

Supporting Information

Control of the Ambident Reactivity of the Nitrite Ion

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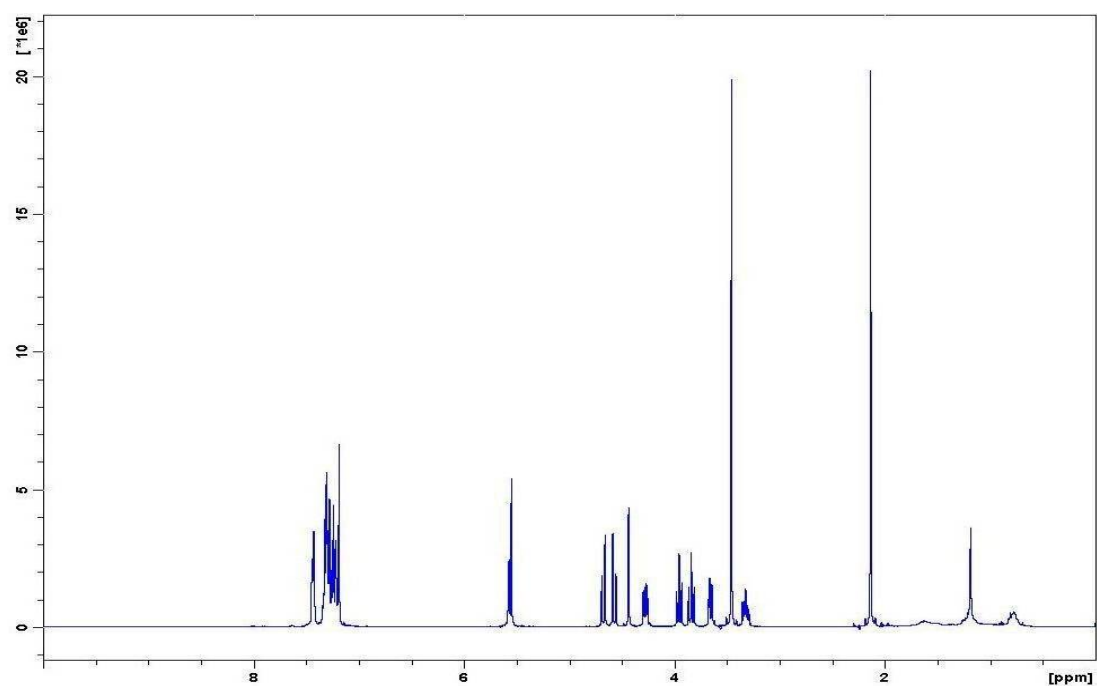
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Contents

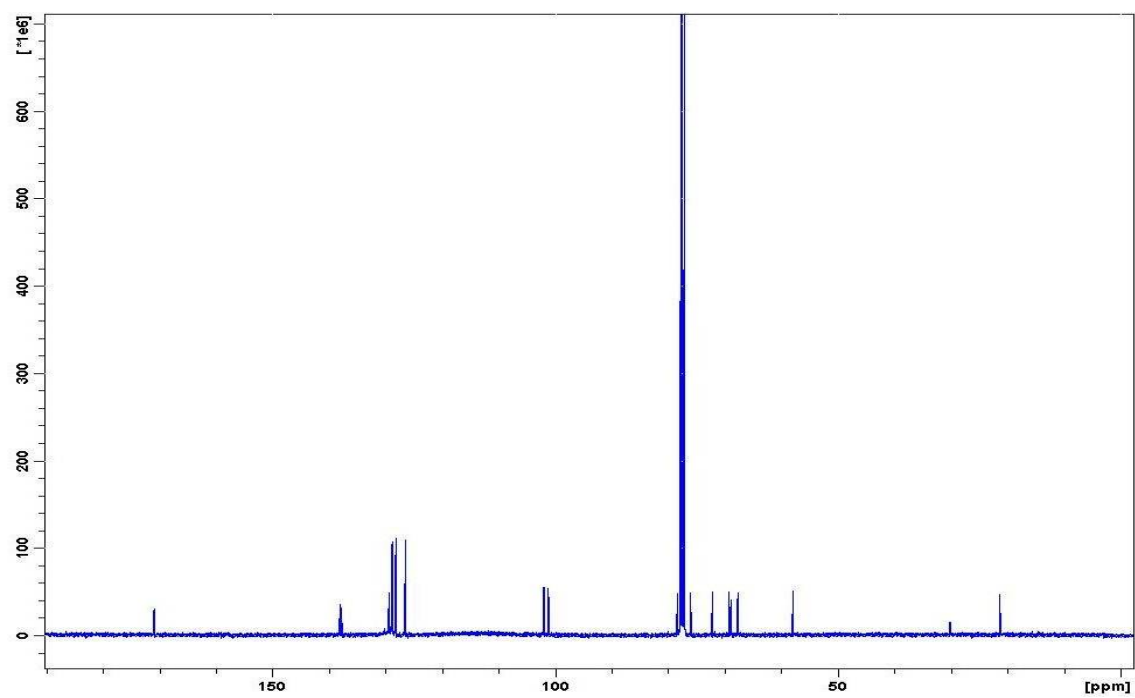
¹ H-NMR spectrum of compound 4	S3
¹³ C-NMR spectrum of compound 4	S3
¹ H-NMR spectrum of compound 5	S4
¹³ C-NMR spectrum of compound 5	S4
¹ H-NMR spectrum of compound 11	S5
¹³ C-NMR spectrum of compound 11	S5
IR spectrum of compound 5	S6
IR spectrum of compound 11	S6
¹ H-NMR spectrum of compound 3	S7
¹ H- ¹ H COSY spectrum of compound 3	S7
¹ H-NMR spectrum of the <i>epi</i> -triflate analog of compound 3	S8
¹ H- ¹ H COSY spectrum of the <i>epi</i> -triflate analog of compound 3	S8
¹ H-NMR spectrum of compound 10	S9
¹ H- ¹ H COSY spectrum of compound 10	S9
¹ H-NMR spectrum of the <i>epi</i> -triflate analog of compound 10	S10

¹ H- ¹ H COSY spectrum of the <i>epi</i> -triflate analog of compound 10	S10
¹ H-NMR spectrum of compound 17	S11
¹ H- ¹ H COSY spectrum of compound 17	S11
Inversion of compound 3	S12
Decompose of nitrite ester 8	S13
¹ H NMR spectrum of inversions with compound 3 and its <i>epi</i> -triflate analog	S14
Decompose of nitrite ester 12	S15
Inversion of triflate of 13	S16
¹ H NMR spectrum of inversions with compound 10 and its <i>epi</i> -triflate analog	S17
Inversion of compound 17	S17
Cartesian coordinates, energies and results of frequency calculations	S19

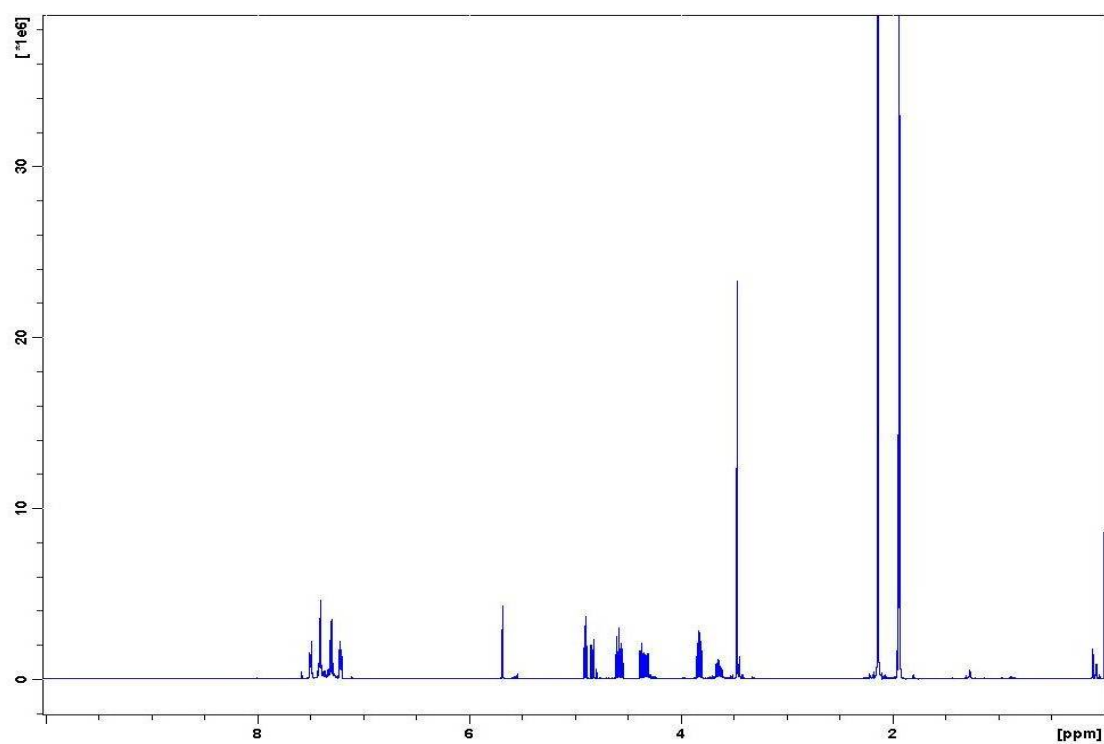
^1H -NMR of **4** (CDCl_3)



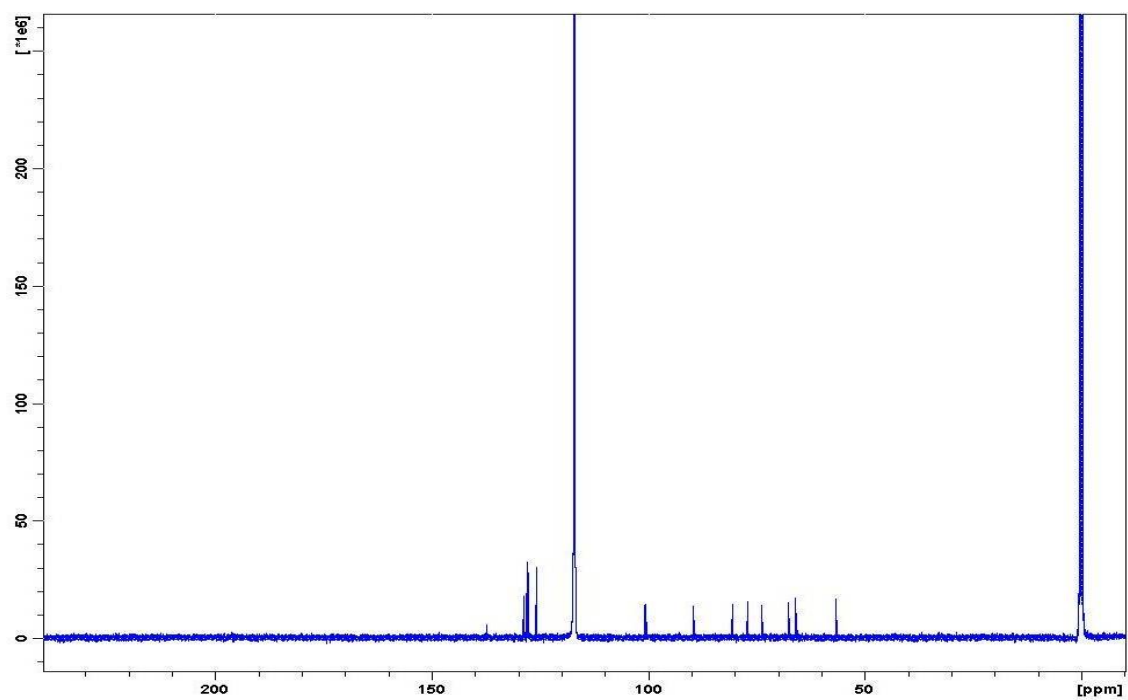
^{13}C -NMR of **4** (CDCl_3)



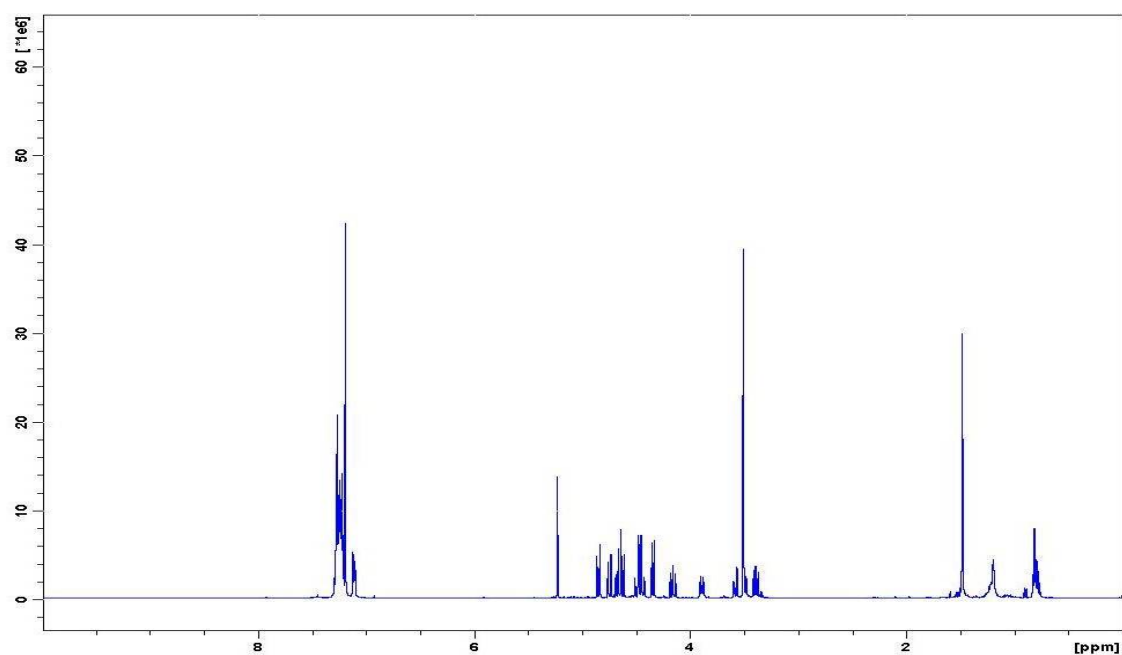
^1H -NMR of **5** (CD_3CN)



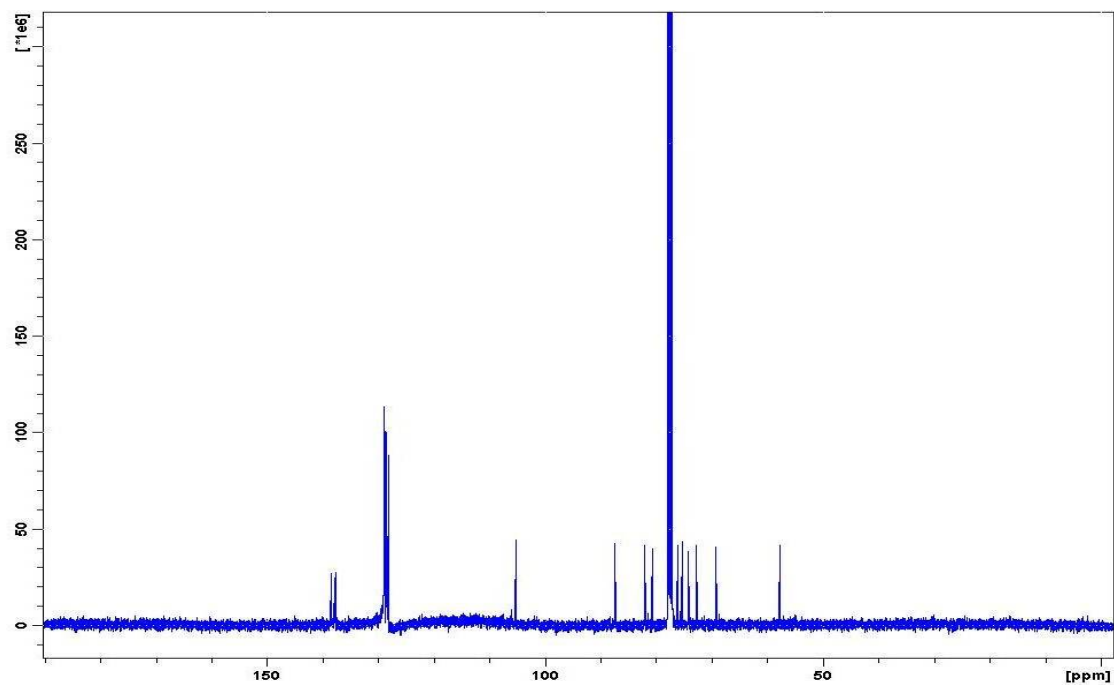
^{13}C -NMR of **5** (CD_3CN)



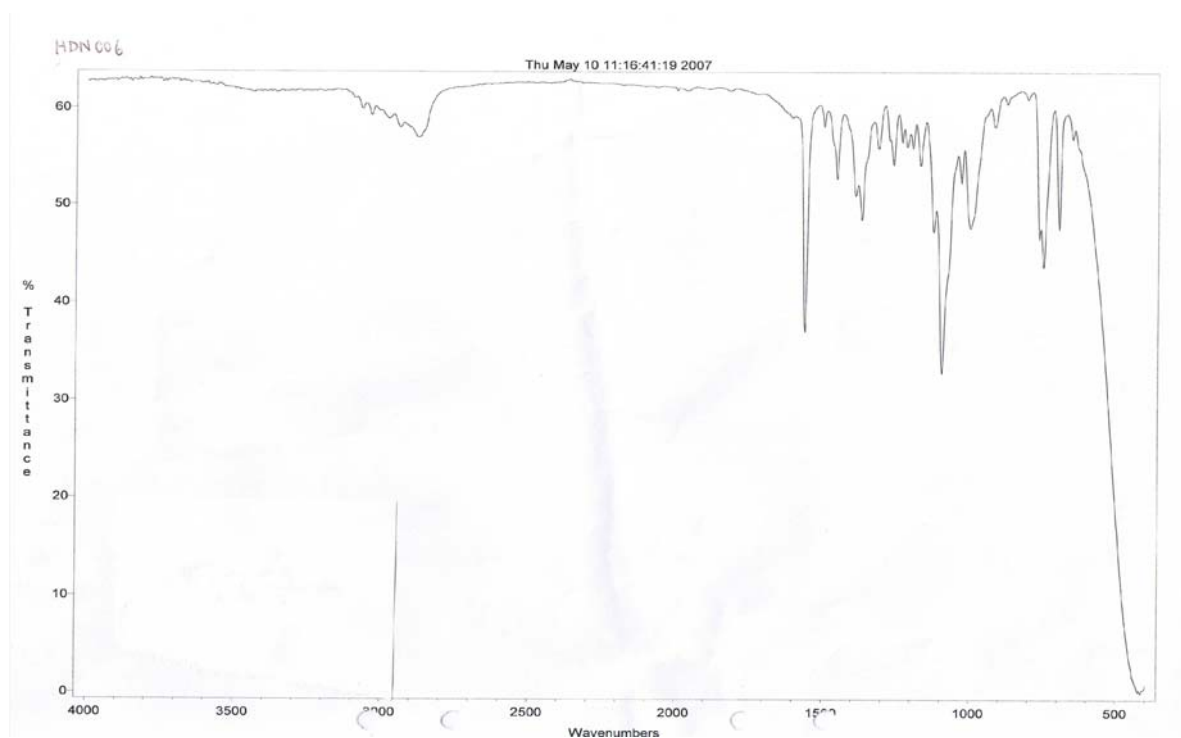
^1H -NMR of **11** (CDCl_3)



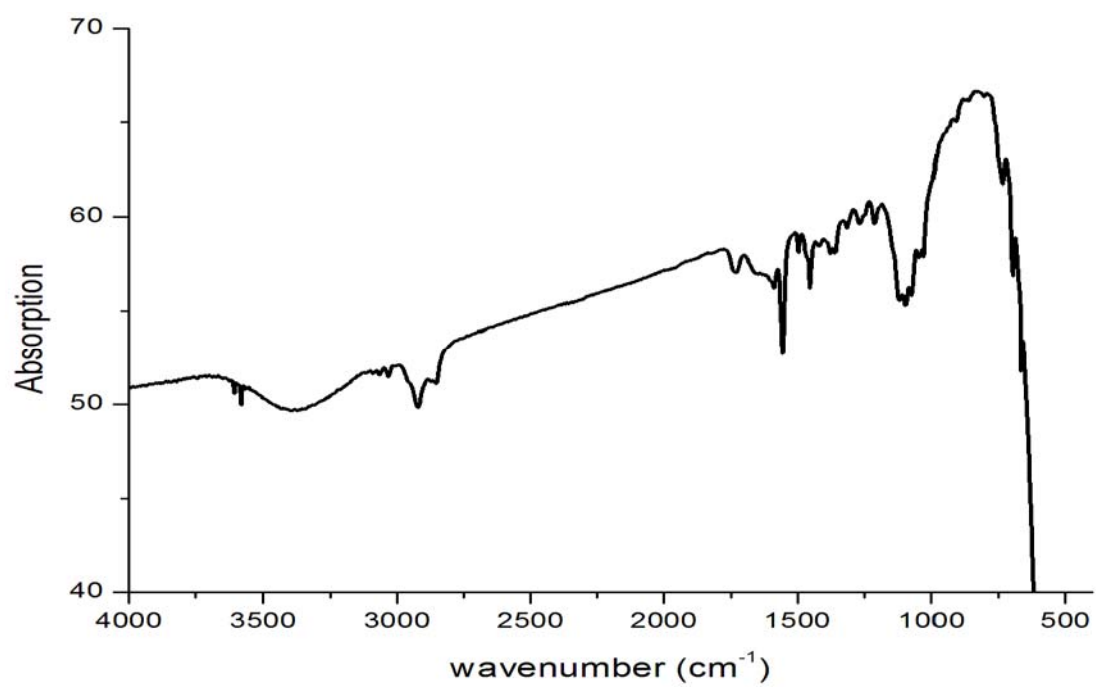
^{13}C -NMR of **11** (CDCl_3)



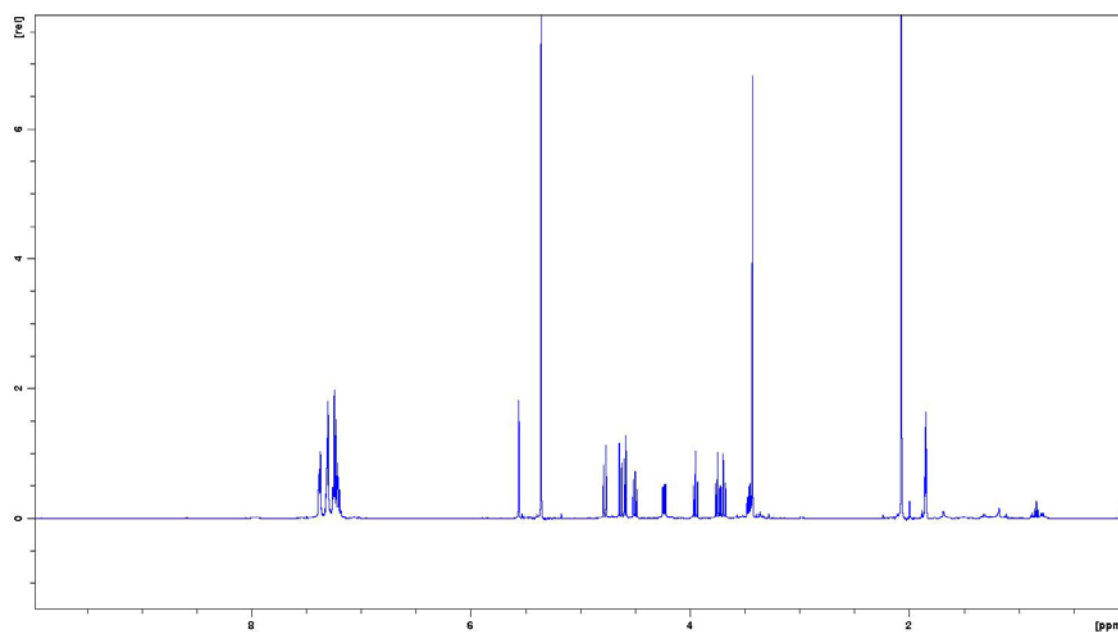
IR spectrum of compound **5**



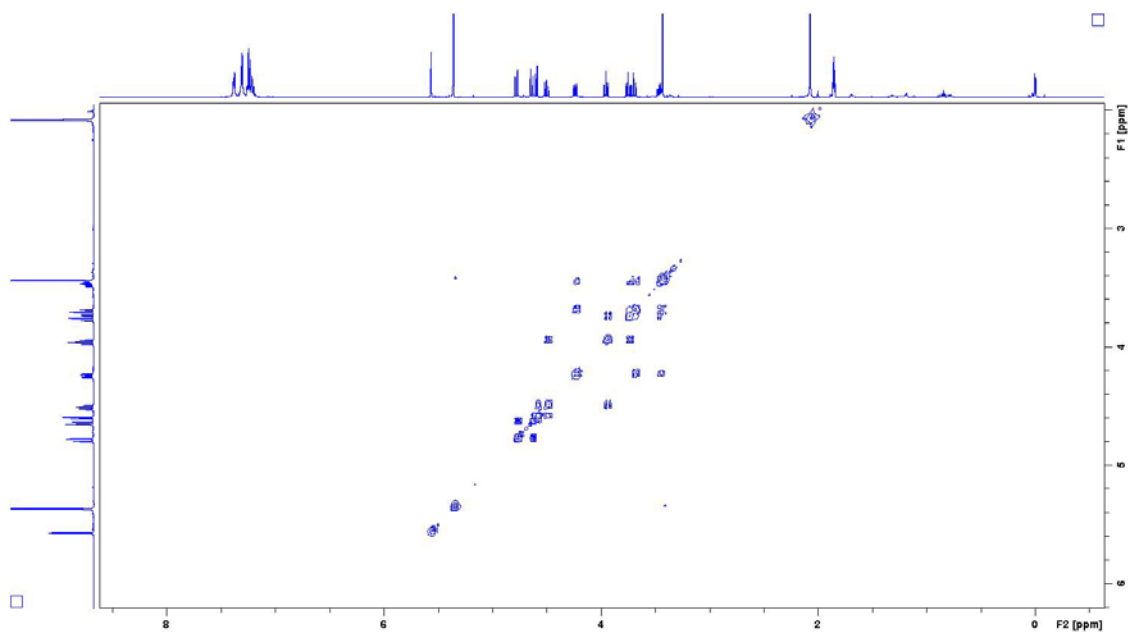
IR spectrum of compound **11**



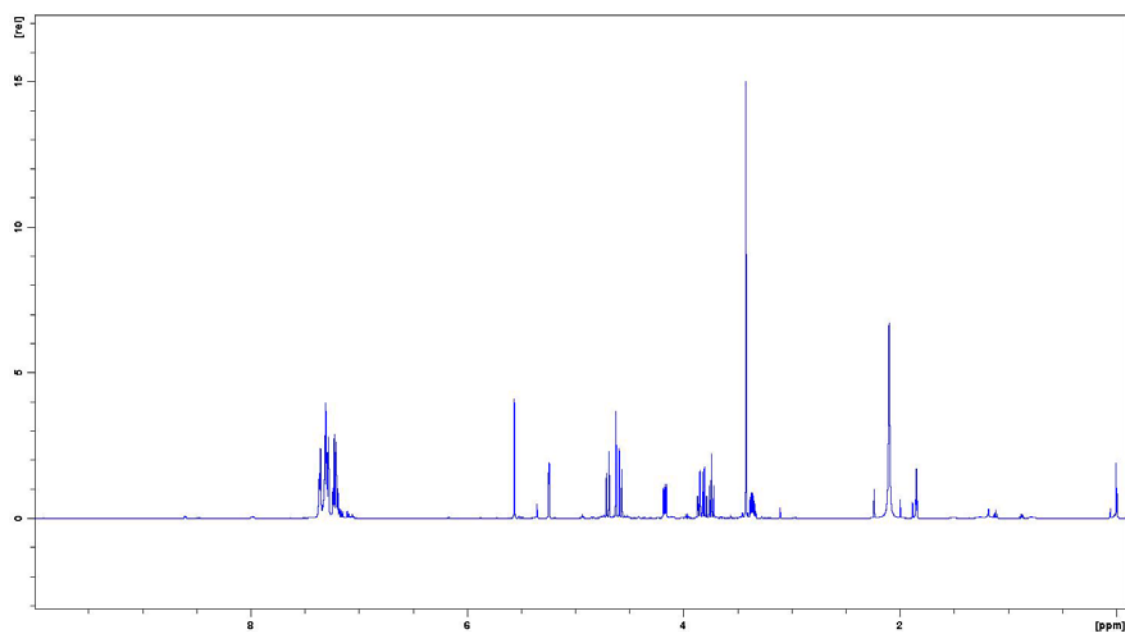
^1H -NMR spectrum of compound **3** (CD_3CN)



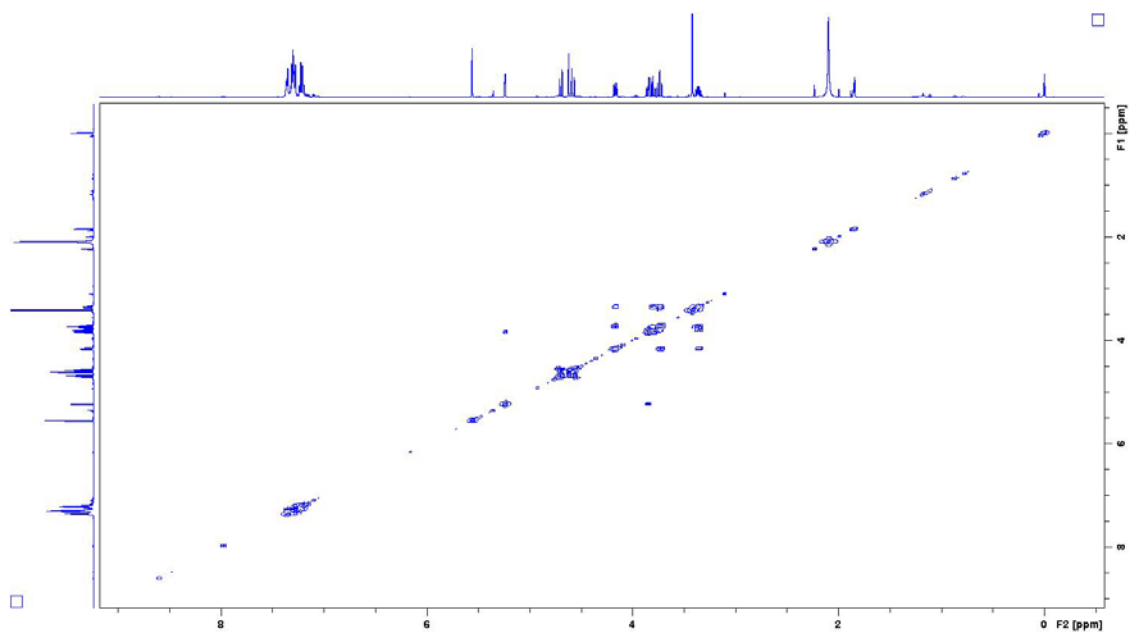
^1H - ^1H COSY spectrum of compound **3** (CD_3CN)



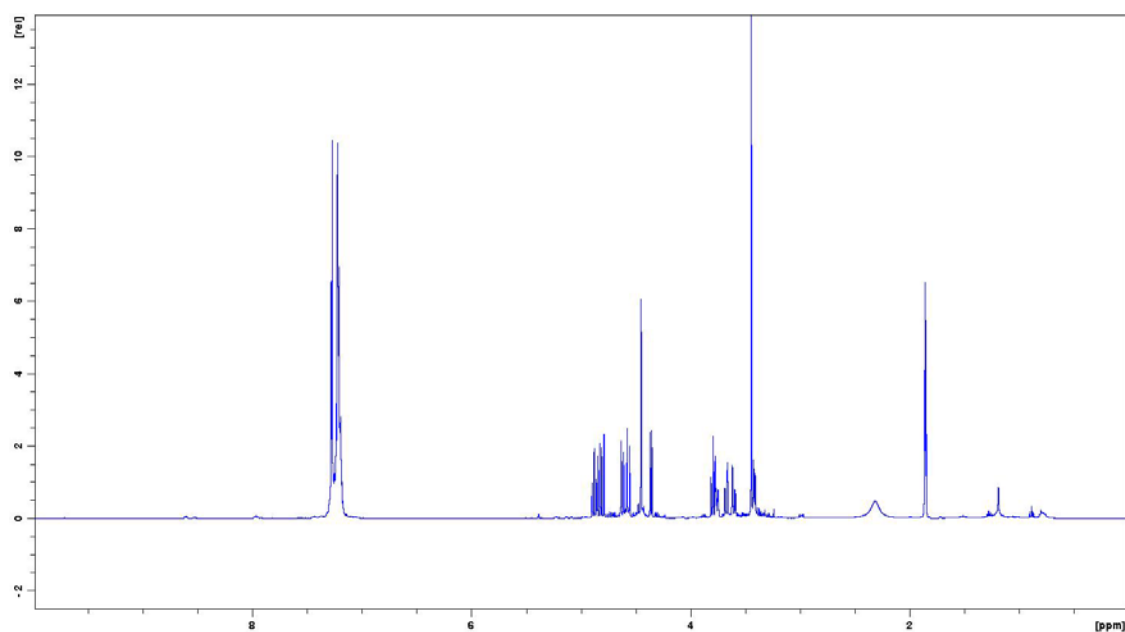
^1H -NMR spectrum of the *epi*-triflate analog of compound **3** (CD_3CN)



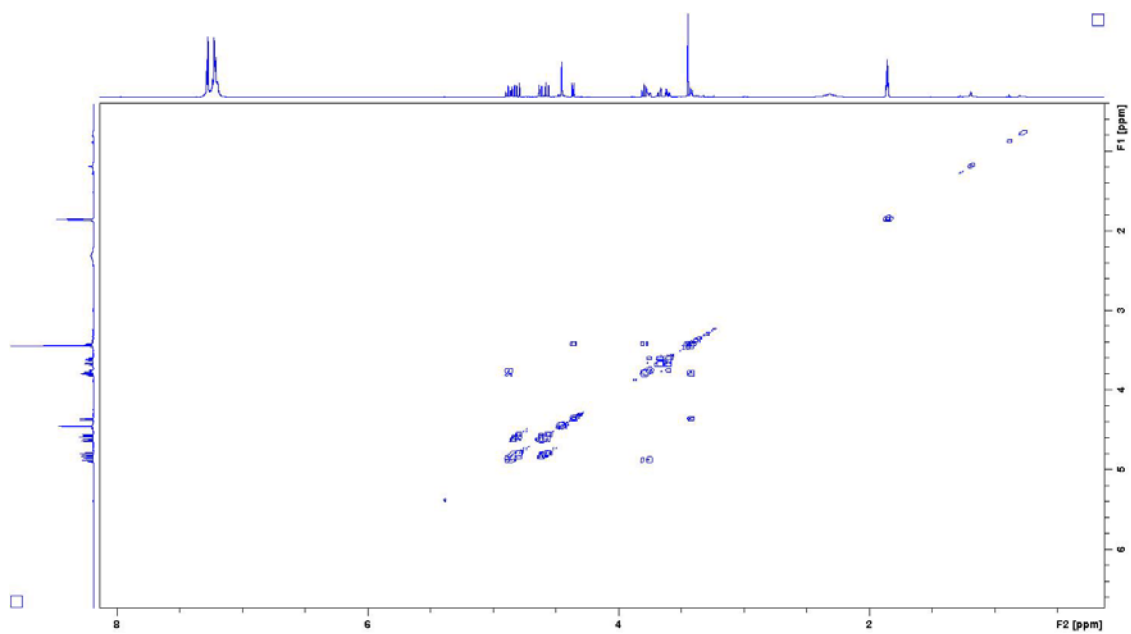
^1H - ^1H COSY spectrum of the *epi*-triflate analog of compound **3** (CD_3CN)



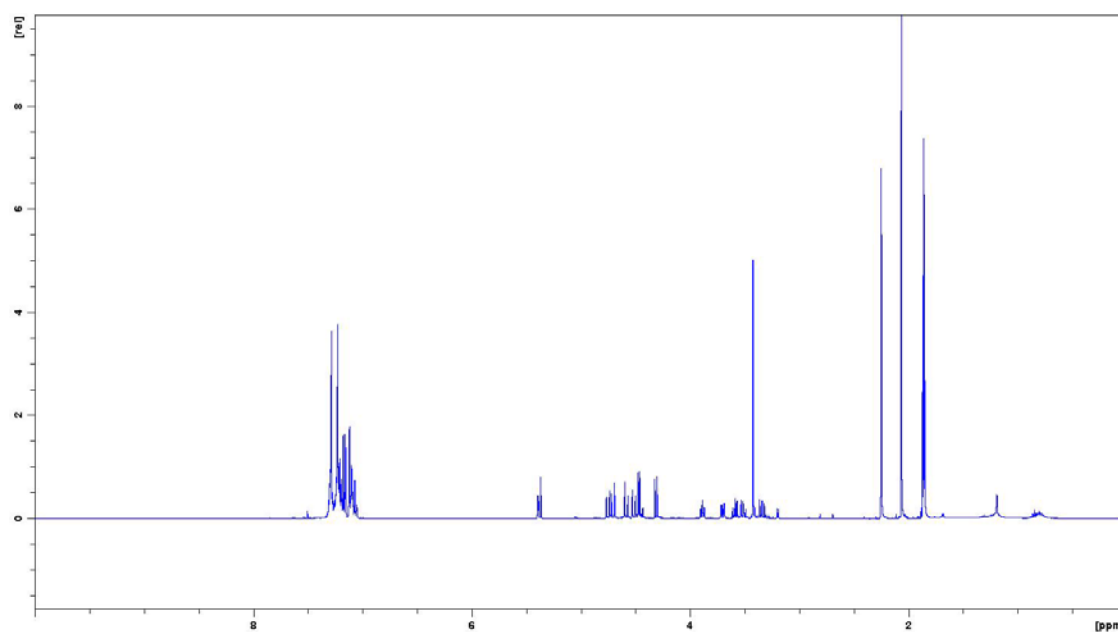
^1H -NMR spectrum of compound **10** (CD_3CN)



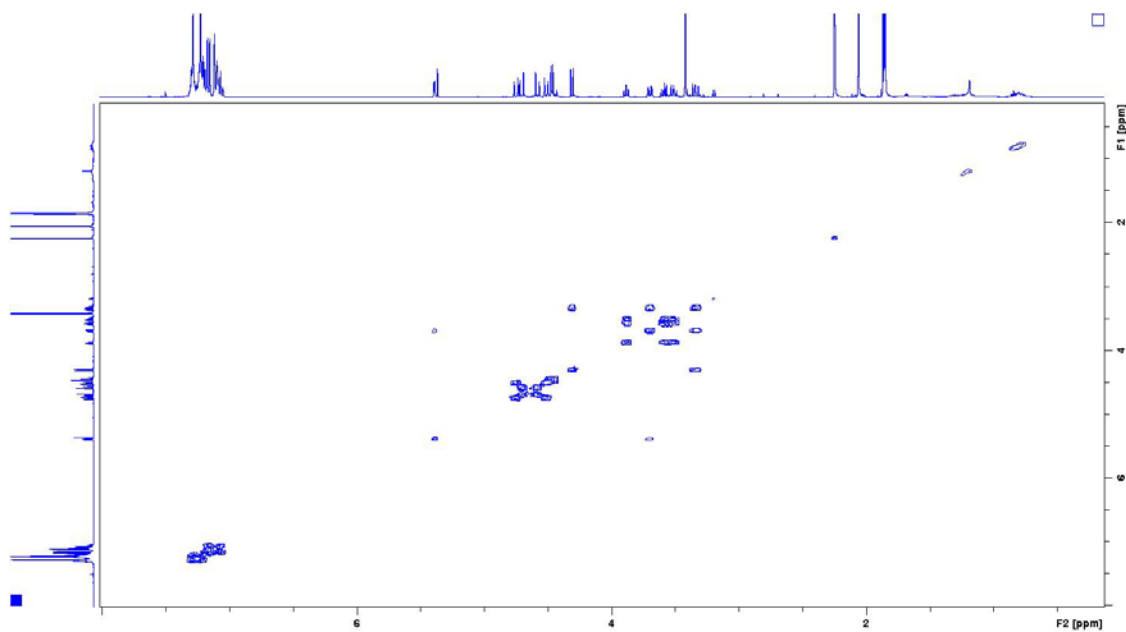
^1H - ^1H COSY spectrum of compound **10** (CD_3CN)



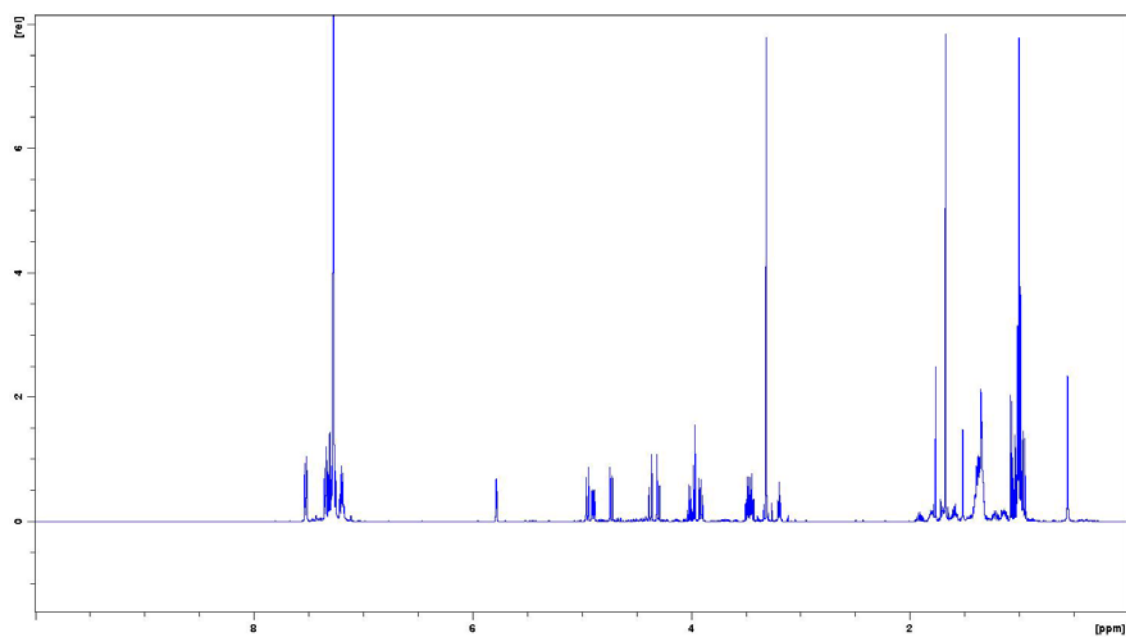
^1H -NMR spectrum of the *epi*-triflate analog of compound **10** (CD_3CN)



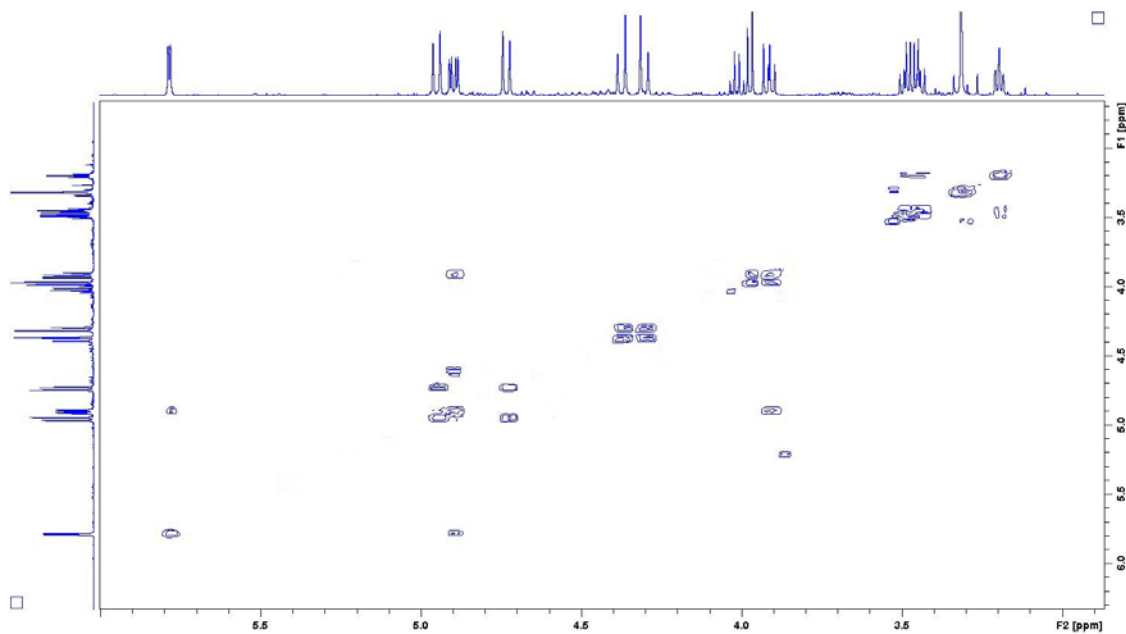
^1H - ^1H COSY spectrum of the *epi*-triflate analog of compound **10** (CD_3CN)



^1H -NMR spectrum of compound 17 (C_6D_6)



^1H - ^1H COSY spectrum of compound 17 (C_6D_6)

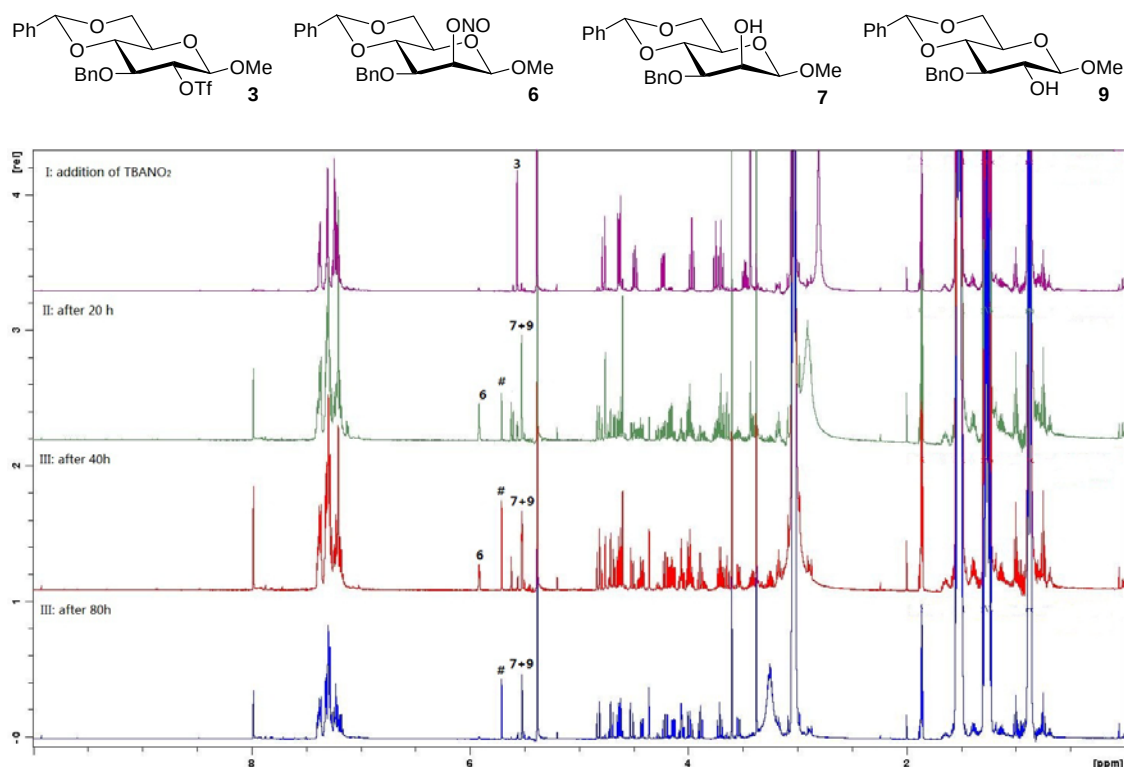


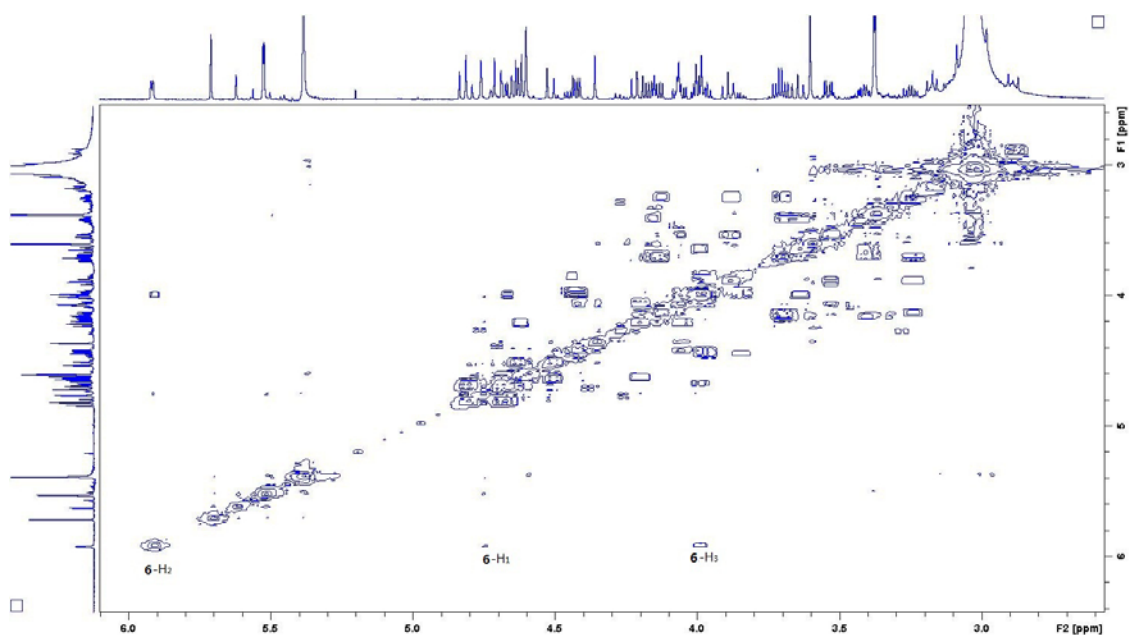
Discrimination of nitrite ester compounds

The nitrite ester compounds in present study cannot be purified due to their unstability. However, the analysis and study of ^1H NMR spectra combined with ^1H - ^1H COSY on them proved their existence.

1. Some of them have the almost same molecule-polarity as their relative nitro-compounds. Thus, usually a mixture of nitrite-ester and its relative nitro-compound was obtained after purification by running a column. The nitrite-ester decomposed to its relative hydroxyl-compound slowly. Finally, a mixture of hydroxyl-compound and nitro-compound was formed. The hydroxyl-compound and nitro-compound could be identified after purification by running a column. Thus, the nitrite ester compound can be discriminated by the analysis and study of NMR.
2. In the ^1H NMR spectra, the protons connecting carbon with nitrite group always appeared larger chemical shift values than the protons connecting carbon with nitro group, and usually they were in the most up-field.
3. When inversion reactions were recorded by ^1H NMR spectra combined with ^1H - ^1H COSY with time, it can be seen that the nitrite esters slowly reached a maximum level and gradually transformed into its relative hydroxyl compounds.

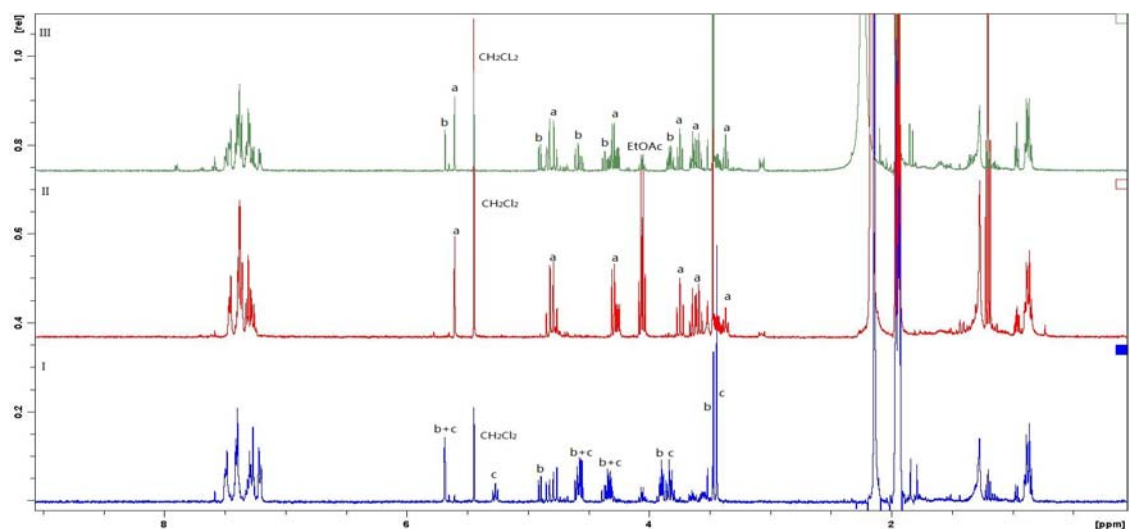
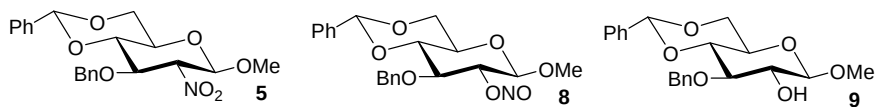
Inversion of compound 3

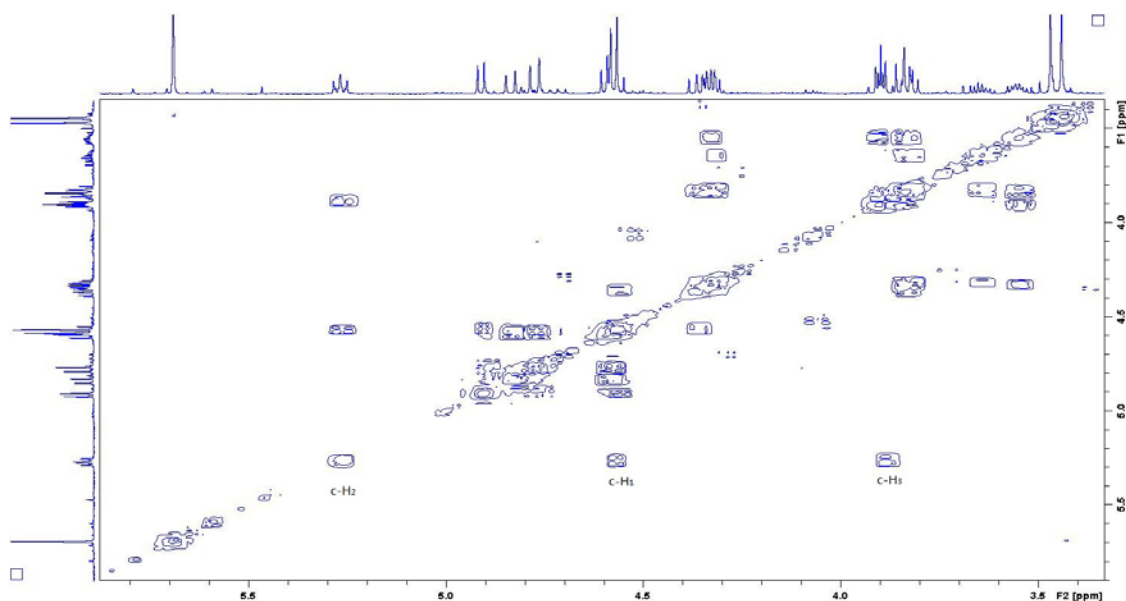




The nitrite ester **6** could be easily discriminated by its characteristic chemical shift (H_2 5.92) from the 1H NMR spectra combined with 1H - 1H COSY. #: fragmentation compound

Decompose of nitrite ester **8**

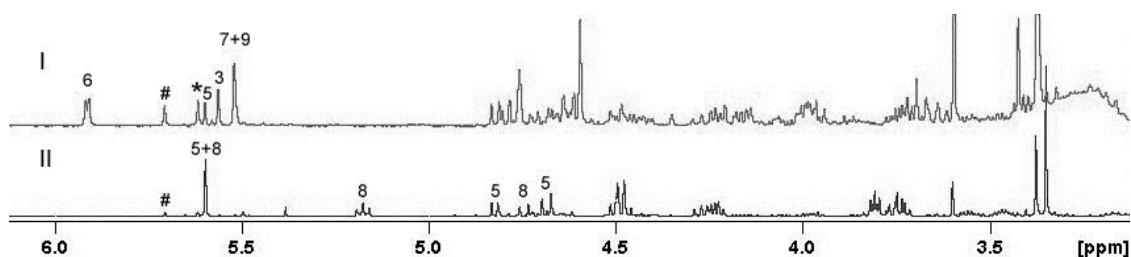




The nitrite ester **8** could be easily discriminated by its characteristic chemical shift (H_2 5.28) from the 1H NMR spectra combined with 1H - 1H COSY.

I: 1H NMR spectra of the purified mixture of nitro compound **5** and nitrite ester **8** (CD_3CN). II: 1H NMR spectra of the purified hydroxyl compound **9** (CD_3CN). III: 1H NMR spectra of the purified mixture of nitro compound **5** and nitrite ester **8** after 24 hours (CD_3CN), all the nitrite ester **8** have decomposed to the hydroxyl compound **9** by that time. a: identified hydroxyl compound **9**; b: identified nitro compound **5**; c: nitrite ester **8**.

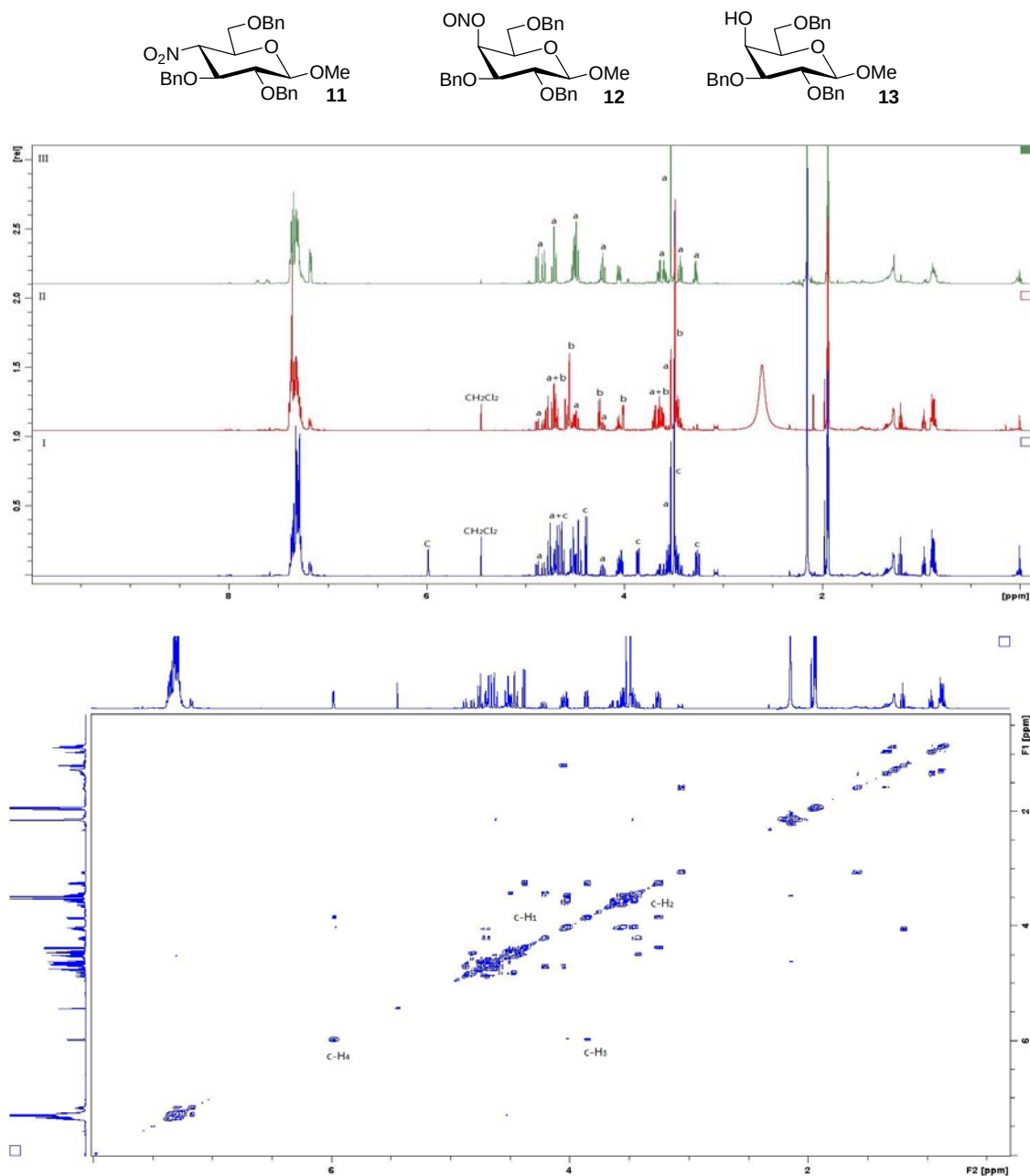
1H NMR spectrum of inversions with compound **3** and its *epi*-triflate analog



I: reaction with **3** for 14 h; II: reaction with the *epi*-triflate analog of **3** for 1 h.

#: fragmentation compound; Nitrite compounds **6** and **8** were always forming compounds **7** and **9** upon purification. *: suggested axial nitro-compound.

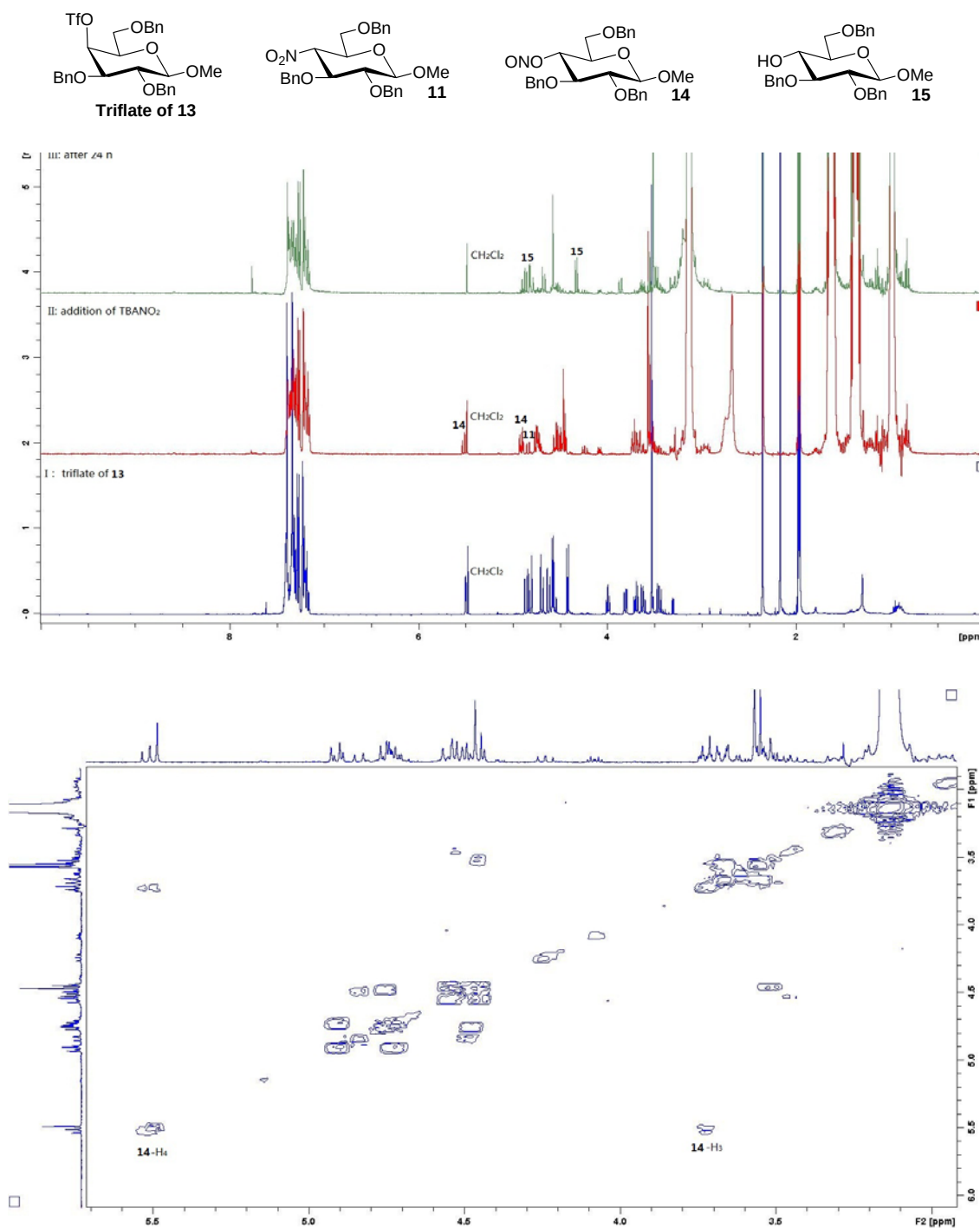
Decompose of nitrite ester **12**



The nitrite ester **12** could be easily discriminated by its characteristic chemical shift (H_4 6.01) from the 1H NMR spectra combined with 1H - 1H COSY.

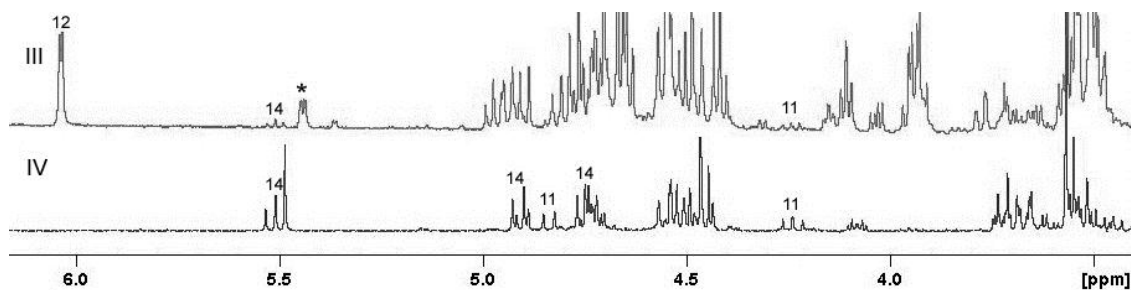
I: 1H NMR spectra of the purified mixture of nitro compound **11** and nitrite ester **12** (CD_3CN). II: 1H NMR spectra of the purified mixture of nitro compound **11** and nitrite ester **12** after 24 hours (CD_3CN), all the nitrite ester **12** have decomposed to the hydroxyl compound **13** by that time. III: 1H NMR spectra of the purified nitro compound **11** (CD_3CN). a: identified nitro compound **11**; b: identified hydroxyl compound **13**; c: nitrite ester **12**.

Inversion of triflate of **13**



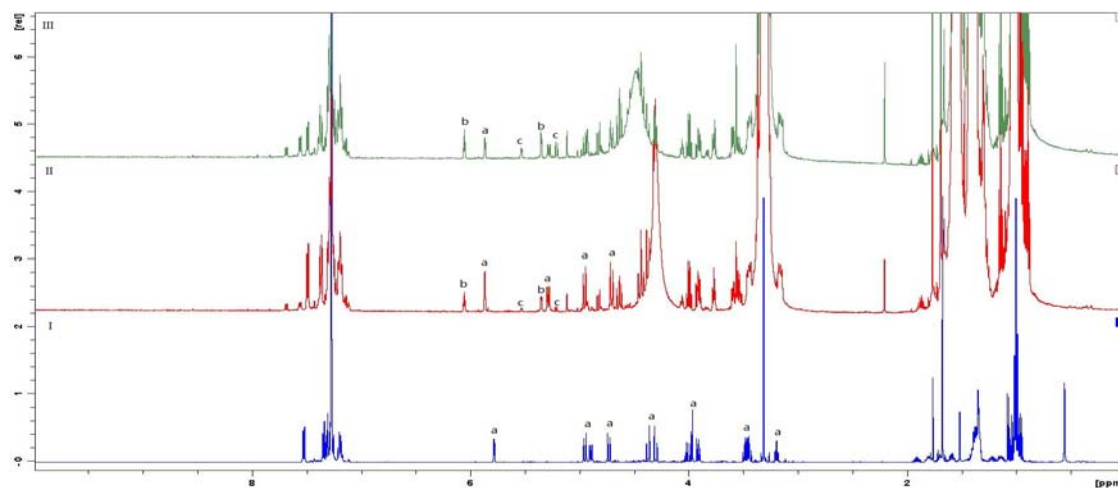
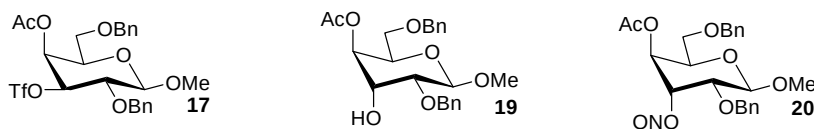
The nitrite ester **14** could be easily discriminated by its characteristic chemical shift (H₄ 5.52) from the ¹H NMR spectra combined with ¹H-¹H COSY. The spectra II indicated the formation of nitro compound **11** and nitrite ester **14** upon addition of nitrite. The spectra III indicated that **14** had totally decomposed to the hydroxyl compound **15** in 24 hours.

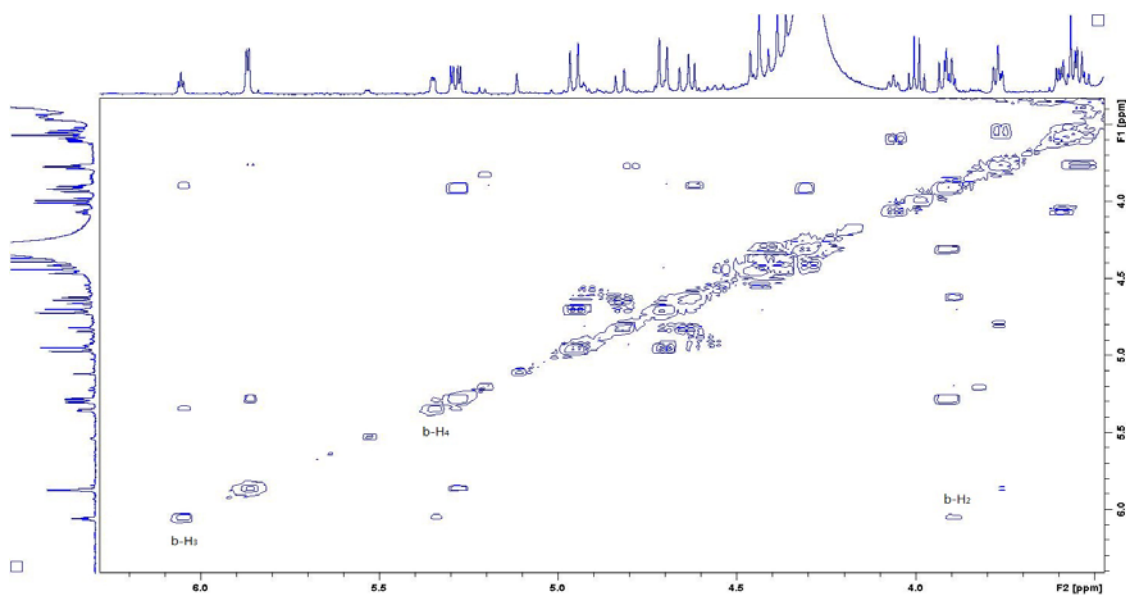
¹H NMR spectrum of inversions with compound **10** and its *epi*-triflate analog



III: reaction with **10** for 10 min; IV: reaction with the *epi*-triflate analog of **10** for 10 min.
*: suggested axial nitro-compound.

Inversion of triflate compound **17**





The nitrite ester **20** could be easily discriminated by its characteristic chemical shift (H_3 6.06) from the 1H NMR spectra combined with 1H - 1H COSY.

I: 1H NMR spectra of the purified triflate compound **17** (C_6D_6). II: 1H NMR spectra of the purified triflate compound **17** with addition of $TBANO_2$ after 1 hours (C_6D_6), the nitrite ester **20** formed and had decomposed to very less the hydroxyl compound **19**. III: 1H NMR spectra of the purified triflate compound **17** with addition of $TBANO_2$ after 3 hours (C_6D_6), the nitrite ester **20** had decomposed to more the hydroxyl compound **19**. a: the triflate compound **17**; b: nitrite ester **20**; c: identified hydroxyl compound **19**.

Cartesian coordinates, energies and results of frequency calculations

TS-N

M062X/6-31+G(d,p): -2047.99169651

M062X/cc-pVTZ: -2048.64820416

SCS-MP2/cc-pVDZ: -2043.608794436

*

C	-0.006449	0.026699	0.002886
C	-0.022815	-0.021952	2.364339
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C	2.194641	-0.350425	1.126742
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H	-0.324268	-1.079464	2.344295
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O	1.628503	-1.694399	3.288273
H	2.177949	-1.440405	1.023709
S	2.842894	-1.996117	4.144352
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O	3.906837	-1.010514	3.979974
C	2.185528	-1.674464	5.839838
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F	1.131972	-2.448104	6.090234
F	3.126669	-1.920925	6.747752
C	1.504930	0.231041	-0.108622
H	1.702317	1.307035	-0.174992
O	-0.490790	0.619569	1.197030
C	4.521716	-0.838045	1.167931
C	5.866444	-0.197980	1.326901
H	5.926277	0.221407	2.335036
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H	5.984720	0.617743	0.611243
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O	2.022219	-0.465086	-1.218649
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C	-0.650769	0.634406	3.574986
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O	2.000180	2.650522	3.280077
O	1.526327	3.061432	1.243881
N	1.664915	2.245698	2.158164

*

TS-O-1

M062X/6-31+G(d,p): -2047.99247804

M062X/cc-pVTZ: -2048.64907225

SCS-MP2/cc-pVDZ: -2043.612552304

*

C	0.025025	-0.047244	0.011643
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C	2.306500	-0.137759	1.049139
H	-0.092462	-1.144796	0.103622
H	-0.289578	-1.045995	2.409981
O	3.518539	0.613943	1.021483
O	1.713678	-1.832133	2.898134
H	2.541330	-1.198751	0.915622
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O	3.196643	-3.275722	4.260429
O	2.533472	-1.004153	5.089558
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F	0.319912	-3.975069	4.362663
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H	1.562277	1.417228	-0.238336
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C	4.518413	0.222513	1.832967
C	5.697957	1.141720	1.722770
H	5.999898	1.238771	0.677865
H	5.401063	2.127920	2.088290
H	6.519975	0.753812	2.321463
O	4.440549	-0.753672	2.545928
O	2.055720	-0.305698	-1.290908
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H	0.055927	0.445995	4.455484
H	-0.453530	1.807555	3.414262
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H	-2.444205	0.342400	-2.065487
H	-2.057494	-1.125825	-1.125443
C	2.094411	0.506776	-2.456443
H	1.087314	0.800349	-2.765786
H	2.700670	1.402929	-2.276682
H	2.560168	-0.093014	-3.239269
C	-2.472851	0.932116	4.846911
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H	-1.954086	0.637393	5.769367
H	-2.454609	2.026620	4.763216
H	2.122960	0.313797	3.241406
O	1.535180	2.186062	2.093654
O	3.141903	2.238301	3.480521
N	2.371869	2.867661	2.747702

*

TS-O-2

M062X/6-31+G(d,p): -2047.99030237

M062X/cc-pVTZ: -2048.64575542

SCS-MP2/cc-pVDZ: -2043.608653081

*

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C	2.274052	-0.152095	1.050169
H	-0.138257	-1.096673	0.068421
H	-0.332946	-1.044960	2.370574
O	3.503326	0.573209	1.025067
O	1.667220	-1.807082	2.903712
H	2.482110	-1.216707	0.905032
S	2.197222	-2.166267	4.275963
O	3.143951	-3.270543	4.251457
O	2.499877	-0.997312	5.095516
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C	1.478184	0.351052	-0.154296
H	1.562047	1.444233	-0.202210
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C	4.497511	0.172201	1.836655
C	5.682211	1.086009	1.732421
H	5.983828	1.190934	0.688414
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H	6.502061	0.690839	2.328918
O	4.407692	-0.796759	2.557844
O	2.036001	-0.260006	-1.293878
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C	-0.582117	0.704088	3.559445
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H	-0.538108	1.790125	3.409016
O	-1.913417	0.268238	3.715777
C	-2.040376	0.079378	-1.156186
H	-2.613332	0.461337	-0.306855
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H	-1.993143	0.586383	5.765452
H	-2.552970	1.949846	4.755458
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O	1.547123	2.132673	2.176038
O	2.693060	3.717266	2.965463
N	2.487424	2.505719	2.940395

*

TS-O-3

M062X/6-31+G(d,p): -2047.98381372

M062X/cc-pVTZ: -2048.64107506

SCS-MP2/cc-pVDZ: -2043.604191553

*

C	0.000000	0.000000	0.000000
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C	1.525495	0.000000	2.378993
C	2.195761	-0.325237	1.070074
H	-0.168282	-1.094610	0.035289
H	-0.318776	-1.051454	2.409788
O	3.606117	-0.176025	1.197844
O	1.750139	-1.767484	3.118982
H	2.066897	-1.404529	0.924450
S	2.091251	-1.961326	4.579473
O	3.124515	-2.964533	4.789928
O	2.189445	-0.700712	5.309245
C	0.543882	-2.755962	5.204083
F	-0.504662	-1.965635	4.972726
F	0.341693	-3.922035	4.594686
F	0.639557	-2.967444	6.515693
C	1.494681	0.314752	-0.135892
H	1.619847	1.397856	-0.149899
O	-0.504222	0.589156	1.186209
C	4.298733	0.904660	0.777855
C	5.708567	0.839281	1.291012
H	5.686080	1.011342	2.370331
H	6.134824	-0.149175	1.109890
H	6.307867	1.608173	0.806509
O	3.853400	1.780081	0.074634
O	2.042344	-0.293629	-1.280399
O	-0.662786	0.555999	-1.076316
C	-0.578237	0.727122	3.564491
H	-0.016152	0.438837	4.465657
H	-0.475598	1.809630	3.414450
O	-1.932597	0.357458	3.688130
C	-2.027009	0.157495	-1.170291
H	-2.596960	0.513259	-0.307880
H	-2.420919	0.604359	-2.082505
H	-2.100413	-0.934767	-1.235060
C	2.117195	0.561290	-2.415314
H	1.118621	0.860348	-2.746575
H	2.713988	1.448821	-2.178523
H	2.610102	-0.011002	-3.202549
C	-2.538279	0.957700	4.815905
H	-3.577013	0.626646	4.843311
H	-2.032573	0.648223	5.740464
H	-2.507160	2.052800	4.743260
H	2.107764	0.398557	3.194079
O	1.532953	2.204658	2.044811
O	3.365439	2.197354	3.111927
N	2.429959	2.857868	2.644684

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M062X/6-31+G(d,p): -1842.83256536

M062X/cc-pVTZ: -1843.41693809

SCS-MP2/cc-pVDZ: -1838.925345204

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C	0.010384	0.007808	0.009342
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C	-0.045662	-0.046771	2.385117
C	1.483213	-0.016068	2.456224
C	2.081200	-0.643494	1.209106
H	-0.367203	-1.031232	-0.002048
H	1.838698	1.010807	2.595903
H	-0.391545	-1.091860	2.346415
O	3.494036	-0.467089	1.273548
O	1.882842	-0.810452	3.607233
H	1.852449	-1.714760	1.191076
S	3.286502	-0.527794	4.309504
O	4.207340	-1.607528	4.043222
O	3.673298	0.855150	4.150369
C	2.676380	-0.756280	6.044125
F	1.810700	0.201534	6.337340
F	2.096810	-1.939495	6.165286
F	3.719513	-0.682776	6.857218
C	1.539352	0.017163	-0.052840
H	1.875140	1.064641	-0.094736
O	-0.418793	0.644093	1.207461
C	4.292279	-1.548192	1.064180
C	5.736161	-1.152461	1.120601
H	5.960518	-0.492360	0.278656
H	5.929330	-0.602752	2.044265
H	6.359701	-2.042957	1.071190
O	3.863022	-2.658229	0.865395
O	2.025319	-0.714965	-1.147451
O	-0.481372	0.721637	-1.061669
C	-0.689218	0.649022	3.565160
H	-0.267327	0.252247	4.499966
H	-0.473188	1.727555	3.512287
O	-2.075269	0.414835	3.511992
C	-1.889033	0.584641	-1.242024
H	-2.431576	0.993865	-0.385622
H	-2.143109	1.143536	-2.141956
H	-2.152935	-0.470511	-1.377842
C	2.294405	0.065286	-2.307030
H	1.386112	0.550466	-2.674144
H	3.055944	0.823250	-2.087421
H	2.677191	-0.622626	-3.061398
C	-2.760329	1.045580	4.577794
H	-3.819567	0.814436	4.463791
H	-2.407377	0.669657	5.546932
H	-2.619604	2.133652	4.543688

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2

M062X/6-31+G(d,p): -1086.65076652#

M062X/cc-pVTZ: -1087.02661247#

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C	-0.021548	-0.045233	-0.038252
C	0.027773	-0.081025	2.324667
C	1.554917	-0.089554	2.368110
C	2.110448	-0.685932	1.074894
H	-0.392608	-1.087749	-0.034458
H	-0.312834	-1.129036	2.307216
O	3.522785	-0.491811	1.000278

H	1.891588	-1.759776	1.065137
C	1.503571	-0.036999	-0.162196
H	1.839116	1.007864	-0.234938
O	-0.421020	0.593591	1.162316
C	4.296301	-1.365891	1.680578
C	5.749893	-1.027770	1.541736
H	6.029201	-1.030794	0.485758
H	5.924388	-0.021969	1.932217
H	6.346544	-1.752001	2.092549
O	3.835918	-2.287297	2.316130
O	1.914350	-0.784997	-1.280524
O	-0.549981	0.655836	-1.103549
C	-0.580760	0.602429	3.531787
H	-0.096459	0.226746	4.446341
H	-0.409450	1.686137	3.465882
O	-1.959506	0.317006	3.550101
C	-1.961667	0.513026	-1.235043
H	-2.477787	0.927963	-0.364976
H	-2.249012	1.062627	-2.130627
H	-2.227341	-0.544243	-1.351841
C	2.191654	-0.007260	-2.438118
H	1.305117	0.545505	-2.761943
H	3.011559	0.693752	-2.239649
H	2.495385	-0.706195	-3.218107
C	-2.618249	0.959920	4.624305
H	-3.671729	0.683768	4.570803
H	-2.205773	0.634210	5.588325
H	-2.523210	2.050666	4.545675
H	1.915719	-0.653804	3.231372
O	1.972701	1.288849	2.477954
N	3.094002	1.588821	3.207005
O	3.665871	0.664455	3.668274

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3

M062X/6-31+G(d,p): -1086.65195468#

M062X/cc-pVTZ: -1087.02818465#

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C	0.002834	-0.039855	-0.038993
C	0.027967	-0.068234	2.316670
C	1.565526	-0.098027	2.394117
C	2.157374	-0.613709	1.082339
H	-0.369773	-1.081035	-0.009705
H	-0.299009	-1.119494	2.277313
O	3.558639	-0.355548	1.019865
H	1.994162	-1.698004	1.078633
C	1.525658	-0.033930	-0.179312
H	1.860464	0.999751	-0.326242
O	-0.387096	0.618329	1.158378
C	4.371456	-1.213894	1.679358
C	5.813192	-0.856877	1.483206
H	6.043902	-0.840193	0.415880
H	5.995650	0.144152	1.881357
H	6.440630	-1.583334	1.995452
O	3.943773	-2.134490	2.337809
O	1.922620	-0.861698	-1.246876

O	-0.535141	0.641550	-1.109896
C	-0.617026	0.586584	3.523040
H	-0.161037	0.191971	4.443408
H	-0.449406	1.674900	3.491482
O	-1.991874	0.297754	3.483279
C	-1.949116	0.502269	-1.224004
H	-2.454209	0.955287	-0.366814
H	-2.240151	1.017616	-2.138595
H	-2.221850	-0.556987	-1.296372
C	2.168559	-0.171177	-2.466026
H	1.265699	0.334399	-2.820454
H	2.973980	0.561290	-2.334391
H	2.479067	-0.923480	-3.191648
C	-2.686601	0.868659	4.577170
H	-3.737272	0.599786	4.467099
H	-2.307363	0.475572	5.529173
H	-2.587973	1.961655	4.576040
H	1.898330	-0.709070	3.233912
N	2.062668	1.289561	2.711774
O	2.156279	2.098467	1.808837
O	2.301493	1.528603	3.883566

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M062X/6-31+G(d,p): -1086.64771556

M062X/cc-pVTZ: -1087.02393675

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C	1.05790600	1.68960000	0.21087600
C	1.42347100	-0.64367800	0.25553600
C	-0.02593400	-0.94678300	-0.14948100
C	-0.94732700	0.20354100	0.25083900
H	1.14879100	1.69294600	1.31301100
H	1.49442400	-0.59473200	1.35373000
O	-2.22687900	0.05365500	-0.37012600
H	-1.07280500	0.20518000	1.33934800
C	-0.40634300	1.55697700	-0.19970800
H	-0.45914700	1.62476100	-1.29674100
O	1.79535700	0.59758900	-0.31311500
C	-3.22827600	-0.50599300	0.34035100
C	-4.48978200	-0.56658600	-0.46829600
H	-4.70361400	0.41076300	-0.90460500
H	-4.34651300	-1.27708900	-1.28731000
H	-5.31322300	-0.89445400	0.16299300
O	-3.08934100	-0.91946900	1.46919100
O	-1.19937300	2.54601900	0.40852200
O	1.56094200	2.85700000	-0.32578900
C	2.38366100	-1.69754700	-0.25418900
H	2.00903300	-2.69607800	0.01316900
H	2.44805400	-1.62799800	-1.35142100
O	3.64270400	-1.46925800	0.33263300
C	2.84839100	3.20611500	0.17581200
H	3.58981200	2.45012300	-0.09709100
H	3.11126700	4.16115900	-0.27785200
H	2.81443400	3.31398800	1.26612300
C	-1.44660700	3.68624500	-0.40484400
H	-0.51322300	4.19120200	-0.66946600

H	-1.98103400	3.39485100	-1.31723900
H	-2.07500900	4.35613700	0.18275900
C	4.60475000	-2.41549400	-0.09222000
H	5.54191400	-2.17298700	0.40952500
H	4.29944200	-3.43434200	0.18006300
H	4.75035400	-2.36506300	-1.17914000
O	-1.65857800	-2.73763900	-1.07981300
O	-0.39625900	-2.14013600	0.56896300
N	-1.24669500	-3.04460200	-0.01764400
H	-0.08814500	-1.12662000	-1.22812600

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TS-ax

M062X/6-31+G(d,p): -1086.63171302

M062X/cc-pVTZ: -1087.00809061

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C	-1.06747900	1.67321200	-0.20490100
C	-1.34308900	-0.64956200	-0.52678600
C	0.12836200	-0.94177400	-0.23576600
C	0.98015100	0.29175600	-0.54952900
H	-1.21130000	1.82745300	-1.29142400
H	-1.45771300	-0.47679700	-1.60956100
O	2.31388600	0.13956000	-0.06449200
H	1.00615900	0.43117200	-1.63739000
C	0.42387200	1.54671200	0.11043400
H	0.53884900	1.46463100	1.20128800
O	-1.75535500	0.50039100	0.19265100
C	3.12421700	-0.70541100	-0.72716500
C	4.48464000	-0.76751300	-0.09990500
H	4.89846600	0.23842400	-0.00585600
H	4.39304500	-1.18930800	0.90428800
H	5.13673800	-1.39210000	-0.70720900
O	2.76255000	-1.33193800	-1.70030800
O	1.13329500	2.65095500	-0.39692100
O	-1.57385800	2.74180900	0.50877600
C	-2.23461600	-1.80345500	-0.11918100
H	-1.82787700	-2.74067000	-0.53084500
H	-2.24817200	-1.88275300	0.97728800
O	-3.53016300	-1.56810100	-0.61814800
C	-2.89510800	3.10899900	0.12287700
H	-3.60106900	2.30132800	0.33421900
H	-3.15768600	3.99041100	0.70675000
H	-2.92512800	3.35409800	-0.94536000
C	1.41150700	3.66184900	0.56303200
H	0.48765900	4.07213000	0.98100500
H	2.03571100	3.26032700	1.37068000
H	1.95908800	4.44679800	0.04043400
C	-4.43750200	-2.58176200	-0.23075300
H	-5.40937300	-2.32762700	-0.65497400
H	-4.11854200	-3.56039200	-0.61318400
H	-4.52052400	-2.63658100	0.86252700
H	0.47240300	-1.77956700	-0.85182800
O	0.28646200	-1.26103900	1.15717900
N	0.78021000	-2.61319800	1.33250600
O	1.94294100	-2.63499800	1.36219700

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TS-eq

M062X/6-31+G(d,p): -1086.63143412

M062X/cc-pVTZ: -1087.00804738

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C	1.03278100	1.70859900	0.19135500
C	1.44956500	-0.61992200	0.26317800
C	0.01148000	-0.95027800	-0.15026300
C	-0.93251100	0.18670900	0.22353600
H	1.09936800	1.72246700	1.29533100
H	1.50773200	-0.56805900	1.36239300
O	-2.19293600	-0.05171600	-0.40160200
H	-1.06451600	0.20544500	1.31047100
C	-0.42265100	1.54359300	-0.24618600
H	-0.45790500	1.59324500	-1.34521600
O	1.80485900	0.62800300	-0.30686100
C	-3.23985800	-0.42568600	0.36461900
C	-4.45574600	-0.66673000	-0.48038900
H	-4.70773000	0.24522600	-1.02663600
H	-4.23822100	-1.44739900	-1.21313200
H	-5.28801300	-0.96707700	0.15295800
O	-3.18299500	-0.53775400	1.56775600
O	-1.25009500	2.52353200	0.33156300
O	1.52655900	2.88176700	-0.34258200
C	2.42666300	-1.66151500	-0.23508800
H	2.05470600	-2.66223400	0.02960000
H	2.50151700	-1.59294800	-1.33201100
O	3.67951000	-1.42547300	0.36263200
C	2.79041200	3.26266400	0.19430000
H	3.55291800	2.51375700	-0.03682000
H	3.05364800	4.21244500	-0.27011000
H	2.71743700	3.39228400	1.28041300
C	-1.47107600	3.66706800	-0.48473800
H	-0.53283600	4.18686800	-0.69737100
H	-1.95345600	3.37597000	-1.42588800
H	-2.13859800	4.32331500	0.07465700
C	4.65087100	-2.36470800	-0.05592700
H	5.58228800	-2.11838200	0.45464100
H	4.34913000	-3.38618100	0.21068800
H	4.80585000	-2.31075900	-1.14146000
O	-0.40787400	-2.13888300	0.53400200
N	-0.84802400	-3.18444800	-0.37579000
O	-1.96722100	-3.05406100	-0.66004900
H	-0.02519600	-1.10892400	-1.23723300

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Nitrite anion

M062X/6-31+G(d,p): -205.182146416

M062X/cc-pVTZ: -205.244910606

SCS-MP2/cc-pVDZ: -204.703602091

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N	0.004458	0.000000	0.002785
O	0.003761	0.000000	1.251750
O	1.126709	0.000000	-0.545361

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Triflate anion

M062X/6-31+G(d,p): -961.405110681

M062X/cc-pVTZ: -961.686779427

SCS-MP2/cc-pVDZ: -959.696854739

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O	0.012464	-0.027996	0.017609
S	-0.004850	-0.012655	1.487597
O	1.318311	-0.010452	2.128146
O	-0.991859	0.894895	2.090509
C	-0.666600	-1.686005	1.910329
F	-1.887333	-1.861715	1.392867
F	0.127987	-2.648762	1.429295
F	-0.752771	-1.845417	3.235553

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