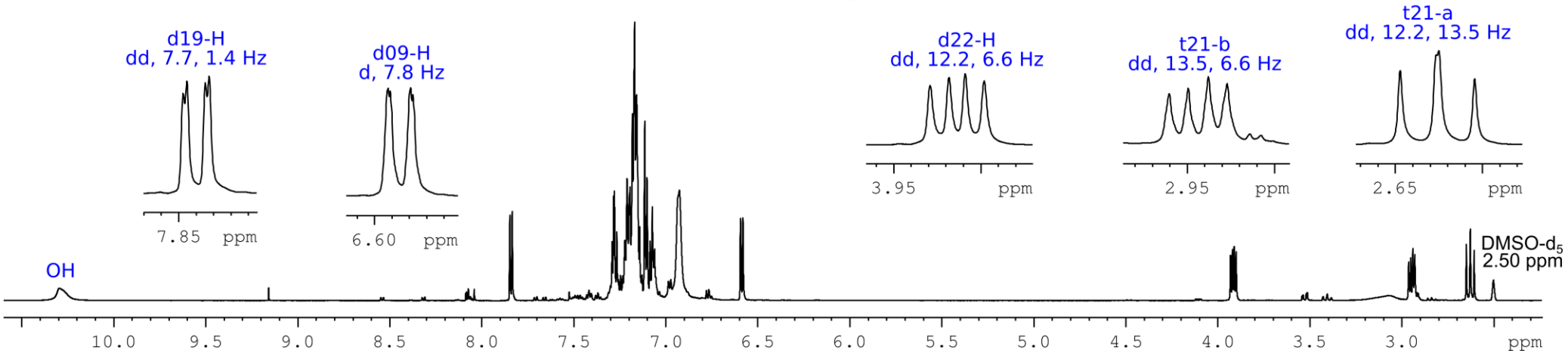
OH-H	10.28
d07-H	6.93 (x2 broad)
d08-H	6.93 (x2 broad)
d09-H	6.59 (d)
d10-H	7.17 (x2 t)
d11-H	7.18 (t)
d12-H	7.21 (x2 t)
d13-H	7.18 (x2 t)
d14-H	7.11 (x2 d)
d15-H	7.28 (t)
d16-H	7.14 (t)
d17-H	7.16 (t)
d18-H	7.07 (t)
d19-H	7.85 (d)
d22-H	3.92
t21-a	2.63
t21-b	2.95

Experiment Bruker_55
2D 1H-1H via Jcoupling (COSY)
d07-H - d12-H
d08-H - d13-H
d12-H - d07-H
d13-H - d08-H
d16-H - d08-H?
d17-H - d07-H?
d22-H - d14-H?(weak) t21-a t21-b
t21-a - d22-H t21-b
t21-b - d22-H t21-a

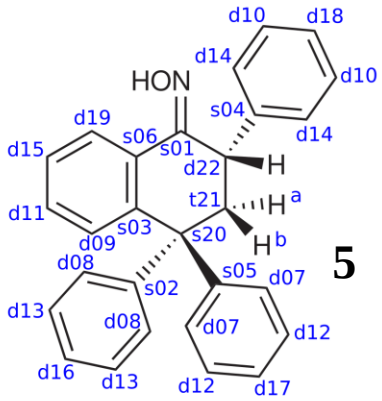
Experiment Bruker_64
2D 1H-1H via Jcoupling (COSY arom)
d07-H - d17-H(weak)
d08-H - d13-H
d09-H - d11-H d15-H
d10-H - d14-H d18-H
d11-H - d09-H d15-H d19-H
d12-H - d07-H? d17-H
d13-H - d08-H
d14-H - d10-H d18-H
d15-H - d09-H d11-H d19-H
d17-H - d07-H d12-H
d18-H - d10-H d14-H
d19-H - d11-H d15-H

Experiment Bruker_65
2D 1H-1H via through-space (NOESY)
d07-H - d09-H d12-H d22-H t21-b
d08-H - d09-H d13-H t21-a
d09-H - d07-H d08-H
d12-H - d07-H
d13-H - d08-H
d14-H - d12-H?(weak) d13-H?(weak) d22-H t21-a t21-b?(weak)
d19-H - OH-H
d22-H - d07-H d14-H OH-H t21-b
OH-H - d14-H? d19-H d22-H
t21-a - d08-H d14-H t21-b
t21-b - d07-H d22-H t21-a





Signal assignment for ^{13}C NMR spectrum of oxime 5 in $CDCl_3$ at 27 ^{o}C (151 MHz, $CDCl_3$-DMSO-d_6 4:1 v/v)



5

Experiment Bruker_56
1D 13C
s01 155.0
s02 146.6
s03 145.1
s04 144.1
s05 143.4
s06 133.2
d07 128.6 (x2 broad)
d08 128.3 (x2 broad)
d09 128.1
d10 127.8 (x2)
d11 127.8
d12 127.7 (x2)
d13 127.4 (x2)
d14 126.8 (x2)
d15 126.6
d16 126.0
d17 125.9
d18 125.3
d19 125.0
s20 52.5
t21 45.5
d22 39.4

Experiment Bruker_54
2D 13C-1H via onebond (HSQC)
d09-H - d09
d12-H - d12
d14-H - d14
d15-H - d15
d18-H - d18
d19-H - d19
d22-H - d22
t21-a - t21
t21-b - t21

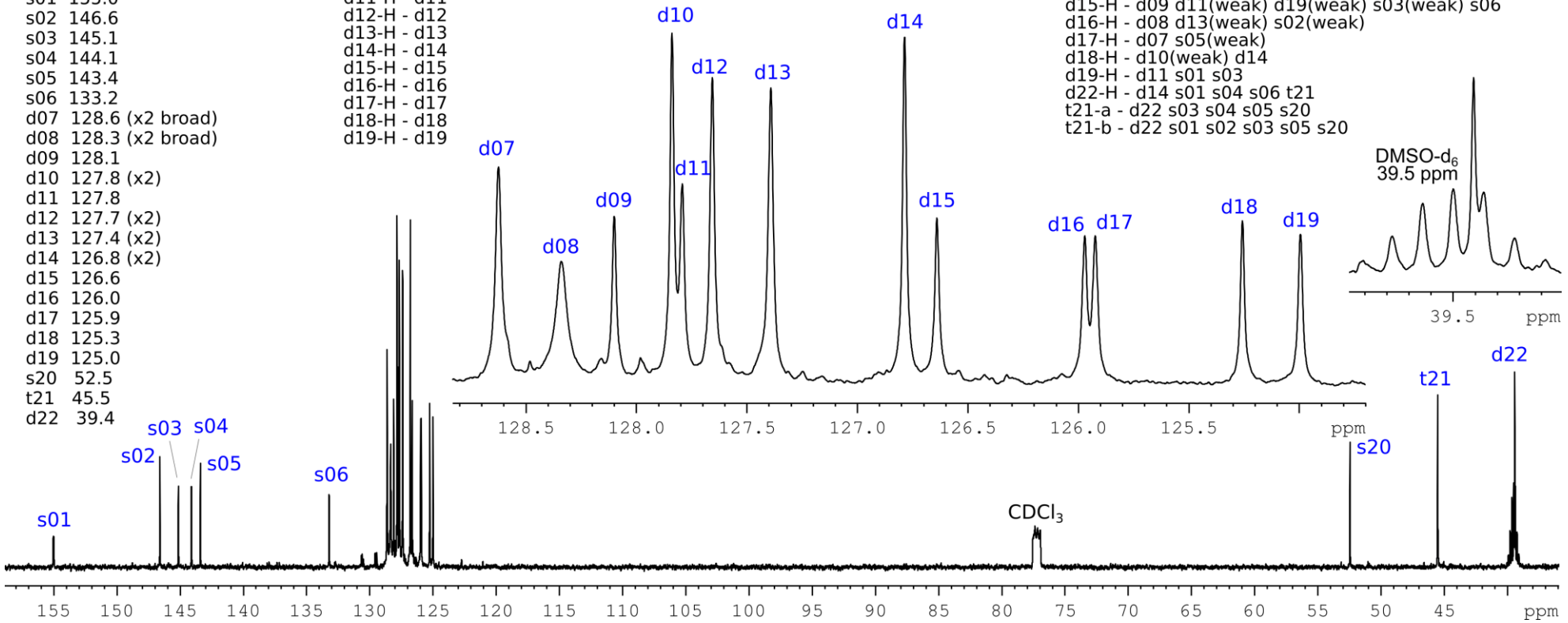
Experiment Bruker_60
2D 13C-1H via onebond (HSQC arom)
d07-H - d07
d08-H - d08
d09-H - d09
d10-H - d10
d11-H - d11
d12-H - d12
d13-H - d13
d14-H - d14
d15-H - d15
d16-H - d16
d17-H - d17
d18-H - d18
d19-H - d19

Experiment Bruker_62
2D 1H-13C via onebond (HXCO)
d07 - d07-H
d08 - d08-H
d09 - d09-H
d10 - d10-H
d11 - d11-H
d12 - d12-H
d13 - d13-H
d14 - d14-H
d15 - d15-H
d16 - d16-H
d17 - d17-H
d18 - d18-H
d19 - d19-H

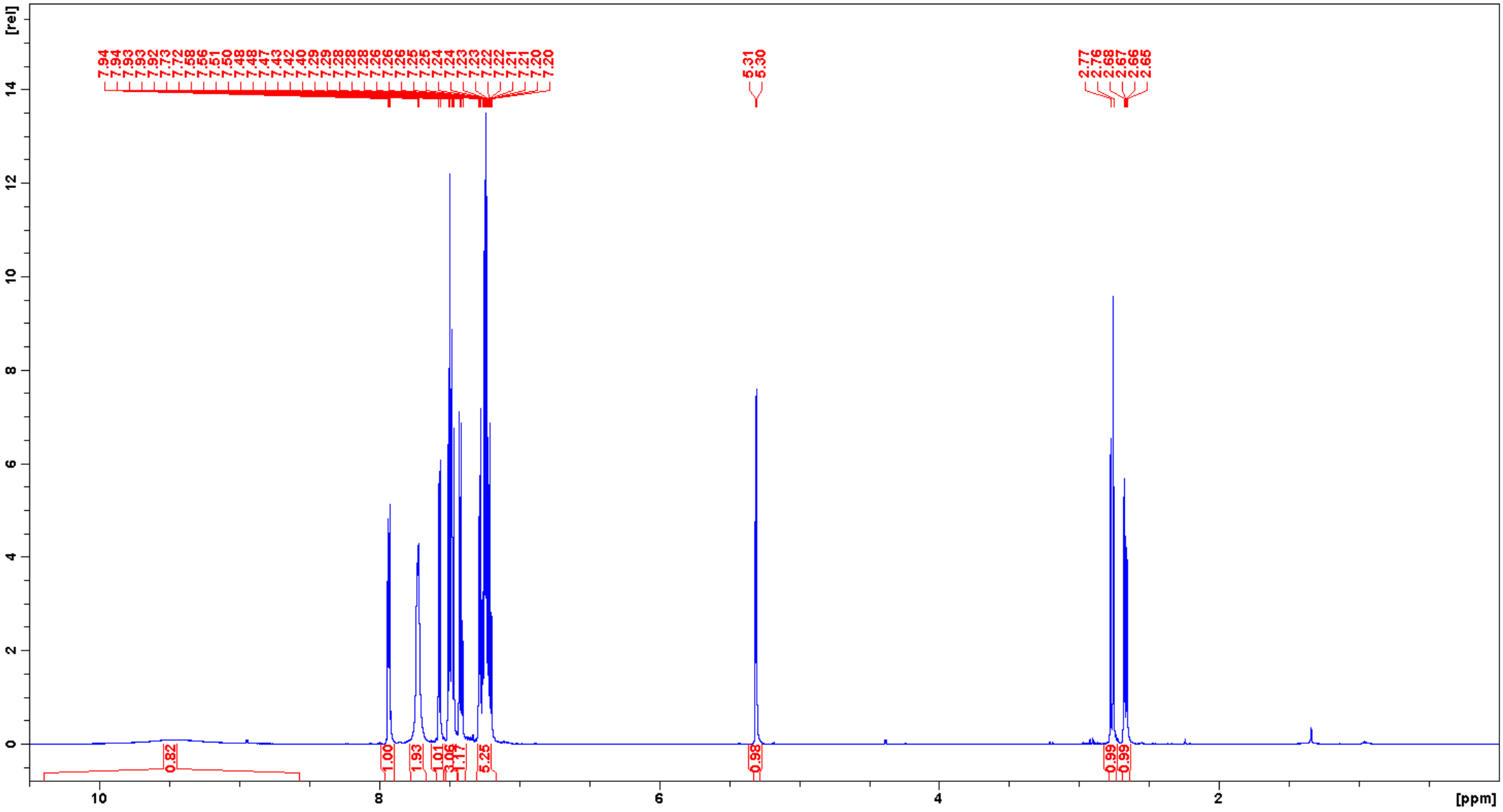
Experiment Bruker_63
2D 1H-13C via Jmultibond (COLOC)
d10 - d14-H
d11 - d19-H
d14 - d14-H
d15 - d09-H
d16 - d08-H
s01 - t21-b
s02 - d13-H
s03 - d19-H t21-a t21-b
s04 - d22-H t21-a
s05 - t21-a
s06 - d09-H

Experiment Bruker_53
2D 13C-1H via Jcoupling (HMBC)
d09-H - d15 s01(weak) s06 s20
d11-H - s03 s06(weak)
d12-H - s05
d13-H - s02
d14-H - d22
d15-H - s03(weak) s06
d18-H - s04(weak)
d19-H - d11 s01 s03
d22-H - d14 s01 s04 s06 t21
t21-a - d22 s03 s04 s05 s20
t21-b - d09(weak) d22 s01 s02 s03 s05 s20

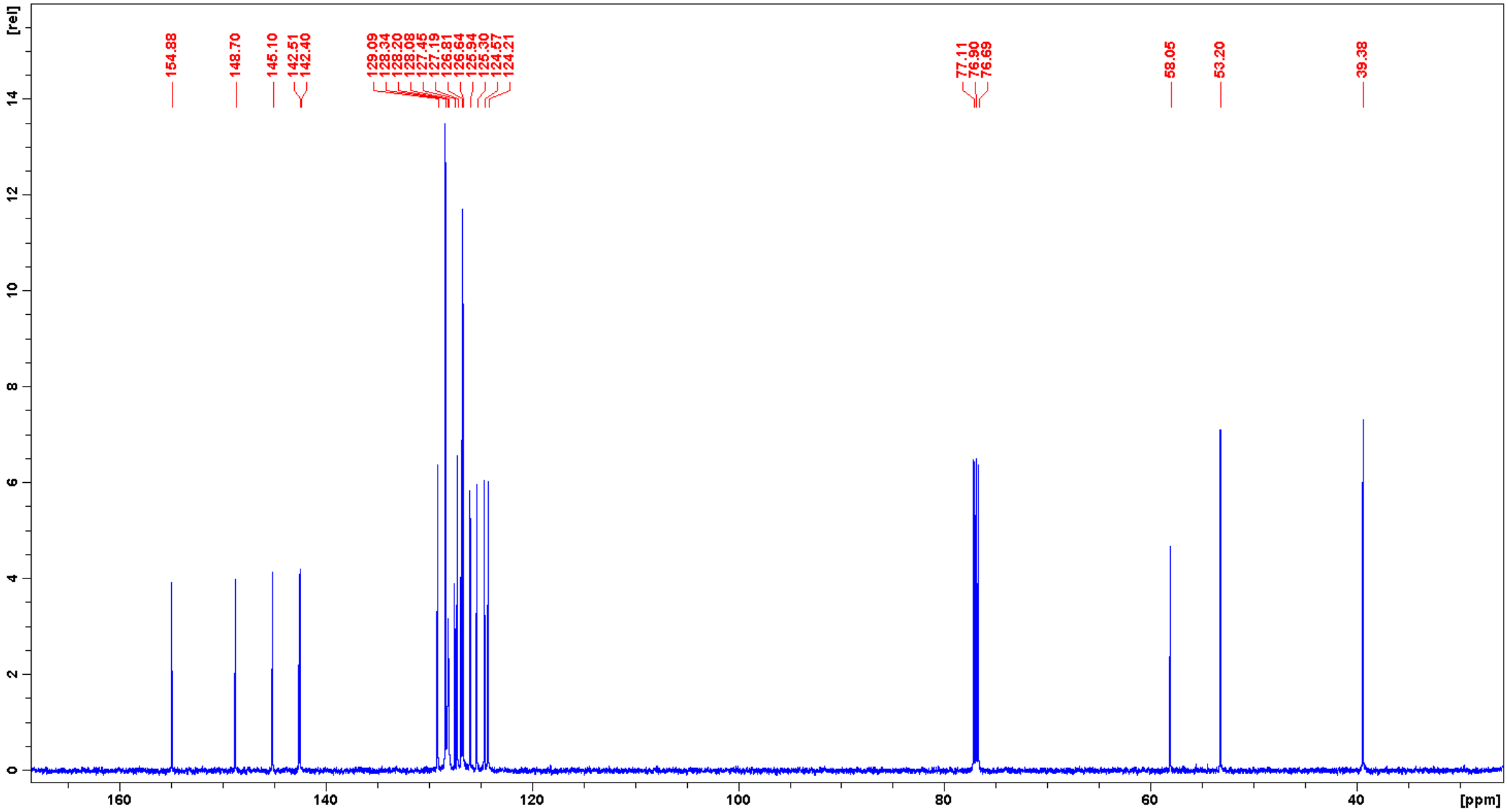
Experiment Bruker_61
2D 13C-1H via Jcoupling (HMBC arom)
d09-H - d15 s01(weak) s06
d10-H - d18(weak) s04
d11-H - d15(weak) d19 s03 s06(weak)
d12-H - d07(weak) d12 d17(weak) s05
d13-H - d08(weak) d13 s02
d14-H - d14 d18 d22
d15-H - d09 d11(weak) d19(weak) s03(weak) s06
d16-H - d08 d13(weak) s02(weak)
d17-H - d07 s05(weak)
d18-H - d10(weak) d14
d19-H - d11 s01 s03
d22-H - d14 s01 s04 s06 t21
t21-a - d22 s03 s04 s05 s20
t21-b - d22 s01 s02 s03 s05 s20



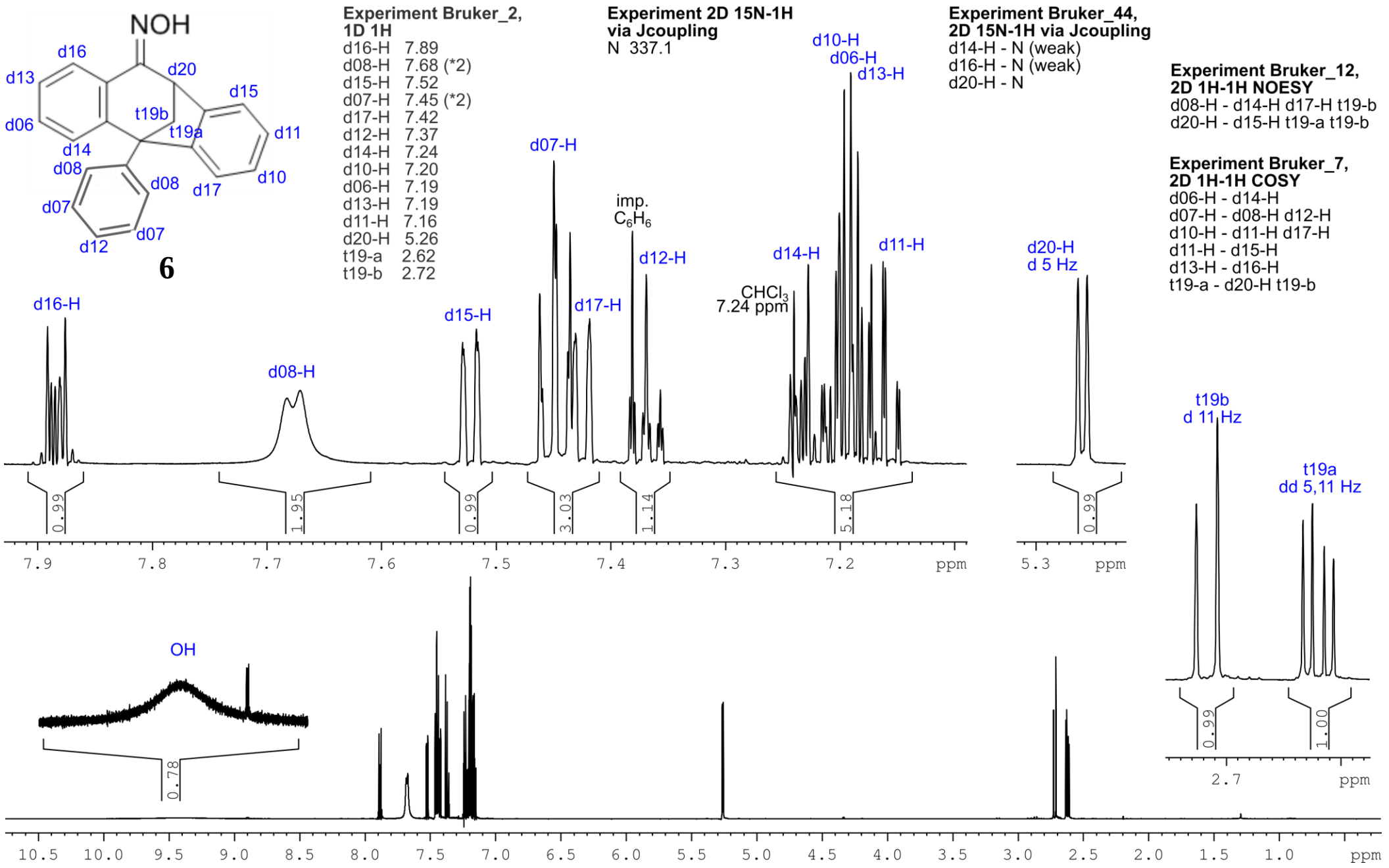
^{1}H NMR spectrum of oxime 6 at 25 ^{o}C (600.3 MHz, $CDCl_3$)



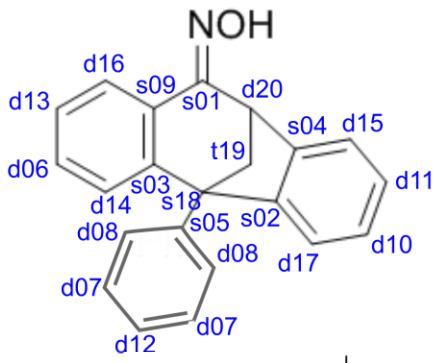
^{13}C NMR spectrum of oxime 6 in $CDCl_3$ at 27 ^{o}C (151 MHz, $CDCl_3$)



Signal assignment for ^{1}H NMR spectrum of oxime 6 at 25 ^{o}C (600.3 MHz, $CDCl_3$)



Signal assignment for ^{13}C NMR spectrum of oxime 6 in $CDCl_3$ at 27 ^{o}C (151 MHz, $CDCl_3$)



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Experiment Bruker_1, 1D 13C:

s01	154.9
s02	148.7
s03	145.1
s04	142.5
s05	142.4
d06	129.1
d07	128.4 (*2)
d08	128.1 (*2)
s09	127.4
d10	127.2
d11	126.8
d12	126.7
d13	126.7
d14	126.0
d15	125.3
d16	124.6
d17	124.2
s18	58.1
t19	53.2
d20	39.4

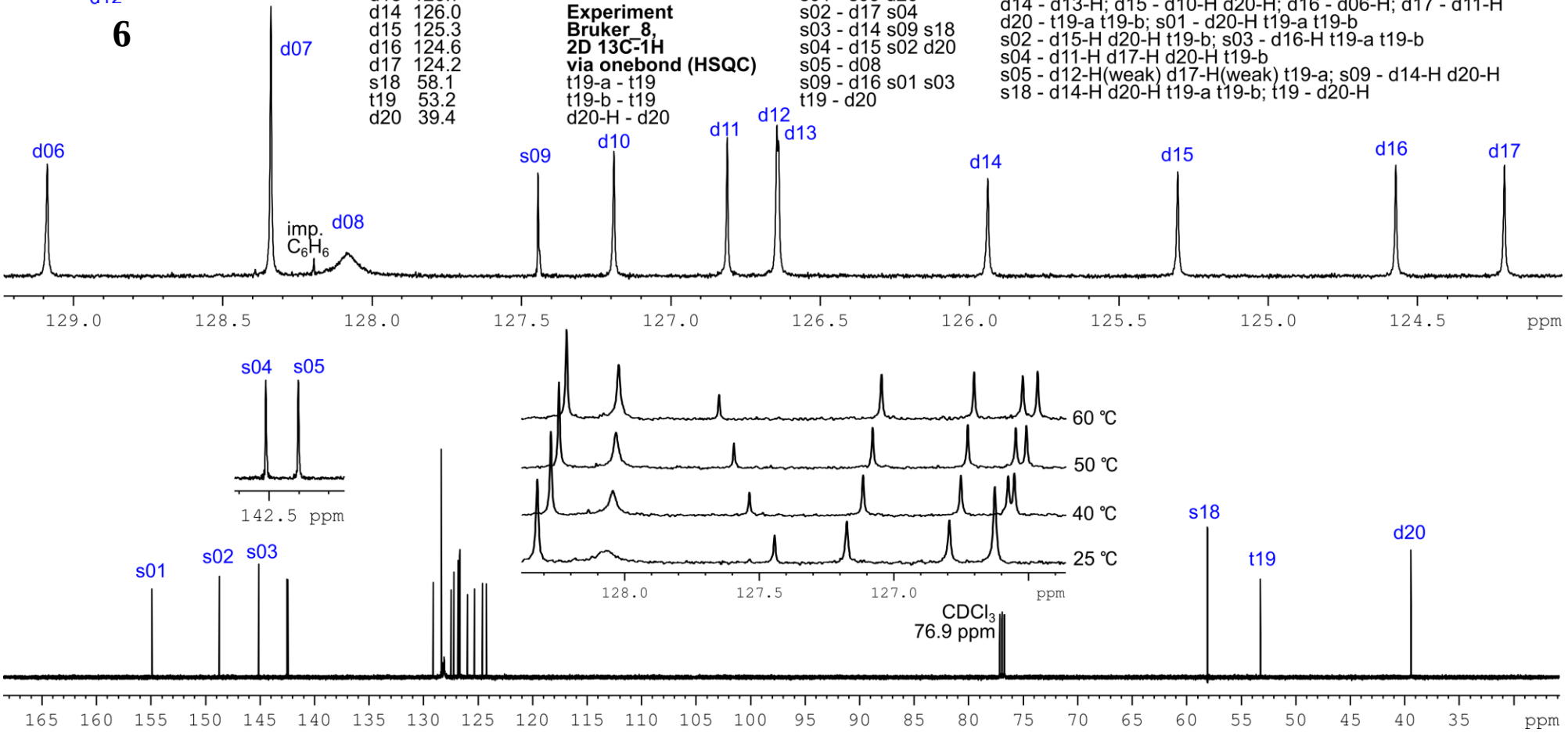
Experiment Bruker_10, 2D 13C-1H via onebond (HSQC)
d06-H - d06
d07-H - d07(*2)
d08-H - d08(*2)
d10-H - d10
d11-H - d11
d12-H - d12
d13-H - d13
d14-H - d14
d15-H - d15
d16-H - d16
d17-H - d17

Experiment Bruker_8, 2D 13C-1H via onebond (HSQC)
t19-a - t19
t19-b - t19
d20-H - d20

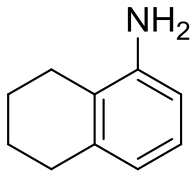
Experiments Bruker_14,25 2D 13C-13C via Jcoupling (INADEQUATE)
d06 - d13 d14
d07 - d12; d08 - s05
d10 - d17; d11 - d15
d12 - d07
d13 - d06 d16
d14 - d06 s03
d15 - d11 s04
d16 - d13 s09
d17 - d10 s02
d20 - s01 s04 t19
s01 - s09 d20
s02 - d17 s04
s03 - d14 s09 s18
s04 - d15 s02 d20
s05 - d08
s09 - d16 s01 s03
t19 - d20

Experiment Bruker_9, 2D 13C-1H via Jcoupling (HMBC)
d06-H - d16 s03; d07-H - d07 s05; d10-H - d15 s02
d11-H - d17 d20(weak) s02(weak) s04
d12-H - d08 s05(weak); d13-H - d14 s09
d14-H - d13 s01(weak) s03(weak) s09 s18
d15-H - d10 d17(weak) d20 s02
d16-H - d06 d14(weak) s01 s03 s09(weak) s18(weak)
d17-H - d11 s04 s18
d20-H - d15 s01 s02 s03(weak) s04 s09 s18 t19
t19-a - d14(weak) d20 s01 s02 s03 s04 s18
t19-b - d15(weak) d17(weak) d20 s01 s02 s03 s04 s18

Experiment Bruker_13, 2D 1H-13C via Jmultibond (COLOC)
d06 - d14-H(weak) d16-H; d07 - d07-H d12-H(weak)
d10 - d15-H; d11 - d17-H; d12 - d08-H; d13 - d14-H
d14 - d13-H; d15 - d10-H d20-H; d16 - d06-H; d17 - d11-H
d20 - t19-a t19-b; s01 - d20-H t19-a t19-b
s02 - d15-H d20-H t19-b; s03 - d16-H t19-a t19-b
s04 - d11-H d17-H d20-H t19-b
s05 - d12-H(weak) d17-H(weak) t19-a; s09 - d14-H d20-H
s18 - d14-H d20-H t19-a t19-b; t19 - d20-H



^{1}H NMR spectrum of compound 7 at 25 ^{o}C (500 MHz, $CDCl_3$)



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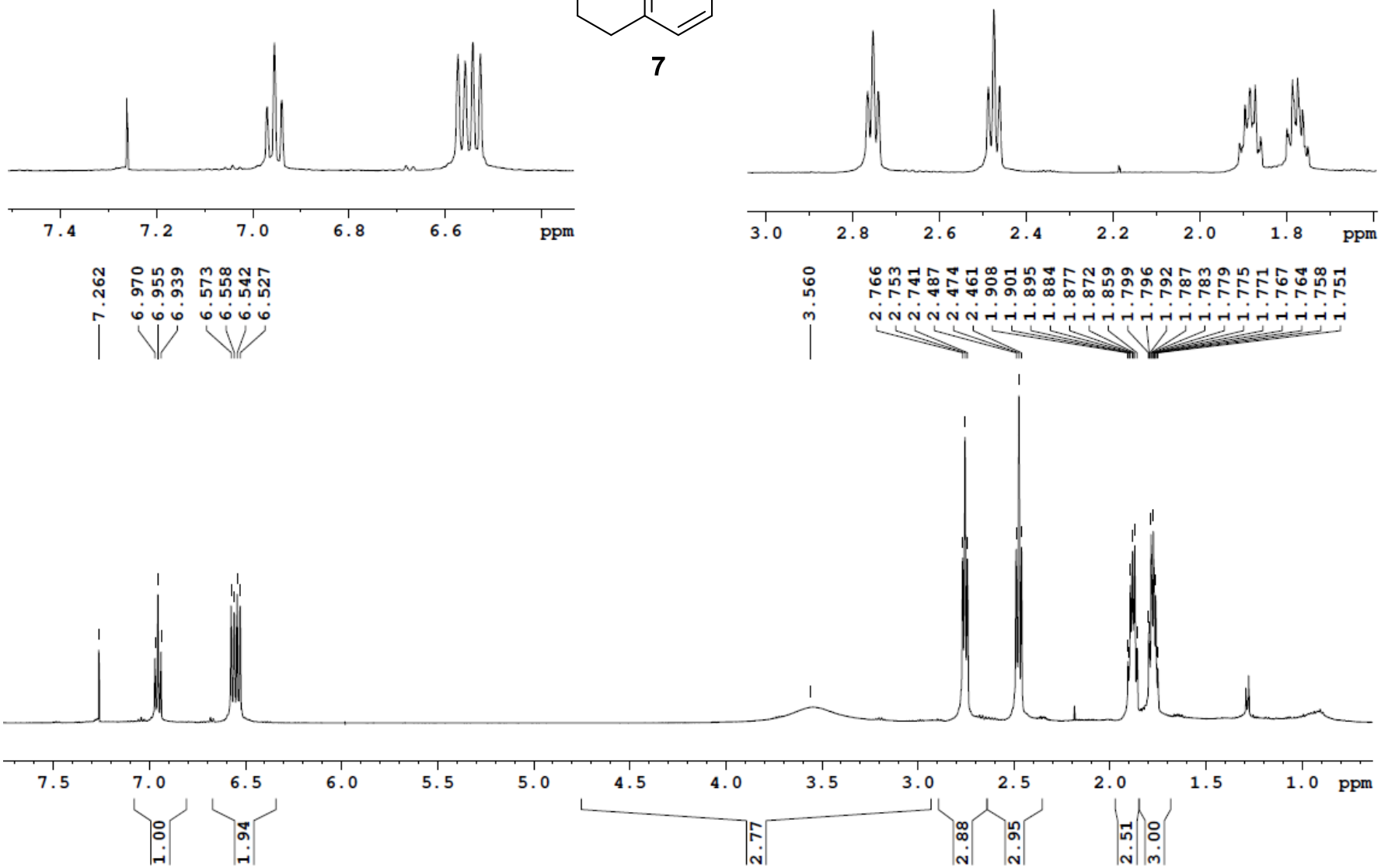
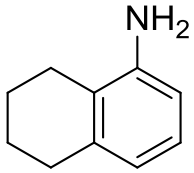


^{13}C NMR spectrum of compound 7 in $CDCl_3$ at 25 ^{o}C (125 MHz, $CDCl_3$)



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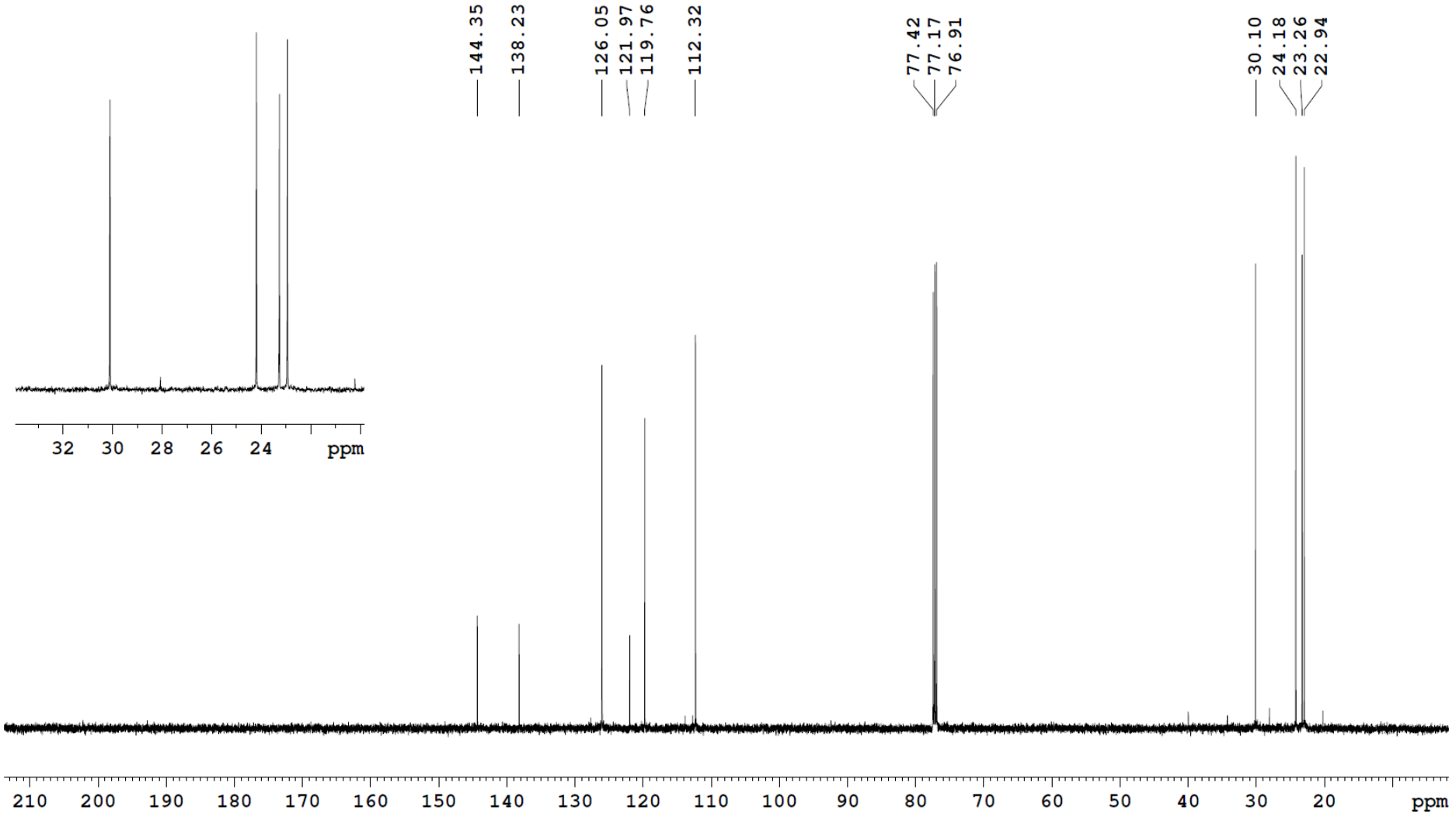
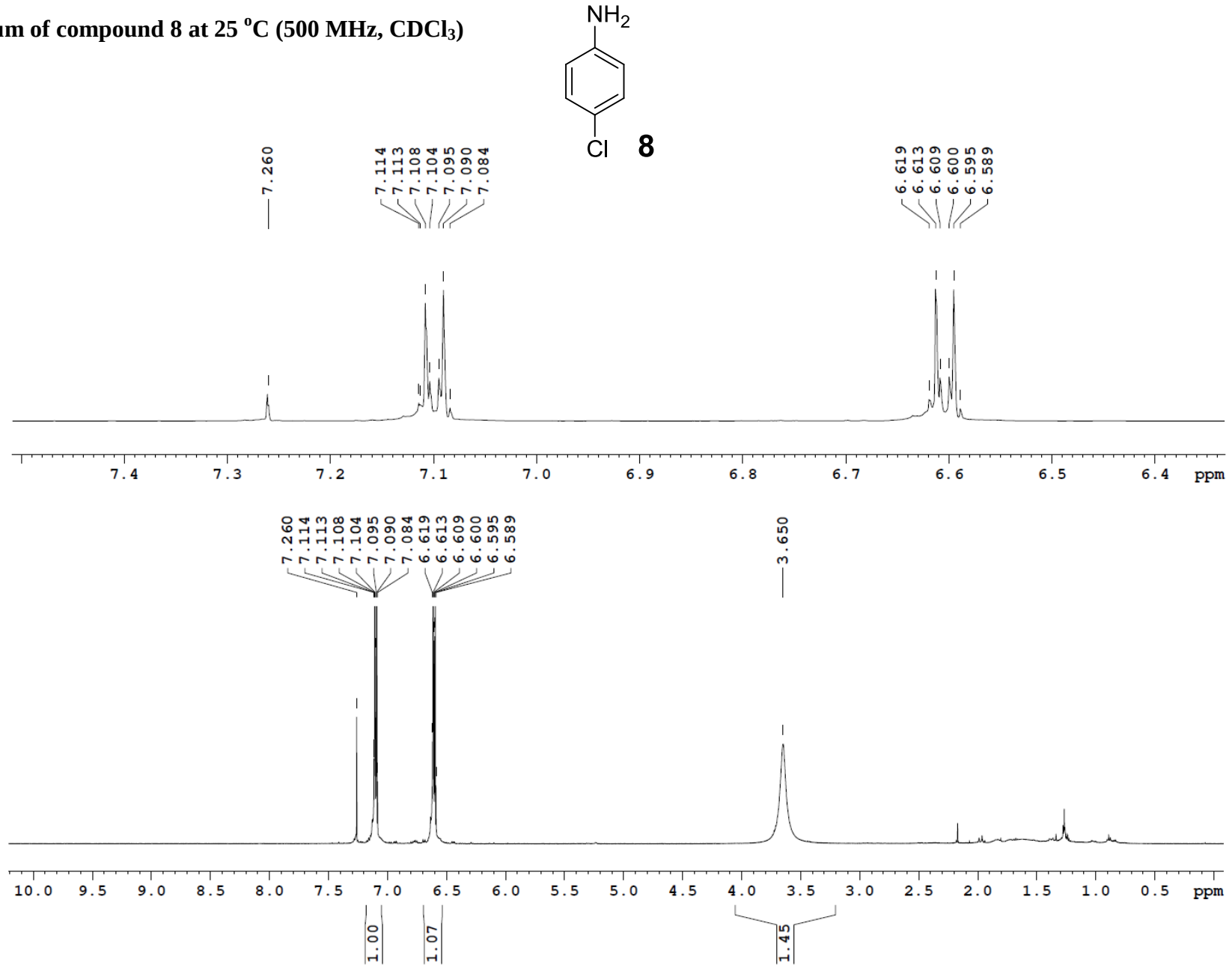
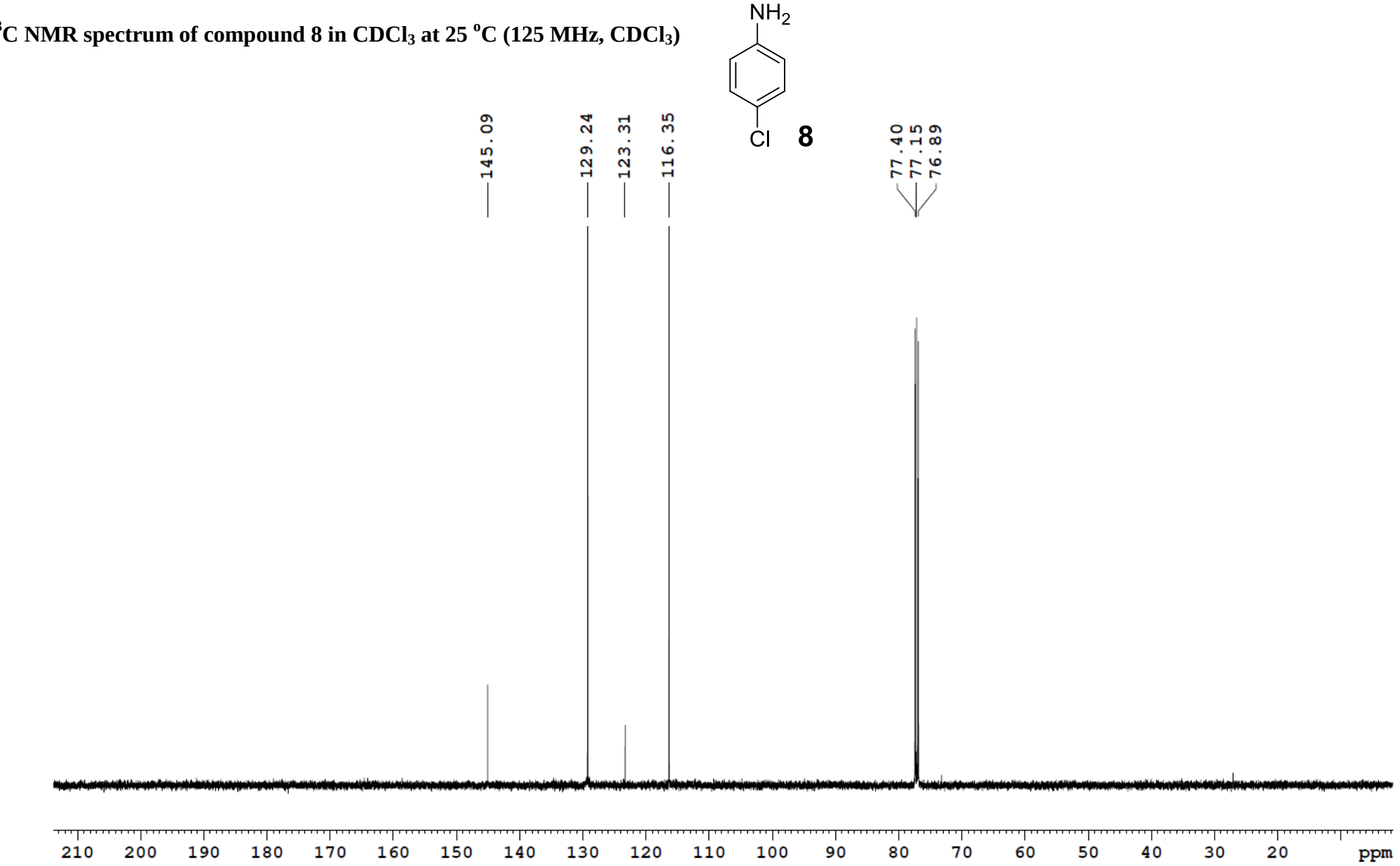


^{1}H NMR spectrum of compound 8 at 25 ^{o}C (500 MHz, $CDCl_3$)

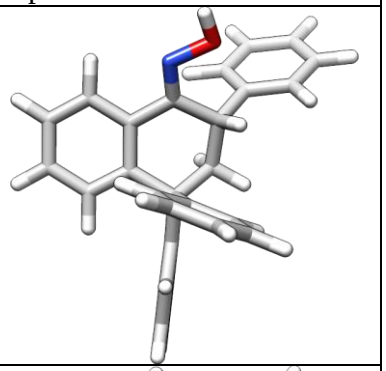
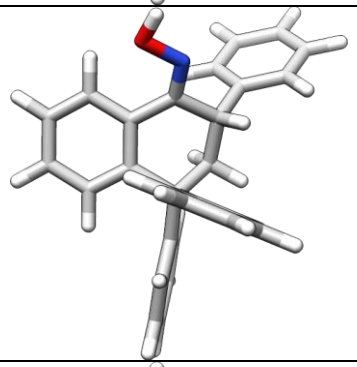
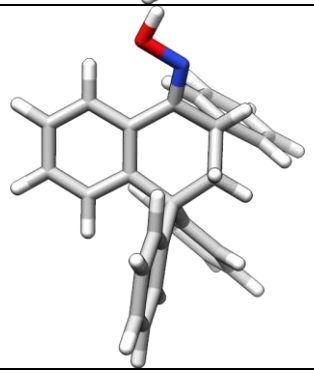
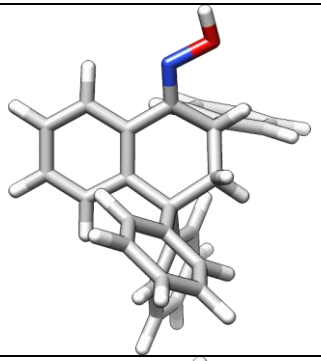
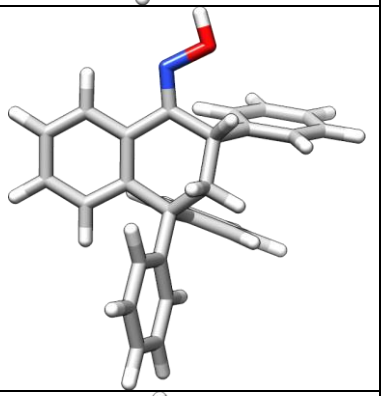
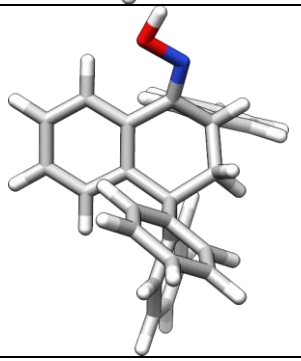


^{13}C NMR spectrum of compound 8 in $CDCl_3$ at 25 ^{o}C (125 MHz, $CDCl_3$)



3. Conformational analysis of oxime 5

Conformers **5a-f** were generated by the molecular mechanics method using ChemAxon Marvin (*conformers* plugin) [S3]. The structures were optimized by DFT/PBE/Λ1. Only structures with the *s-trans* fragment C=N-O-H are reported (*s-cis* ones are less stable).

Conformer	$\Delta E_{DFT}+\Delta G_{298}$, kcal/mol	Spatial structure
5a	0	
5b	3.7	
5c	4.5	
5d	6.8	
5e	8.8	
5f	9.0	

[S3] Imre, G., Jakli, I., Kalaszi, A., and Farkas, O., *Advanced Automatic Generation of 3D Molecular Structures. 1st European Chemistry Congress*, Budapest, Hungary, August 27–31, 2006.

53 Oxime **5,** conformer **5a**

Energy -1209.546778789 Dipole 0.395766 ZPE 0.421482 G(298.15) 229.23

C	-0.04484931	-1.92656230	-2.90782243
C	0.95752462	-1.65471169	-3.83322748
C	1.84055420	-0.59548676	-3.60507014
C	1.71596063	0.17992593	-2.45094772
C	0.71428453	-0.07989515	-1.50756313
C	-0.18433585	-1.14673544	-1.74544166
C	-1.28815177	-1.40041864	-0.80004707
C	0.53699633	0.76694994	-0.23755388
C	0.18517453	-0.24307675	0.89664583
C	-1.13727220	-0.99732255	0.65597183
N	-2.36379445	-1.90937360	-1.30512799
O	-3.36788688	-2.08971004	-0.32603710
C	-1.22170645	-2.17901650	1.61700571
C	-0.62067529	1.77713956	-0.39084516
C	-0.53607760	-4.41244614	2.29405939
C	-0.50663562	-3.36099400	1.37626316
C	-1.96262572	-2.07429529	2.80092790
C	-1.99060592	-3.12198931	3.72387743
C	-1.27676543	-4.29616783	3.47336943
C	-1.23858718	2.03009290	-1.62195003
C	-2.27879330	2.95948023	-1.72837930
C	-2.72192906	3.65432242	-0.60356128
C	-2.11140467	3.41563769	0.63141423
C	-1.07338140	2.48999332	0.73371826
C	1.85184367	1.50143826	0.10754538
C	2.01265717	2.87479218	-0.13138349
C	2.95385292	0.79474484	0.62003076
C	4.15905282	1.43871327	0.90277232
C	4.29884962	2.80892618	0.66974079
C	3.22040942	3.52187938	0.14605258
H	-0.74911760	-2.74655449	-3.06467155
H	1.05553638	-2.27201061	-4.73018693
H	2.63388810	-0.37369606	-4.32385148
H	2.41076109	1.00429199	-2.27531089
H	0.99680504	-0.98305983	0.96714382
H	0.13728260	0.27025245	1.86983646
H	-1.98697017	-0.32753968	0.88093814
H	-4.09584609	-2.43937784	-0.87112628
H	0.02219321	-5.32945236	2.08631152
H	0.07218994	-3.46327621	0.45291430
H	-2.53355288	-1.16083672	2.99548481
H	-2.57754744	-3.02217836	4.64107354
H	-1.30007121	-5.11920337	4.19246699
H	-0.90522637	1.49196287	-2.51209660
H	-2.74397423	3.13644371	-2.70194734
H	-3.53619139	4.37910655	-0.68571138
H	-2.44314679	3.95707217	1.52167470
H	-0.59379573	2.33356884	1.70396031
H	1.17964723	3.45047200	-0.54017901
H	2.88317554	-0.28144516	0.79272036
H	4.99637320	0.86188841	1.30499208
H	5.24246602	3.31423165	0.89178450
H	3.31343915	4.59350591	-0.05065723

53 Oxime **5,** conformer **5b**

Energy -1209.540888852 Dipole 0.478739 ZPE 0.421578 G(298.15) 229.21

C	-1.25752060	-0.07164520	-3.17088732
C	-1.63690590	1.16801912	-3.67978094
C	-1.62409501	2.29091550	-2.85176619
C	-1.20783087	2.17251558	-1.52389647
C	-0.80456964	0.94069523	-0.99850766
C	-0.84412021	-0.20862877	-1.83169379
C	-0.45291408	-1.51347681	-1.26357810
C	-0.29477387	0.78980049	0.44434015
C	0.96225735	-0.12355345	0.32512011
C	0.62032533	-1.54140683	-0.16668947
N	-0.92413913	-2.68688260	-1.52534287
O	-1.94505125	-2.70459140	-2.51068565
C	1.88588533	-2.26286817	-0.60996044
C	0.08994418	2.16455455	1.03382206
C	3.72095631	-2.55358835	-2.18119829
C	2.54030104	-1.91459991	-1.80180616
C	2.44545036	-3.26679282	0.19002139
C	3.62941578	-3.90773255	-0.18532373
C	4.27188544	-3.55251151	-1.37256100
C	1.32852126	2.76324139	0.75018846
C	1.65382227	4.02521167	1.25234682
C	0.74331081	4.72627759	2.04505283
C	-0.49620579	4.15011695	2.32754060
C	-0.81608340	2.88503982	1.82920403
C	-1.33611866	0.10824329	1.35775497
C	-0.96621079	-0.26942522	2.66049148
C	-2.65371888	-0.13351080	0.95021249
C	-3.57332638	-0.74018645	1.81253136
C	-3.19072108	-1.11810076	3.09904337
C	-1.87924015	-0.87806427	3.52079043
H	-1.28012704	-0.95537758	-3.80722765
H	-1.94830328	1.25411974	-4.72411929
H	-1.93146274	3.26652987	-3.23793808
H	-1.18547838	3.05743949	-0.88448174
H	1.66037847	0.33795388	-0.39017579
H	1.48701422	-0.19222030	1.29113907
H	0.18996222	-2.10769406	0.67568128
H	-2.17487783	-3.65142841	-2.50272658
H	4.21376087	-2.27271113	-3.11607024
H	2.11179149	-1.14112101	-2.44717024
H	1.94071290	-3.55435413	1.11777880
H	4.04830918	-4.69132996	0.45200817
H	5.19640362	-4.05408730	-1.67041966
H	2.05827672	2.24844617	0.12211406
H	2.62851872	4.46218914	1.01859202
H	0.99824025	5.71368362	2.43886502
H	-1.22358267	4.68555740	2.94393085
H	-1.78805292	2.44595334	2.06571617
H	0.04846693	-0.06702528	3.01501842
H	-2.96798153	0.15285378	-0.05603333
H	-4.59616332	-0.91754860	1.46917623
H	-3.90821174	-1.59436466	3.77242791
H	-1.56612392	-1.16252931	4.52913212

53 Oxime **5**, conformer **5c**

Energy -1209.535390345 Dipole 0.378821 ZPE 0.421908 G(298.15)

C	1.23175027	-3.26140304	0.55906173
C	2.46640337	-3.27741915	-0.07753990
C	3.05193032	-2.07533320	-0.48368436
C	2.38253977	-0.87615638	-0.26044496
C	1.11996253	-0.83436094	0.35192669
C	0.53647361	-2.05134570	0.78698602
C	-0.79069026	-2.03751987	1.43360794
C	0.45757307	0.54439364	0.54908946
C	-0.83698312	0.42157390	1.41230790
C	-1.67797911	-0.84427243	1.14186939
N	-1.32270325	-2.86354778	2.27553360
O	-0.49902835	-3.96551966	2.63389726
H	-2.46819851	-0.86933566	1.91440455
C	0.06427638	1.18797126	-0.80299527
C	0.18084146	0.52722559	-2.03136210
C	-0.23055620	1.13573080	-3.22154794
C	-0.76374365	2.42337938	-3.21087127
C	-0.88950435	3.09722805	-1.99286041
C	-0.48574834	2.48366371	-0.80812995
C	1.49469498	1.41484597	1.31597240
C	2.17141326	2.49405570	0.73020068
C	1.84732310	1.06154222	2.63111856
C	2.80586108	1.77992707	3.34400495
C	3.45341879	2.86902661	2.75402357
C	3.13670075	3.21523765	1.44142951
H	0.77830270	-4.19305546	0.89202324
H	2.97755527	-4.22849487	-0.24808466
H	4.03182862	-2.07038391	-0.96846430
H	2.84951001	0.06478726	-0.56266821
H	-0.56398525	0.39692674	2.47828719
H	-1.44810819	1.32488127	1.26651008
C	-2.39261578	-0.90427244	-0.20854485
H	-1.07925954	-4.41294667	3.27633210
H	0.58359618	-0.48619127	-2.06542488
H	-0.13698562	0.58788557	-4.16294552
H	-1.08424281	2.89873501	-4.14161474
H	-1.30619324	4.10787096	-1.96339833
H	-0.58832676	3.03097991	0.13346756
H	1.94450773	2.78158371	-0.29809897
H	1.38560004	0.18981229	3.10310699
H	3.05531023	1.47973680	4.36536409
H	4.20538585	3.43395727	3.31107728
H	3.64402425	4.05391452	0.95654211
C	-3.27339449	0.12754994	-0.56867699
C	-3.98784888	0.07966721	-1.76480062
C	-3.84210724	-1.01022080	-2.62773654
C	-2.98174670	-2.04999118	-2.27480635
C	-2.26773154	-1.99817142	-1.07433437
H	-3.40431733	0.98566572	0.09724906
H	-4.66505904	0.89792583	-2.02410808
H	-4.40170028	-1.04950563	-3.56599180
H	-2.86446361	-2.91352751	-2.93539983
H	-1.60356220	-2.82470659	-0.81085871

53 Oxime **5**, conformer **5d**

Energy -1209.537188853 Dipole 0.303762 ZPE 0.421751 G(298.15) 230.05

C	2.73153450	-0.64299996	2.05103138
C	2.45387110	-0.03787717	3.26879057
C	1.33140261	0.79003225	3.38278848
C	0.52502571	1.02159273	2.27168614
C	0.80480850	0.44562862	1.02124392
C	1.91740603	-0.41805938	0.92106643
C	2.18940663	-1.15398003	-0.32546845
C	-0.03061901	0.85726538	-0.20614508
C	0.24534064	-0.07338024	-1.45507081
C	1.02621546	-1.39805367	-1.25184882
N	3.39942744	-1.56236875	-0.51958395
O	3.52151107	-2.33986543	-1.69909653
C	0.17525742	-2.60693372	-0.86353689
C	-1.52659594	0.84008446	0.19403673
C	0.38337181	2.27844823	-0.67066939
C	-0.64896744	-3.17880117	-1.84736873
C	-1.46408149	-4.27324656	-1.55896823
C	-1.46435964	-4.82697239	-0.27528678
C	-0.63890442	-4.27807604	0.70688733
C	0.17478969	-3.17889834	0.41583564
C	-0.33713133	2.88589970	-1.71660402
C	0.03285154	4.13178101	-2.21987140
C	1.14038410	4.80345805	-1.69229719
C	1.86707160	4.21035738	-0.66141941
C	1.49258469	2.95979829	-0.15567518
C	-2.25116832	-0.36213602	0.20362870
C	-3.58558163	-0.39889225	0.61297153
C	-4.23033251	0.76709908	1.03042485
C	-3.52173293	1.96914401	1.03598616
C	-2.18690797	2.00378816	0.62347238
H	3.57875159	-1.32326105	1.93826240
H	3.09393559	-0.22713077	4.13457725
H	1.08193794	1.25486224	4.34031889
H	-0.34630482	1.67259922	2.36984710
H	-0.71366123	-0.29361257	-1.94996577
H	0.83807160	0.51787950	-2.16788604
H	1.45746330	-1.64469337	-2.23616404
H	4.48295983	-2.49693021	-1.71351862
H	-0.64740315	-2.75816654	-2.85848708
H	-2.09598361	-4.70111268	-2.34211129
H	-2.09984544	-5.68630822	-0.04575915
H	-0.62525499	-4.70589313	1.71300146
H	0.80897534	-2.75910892	1.19976876
H	-1.21031608	2.37667626	-2.13433973
H	-0.54885304	4.58231804	-3.02887870
H	1.43242148	5.78091319	-2.08516211
H	2.73821281	4.71964735	-0.24019260
H	2.07894507	2.51267626	0.64937680
H	-1.77016538	-1.29300890	-0.10291827
H	-4.12128428	-1.35201983	0.60581666
H	-5.27573763	0.73886329	1.34898313
H	-4.00822282	2.89324768	1.36041574
H	-1.65452000	2.95772694	0.62407581

53 Oxime **5**, conformer **5e**

Energy -1209.541736151 Dipole 0.233523 ZPE 0.421784 G(298.15) 230.55

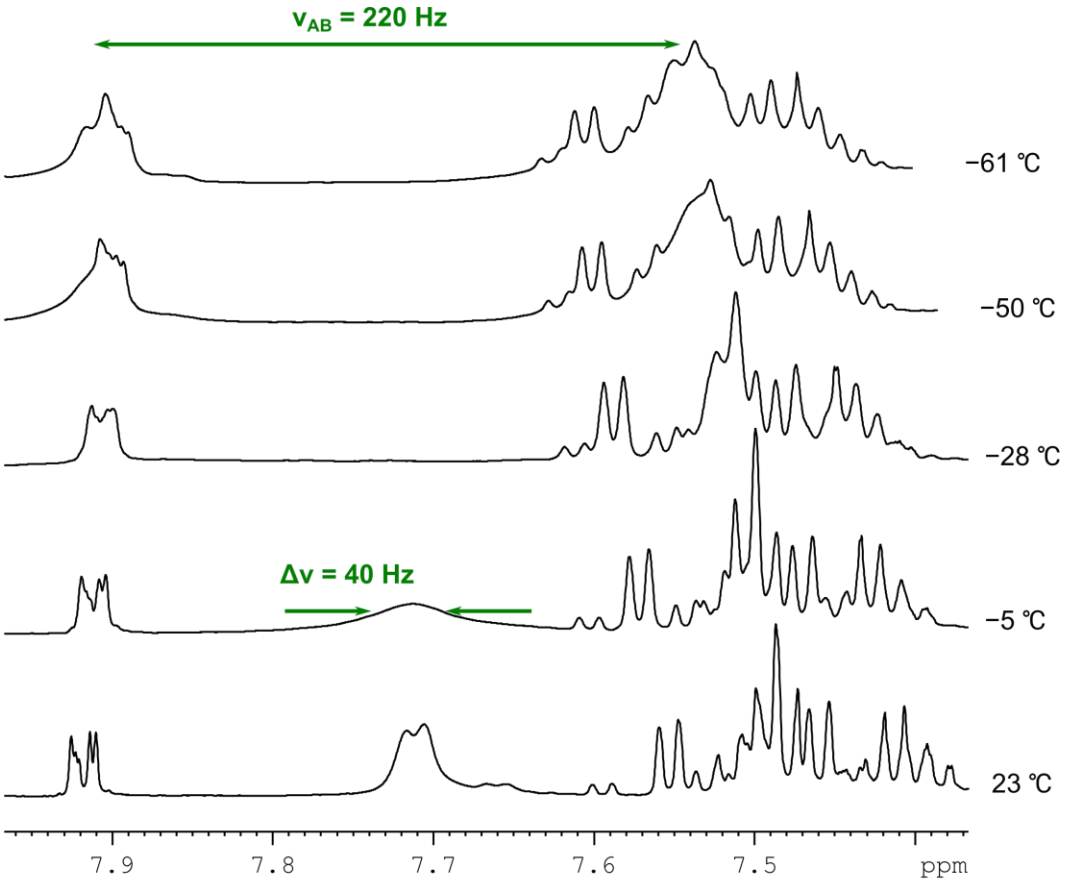
C	1.38288469	-3.42766063	0.72511756
C	2.74838346	-3.46930431	0.48762485
C	3.45181116	-2.27580462	0.28592138
C	2.77115888	-1.06277267	0.32663552
C	1.38616175	-0.99799239	0.55719694
C	0.67717278	-2.20435298	0.75967514
C	-0.77835481	-2.21413412	1.01961022
C	0.67688166	0.36603225	0.54657220
C	-0.59777962	0.26054255	1.43487153
C	-1.54637102	-0.91593793	1.11994290
N	-1.32407545	-3.37333374	1.20508322
O	-2.70614334	-3.26921586	1.47781103
H	-2.19775510	-1.03447369	2.00611670
C	0.31105509	0.77762424	-0.90000292
C	0.84814167	0.12855638	-2.02004252
C	0.52501934	0.53600606	-3.31807184
C	-0.34504171	1.60499448	-3.52624669
C	-0.88528090	2.26664246	-2.42064545
C	-0.55824272	1.85878776	-1.12825861
C	1.60379098	1.42545839	1.20249490
C	2.04005307	2.57900995	0.53790946
C	2.05229870	1.22135382	2.52085596
C	2.88064413	2.14435479	3.15668815
C	3.29346220	3.29924862	2.48538661
C	2.87385166	3.50698355	1.17268462
H	0.81432512	-4.34441369	0.89277796
H	3.26981045	-4.42992832	0.46342468
H	4.52935582	-2.29058249	0.10204453
H	3.32173363	-0.13001563	0.18120289
H	-0.26443479	0.14660034	2.47814093
H	-1.16249928	1.20436408	1.39153100
C	-2.50834174	-0.66538624	-0.04281556
H	-2.94146371	-4.20702105	1.59845578
H	1.52549463	-0.71626320	-1.88220617
H	0.95821926	0.00565461	-4.17065958
H	-0.60320406	1.92145893	-4.54026268
H	-1.57072378	3.10625914	-2.56325746
H	-0.98867343	2.40117405	-0.28330681
H	1.73067404	2.75891362	-0.49316388
H	1.77012510	0.30895073	3.05375643
H	3.21219464	1.95624440	4.18157023
H	3.94365001	4.02459970	2.98154742
H	3.19732554	4.39771153	0.62699282
C	-3.58659756	0.20900681	0.15944315
C	-4.48942215	0.48787770	-0.86697171
C	-4.33162791	-0.11258188	-2.11885997
C	-3.26998688	-0.99513193	-2.32662449
C	-2.36899545	-1.27148627	-1.29599466
H	-3.72528620	0.67326844	1.14189541
H	-5.32497172	1.16976555	-0.68578152
H	-5.03755834	0.10115961	-2.92576397
H	-3.13884591	-1.47452273	-3.30040803
H	-1.54400186	-1.96628815	-1.47163759

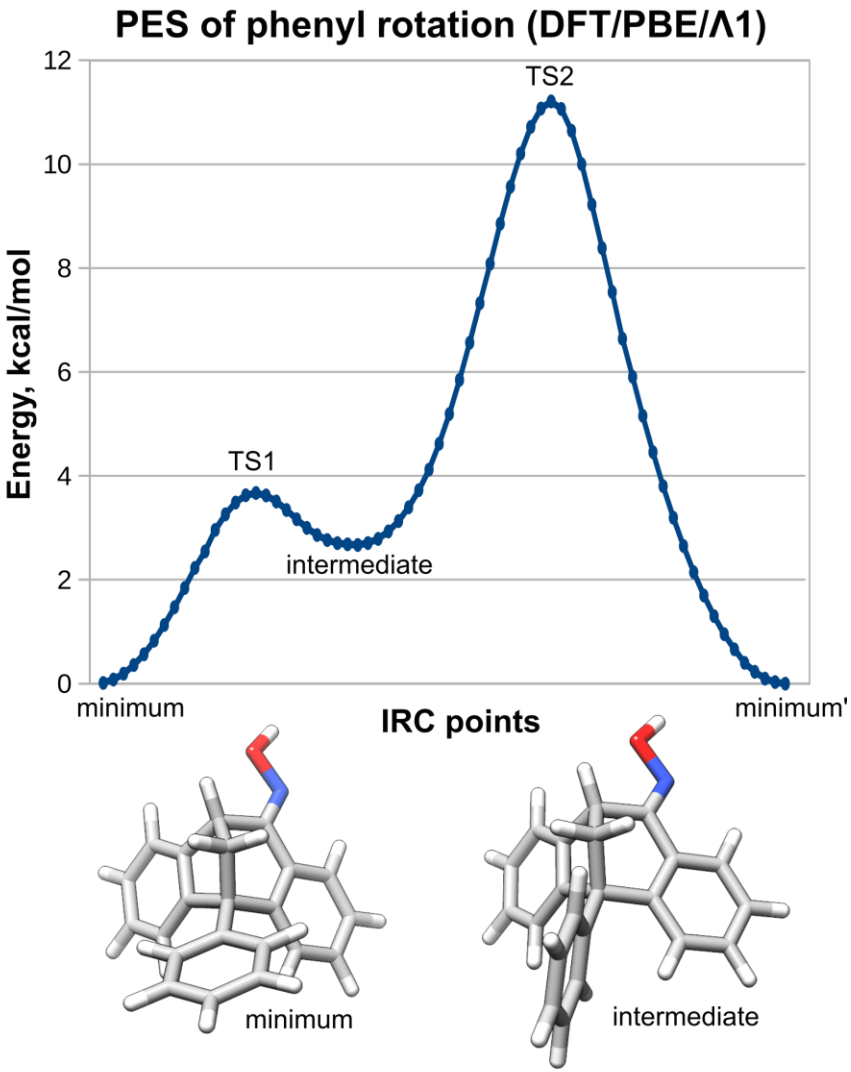
53 Oxime **5**, conformer **5f**

Energy -1209.533937769 Dipole 0.179723 ZPE 0.421752 G(298.15) 230.15

C	-2.82940039	0.64265407	-1.74683718
C	-2.50346954	0.28657690	-3.05071037
C	-1.29619758	-0.36912129	-3.30485628
C	-0.43655805	-0.67453892	-2.25143153
C	-0.74656561	-0.33354211	-0.92647031
C	-1.95945991	0.35201338	-0.67520819
C	-2.22522084	0.85726672	0.68277690
C	0.16716990	-0.81522112	0.21697757
C	-0.05998510	0.00723356	1.55268499
C	-1.00358580	1.23508641	1.49151576
N	-3.34389153	1.01799753	1.30799729
O	-4.48246137	0.60651820	0.56223458
C	-0.32327456	2.54122699	1.08110069
C	1.63895992	-0.69523865	-0.25051717
C	-0.17030342	-2.28863185	0.56442575
C	-0.54226095	3.19792199	-0.13718619
C	0.12011819	4.39301622	-0.43562188
C	1.01074697	4.95716107	0.47811758
C	1.22861659	4.31990447	1.70316174
C	0.56538050	3.12921093	1.99832912
C	-1.21116448	-3.00300740	-0.03996983
C	-1.50132503	-4.31724461	0.34619614
C	-0.75460931	-4.94378457	1.34204412
C	0.28830859	-4.24204802	1.95548009
C	0.57261997	-2.93277330	1.57242911
C	2.26594305	0.56153299	-0.27836410
C	3.57370245	0.70564684	-0.74362434
C	4.28803013	-0.40441627	-1.20091169
C	3.67432839	-1.65704725	-1.19269802
C	2.36422594	-1.79953860	-0.72475494
H	-3.76122650	1.16613892	-1.53422525
H	-3.18680853	0.52790323	-3.86912781
H	-1.02247701	-0.64843847	-4.32584574
H	0.50104233	-1.19504360	-2.45832358
H	-0.49798428	-0.68153956	2.28887398
H	0.91884547	0.32037957	1.94762916
H	-1.36740931	1.39459095	2.52177796
H	-5.18762762	0.77566753	1.21290547
H	-1.23140867	2.77335775	-0.86945111
H	-0.06520738	4.88438761	-1.39468415
H	1.52715150	5.89136696	0.24244019
H	1.91293238	4.75625542	2.43597185
H	0.73592103	2.64405393	2.96532192
H	-1.81288410	-2.53228737	-0.81962108
H	-2.32291864	-4.84944881	-0.14100437
H	-0.98099888	-5.97040645	1.64174936
H	0.88597813	-4.71843579	2.73757093
H	1.39733976	-2.40098528	2.05573657
H	1.72404661	1.44908477	0.05714236
H	4.03404553	1.69737985	-0.75041850
H	5.31331591	-0.29232235	-1.56341421
H	4.21495772	-2.53694193	-1.55241850
H	1.90295742	-2.78953119	-0.72489490

4. Experimental and theoretical evaluation of the rotational barrier of phenyl group in oxime 6





DNMR formula for fast exchange

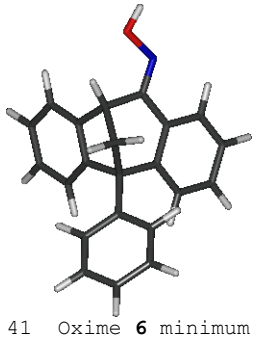
$$k = \frac{\pi\, \nu_{AB}^{\,2}}{2(\Delta\nu - \Delta\nu_{ref})} = 1900\ s^{-1}$$

Euring equation

$\Delta G^{\ddagger} = 1.987\ T\ (23.76 + \ln(T/k)) = 11.6$ kcal/mol (−5 ℃)

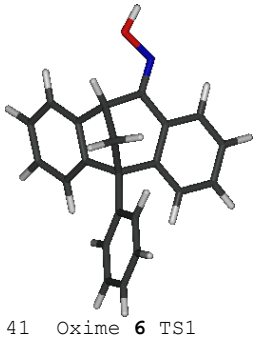
Energy + ΔG(268 K), kcal/mol	
minimum	0.0
TS1	4.4
intermediate	2.9
TS2	11.6

Stationary points on PES of the phenyl rotation in oxime 6



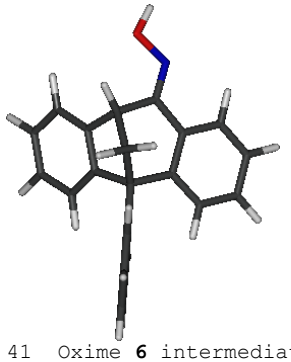
41 Oxime **6** minimum
Energy -977.5443320587 Dipole 0.318311 ZPE 0.322201 G(268) 177.49 kcal

C	-0.96590660	-1.18716444	-1.68161364
C	-1.60892960	0.16902591	-1.43180424
C	-0.78203656	0.92622844	-0.58474930
C	0.46236228	0.09250806	-0.23105501
C	0.52228992	-0.85675963	-1.46640539
C	-1.38201248	-2.13409742	-0.57117743
C	0.02943276	-0.75036273	0.98245426
C	-0.86390365	-1.83551321	0.78500601
C	1.79117590	0.82115275	-0.08028782
C	2.89815004	0.15688622	0.47704435
C	4.15313994	0.76431295	0.52680342
C	4.33360876	2.05140021	0.01356373
C	3.24857701	2.71522610	-0.56006862
C	1.99251715	2.10398736	-0.61071578
C	-2.84602670	0.65305589	-1.84678440
C	-3.25408224	1.91956648	-1.40887831
C	-2.44547464	2.66472976	-0.54536317
C	-1.20787176	2.16711938	-0.11527967
C	0.41877163	-0.42520934	2.28784526
C	-0.01925717	-1.17305505	3.38070015
C	-0.86902737	-2.26562587	3.18153558
C	-1.29166401	-2.58417361	1.89614554
N	-2.15410304	-3.15888900	-0.70867645
O	-2.62294256	-3.30705859	-2.04059809
H	-1.20299299	-1.62246573	-2.66129020
H	1.14639638	-1.74330526	-1.27374010
H	0.92429963	-0.30808423	-2.33310522
H	2.77217307	-0.85173103	0.87984640
H	4.99667591	0.22613504	0.96782521
H	5.31564800	2.52987864	0.05500147
H	3.37692114	3.71786906	-0.97714645
H	1.15830338	2.63005948	-1.08023448
H	-3.48812867	0.05412648	-2.49885731
H	-4.21591211	2.32368264	-1.73561672
H	-2.78303121	3.64468291	-0.19737195
H	-0.59200864	2.74828710	0.57640806
H	1.08654571	0.42482766	2.44646264
H	0.30331252	-0.90090755	4.38927473
H	-1.21351070	-2.85903240	4.03252700
H	-1.97800914	-3.41500141	1.71924314
H	-3.14346929	-4.12631203	-1.95686720



41 Oxime **6** TS1
Energy -977.5384782904 Dipole 0.309809 ZPE 0.322182 G(268) 178.20 kcal

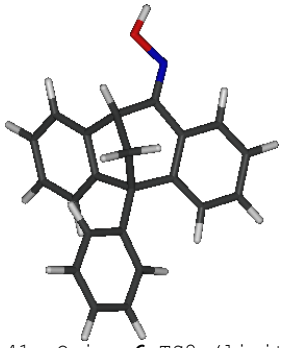
C	-0.92979068	-2.04902116	0.49962808
C	0.58494555	-2.09254477	0.47116921
C	1.09392691	-0.77980864	0.44608449
C	-0.10241858	0.21194521	0.49168069
C	-1.17691150	-0.69165027	1.17104395
C	-1.42029932	-1.96481928	-0.93378084
C	-0.56103359	0.39783904	-0.97283409
C	-1.19835139	-0.68163570	-1.63951717
C	0.05508348	1.54634995	1.22630660
C	1.25347706	2.27528461	1.28027521
C	1.33330411	3.50416335	1.94167057
C	0.20946158	4.04741124	2.56283325
C	-0.99653965	3.34675877	2.50825132
C	-1.06942536	2.11932273	1.84895808
C	1.41340073	-3.20705436	0.39090080
C	2.79485345	-3.01428387	0.28555952
C	3.31218924	-1.71938130	0.22328027
C	2.46954592	-0.60091183	0.28580535
C	-0.35152350	1.59336951	-1.66870358
C	-0.75602813	1.73731576	-2.99643665
C	-1.38575486	0.67573718	-3.65227403
C	-1.60275288	-0.51970845	-2.97642136
N	-1.99331332	-2.92081021	-1.58425886
O	-2.11278783	-4.10416214	-0.80776083
H	-1.39322125	-2.90345994	1.01028001
H	-2.20041840	-0.32553211	1.00178078
H	-0.98127676	-0.75846813	2.25338681
H	2.15129019	1.89466930	0.79853092
H	2.28698370	4.03851167	1.96592148
H	0.27102670	5.00787553	3.08100264
H	-1.89253345	3.75649035	2.98241916
H	-2.03030033	1.60244395	1.81859077
H	0.98560588	-4.21345094	0.40448059
H	3.46681740	-3.87507499	0.23640609
H	4.38979822	-1.56900712	0.11681297
H	2.91989159	0.38675637	0.19574615
H	0.12631310	2.43061041	-1.15494786
H	-0.58280809	2.68323538	-3.51653264
H	-1.70767728	0.78158897	-4.69158828
H	-2.09037354	-1.36390004	-3.46863592
H	-2.58237511	-4.68299402	-1.43511369



41 Oxime **6** intermediate

Energy -977.5400712513 Dipole 0.466370 ZPE 0.322499 G(268) 177.72 kcal

C	-0.92964416	-2.06554130	0.43767706
C	0.58746250	-2.06499785	0.43166202
C	1.05074953	-0.73845307	0.43371786
C	-0.17321952	0.21909698	0.44374490
C	-1.22265846	-0.71446560	1.11610531
C	-1.39139383	-2.00825452	-1.00199032
C	-0.66775982	0.40178042	-1.01697812
C	-1.24265261	-0.70899282	-1.69320005
C	0.05088403	1.53517441	1.18335454
C	1.09149308	2.41424675	0.82700115
C	1.29953526	3.61217897	1.51254108
C	0.46487913	3.97156556	2.57264394
C	-0.58186937	3.12200704	2.92989236
C	-0.78447066	1.92224639	2.24252930
C	1.46321844	-3.14530028	0.39857053
C	2.84006353	-2.89347388	0.39071022
C	3.31126137	-1.57892865	0.40946575
C	2.42282522	-0.49435713	0.42759205
C	-0.60539096	1.62604559	-1.69337067
C	-1.05693759	1.76020929	-3.00722383
C	-1.59436183	0.65910150	-3.67733941
C	-1.69032842	-0.55997357	-3.01775716
N	-1.87825444	-2.99962025	-1.66962438
O	-1.94408041	-4.18809181	-0.89364393
H	-1.37161196	-2.93308432	0.94543255
H	-2.25568217	-0.36698997	0.95771849
H	-1.01935904	-0.80218971	2.19557797
H	1.74203105	2.17203027	-0.01572920
H	2.11865060	4.27063468	1.21071900
H	0.62648179	4.90901172	3.11102713
H	-1.25148085	3.39097592	3.75130967
H	-1.61547611	1.28154919	2.54352804
H	1.07857053	-4.16895488	0.38725596
H	3.54774076	-3.72661662	0.37887182
H	4.38779009	-1.38830950	0.41646209
H	2.82373275	0.51913721	0.46330577
H	-0.21231042	2.50334416	-1.17844157
H	-0.99370793	2.73281305	-3.50258901
H	-1.94863539	0.75485449	-4.70702494
H	-2.12294138	-1.43408918	-3.50909454
H	-2.35314235	-4.79731869	-1.53440942



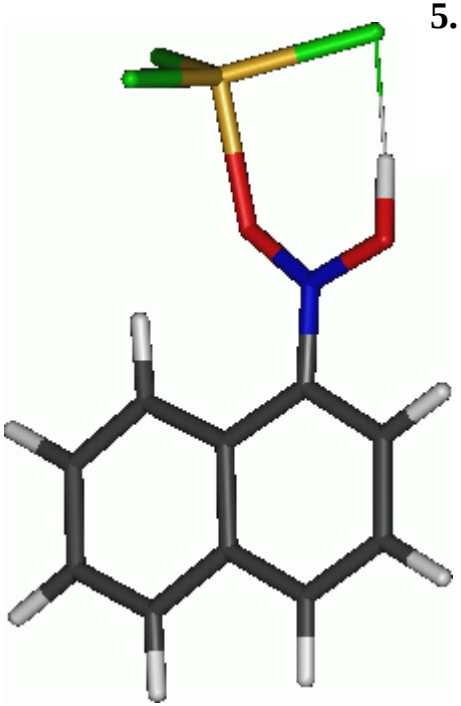
41 Oxime **6** TS2 (limited)

Energy -977.5264658069 Dipole 0.441111 ZPE 0.321997 G(268) 177.91 kcal

C	-0.99557894	-1.95948776	0.46609447
C	0.52265289	-1.91239469	0.47801203
C	0.93656023	-0.58021839	0.35157295
C	-0.29272778	0.35507464	0.31684678
C	-1.36501595	-0.56296331	0.99841508
C	-1.42053544	-2.02373143	-0.97947545
C	-0.76029625	0.42410034	-1.17119673
C	-1.29115475	-0.76966823	-1.75766784
C	0.01662228	1.61391462	1.16635442
C	0.33256819	2.90253901	0.70301208
C	0.66245566	3.94789444	1.57376213
C	0.71265003	3.74253113	2.94874598
C	0.45282616	2.46083392	3.43640212
C	0.12299423	1.42744594	2.56288479
C	1.45131036	-2.94934067	0.51794665
C	2.81334069	-2.63118033	0.44439007
C	3.22687028	-1.30071341	0.31691980
C	2.28854973	-0.26178266	0.26709765
C	-0.69542888	1.54950945	-2.00551340
C	-1.11718716	1.53143475	-3.33637566
C	-1.62517427	0.36059307	-3.89450186
C	-1.70714461	-0.77444991	-3.10048253
N	-1.86267680	-3.07554339	-1.58261268
O	-1.90409382	-4.20573813	-0.72307898
H	-1.42729492	-2.79424295	1.03432521
H	-2.38648832	-0.25299829	0.72856803
H	-1.27563120	-0.55813720	2.09134477
H	0.35364951	3.13461703	-0.35544410
H	0.88940274	4.93213995	1.15499825
H	0.96779849	4.55944929	3.62847050
H	0.51567568	2.25488351	4.50835830
H	-0.02729139	0.43610713	2.99201815
H	1.12260154	-3.98866678	0.60577057
H	3.55976073	-3.42879147	0.48844698
H	4.29376403	-1.06823280	0.26254312
H	2.61380499	0.77901566	0.18341860
H	-0.31861998	2.49275823	-1.63160649
H	-1.04407862	2.44590354	-3.93105999
H	-1.95590244	0.33258597	-4.93583139
H	-2.10164297	-1.71179010	-3.49811734
H	-2.28189392	-4.87325973	-1.32375503

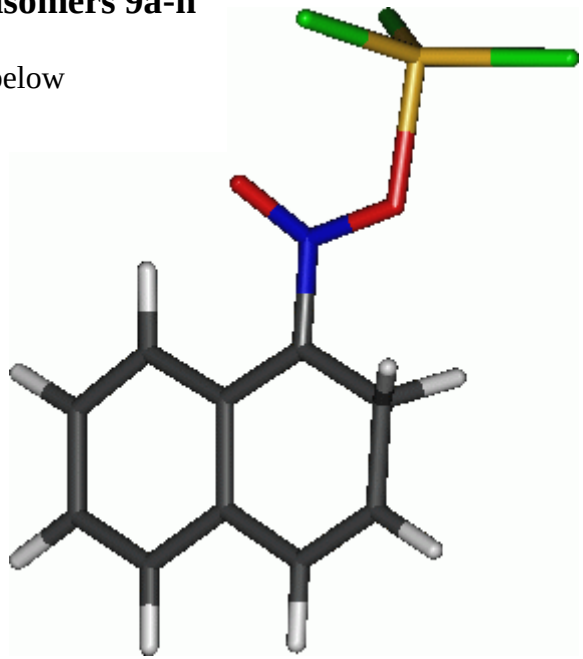
5. DFT calculations on structural and electronic properties of isomers 9a-h

The most stable stereoisomers are provided. For other stereoisomers see below



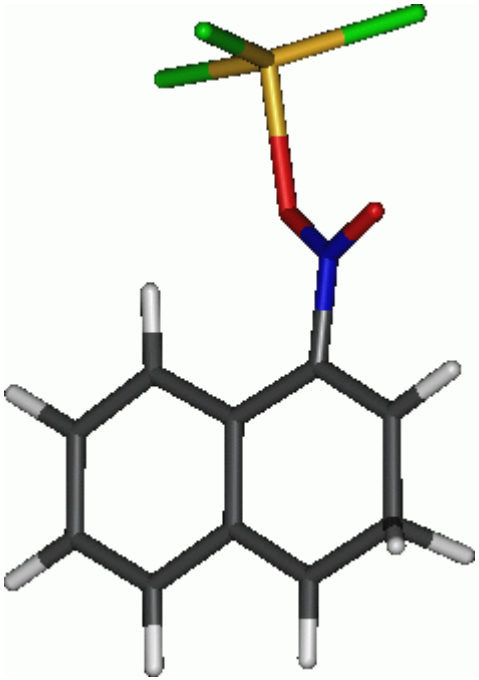
25 **9a**
Energy -2212.812233509 Charge 1 Dipole 4.601421 ZPE 0.161532 G(298) 70.90

C	-0.90411418	0.35570079	-0.19403687
C	-1.70444888	1.51962162	-0.31947846
C	-1.13136896	2.77503823	-0.25305251
C	0.24812335	2.89428745	-0.06186714
C	2.48061243	1.95611538	0.23782853
C	3.33412939	0.87490540	0.34565350
C	2.80324629	-0.42072130	0.26719021
C	1.43613475	-0.64687808	0.08800442
C	0.53719698	0.43020466	-0.01676450
C	1.08403163	1.76676939	0.05452769
H	3.46838776	-1.28454505	0.34476397
H	1.09014744	-1.67364608	0.02453811
H	2.86540174	2.97803151	0.29045131
H	4.40652357	1.02486960	0.48635900
H	0.70138516	3.88872862	-0.00538445
H	-1.75723388	3.66393664	-0.34950032
H	-2.77873768	1.41389038	-0.46617947
N	-1.58031778	-0.85204417	-0.23721867
O	-0.99337797	-1.96346102	-0.17274190
O	-2.91620175	-0.80526499	-0.32768313
Al	-1.72305602	-3.87072722	0.18710063
Cl	-0.21574322	-4.96967544	-0.76838625
Cl	-1.90784211	-3.69507126	2.27903927
Cl	-3.60143047	-3.56963890	-0.89480387
H	-3.24144761	-1.79042618	-0.53835909



25 **9b**
Energy -2212.764414704 Charge 1 Dipole 8.615937 ZPE 0.160349 G(298.15) 69.85

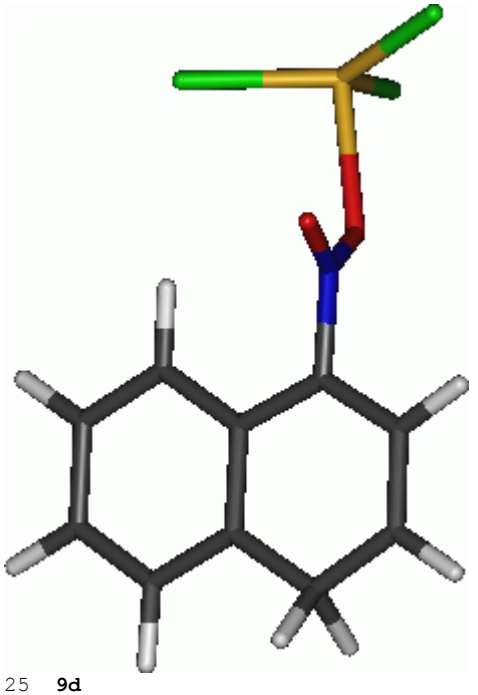
C	-0.85159605	-0.27847482	-0.03405294
C	-1.64279334	-1.52100979	0.02863683
C	-0.88385575	-2.77680321	0.12474810
C	0.47554413	-2.77655958	0.12572696
C	2.62304704	-1.60039094	0.00337106
C	3.36483721	-0.43609733	-0.11404651
C	2.72487110	0.82543928	-0.21998082
C	1.35602573	0.92531089	-0.19197030
C	0.54248165	-0.25295438	-0.06073485
C	1.21898754	-1.56046428	0.02510680
H	3.32867639	1.72970512	-0.32460972
H	0.88027827	1.89992981	-0.26447537
H	3.12547510	-2.56811137	0.07394954
H	4.45684086	-0.48829600	-0.13265334
H	1.03042001	-3.71568409	0.19781825
H	-1.45344672	-3.70712165	0.19525458
H	-2.33027178	-1.55646817	-0.84833674
N	-1.70379865	0.90760717	-0.10055311
O	-1.17162222	2.03381616	0.20311901
O	-2.87811293	0.78031806	-0.39786400
Al	-2.32884896	3.69456828	0.20911335
Cl	-0.82148187	5.05424073	0.82522373
Cl	-2.90347969	3.73938114	-1.84420288
Cl	-3.78178527	3.09940947	1.65650821
H	-2.37639177	-1.45129050	0.86490415



25 **9c**

Energy -2212.767946269 Charge 1 Dipole 12.724643 ZPE 0.160462 G(298) 69.23

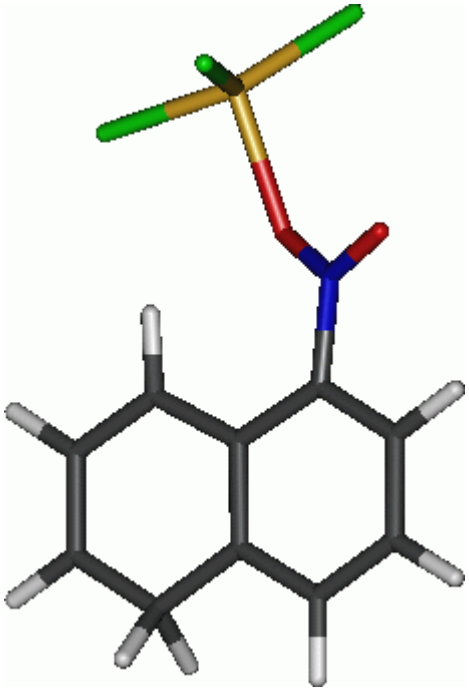
C	-0.77816193	0.72476285	-0.01641998
C	-2.13237181	0.72303738	0.02902850
C	-2.88576042	-0.54090593	0.08642800
C	-2.08722257	-1.76795843	0.07239349
C	0.00558649	-2.99877104	-0.04093292
C	1.37593480	-3.01189520	-0.14146148
C	2.06882485	-1.78397568	-0.20293782
C	1.41656386	-0.54813769	-0.15282908
C	0.02285717	-0.48718543	-0.04699268
C	-0.70900232	-1.75477685	0.00036875
H	3.15938721	-1.78829571	-0.28941652
H	2.01747086	0.35960641	-0.18303666
H	-0.56596348	-3.92987884	0.00173642
H	1.92606033	-3.95446099	-0.17724944
H	-2.61790317	-2.72570653	0.11344962
H	-3.63281583	-0.58044798	-0.74265261
H	-2.67496458	1.67230944	0.02711952
N	-0.16488031	2.08457201	-0.04218833
O	1.00800981	2.14786836	0.43377691
O	-0.79370131	3.01768693	-0.48157510
Al	2.25468577	3.78692180	0.23149871
Cl	3.97682897	2.67360769	0.80564673
Cl	2.00721771	4.10011417	-1.85963814
Cl	1.36818767	5.13144892	1.60368660
H	-3.56486777	-0.54953966	0.97219751



25 **9d**

Energy -2212.76905673 Charge 1 Dipole 10.375099 ZPE 0.160371 G(298) 69.58

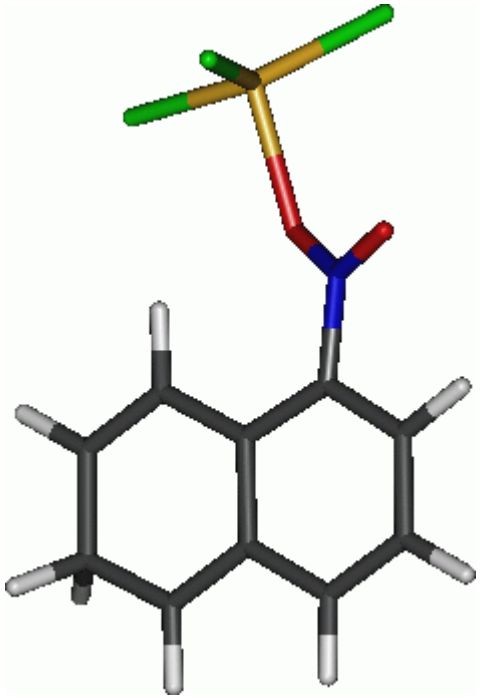
C	0.18130525	1.02503006	-0.01600818
C	-0.48444370	2.22956896	0.28615813
C	-1.83862805	2.18620643	0.48400960
C	-2.60039499	0.93417027	0.36955257
C	-2.48392930	-1.52901308	-0.14437740
C	-1.74708185	-2.66603174	-0.48167160
C	-0.35081850	-2.60573595	-0.67126485
C	0.31935591	-1.41031571	-0.51801010
C	-0.41714396	-0.23909221	-0.17355729
C	-1.84462182	-0.30252975	0.01192506
H	0.20215341	-3.50945250	-0.93614481
H	1.40458701	-1.37144527	-0.66239483
H	-3.56582220	-1.60392106	-0.00489622
H	-2.26389161	-3.62205553	-0.60125161
H	-3.43668052	1.09902366	-0.34748464
H	-2.38934539	3.09794846	0.73894873
H	0.08131807	3.16076800	0.36684152
N	1.64153362	1.13069654	-0.23193123
O	2.33733105	0.66148446	0.70524655
O	2.02720392	1.61973607	-1.26832216
Al	4.43109491	0.29465229	0.48008242
Cl	4.72269456	-0.54942662	2.38949585
Cl	4.10874476	-1.05843400	-1.15190170
Cl	5.11857074	2.24711591	0.05131255
H	-3.15309133	0.78105231	1.32564361



25 **9e**

Energy -2212.776835591 Charge 1 Dipole 11.583958 ZPE 0.160699 G(298) 70.32

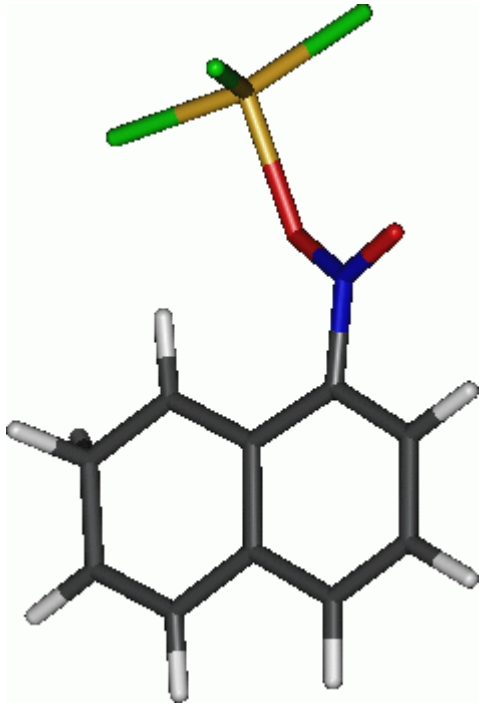
C	0.22402122	-1.25716216	-0.02175088
C	-0.53109188	-2.41251264	0.02199860
C	-1.93275416	-2.33119115	0.04294866
C	-2.56532758	-1.09474687	0.03493789
C	-2.51105353	1.40583087	0.03317472
C	-1.68187743	2.61375415	0.05128958
C	-0.31176257	2.53275982	0.05584651
C	0.32570867	1.27896475	0.02688396
C	-0.38094718	0.04410068	-0.01159523
C	-1.81381860	0.08685494	0.01625753
H	0.30778674	3.43236734	0.08055093
H	1.42081827	1.28206441	0.02794296
H	-3.20755455	1.47428407	-0.83503452
H	-2.18801667	3.58459907	0.06539621
H	-3.65759412	-1.04235755	0.05040979
H	-2.52221715	-3.25082571	0.06169283
H	-0.02305636	-3.37904025	0.02773169
N	1.68662771	-1.47370380	-0.06764884
O	2.36127660	-0.50316124	-0.54215653
O	2.15714564	-2.51423112	0.32586840
Al	4.32759671	-0.08919875	-0.15491905
Cl	3.92827093	2.02183352	-0.26748132
Cl	4.47236003	-0.83094192	1.83420786
Cl	5.33705770	-1.03162122	-1.74667328
H	-3.22159844	1.45328076	0.89012153



25 **9f**

Energy -2212.769837732 Charge 1 Dipole 12.856004 ZPE 0.160224 G(298) 69.53

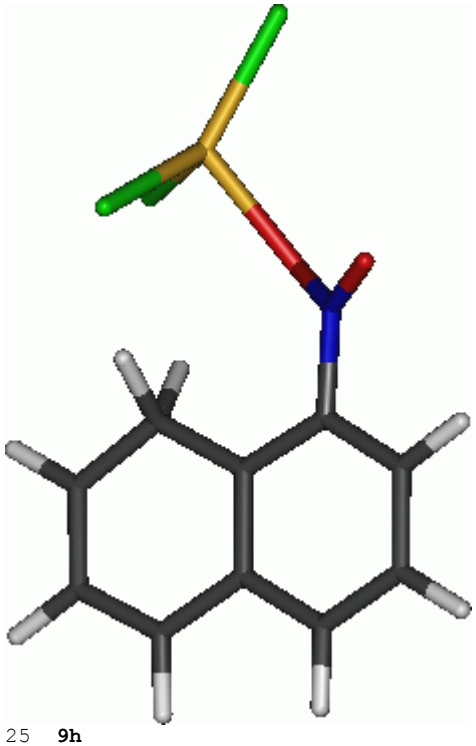
C	1.15445979	0.52134577	0.02825465
C	1.72046061	1.79090708	0.01500778
C	0.92632963	2.95367840	0.01770848
C	-0.44142326	2.82719734	0.00597360
C	-2.43584518	1.43297851	-0.04626830
C	-3.11966029	0.14559940	-0.08406410
C	-2.26513155	-1.05138966	-0.08974967
C	-0.90578919	-0.96547358	-0.04257838
C	-0.24895792	0.31002345	0.00444846
C	-1.05479454	1.53200262	-0.01237724
H	-2.74673734	-2.03258893	-0.12905895
H	-0.32013863	-1.88562726	-0.02736616
H	-3.04263193	2.34509733	-0.04546661
H	-3.82549586	0.13295653	-0.95075292
H	-1.08548826	3.71085786	0.00516145
H	1.40434848	3.93494744	0.02748889
H	2.81145048	1.86466668	0.00599949
N	2.14161996	-0.58576790	0.02887831
O	1.72311132	-1.67935474	0.51722925
O	3.25067400	-0.39719469	-0.41449127
Al	2.52393729	-3.54766333	0.16698000
Cl	0.61707748	-4.47178319	0.47590887
Cl	3.07115616	-3.30409822	-1.87524227
Cl	4.00466685	-3.68281370	1.66319001
H	-3.85719811	0.10149679	0.75518664



25 **9g**

Energy -2212.772188546 Charge 1 Dipole 10.278594 ZPE 0.160060 G(298) 69.55

C	1.08523853	-0.74821130	0.02717732
C	2.45162136	-0.62502649	-0.02749208
C	3.04545950	0.65850605	-0.05588242
C	2.26639511	1.79890880	-0.04443087
C	0.07513853	2.91452184	-0.03918833
C	-1.28427747	2.87736673	-0.04633605
C	-1.98197384	1.58480860	-0.04023924
C	-1.17998935	0.36650981	-0.00504790
C	0.21094741	0.40469511	0.01891821
C	0.85542282	1.71237022	-0.01854742
H	-2.69045045	1.50470310	-0.90265860
H	-1.73608357	-0.57744907	0.00600270
H	0.60668859	3.86959342	-0.05422240
H	-1.87748033	3.79548894	-0.06156237
H	2.73686817	2.78518946	-0.06345250
H	4.13519435	0.73684311	-0.08243262
H	3.06779933	-1.52677346	-0.03588387
N	0.58482152	-2.13814397	0.07935413
O	-0.59424674	-2.26610062	0.54340362
O	1.27993607	-3.04898371	-0.30395532
Al	-1.90037973	-3.78981138	0.15010984
Cl	-3.56017091	-2.42530529	0.27506771
Cl	-1.30834815	-4.25129719	-1.84128114
Cl	-1.56103986	-5.14167223	1.72967101
H	-2.72709089	1.52926954	0.79290858



25 **9h**

Energy -2212.786570913 Charge 1 Dipole 8.059128 ZPE 0.160495 G(298) 71.42

C	0.06198266	-1.35112963	0.14814623
C	0.98298711	-2.39554310	0.11868556
C	2.35405295	-2.12067877	0.04808547
C	2.77842142	-0.80753644	-0.03864982
C	2.29443325	1.59777660	-0.20931874
C	1.43274882	2.69272066	-0.27744832
C	0.07098519	2.47586775	-0.16913331
C	-0.49683502	1.15545527	0.00463811
C	0.43614150	0.00689227	0.06612528
C	1.84080051	0.25975227	-0.05252366
H	-0.63083990	3.31583867	-0.20372089
H	-1.29608397	0.98953996	-0.80205654
H	3.37439833	1.76317597	-0.28731222
H	1.83253609	3.70064283	-0.40578048
H	3.84435104	-0.57539789	-0.11220039
H	3.07295712	-2.94207022	0.05221423
H	0.61752964	-3.42456730	0.16149387
N	-1.35260200	-1.74554909	0.19615825
O	-2.10310519	-0.94023292	0.84687493
O	-1.73040319	-2.74632960	-0.35836693
Al	-3.88556841	-0.21440392	0.23915907
Cl	-3.68813337	1.52269474	1.47721153
Cl	-3.16364016	0.21390666	-1.77548164
Cl	-5.41054314	-1.62415075	0.48162246
H	-1.23657129	1.19332597	0.85157795

Cartesian coordinates for the less stable stereoisomers of 9a-h

For their spatial structures see, please,

http://limor1.nioch.nsc.ru/quant/$ArNO_2$

25 **9a′**

Energy -2212.810811722 Charge 1 Dipole 4.121100 ZPE 0.161129 G(298)

C	0.40617595	-0.43899483	-0.05884272
C	1.77140281	-0.58552885	-0.41244545
C	2.58340229	0.52157928	-0.56401162
C	2.05020512	1.79693394	-0.36195391
C	0.22473802	3.31762490	0.18475427
C	-1.08993619	3.55551950	0.53574524
C	-1.95616931	2.46498508	0.69949955
C	-1.52664650	1.14945559	0.51347836
C	-0.19435066	0.86767257	0.15767825
C	0.70045995	1.99251258	-0.00873297
H	-2.99877490	2.63879035	0.97714755
H	-2.24966619	0.35194262	0.64752140
H	0.92485128	4.14644533	0.05066178
H	-1.45071860	4.57539389	0.68386939
H	2.69095496	2.67594128	-0.48143143
H	3.63087038	0.39398386	-0.84306057
H	2.16900459	-1.58831786	-0.56958623
N	-0.28082116	-1.64097965	0.05929463
O	-1.58457036	-1.60486299	0.29837882
O	0.30868784	-2.75282918	-0.06266483
Al	-0.39487181	-4.63497557	-0.45588760
Cl	1.06211491	-5.79251336	0.50081147
Cl	-2.29946237	-4.36593118	0.61768323
Cl	-0.58423277	-4.42270566	-2.54506458
H	-1.91264727	-2.62114162	0.43715797

25 **9a″**

Energy -2212.785727331 Charge 1 Dipole 5.991728 ZPE 0.161928 G(298) 70.24

C	0.24368003	-0.53578651	0.22523396
C	1.60832989	-0.84542493	0.02712892
C	2.50956303	0.17115767	-0.25335011
C	2.06283363	1.48992594	-0.33230580
C	0.32630268	3.20763314	-0.08220254
C	-0.95936297	3.57748193	0.26725694
C	-1.87562403	2.59208307	0.66945900
C	-1.53279446	1.24137322	0.66881917
C	-0.24778711	0.82668176	0.26112199
C	0.71787131	1.84418849	-0.07459860
H	-2.87450101	2.88356936	1.00327381
H	-2.26746596	0.52674433	1.04645191
H	1.06917707	3.96440514	-0.34787812
H	-1.25310570	4.62920806	0.26236338
H	2.77063981	2.28531534	-0.58509232
H	3.55623715	-0.07278086	-0.44511351
H	1.91926125	-1.89433450	0.02111363
N	-0.58903858	-1.64765394	0.31544017
O	-1.92762644	-1.55296409	0.00186497
O	-0.20402961	-2.77355960	0.61095001
Al	-0.28890681	-4.71681690	-0.58097068
Cl	1.78470367	-4.42700839	-1.00130680
Cl	-0.89659512	-6.00972221	0.94791142
Cl	-1.61851168	-4.03195749	-2.08107736
H	-2.03325005	-0.73175802	-0.54449344

25 **9b′**

Energy -2212.764414704 Charge 1 Dipole 8.615937 ZPE 0.160349 G(298) 69.85

C	-0.85159605	-0.27847482	-0.03405294
C	-1.64279334	-1.52100979	0.02863683
C	-0.88385575	-2.77680321	0.12474810
C	0.47554413	-2.77655958	0.12572696
C	2.62304704	-1.60039094	0.00337106
C	3.36483721	-0.43609733	-0.11404651
C	2.72487110	0.82543928	-0.21998082
C	1.35602573	0.92531089	-0.19197030
C	0.54248165	-0.25295438	-0.06073485
C	1.21898754	-1.56046428	0.02510680
H	3.32867639	1.72970512	-0.32460972
H	0.88027827	1.89992981	-0.26447537
H	3.12547510	-2.56811137	0.07394954
H	4.45684086	-0.48829600	-0.13265334
H	1.03042001	-3.71568409	0.19781825
H	-1.45344672	-3.70712165	0.19525458
H	-2.33027178	-1.55646817	-0.84833674
N	-1.70379865	0.90760717	-0.10055311
O	-1.17162222	2.03381616	0.20311901
O	-2.87811293	0.78031806	-0.39786400
Al	-2.32884896	3.69456828	0.20911335
Cl	-0.82148187	5.05424073	0.82522373
Cl	-2.90347969	3.73938114	-1.84420288
Cl	-3.78178527	3.09940947	1.65650821
H	-2.37639177	-1.45129050	0.86490415

25 **9c'**
Energy -2212.767608318 Charge 1 Dipole 12.4938 ZPE 0.160486 G(298) 69.66

C	-0.38104283	0.52471763	-0.12687608
C	-1.73560625	0.54534668	-0.17152062
C	-2.50426677	-0.71219532	-0.16652598
C	-1.72451847	-1.95008741	-0.09809451
C	0.36212190	-3.19738718	0.07011541
C	1.73330884	-3.21350055	0.16876608
C	2.43725379	-1.98985125	0.17439545
C	1.79097304	-0.75577830	0.06605899
C	0.39795244	-0.69499317	-0.04183114
C	-0.34480692	-1.95329942	-0.02830867
H	3.52717730	-2.00141104	0.26435306
H	2.38643255	0.15582107	0.05827866
H	-0.21399125	-4.12659969	0.07319176
H	2.27666153	-4.15735920	0.24808034
H	-2.26957218	-2.90047303	-0.09446159
H	-3.19202473	-0.75083908	-1.04462733
H	-2.27002304	1.49741972	-0.22034693
N	0.30156600	1.84091776	-0.20347087
O	1.38813313	1.94220636	-0.72955259
O	-0.36251370	2.80255703	0.29110533
Al	0.34464548	4.74246658	0.21940644
Cl	-1.31885333	5.62826370	1.18688121
Cl	2.13943261	4.48065962	1.33182075
Cl	0.47629383	4.94385394	-1.89668888
H	-3.24473298	-0.70045544	0.66985171

25 **9d'**
Energy -2212.76859925 Charge 1 Dipole 9.798942 ZPE 0.160364 G(298) 69.39

C	0.15629499	0.72364554	-0.35139657
C	-0.60825633	1.90267151	-0.46502570
C	-1.97162008	1.80980942	-0.38252260
C	-2.64679834	0.52560961	-0.15224615
C	-2.34049086	-1.93048184	0.28568427
C	-1.51875971	-3.04596649	0.44928087
C	-0.11665642	-2.93937391	0.34579113
C	0.46851846	-1.72236596	0.06756475
C	-0.35310980	-0.57031079	-0.10728863
C	-1.78533740	-0.68253693	0.01379906
H	0.50793347	-3.82404446	0.48596247
H	1.55372823	-1.64611106	-0.01608689
H	-3.42495420	-2.03633448	0.37678502
H	-1.96989635	-4.01783497	0.66620706
H	-3.37344544	0.36508977	-0.98269939
H	-2.58938504	2.70661654	-0.49154545
H	-0.10390035	2.85775731	-0.62657428
N	1.61264177	0.89631199	-0.50884928
O	2.22088324	0.22866159	-1.31503394
O	2.10507693	1.77147682	0.26720089
Al	4.17317071	1.99342690	0.41138546
Cl	4.19429467	3.26196338	2.09852615
Cl	4.62858051	-0.07378114	0.72983746
Cl	4.50929734	2.80854794	-1.52058803
H	-3.32780998	0.63755371	0.72183233

25 **9e'**
Energy -2212.775324349 Charge 1 Dipole 12.416 ZPE 0.160677 G(298) 70.03

C	0.27599542	-0.76449594	0.10250410
C	-0.43076257	-1.95319755	0.09915318
C	-1.83410456	-1.92319543	0.08976675
C	-2.51815271	-0.71237867	0.06740305
C	-2.55778077	1.79293311	-0.00565679
C	-1.76396382	3.02517246	-0.07163771
C	-0.39190922	2.98889193	-0.09427451
C	0.28354510	1.75593192	-0.03477610
C	-0.38384856	0.50712545	0.05803120
C	-1.81706666	0.49754144	0.04320164
H	0.19179466	3.90969354	-0.16009975
H	1.37459864	1.76236862	-0.05730899
H	-3.27953185	1.79237983	-0.85423867
H	-2.29984429	3.97904042	-0.10973708
H	-3.61174995	-0.70637081	0.06342953
H	-2.38705959	-2.86533651	0.10731492
H	0.10940976	-2.90092679	0.12437799
N	1.74007296	-0.85911293	0.18024318
O	2.41283311	0.05497474	0.61730537
O	2.22292219	-1.96628210	-0.22545215
Al	4.24119237	-2.27716843	-0.20111257
Cl	4.21854985	-4.23569061	-1.01193374
Cl	4.84521091	-0.68528112	-1.48641391
Cl	4.60385748	-2.08321485	1.88986895
H	-3.24420792	1.86659828	0.87004211

25 **9f'**
Energy -2212.768831805 Charge 1 Dipole 13.564 ZPE 0.160260 G(298) 69.77

C	0.78163932	0.20917124	-0.15135649
C	1.39977245	1.45668645	-0.16379736
C	0.64383681	2.64450960	-0.14390414
C	-0.72758498	2.57023694	-0.08409684
C	-2.76902843	1.24049623	0.04465920
C	-3.49049460	-0.02731493	0.11286737
C	-2.66998717	-1.25072892	0.09928767
C	-1.31336119	-1.20094441	0.00280221
C	-0.62309820	0.05536931	-0.07760340
C	-1.38740226	1.29948039	-0.03751461
H	-3.18131652	-2.21473753	0.16806504
H	-0.73628495	-2.12385612	-0.02114587
H	-3.34883768	2.16977743	0.06051160
H	-4.25495150	-0.05470955	-0.70228925
H	-1.33705316	3.47786792	-0.06688826
H	1.15595978	3.60808500	-0.17612591
H	2.49118246	1.49677842	-0.19921268
N	1.67545271	-0.96546377	-0.21773892
O	1.30121389	-2.01276444	-0.70122505
O	2.83960826	-0.75967533	0.24993753
Al	4.26958366	-2.24322736	0.24671962
Cl	5.79401421	-1.10607299	1.17988263
Cl	3.24306875	-3.69082291	1.42686680
Cl	4.40919360	-2.56301346	-1.85241284
H	-4.16512522	-0.01512721	1.00371197

25 **9g'**

Energy -2212.770195419 Charge 1 Dipole 11.2056 ZPE 0.160178 G(298) 69.72

C	0.61245122	-0.56621864	-0.06822975
C	1.98714139	-0.50218446	-0.04055553
C	2.63348404	0.75427010	-0.03216564
C	1.90609486	1.93106048	-0.03828358
C	-0.23828168	3.13861776	-0.02215716
C	-1.59726553	3.15486784	0.00246217
C	-2.35332091	1.89233887	0.02003410
C	-1.59192669	0.64418722	-0.01205216
C	-0.20532366	0.62789543	-0.05652830
C	0.49567003	1.90731813	-0.04141415
H	-3.10398641	1.86818954	-0.80815356
H	-2.15017965	-0.29306717	-0.00193230
H	0.32940201	4.07280771	-0.02393043
H	-2.15268755	4.09627170	0.01392388
H	2.42145323	2.89481218	-0.03644695
H	3.72595935	0.78412786	-0.02758501
H	2.56867483	-1.42548663	-0.04320398
N	0.00775494	-1.90034068	-0.12862921
O	-1.14711615	-2.06358965	-0.47691258
O	0.78668558	-2.85696553	0.19911134
Al	0.10460919	-4.77460576	0.18086407
Cl	1.89166076	-5.70264130	0.84133309
Cl	-1.48879935	-4.58705988	1.58877757
Cl	-0.39517437	-4.95309329	-1.88445164
H	-3.04697949	1.85848818	0.89612570

25 **9h'**

Energy -2212.778103576 Charge 1 Dipole 12.536 ZPE 0.160779 G(298) 70.23

C	-0.08276878	-0.75174941	-0.05956939
C	0.73328809	-1.88803250	-0.03913905
C	2.12617374	-1.76085957	-0.01971602
C	2.69372541	-0.50016507	-0.01152742
C	2.47341071	1.94280956	-0.00471151
C	1.74407794	3.14103397	-0.00710923
C	0.37129350	3.08011219	-0.03024015
C	-0.36146732	1.80957314	-0.06445940
C	0.44245101	0.55144166	-0.05477365
C	1.87234419	0.65939071	-0.02471514
H	-0.22711371	3.99707182	-0.03043794
H	-1.04768731	1.82477986	-0.94202517
H	3.56778167	1.99055664	0.01547790
H	2.26640631	4.09982861	0.01120634
H	3.78026538	-0.37981181	0.00580272
H	2.75050166	-2.65640900	-0.01095723
H	0.25943182	-2.87181001	-0.04145985
N	-1.53949791	-0.97297855	-0.08374459
O	-2.30304623	-0.05327329	-0.30829762
O	-1.90808615	-2.16569398	0.14579346
Al	-3.90512235	-2.66540196	0.19122911
Cl	-3.62675636	-4.71753880	0.63938224
Cl	-4.52576883	-1.37813287	1.77237798
Cl	-4.43820514	-2.14669959	-1.80314532
H	-1.11563135	1.81195824	0.75475893

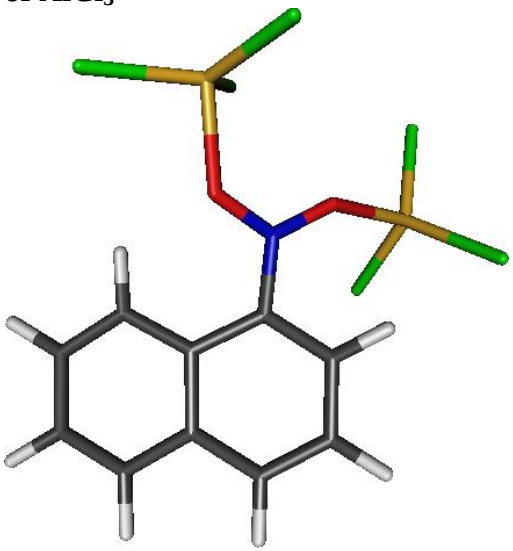
Energy of the LUMO (eV) and sum of the squares of the coefficients on carbon atoms (c_i^2) in the complexes **1**-$AlCl_3$ (**9**) calculated by DFT/PBE/cc-pVDZ.

	ε_{LUMO}	C1	C2	C3	C4	C5	C6	C7	C8	C8a	C4a
E_C2 (**9b**)	-0.3551	0.15	0.01	0.05	0.02	0.00	0.06	0.01	0.03	0.03	0.06
E_C3 (**9c′**)	-0.3408	0.01	0.04	0.01	0.28	0.09	0.00	0.12	0.00	0.11	0.00
E_C4 (**9d′**)	-0.3478	0.20	0.01	0.15	0.01	0.00	0.05	0.00	0.03	0.03	0.06
E_C5 (**9e′**)	-0.3426	0.04	0.01	0.06	0.01	0.01	0.18	0.00	0.22	0.00	0.07
E_C6 (**9f′**)	-0.3403	0.00	0.12	0.00	0.09	0.27	0.01	0.06	0.01	0.10	0.00
E_C7 (**9g′**)	-0.3427	0.07	0.02	0.08	0.02	0.01	0.05	0.01	0.19	0.00	0.08
E_Oa (**9a′**)	-0.3348	0.01	0.09	0.01	0.11	0.03	0.00	0.04	0.01	0.02	0.00
E_Ob (**9a″**)	-0.3408	0.01	0.09	0.00	0.10	0.02	0.00	0.02	0.01	0.03	0.00
Z_C2 (**9b′**)	-0.3549	0.15	0.01	0.05	0.02	0.00	0.06	0.01	0.03	0.03	0.07
Z_C3 (**9c**)	-0.3418	0.01	0.04	0.01	0.29	0.09	0.00	0.12	0.00	0.11	0.00
Z_C4 (**9d**)	-0.3441	0.24	0.00	0.18	0.01	0.00	0.06	0.00	0.04	0.02	0.07
Z_C5 (**9e**	-0.3431	0.05	0.02	0.06	0.01	0.01	0.19	0.00	0.23	0.00	0.07
Z_C6 (**9f**)	-0.3414	0.00	0.12	0.00	0.09	0.27	0.01	0.06	0.01	0.10	0.00
Z_C7 (**9g**)	-0.3424	0.08	0.02	0.09	0.02	0.01	0.05	0.01	0.20	0.01	0.09
Z_C8 (**9h**)	-0.3245	0.00	0.08	0.00	0.05	0.24	0.01	0.21	0.03	0.05	0.00
Z_Oa (**9a**)	-0.3351	0.01	0.09	0.01	0.11	0.03	0.00	0.04	0.01	0.02	0.00

NBO charges on carbon atoms (q_i) in the complexes **1**-$AlCl_3$ (**9**) calculated by DFT/PBE/cc-pVDZ.

	C1	C2	C3	C4	C5	C6	C7	C8	C8a	C4a
E_C2 (**9b**)	0.26	0.15	0.20	0.08	0.07	0.17	0.10	0.13	-0.06	0.03
E_C3 (**9c′**)	0.08	0.22	0.14	0.31	0.15	0.08	0.19	0.09	0.00	-0.09
E_C4 (**9d′**)	0.24	0.05	0.27	0.14	0.06	0.16	0.09	0.12	-0.08	0.06
E_C5 (**9e′**)	0.13	0.13	0.15	0.08	0.14	0.27	0.04	0.27	-0.09	0.06
E_C6 (**9f′**)	0.09	0.20	0.08	0.17	0.31	0.14	0.20	0.08	0.03	-0.10
E_C7 (**9g′**)	0.14	0.14	0.16	0.10	0.07	0.19	0.14	0.31	-0.11	0.03
E_Oa (**9a′**)	0.14	0.15	0.07	0.21	0.13	0.07	0.13	0.09	-0.06	-0.07
E_Ob (**9a″**)	0.11	0.16	0.07	0.20	0.13	0.08	0.12	0.02	-0.07	-0.07
Z_C2 (**9b′**)	0.26	0.14	0.20	0.08	0.07	0.18	0.10	0.14	-0.06	0.03
Z_C3 (**9c**)	0.08	0.21	0.15	0.31	0.16	0.08	0.20	0.10	0.00	-0.09
Z_C4 (**9d**)	0.25	0.04	0.28	0.14	0.06	0.17	0.09	0.12	-0.09	0.06
Z_C5 (**9e**	0.13	0.12	0.15	0.08	0.14	0.28	0.05	0.29	-0.09	0.06
Z_C6 (**9f**)	0.08	0.19	0.08	0.17	0.31	0.14	0.21	0.09	0.03	-0.10
Z_C7 (**9g**)	0.14	0.13	0.16	0.10	0.07	0.20	0.15	0.34	-0.11	0.04
Z_C8 (**9h**)	0.08	0.15	0.09	0.15	0.24	0.04	0.29	0.14	0.06	-0.08
Z_Oa (**9a**)	0.14	0.15	0.07	0.21	0.13	0.07	0.13	0.09	-0.06	-0.07

6. DFT calculations on coordination of compound 1 with two molecules of $AlCl_3$



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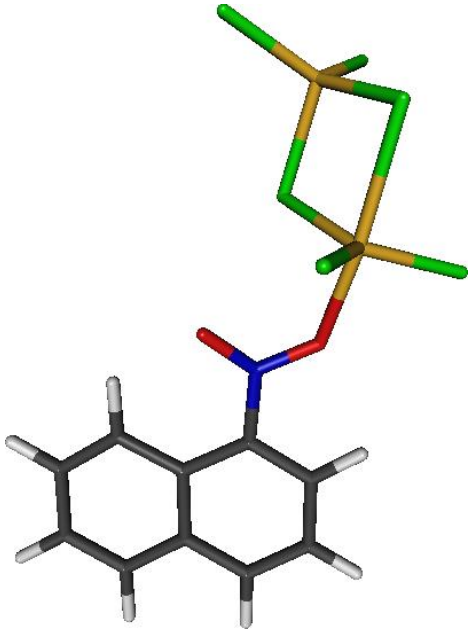
28
 Energy -3835.1052679  Dipole 12.980908  ZPE 0.157121  G(298.15) 61.27
 C    0.34342099  -0.17038264  -0.47314459
 C    1.59699036  -0.42909541  -1.03725218
 C    2.60602785   0.53207876  -0.98572844
 C    2.37006299   1.73648068  -0.34638399
 C    0.93579404   3.26905173   0.91830293
 C   -0.26462526   3.57484804   1.52395739
 C   -1.31658351   2.64217365   1.47590087
 C   -1.17979248   1.42658047   0.82111223
 C    0.03708980   1.07862319   0.19180762
 C    1.12036313   2.03059948   0.25093656
 H   -2.27088663   2.87418430   1.95509471
 H   -2.03295108   0.75397110   0.78925184
 H    1.77273539   3.97191658   0.94852925
 H   -0.39903914   4.52900914   2.03826554
 H    3.15890050   2.49292480  -0.29488353
 H    3.57037331   0.32077668  -1.45114786
 H    1.77911441  -1.36891876  -1.56837146
 N   -0.61233354  -1.20860087  -0.60284093
 O   -1.84113303  -0.90089421  -0.52918510
 O   -0.29233688  -2.41510327  -0.81572972
Al    1.15066933  -3.72783390  -0.26471925
Cl    2.31518073  -3.75749257  -2.06480384
Cl    2.04505309  -2.66432470   1.36354327
Cl    0.04747289  -5.46808993   0.18236959
Al   -3.42602947  -2.14992566  -0.52370071
Cl   -3.30418548  -3.09462037  -2.42408868
Cl   -3.03448883  -3.28219372   1.23509549
Cl   -4.87486349  -0.59574261  -0.31218702
```



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28
 Energy -3835.112316903  Dipole 14.046262  ZPE 0.157189  G(298.15) 61.15
 C    0.76375519   0.40750806  -0.24129329
 C    2.11401706   0.15210151  -0.45104465
 C    3.04008744   1.20238538  -0.44722371
 C    2.60737175   2.49426791  -0.21832448
 C    0.83243871   4.12328650   0.26606445
 C   -0.48906932   4.42636069   0.50820399
 C   -1.44897529   3.39352755   0.50737650
 C   -1.09425911   2.08002794   0.25757623
 C    0.25603948   1.73058622   0.00218628
 C    1.24092267   2.78687908   0.01454939
 H   -2.49762207   3.63022413   0.70392295
 H   -1.85978151   1.30912512   0.24756022
 H    1.59496347   4.90700366   0.26792279
 H   -0.79385604   5.45724367   0.70267206
 H    3.32307224   3.32164896  -0.21348032
 H    4.09518984   0.98971713  -0.62961150
 H    2.43344706  -0.87433536  -0.63224761
 N   -0.11906268  -0.74558173  -0.29382271
 O   -1.32623074  -0.63729661  -0.40368143
 O    0.46998672  -1.89089397  -0.22817768
Al   -0.38079564  -3.66993552  -0.72748414
Cl    1.48931655  -4.64822558  -0.40831681
Cl   -1.70842933  -3.49081766   1.16435387
Cl   -1.10304271  -2.99982287  -2.62502969
Al   -2.76541130  -5.55293069   0.85783166
Cl   -4.82324877  -5.16122280   0.53316384
Cl   -1.62782924  -5.94153150  -0.99642675
Cl   -2.22299442  -6.79929923   2.48278052
```