Predicting the Catalytic Activity of Azolium-Based Halogen Bond Donors: An Experimentally-Verified Theoretical Study

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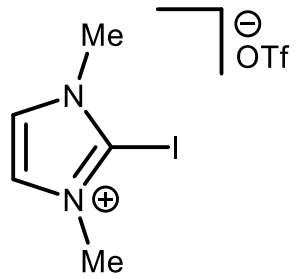
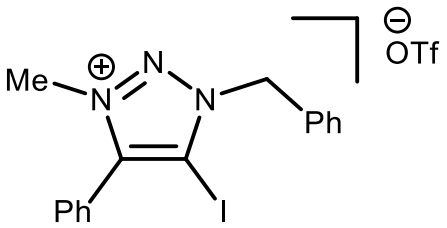
Table of contents

Synthesis and characterization of [6–7]OTf.



A solution of MeI (2.73 mL; 43.90 mmol) in CH_3CN (1 mL) was added to a stirred solution of 1-methylimidazole (3.000 g; 36.58 mmol) in CH_3CN (4 mL). The resulting solution was stirred at 60 °C for 3 h. The solvent was evaporated *in vacuo* at 40 °C and then the residue was crystallized under EtOAc. The precipitate formed was filtered off, washed with Et_2O (10 mL), dried at 50 °C for 2 h in air and then at RT in air to give the 1,3-dimethylimidazolium iodide in 92 % (7.550 g) yield as a colorless solid. A solution of NIS (540 mg; 2.40 mmol) in anhydrous CH_2Cl_2 (1 mL) was added to a stirred solution of 1,3-dimethylimidazolium iodide (448 mg, 2.00 mmol) in anhydrous CH_2Cl_2 (4 mL). The resulting solution was refluxed for 24 h. The solvent was evaporated *in vacuo* at RT, and 2-iodo-1,3-dimethylimidazolium iodide was isolated via column chromatography in 70 % (490 mg) yield as a colorless solid. A solution of AgOTf (162 mg; 0.63 mmol) in MeOH (2 mL) was added to a stirred solution of 2-iodo-1,3-dimethylimidazolium iodide (210 mg; 0.63 mmol) in MeOH (3 mL). The suspension was stirred for 15 min at RT and the precipitate formed was filtered off and washed with MeOH (15 mL). The combined organic layers were evaporated *in vacuo* at 40 °C and the residue was recrystallized from EtOAc (5 mL) to give [**6**]OTf as a colorless solid.

[**6**]OTf. Yield: 60 % (127 mg). M.p.: 162–164 °C. Λ_M (CH_3OH, 9.5×10^{-4} *M*): 168.3 $Ohm^{-1}\cdot cm^{-1}\cdot mol^{-1}$. ^1H NMR (400.13 MHz, CD_3CN): δ = 7.60 (s, 2H, C*H*), 3.81(s, 6H, CH_3). $^{13}C\{^1H\}$ NMR (101.61 MHz, CD_3CN): δ = 126.25 (*C*H), 120.69 (q, $^1J_{CF}$ = 319.2 Hz, *C*F_3), 39.33 (*C*H_3). HRMS (ESI-TOF): *m*/*z* calcd for $C_5H_8N_2I^+$: 222.9727; found: 222.9725. IR (KBr, selected bands): $\tilde{\nu}$ = 3087 (w, C−H), 2954 (w, C−H), 1648 (m, C=N), 1570 (m, C=C), 1254 (s, C−F), 1227 (s, S=O or C−F), 1171 (s, C−F), 1033 (s, S=O or C−F), 638 (s, C−I), 519 (m, C−I).



A suspension of I_2 (4.900 g; 19.00 mmol) in benzene (5 mL) was added to a stirred solution of morpholine (4.600 mL; 52.80 mmol) in benzene (10 mL). The resulting suspension was stirred for 30 min at RT. A solution of phenylacetylene in benzene (10 mL) was added dropwise to the reaction mixture. The resulting suspension was stirred for 24 h at 45 °C and then the precipitate formed was filtered off and then washed with Et_2O (20 mL). The combined organic layers were consequently washed with saturated aqueous solutions of NH_4Cl (20 mL), $NaHCO_3$ (20 mL) and H_2O (20 mL). The organic layer was dried over Na_2SO_4 and filtered. Solvent was evaporated *in vacuo* at 50 °C to give 1-iodo-2-phenylethyne in 66 % (2.440 g) yield, which was used without additional purification. A suspension of NaN_3 (1.000 g, 15.00 mmol) in DMSO (2 mL) was added to a stirred solution of BnBr (1.665 mL, 14.00 mmol) in DMSO (4 mL). The resulting solution was stirred for 24 h at 90 °C. Next, H_2O (50 mL) was added to the reaction mixture. The product was extracted with Et_2O (3×20 mL). The combined organic layers were dried over Na_2SO_4, filtered and solvent was evaporated *in vacuo* at 50 °C. The resulting benzyl azide in 86 % (1.596 g) yield was used without additional purification. A suspension of CuI (36 mg, 0.19 mmol) and 1-iodo-2-phenylethyne (857 mg, 3.76 mmol) in glycerol (1 mL) was added to a stirred solution of BnN_3 (500 mg, 3.76 mmol) in glycerol (4 mL). The resulting suspension was stirred for 24 h at RT and then H_2O (10 mL) was added to the reaction mixture. The precipitate formed was filtered off, washed with MeOH (5 mL), dried at 50 °C for 2 h in air and then at RT in air to give 1-benzyl-4-phenyl-5-iodo-1,2,3-triazole in 85 % (1.154 mg) yield as a colorless solid. A solution of MeI (2.730 mL, 43.90 mmol) in CH_3CN (1 mL) was added to a stirred solution of 1-benzyl-4-phenyl-5-iodo-1,2,3-triazole (430 mg, 1.19 mmol) in CH_3CN (4 mL). The resulting solution was stirred for 48 h at 60 °C and the solvent was evaporated *in vacuo* at 40 °C, the product was crystallized under EtOAc, and the precipitate formed was filtered off, washed with Et_2O (10 mL), dried at 50 °C for 2 h in air and then at RT in air

to give 1-benzyl-3-methyl-4-phenyl-5-iodo-1,2,3-triazolium iodide in 95 % (600 mg) yield as a colorless solid. A solution of AgOTf (175 mg; 0.70 mmol) in MeOH (2 mL) was added to a stirred solution of 1-benzyl-3-methyl-4-phenyl-5-iodo-1,2,3-triazolium iodide (350 mg, 0.70 mmol) in MeOH (3 mL). The suspension was stirred for 15 min at RT and the precipitate formed was filtered off, washed with MeOH (15 mL), and the solvent from combined organic layers was evaporated *in vacuo* at 40 °C. Recrystallization from EtOAc (5 mL) gave [**7**]OTf in 83 % (303 mg) yield as a colorless solid.

[**7**]OTf. Yield: 83 % (303 mg). M.p.: 133–134 °C. Λ_M (CH_3OH, 1.01×10^{-3} *M*): 66.9 $Ohm^{-1} \cdot cm^{-1} \cdot mol^{-1}$. ^1H NMR (400.13 MHz, CD_3OD): δ = 7.74−7.64 (m, 5H, Ph), 7.57−7.54 (m, 2H, Ph), 7.51−7.44 (m, 3H, Ph), 5.96 (s, 2H, C*H*$_2$), 4.26 (s, 3H, C*H*$_3$). $^{13}C\{^1H\}$ NMR (101.61 MHz, CD_3OD): δ = 147.43 (*C*−I); 131.80 (*C*−Ph); 129.98, 129.32, 129.20, 128.95, 128.65 и 122.90 (Ph), 120.44 (q, $^1J_{CF}$ = 319.0 Hz, *C*F$_3$), 89.91 (Ph), 57.75 (*C*H$_2$), 38.29 (*C*H$_3$). HRMS (ESI-TOF): *m*/*z* calcd for $C_{16}H_{15}N_3I^+$: 376.0305; found: 376.0304. IR (KBr, selected bands): $\tilde{\upsilon}$ = 3075 (w, C−H), 3039 (w, C−H), 1557 (m, C=N), 1280 (s, C−F), 1245 (s, S=O or C−F), 1029 (s, S=O or C−F), 637 (s, C−I), 516 (m-s, C−I).

Spectra of [1-7]OTf

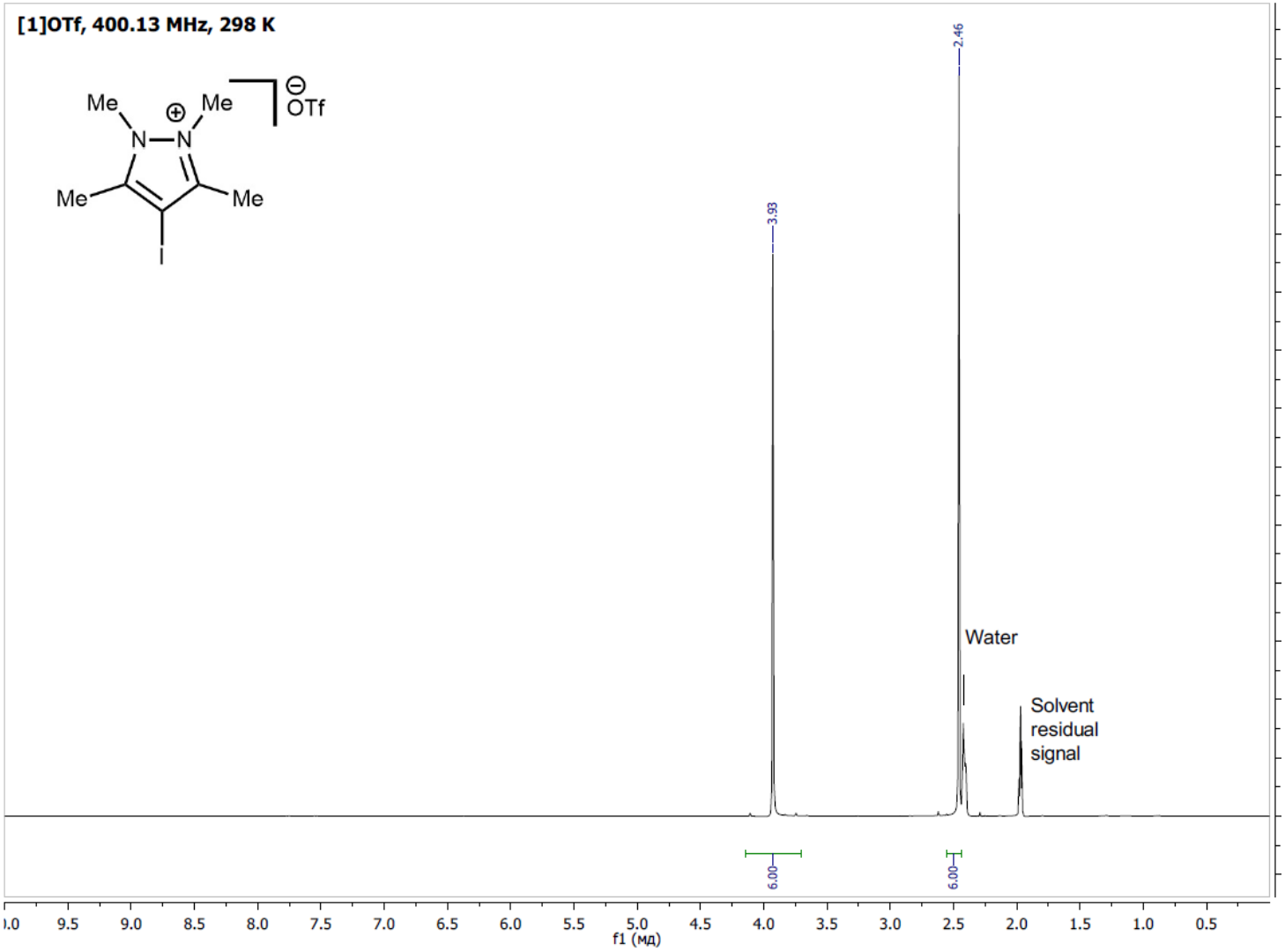


Figure S1. ^{1}H NMR spectrum of [**1**]OTf.

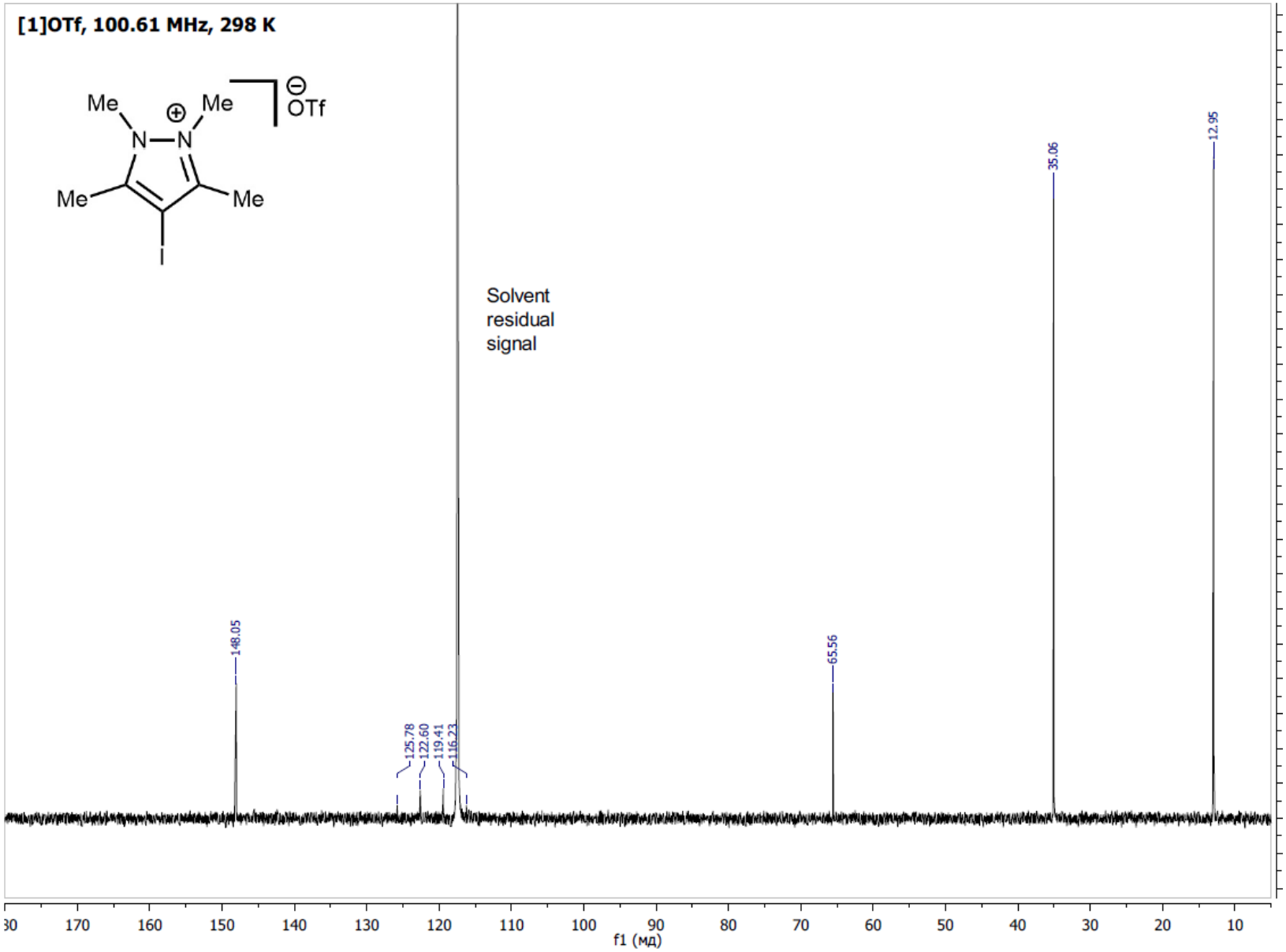


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of [**1**]OTf.

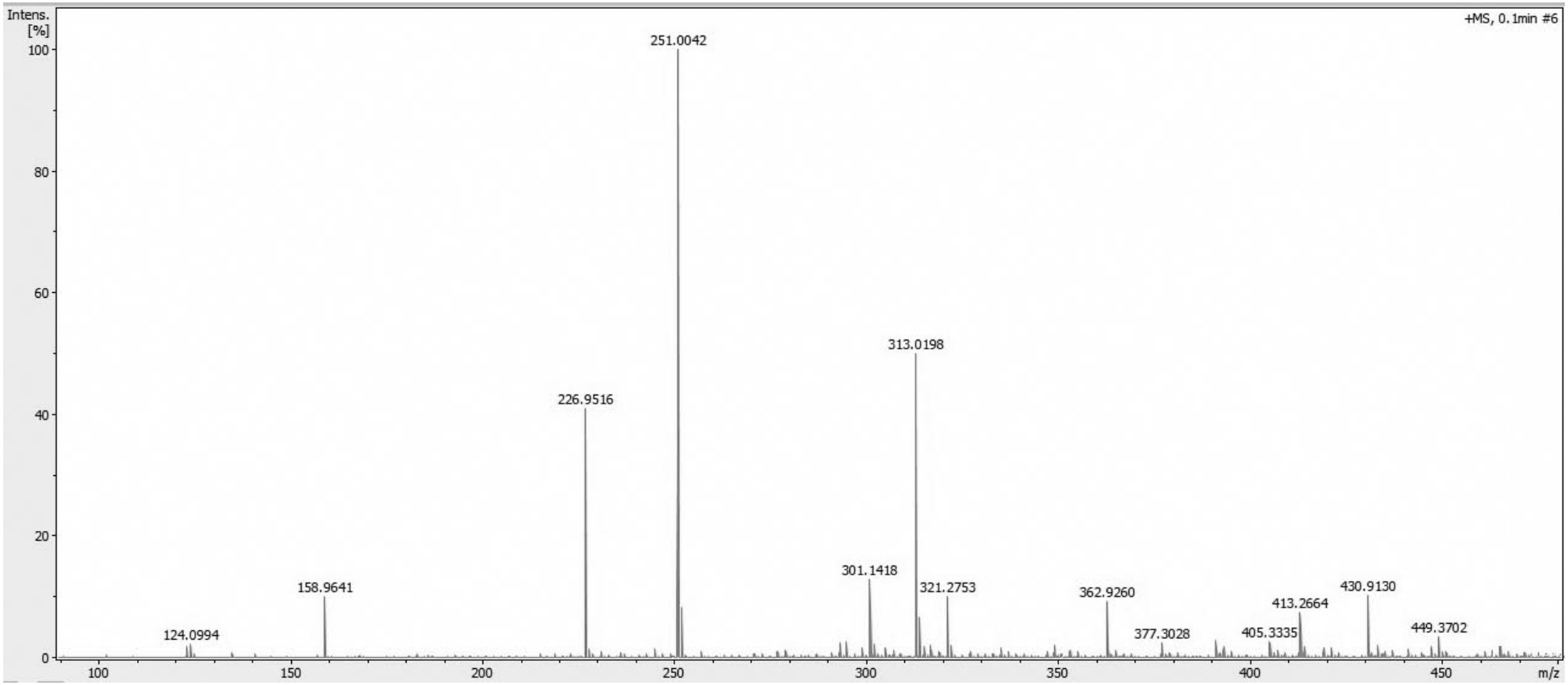


Figure S3. HRMS^{+}-MS of [**1**]OTf.

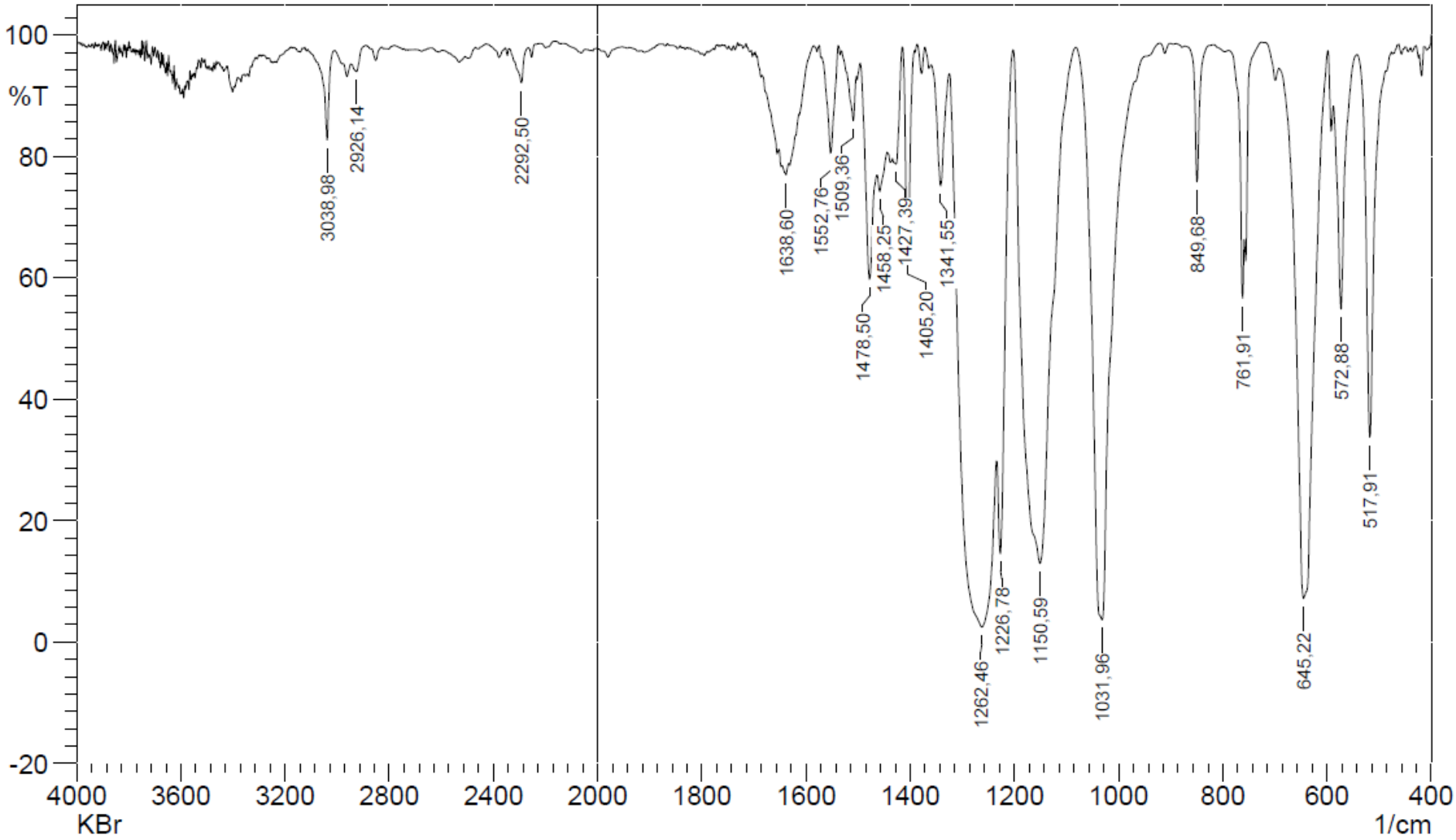


Figure S4. IR spectrum of [**1**]OTf.

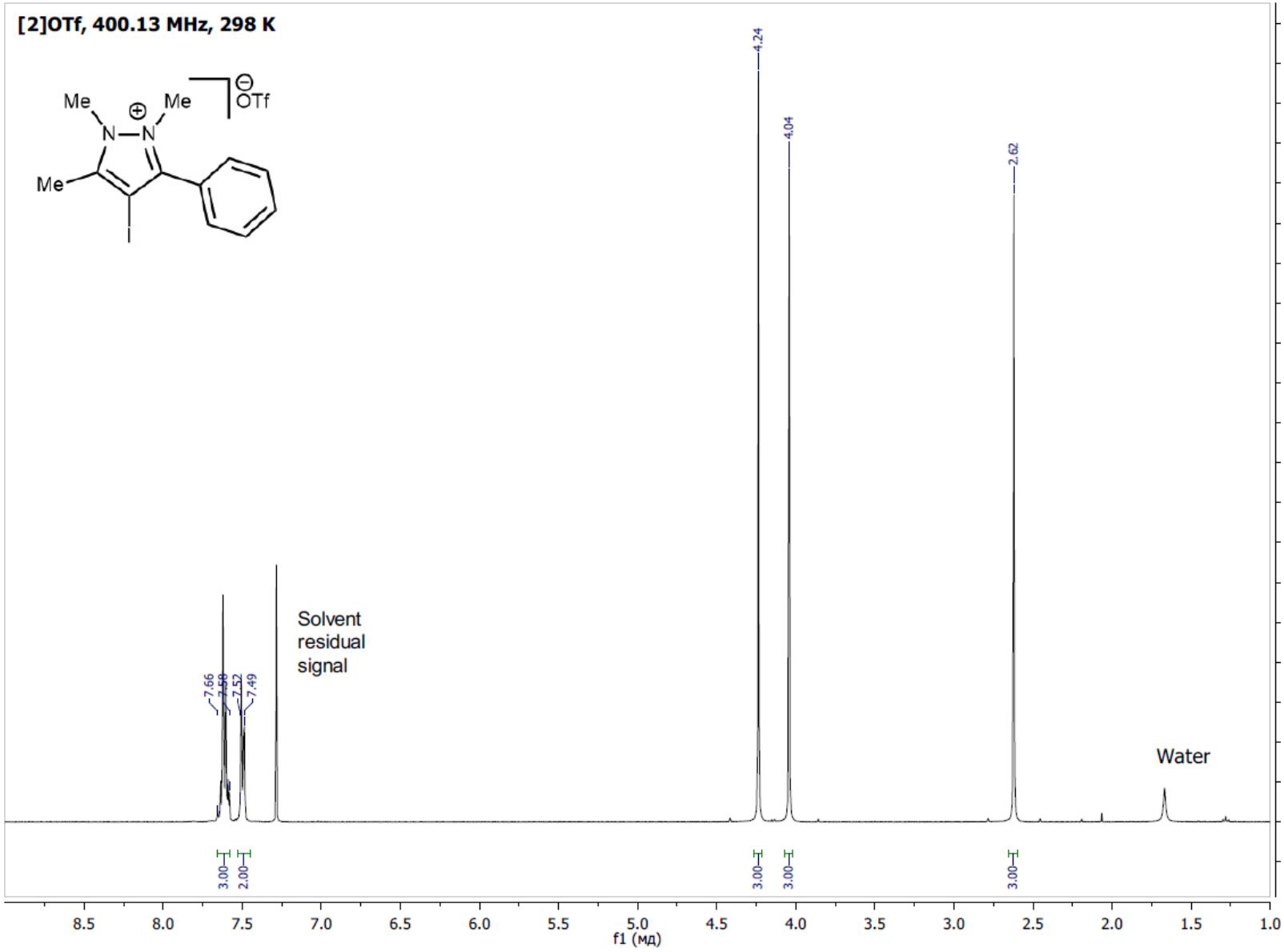


Figure S5. ^{1}H NMR spectrum of [**2**]OTf.

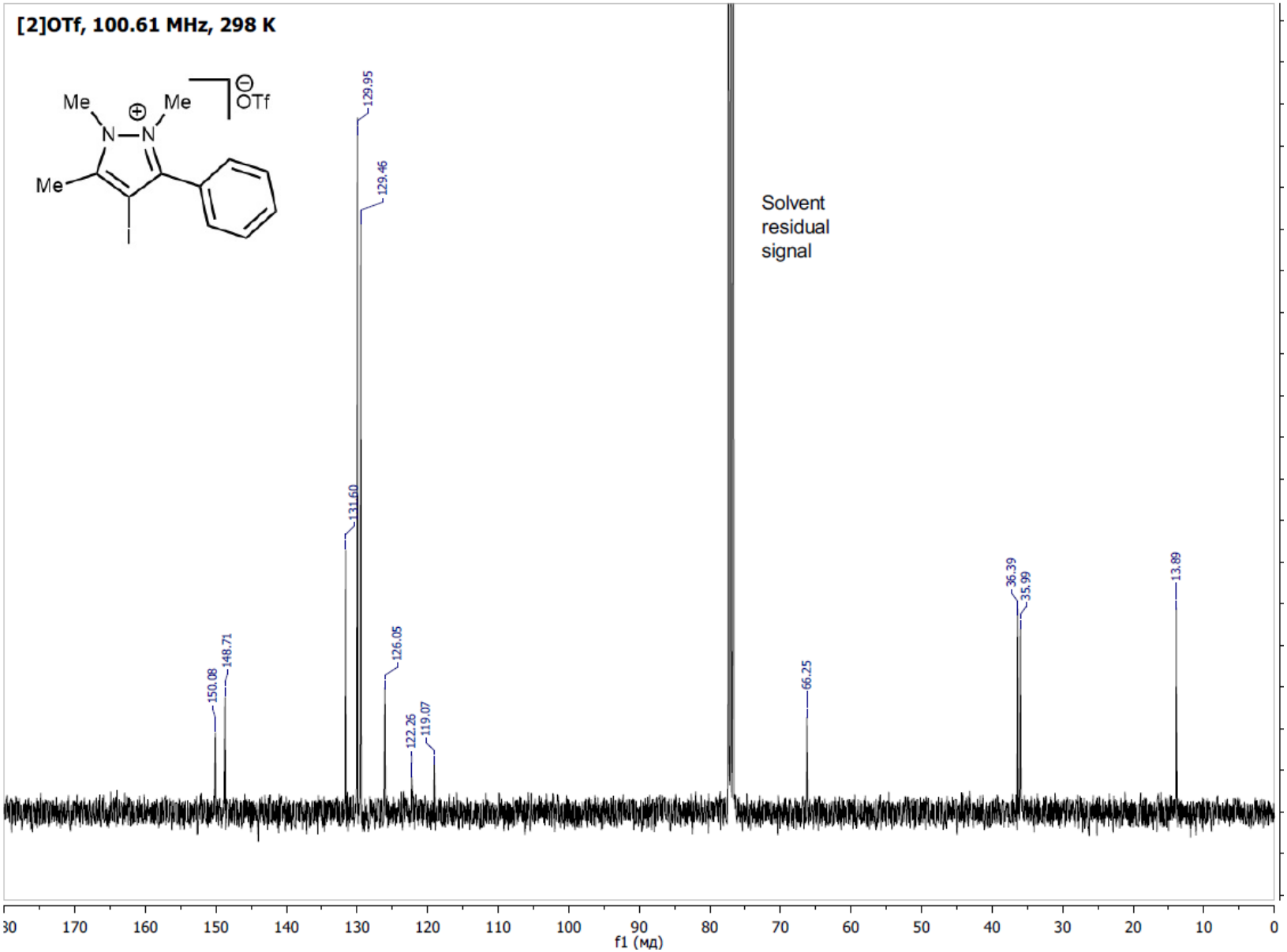


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of [**2**]OTf.

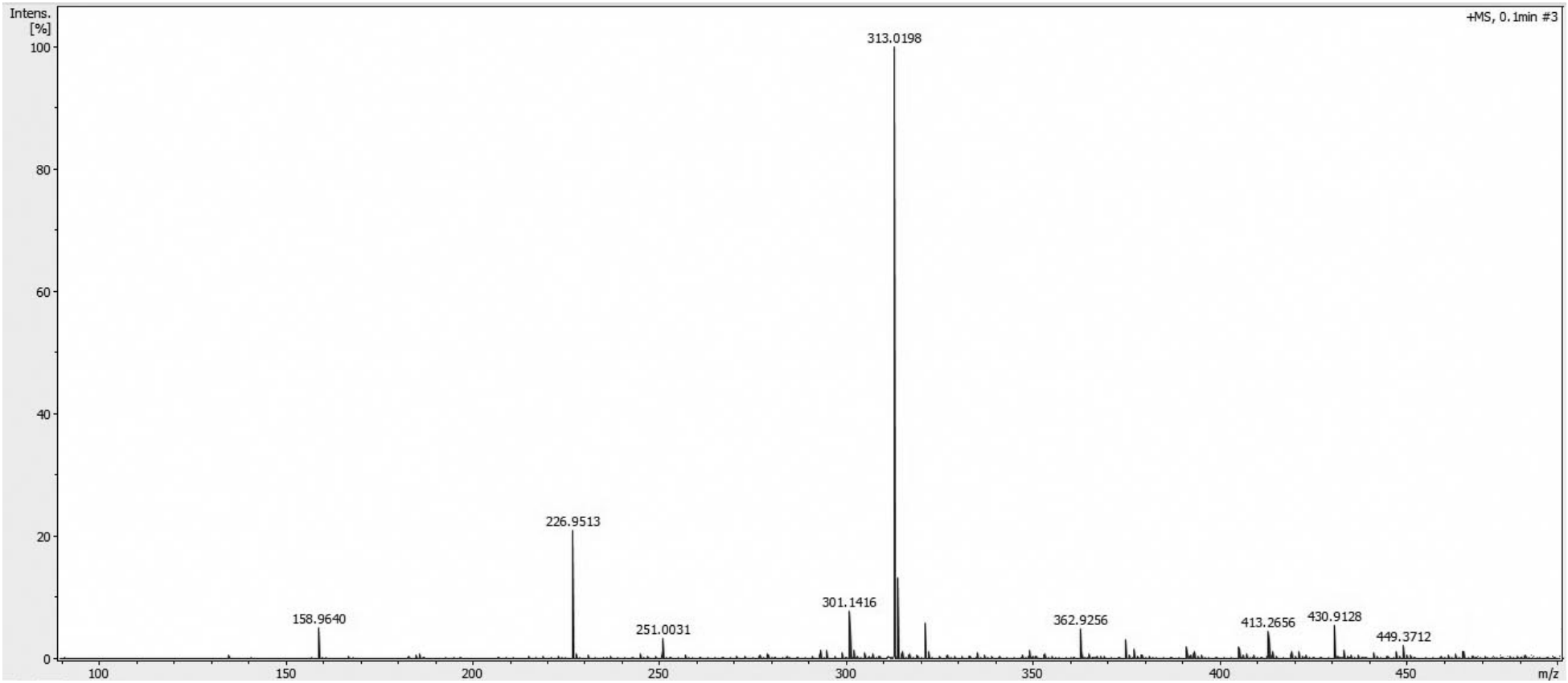


Figure S7. HRMS^{+}-MS of [**2**]OTf.

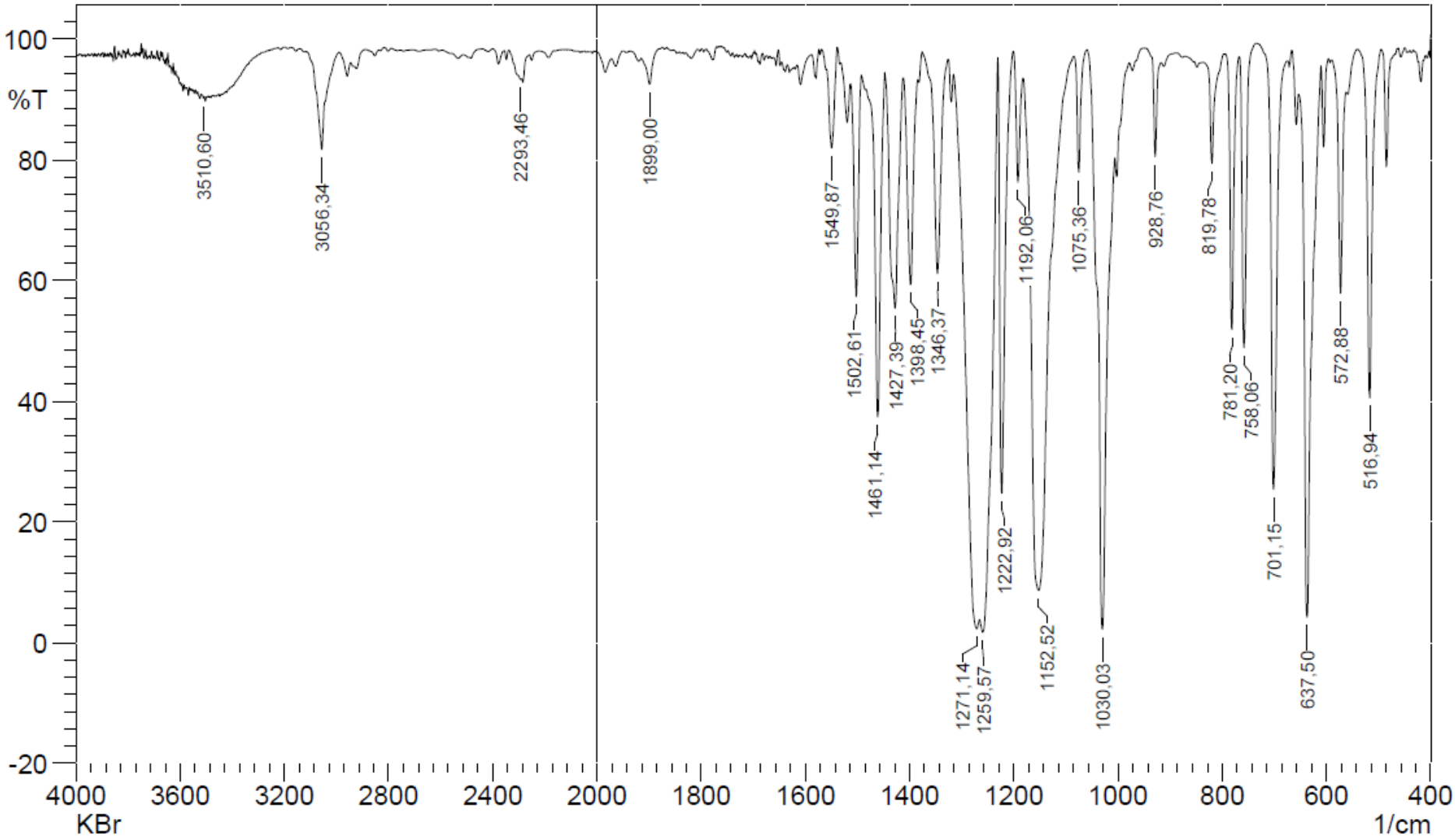


Figure S8. IR spectrum of [**2**]OTf.

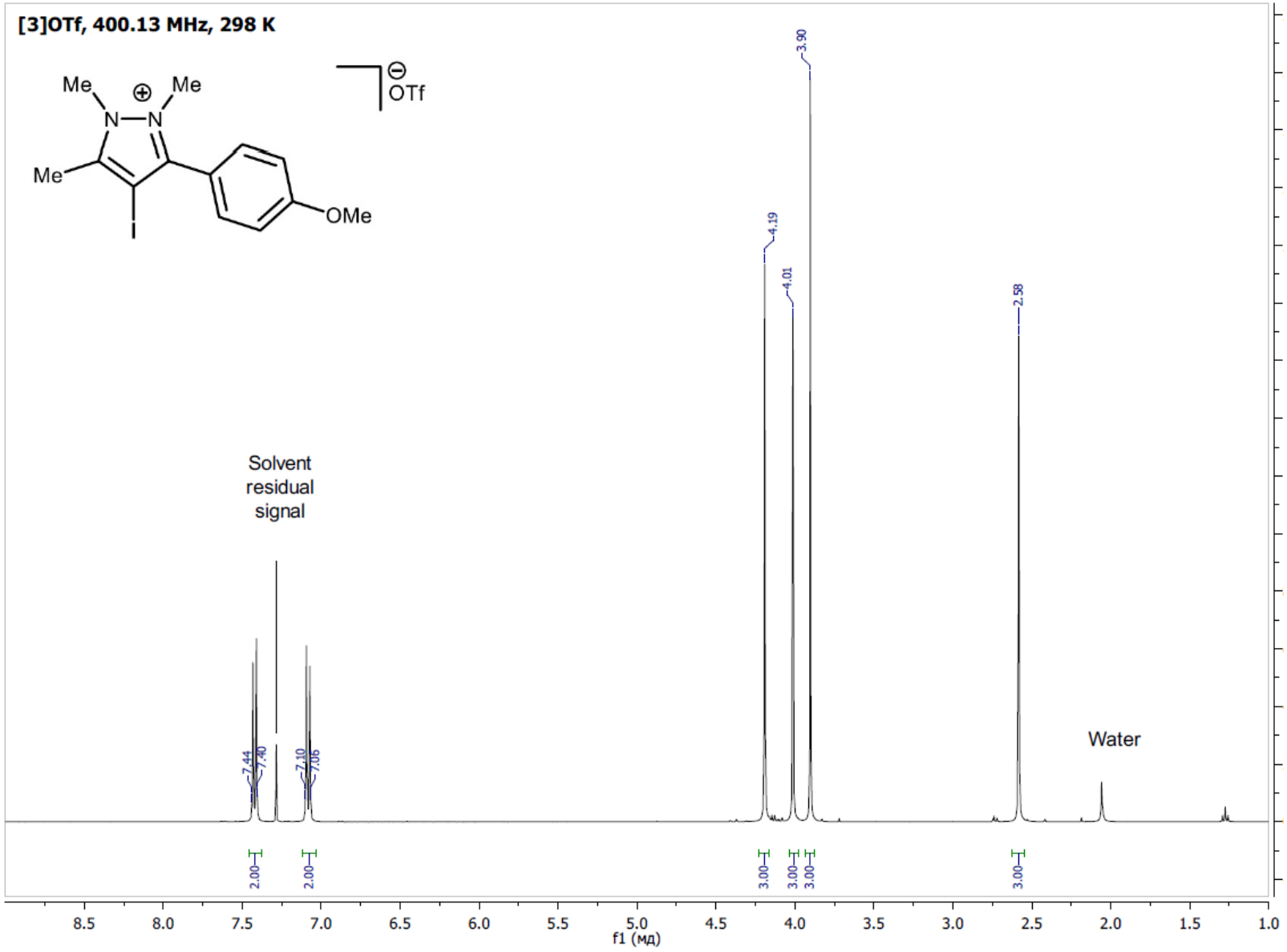


Figure S9. ^{1}H NMR spectrum of [**3**]OTf.

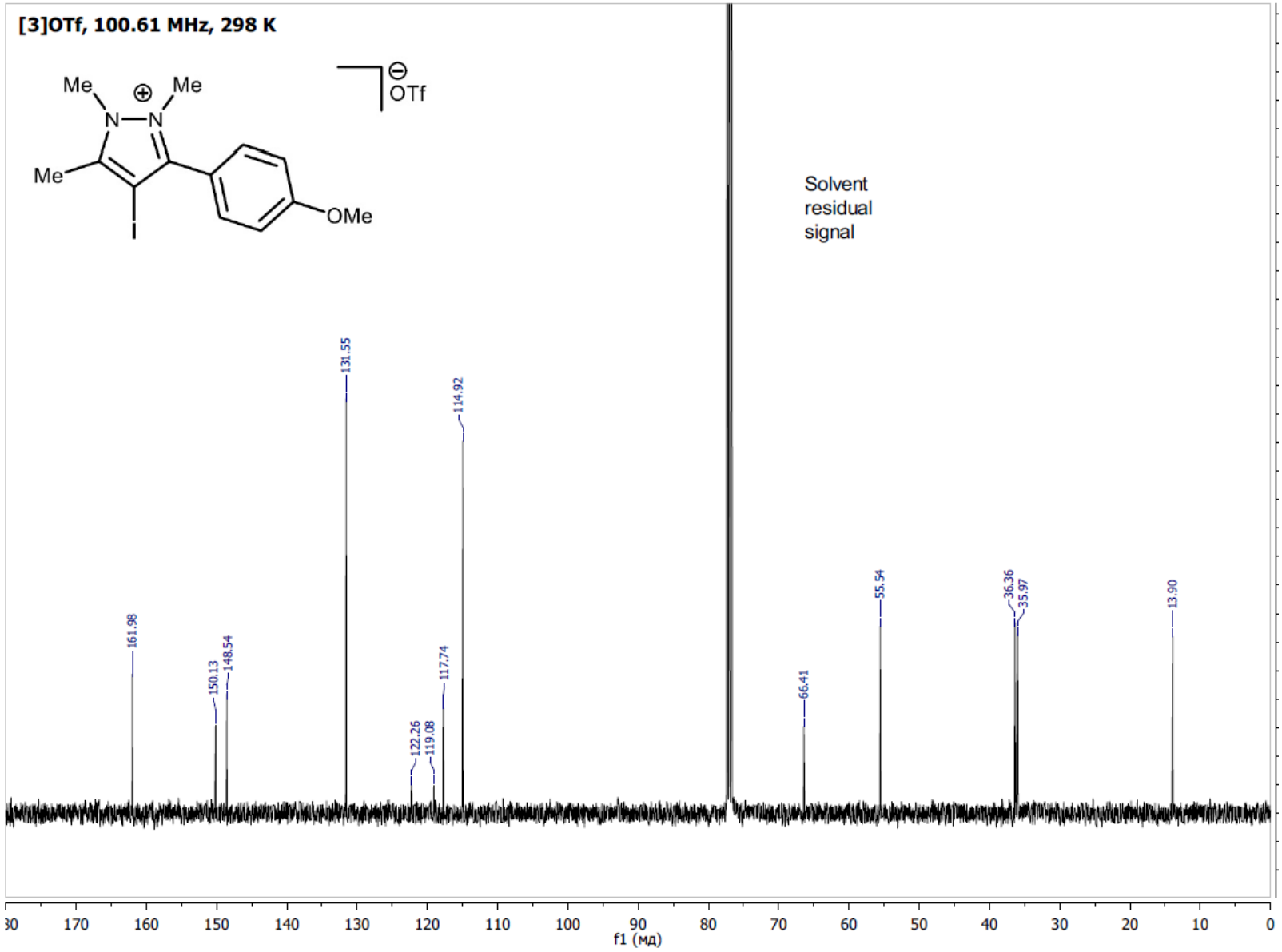


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of [**3**]OTf.

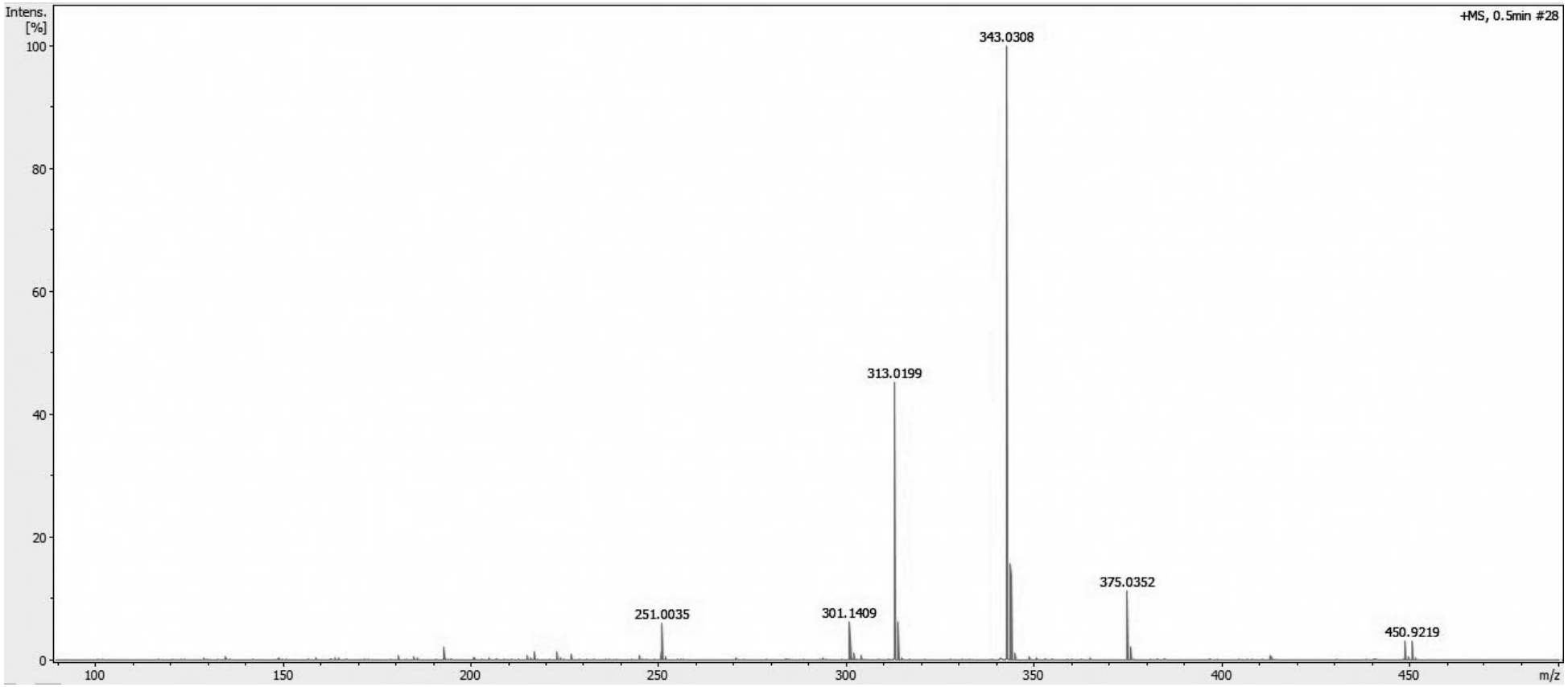


Figure S11. HRMS^{+}-MS of [**3**]OTf.

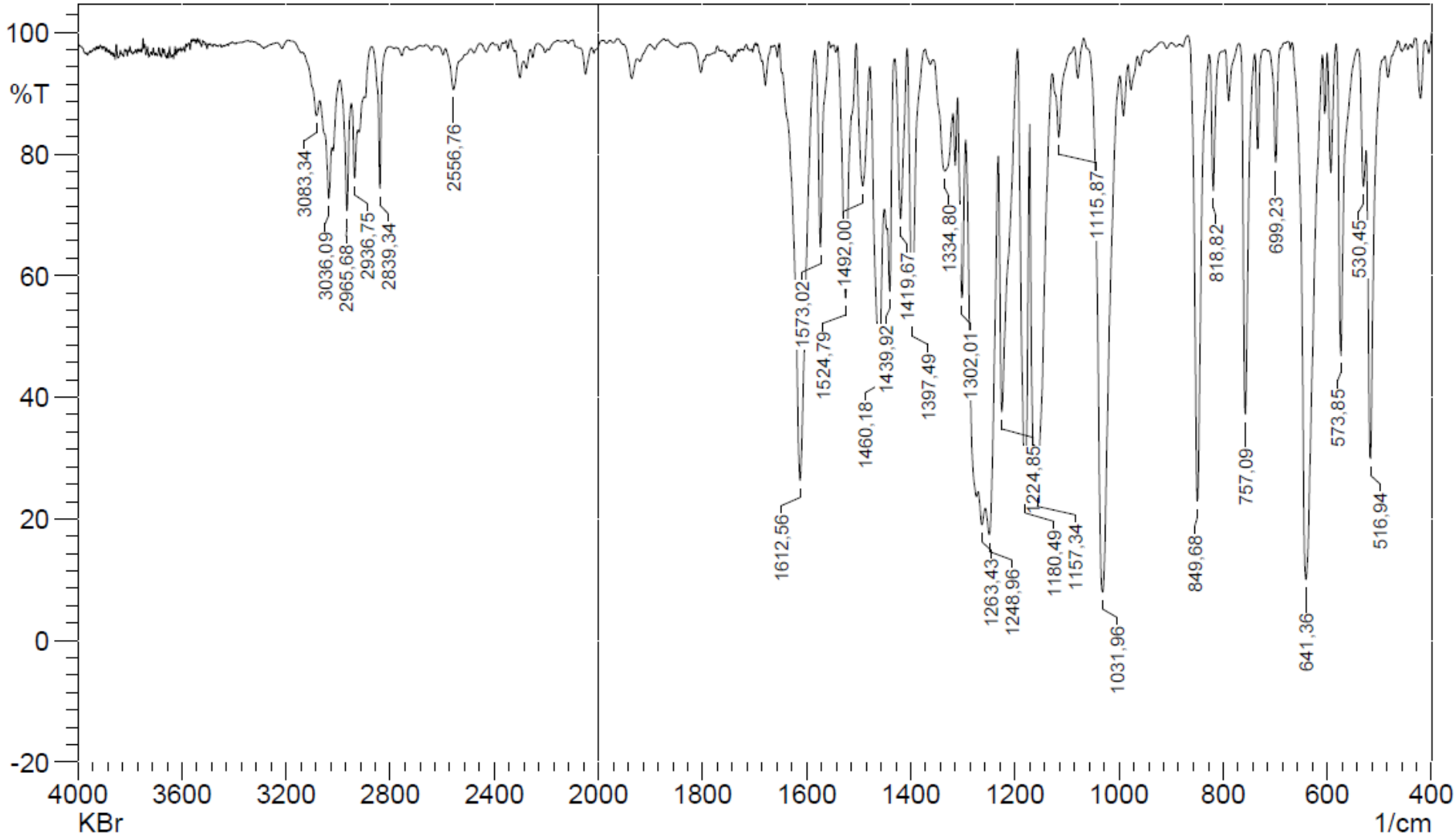


Figure S12. IR spectrum of [**3**]OTf.

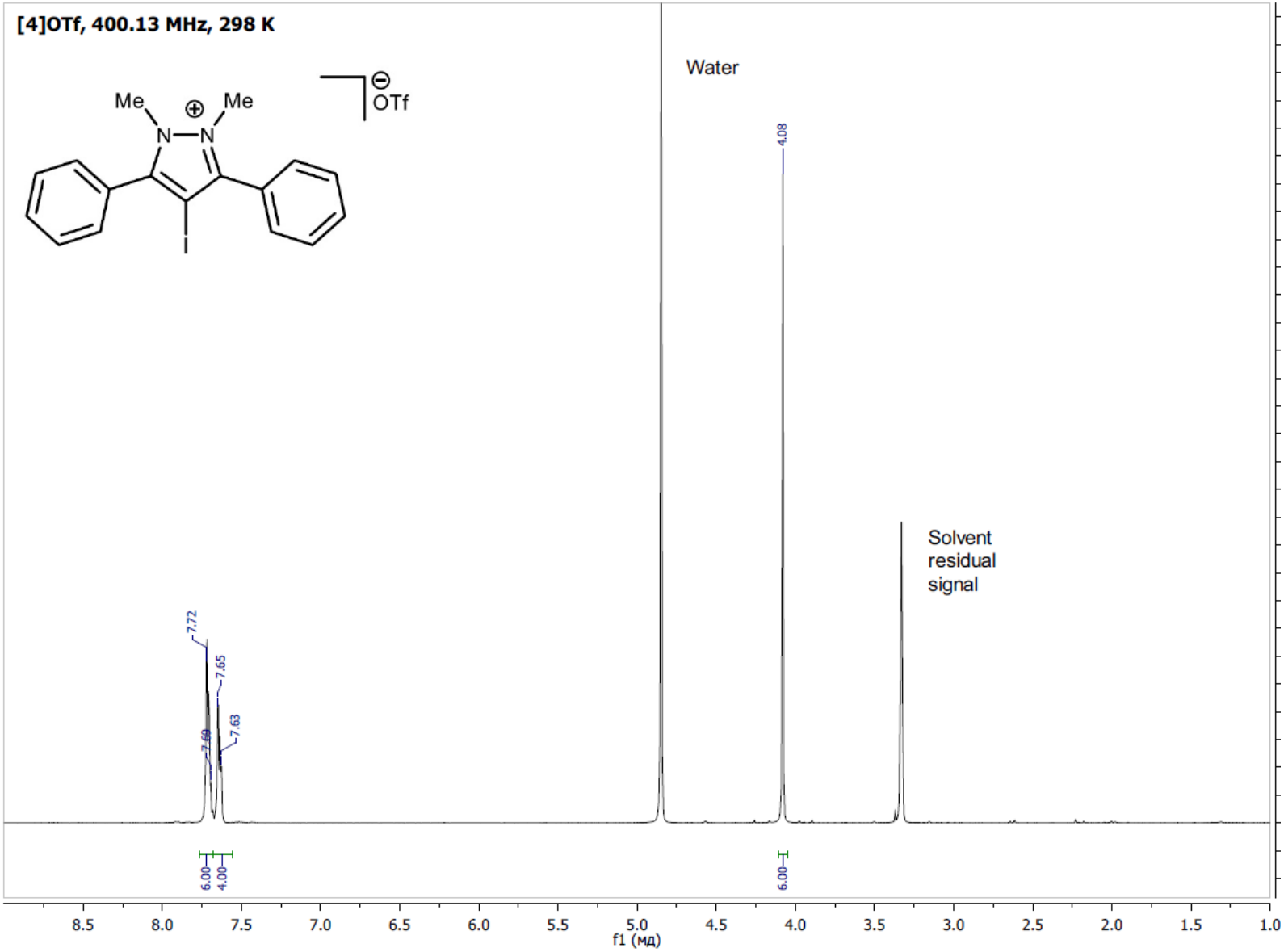


Figure S13. ^{1}H NMR spectrum of [**4**]OTf.

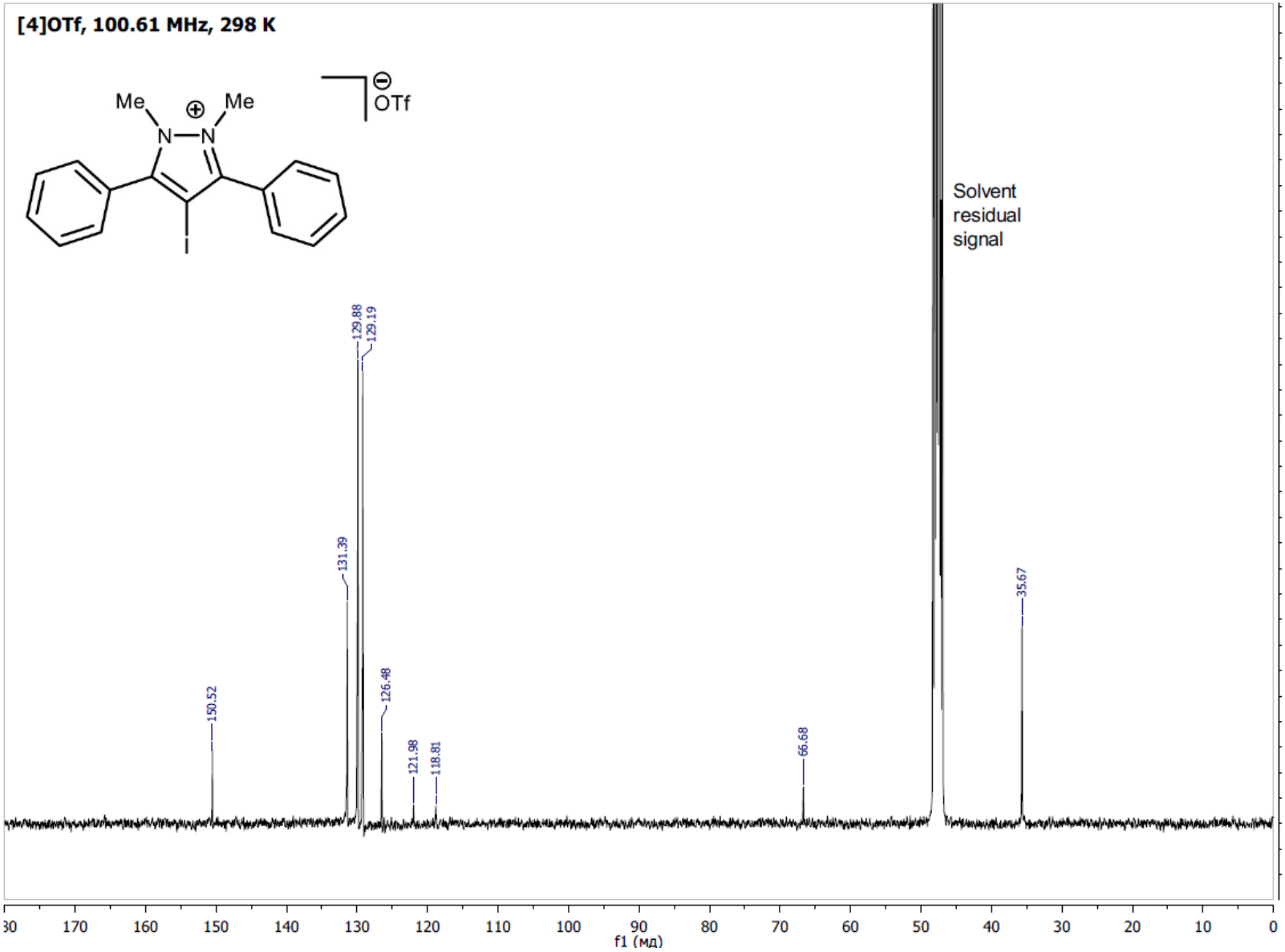


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of [**4**]OTf.

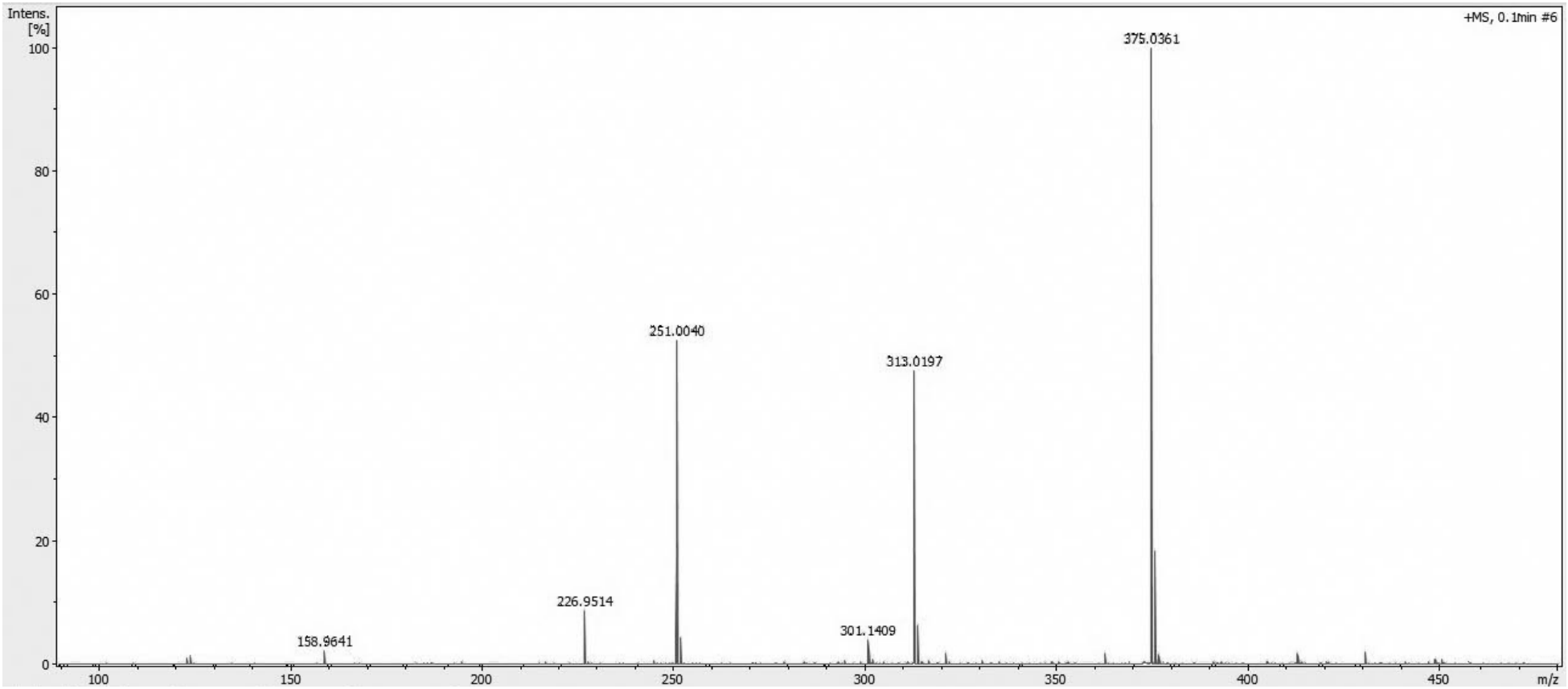


Figure S15. HRMS^{+}-MS of [**4**]OTf.

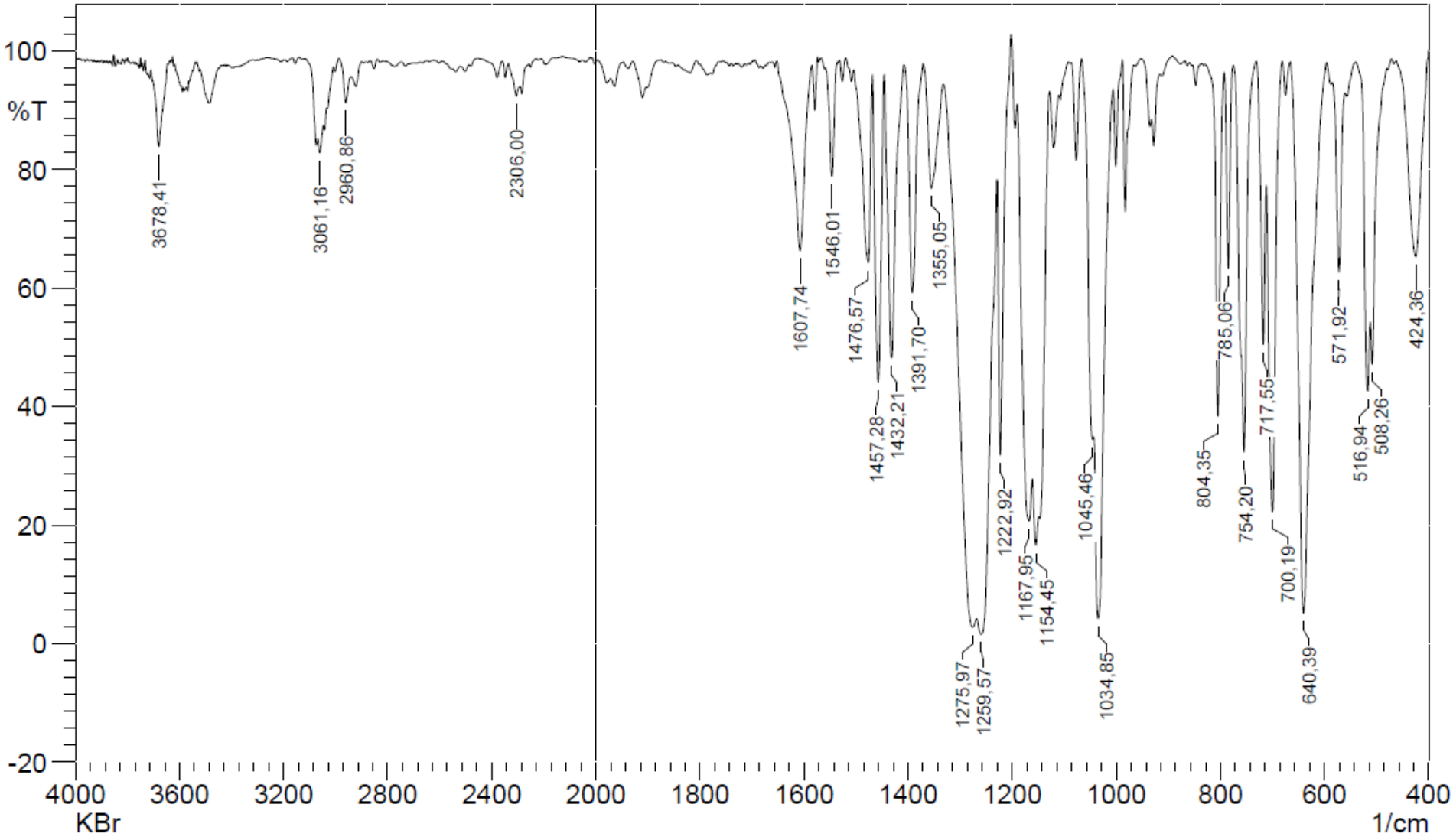


Figure S16. IR spectrum of [**4**]OTf.

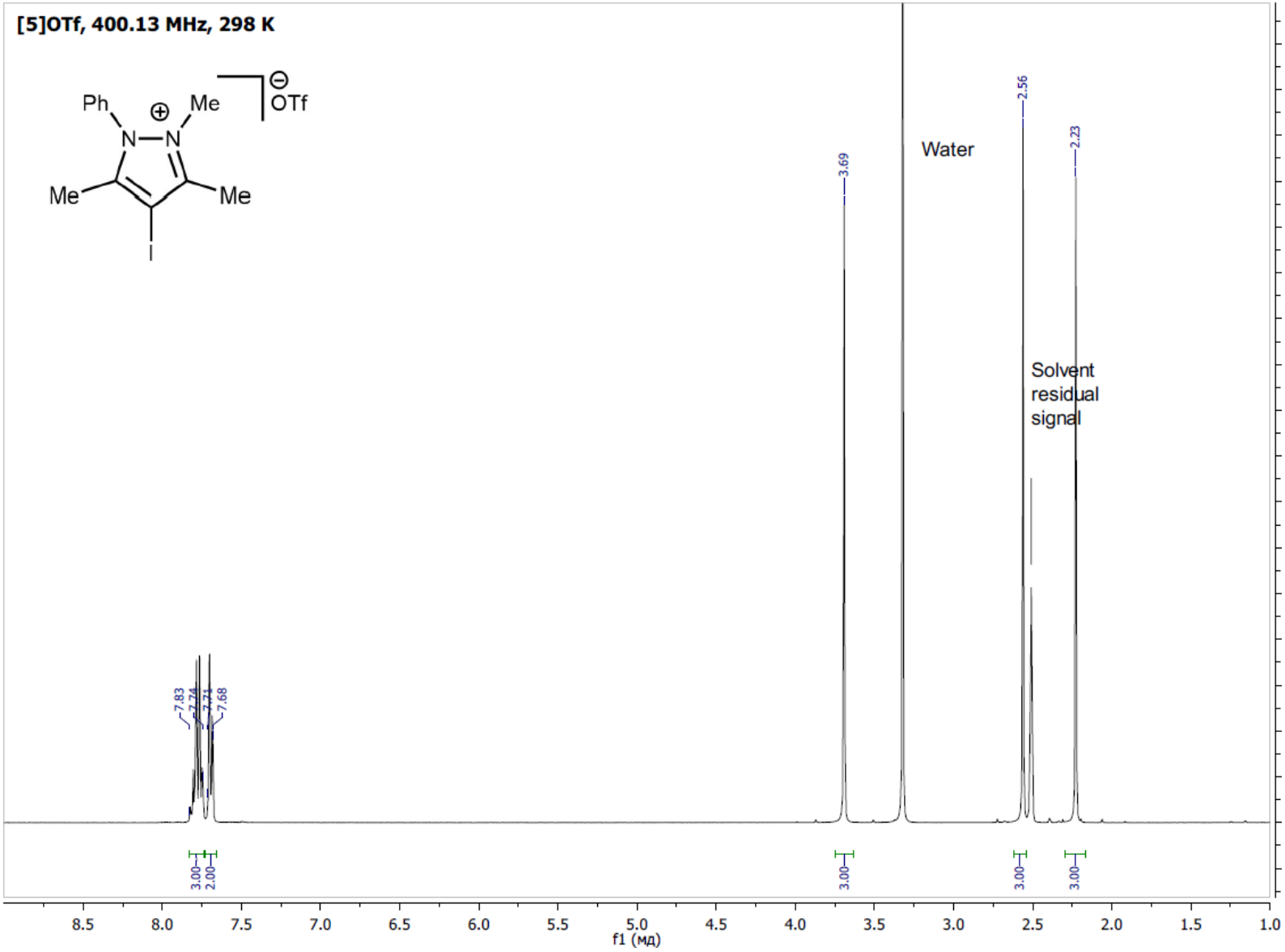


Figure S17. ^{1}H NMR spectrum of [**5**]OTf.

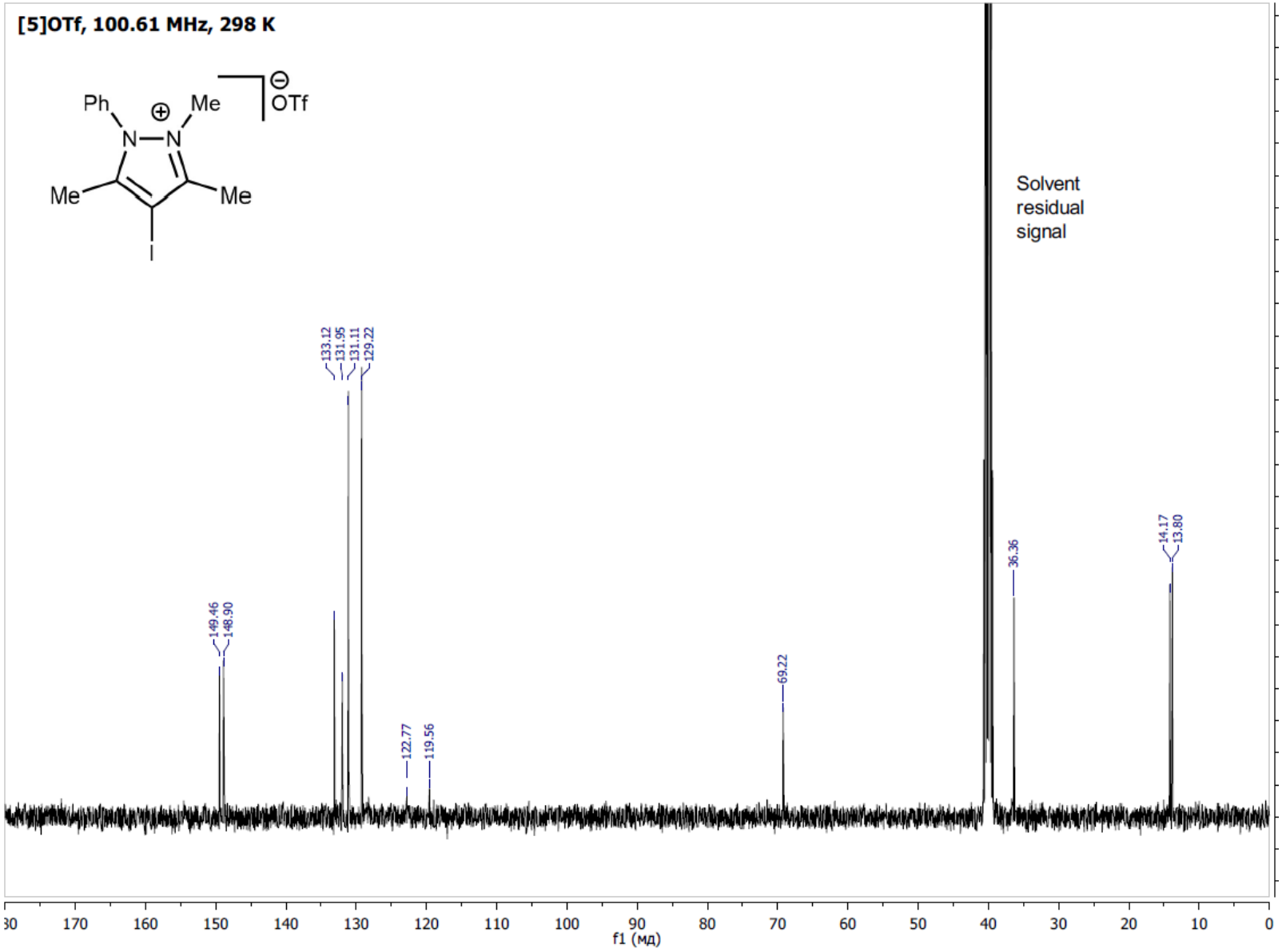


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of [**5**]OTf.

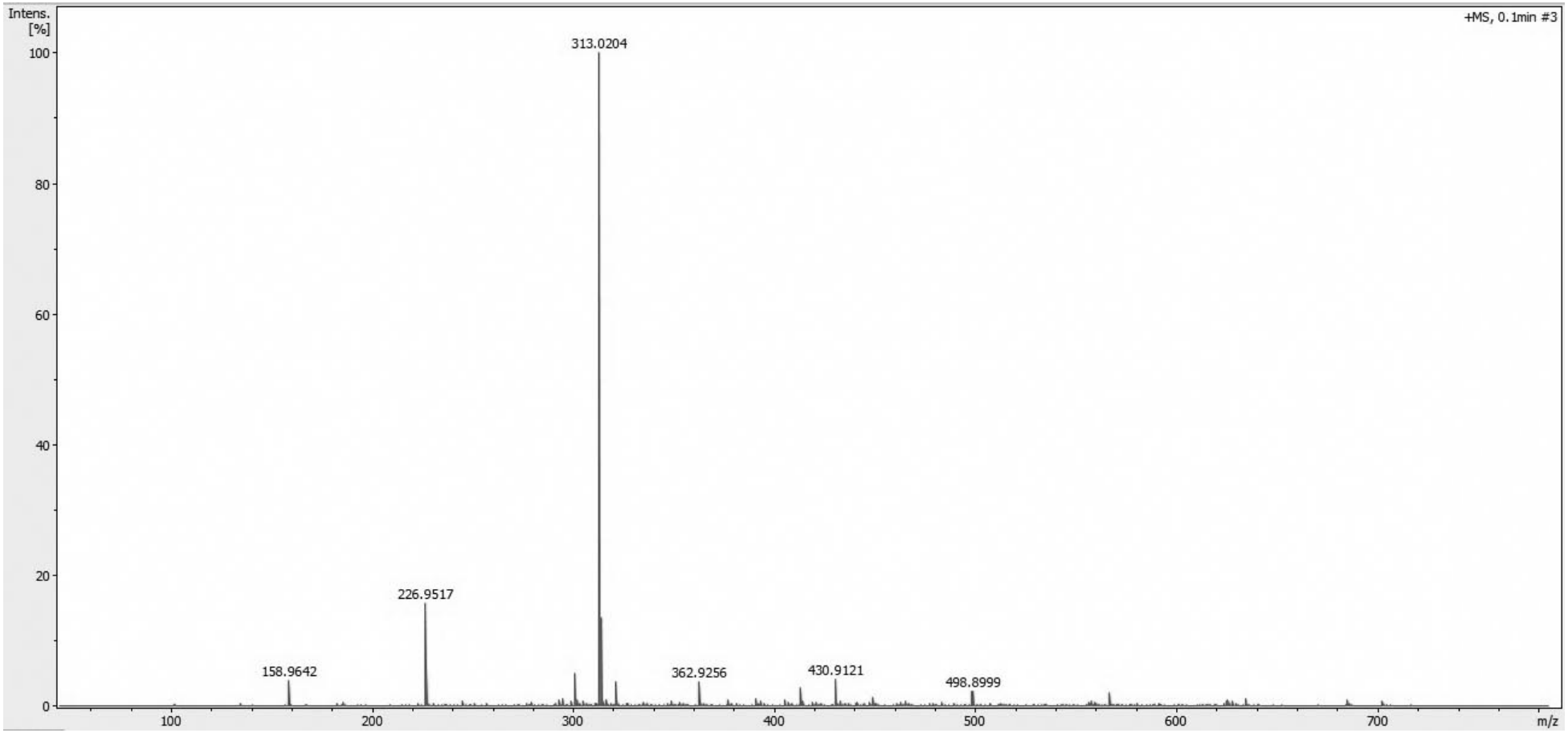


Figure S19. HRMS^{+}-MS of [**5**]OTf.

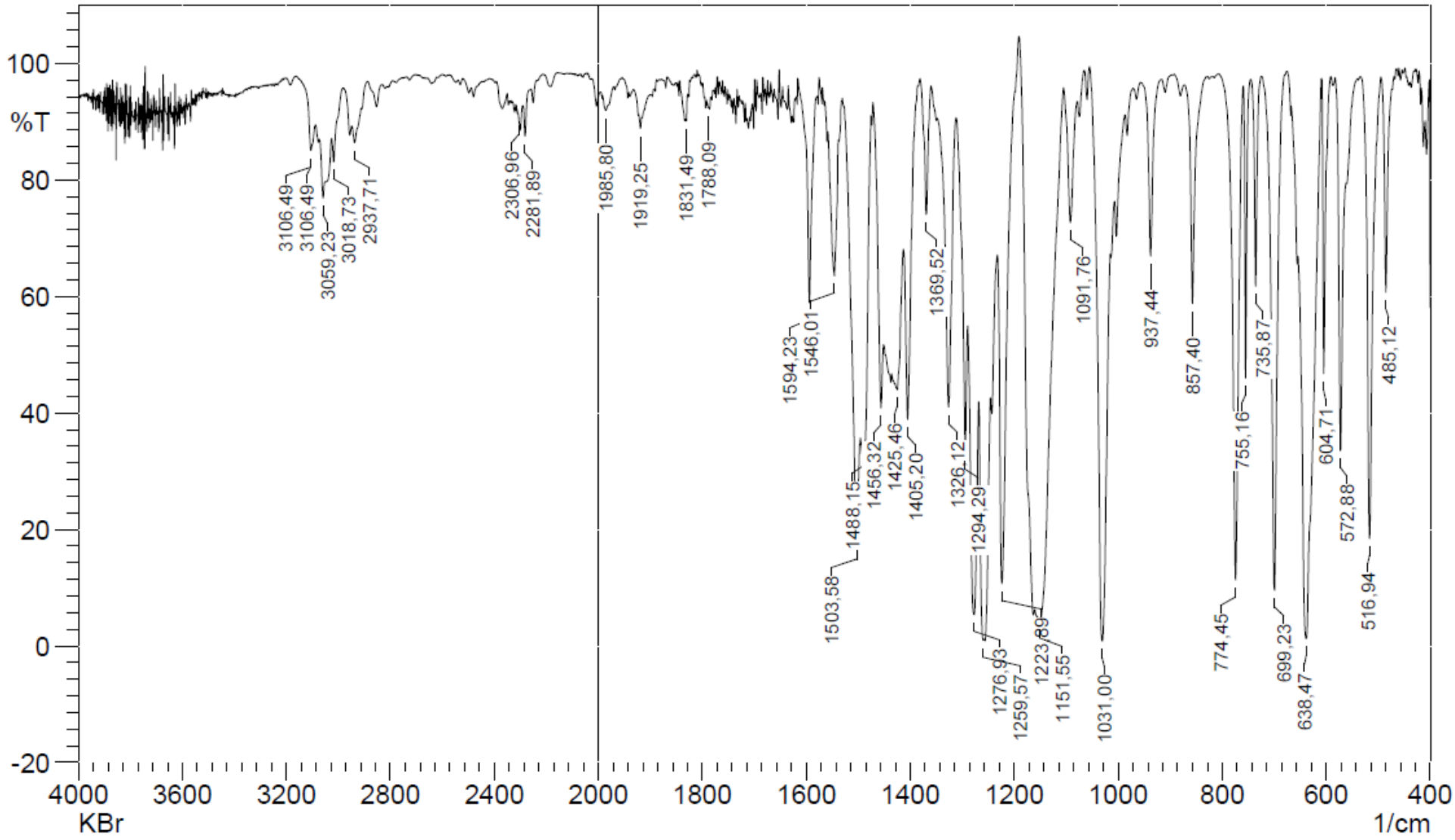


Figure S20. IR spectrum of [**5**]OTf.

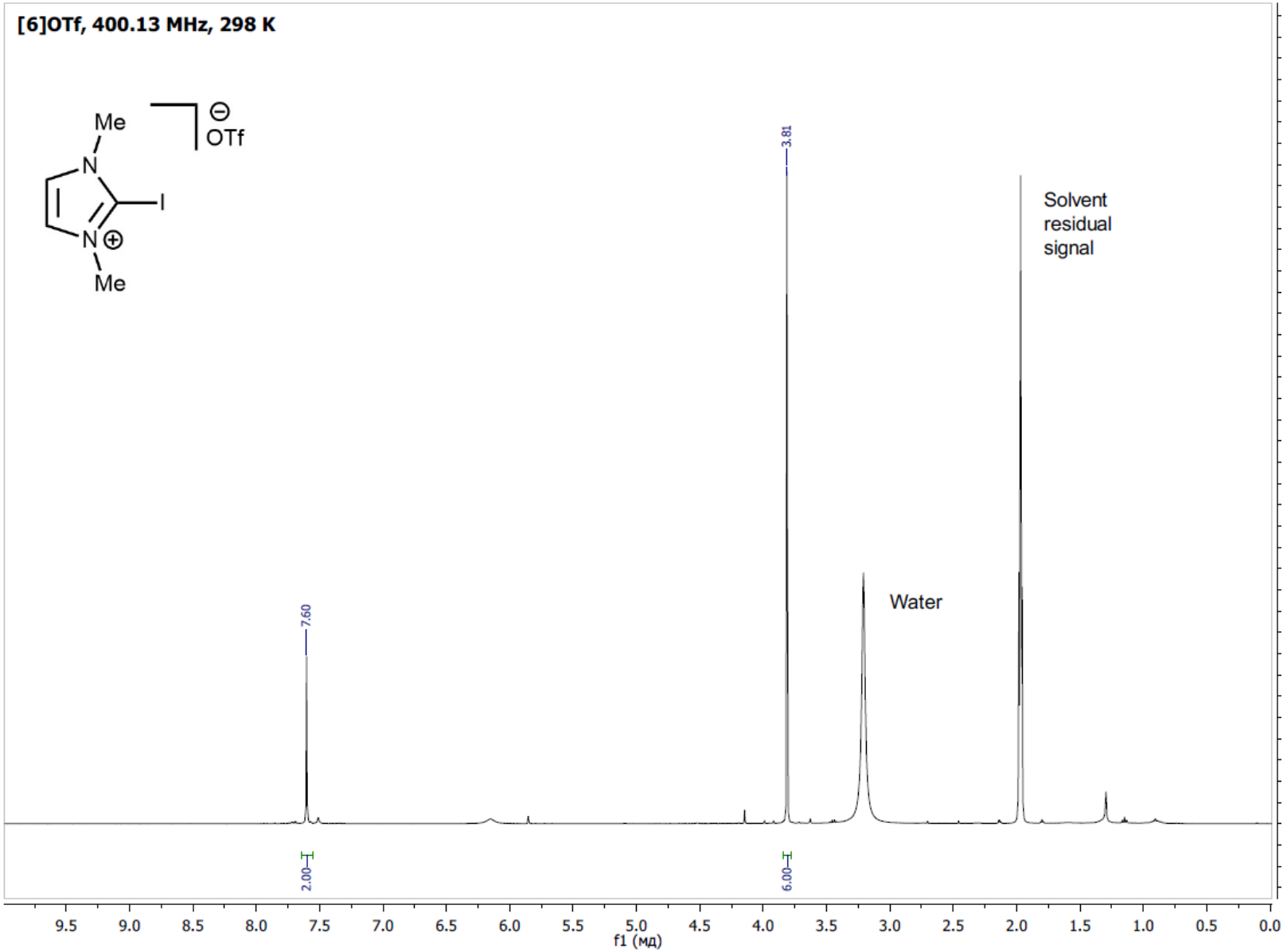


Figure S21. ^{1}H NMR spectrum of [**6**]OTf.

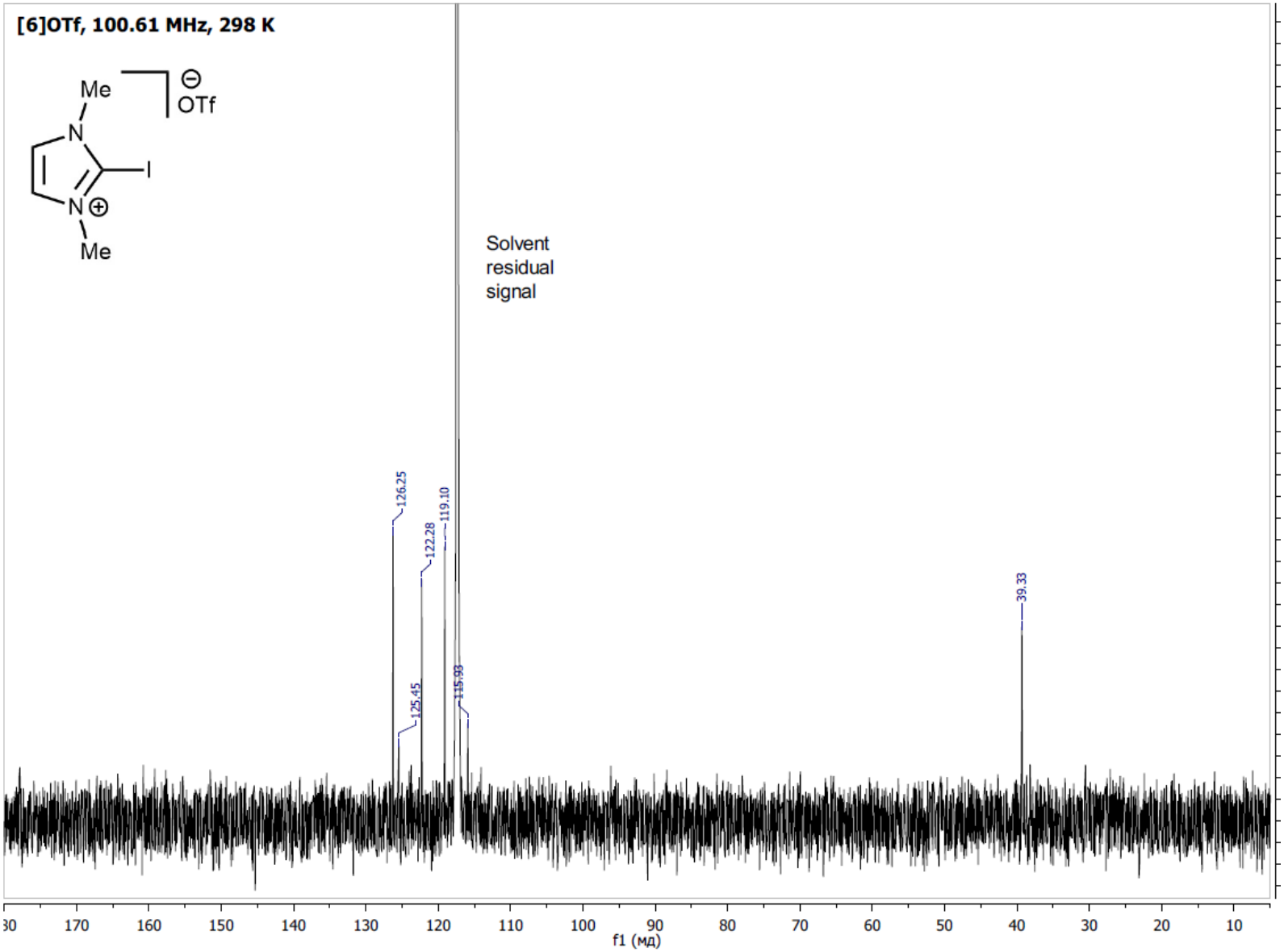


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of [**6**]OTf.

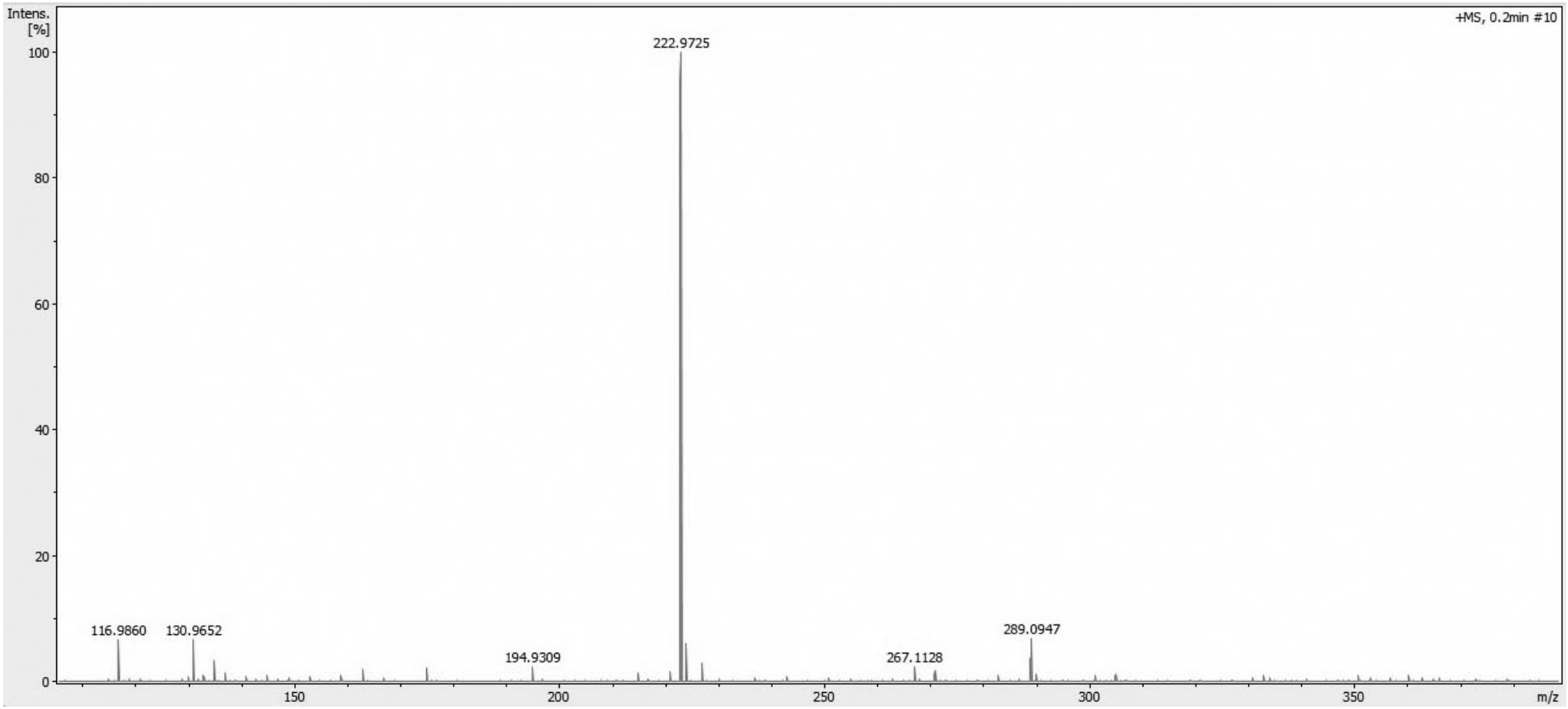


Figure S23. HRMS^{+}-MS of [**6**]OTf.

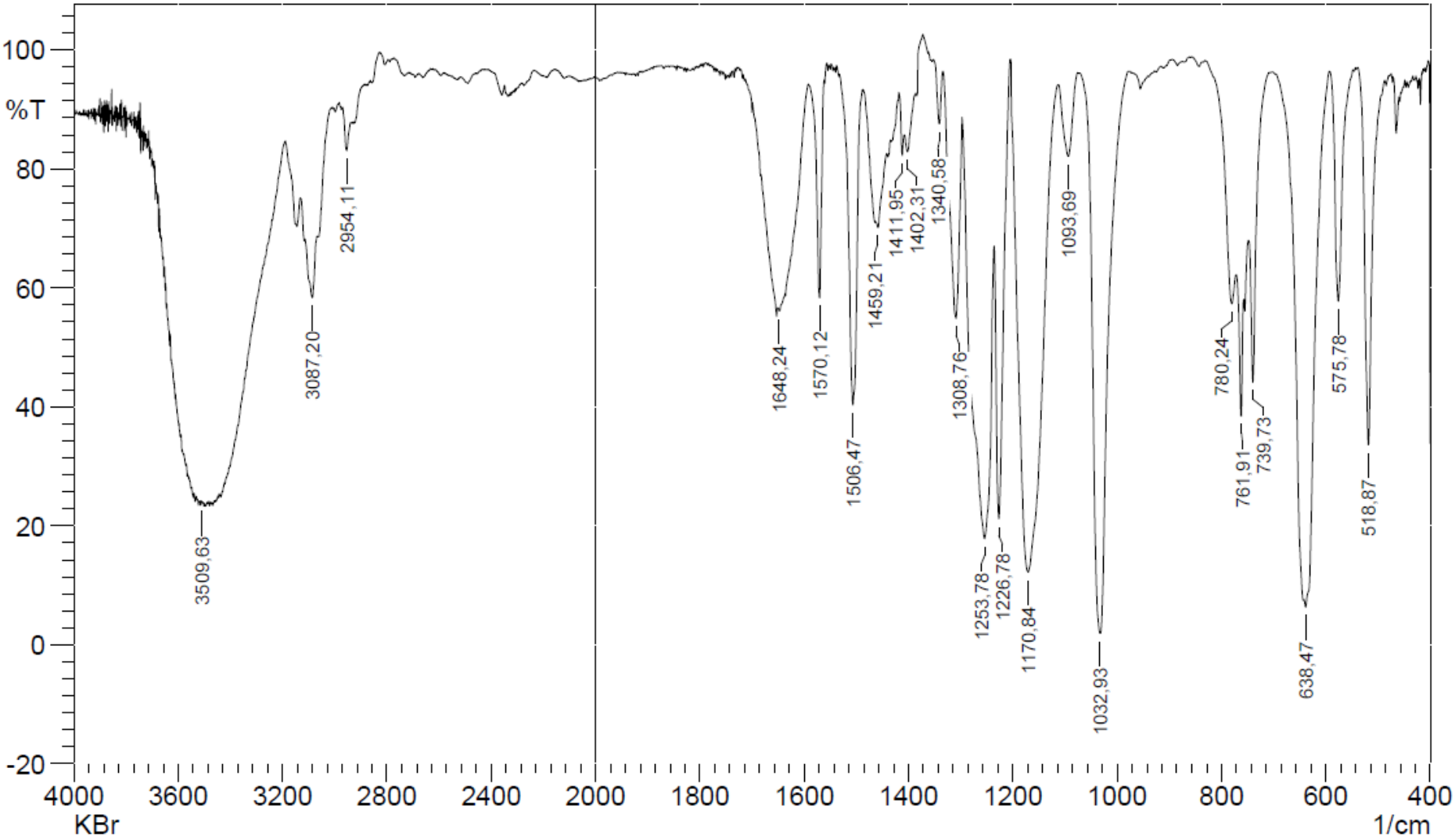


Figure S24. IR spectrum of [**6**]OTf.

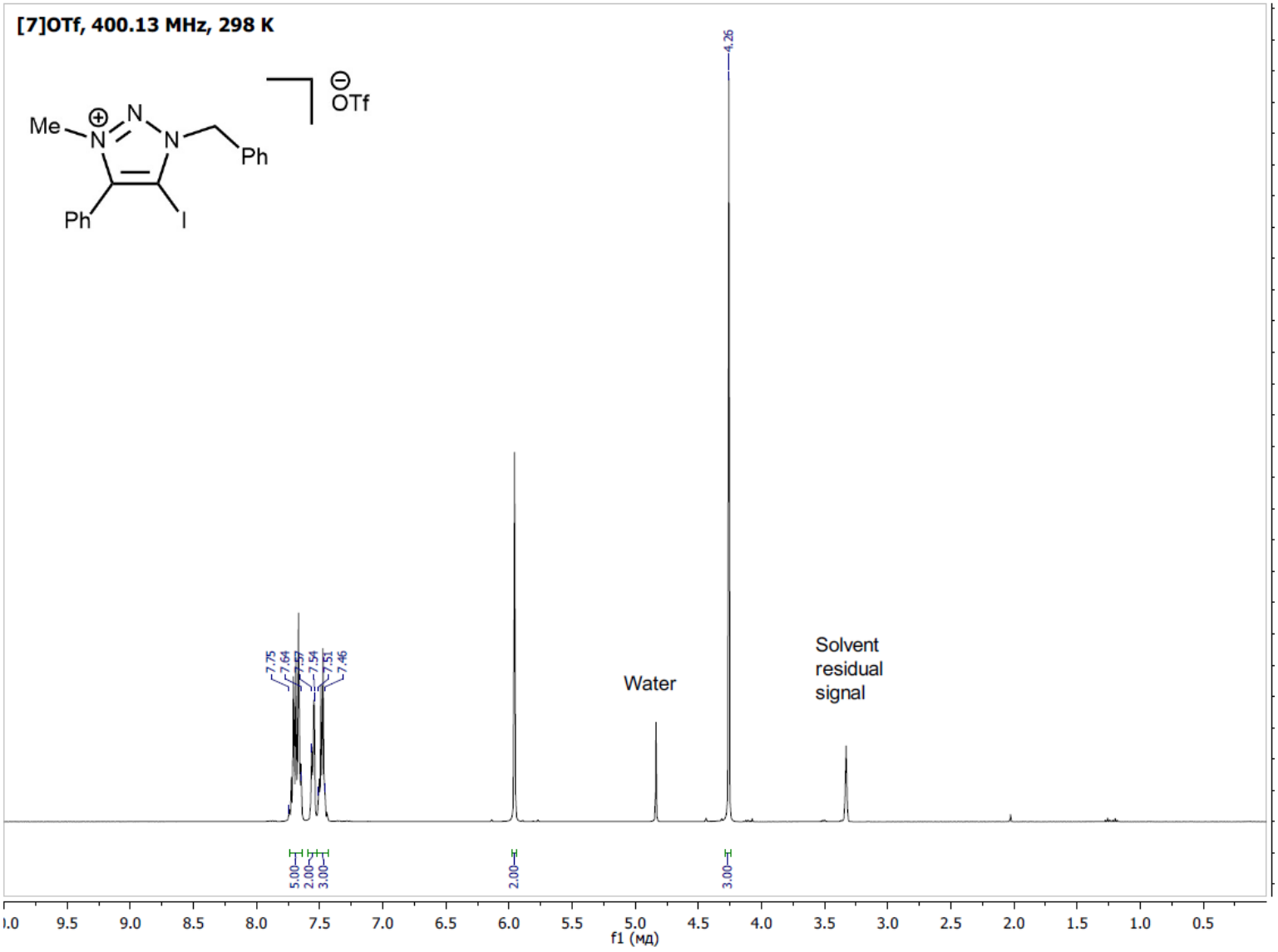


Figure S25. ^{1}H NMR spectrum of [**7**]OTf.

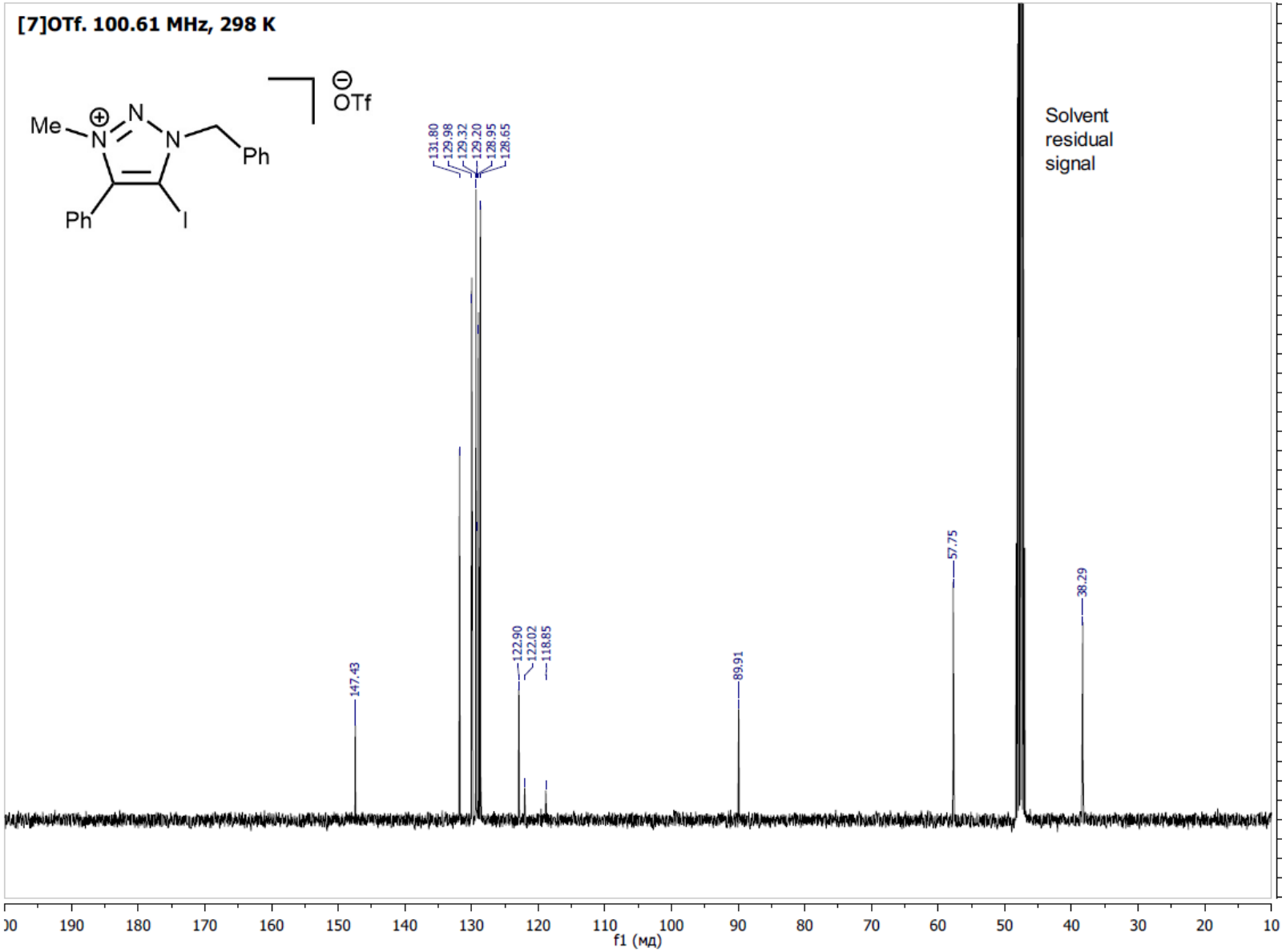


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of [**7**]OTf.

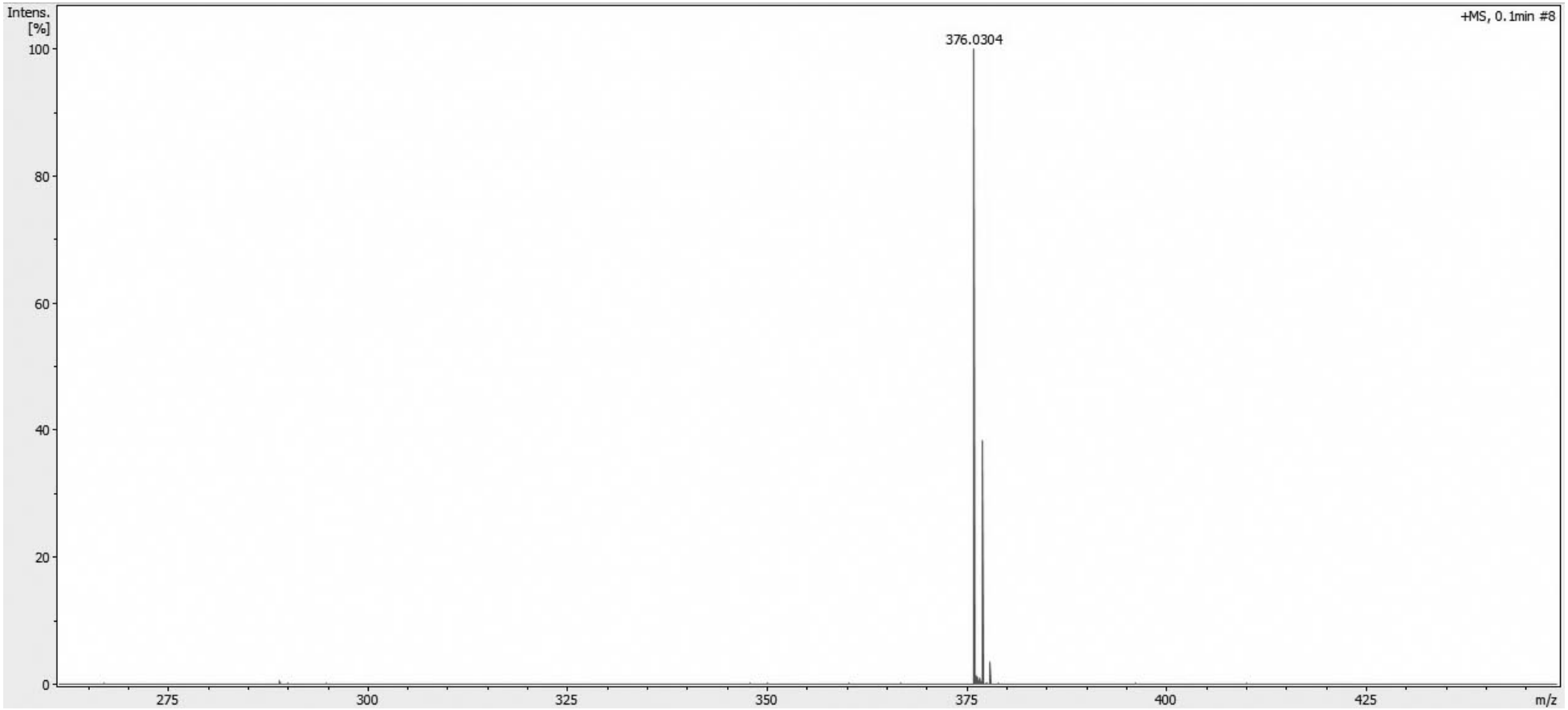


Figure S27. HRMS^{+}-MS of [**7**]OTf.

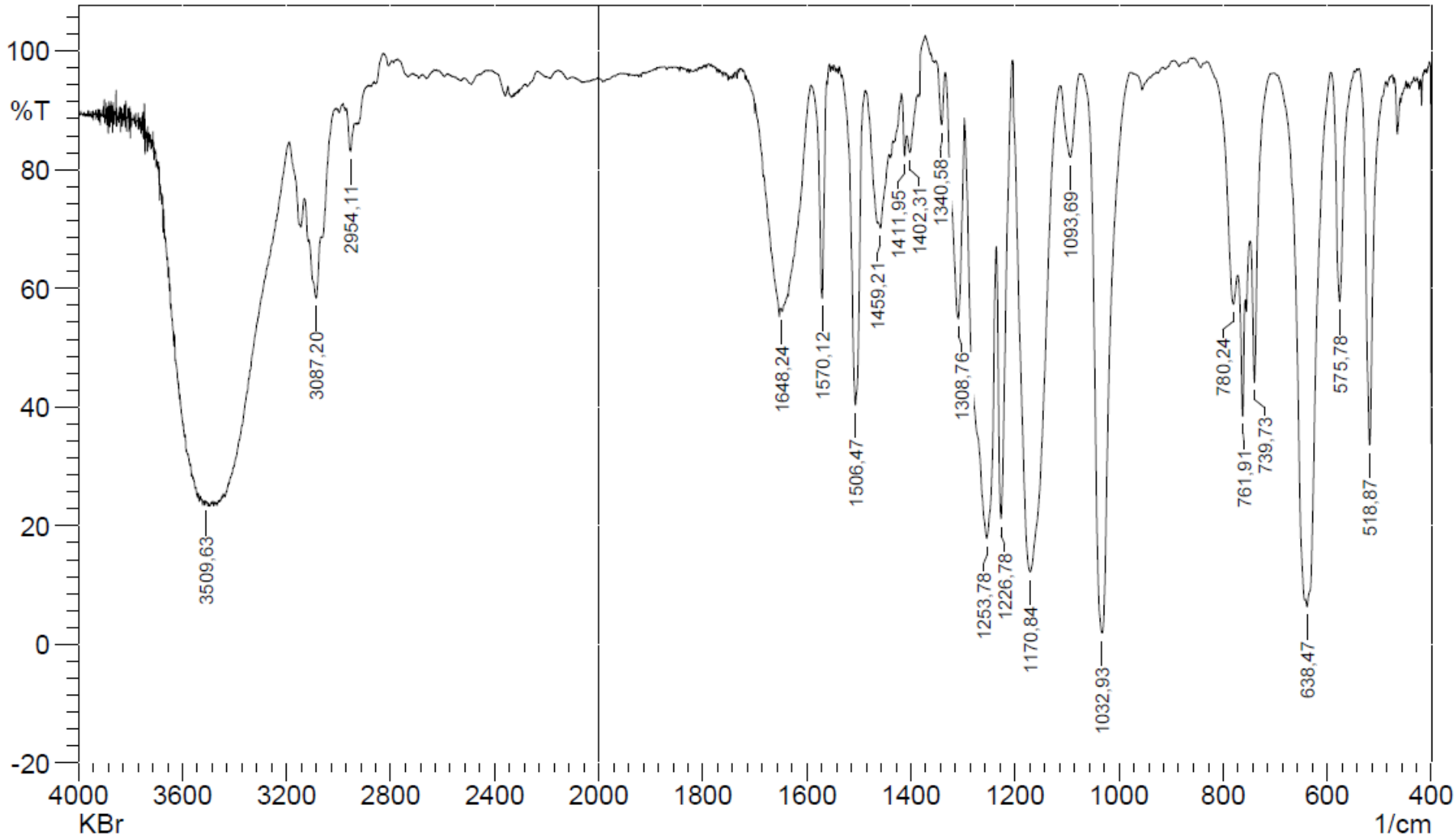


Figure S28. IR spectrum of [**7**]OTf.

Table S1. Crystal data for [**5**]OTf, [**5**]I and [**1**]I.

Identification code	[**5**]I	[**5**]OTf	[**1**]I
Empirical formula	$C_{12}H_{14}I_2N_2$	$C_{13}H_{14}F_3IN_2O_3S$	$C_7H_{12}I_2N_2$
Formula weight	440.05	462.22	377.99
Temperature/K	100(2)	100(2)	100(2)
Crystal system	orthorhombic	monoclinic	monoclinic
Space group	Pnma	$P2_1/c$	C2/c
a/Å	12.7742(2)	8.3762(4)	14.6499(2)
b/Å	7.18240(10)	14.1584(7)	16.45897(18)
c/Å	15.7199(2)	14.0266(7)	28.2119(4)
α/°	90	90	90
β/°	90	97.152(4)	95.4830(12)
γ/°	90	90	90
Volume/Å^3	1442.29(4)	1650.52(14)	6771.38(15)
Z	4	4	24
ρ_{calc}g/cm^3	2.027	1.860	2.225
μ/mm^{-1}	34.066	16.867	43.377
F(000)	824.0	904.0	4176.0
Crystal size/mm^3	0.2 × 0.15 × 0.15	0.14 × 0.08 × 0.06	0.301 × 0.191 × 0.093
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.92 to 139.958	8.91 to 139.978	6.294 to 141.028
Index ranges	$-15 \le h \le 15$, $-8 \le k \le 8$, $-19 \le l \le 19$	$-9 \le h \le 10$, $-17 \le k \le 17$, $-17 \le l \le 16$	$-17 \le h \le 15$, $-20 \le k \le 20$, $-34 \le l \le 34$
Reflections collected	25810	16922	38003
Independent reflections	1483 [R_{int} = 0.0749, R_{sigma} = 0.0223]	3129 [R_{int} = 0.0506, R_{sigma} = 0.0317]	6461 [R_{int} = 0.1082, R_{sigma} = 0.0462]
Data/restraints/parameters	1483/0/93	3129/0/211	6461/0/311
Goodness-of-fit on F^2	1.062	1.049	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0216, wR_2 = 0.0530	R_1 = 0.0252, wR_2 = 0.0653	R_1 = 0.0423, wR_2 = 0.1134
Final R indexes [all data]	R_1 = 0.0222, wR_2 = 0.0535	R_1 = 0.0260, wR_2 = 0.0659	R_1 = 0.0441, wR_2 = 0.1154
Largest diff. peak/hole / e Å^{-3}	1.53/-0.71	0.61/-0.58	1.67/-0.89
CCDC number	2085430	2085431	2085432

Table S2. Calculated Gibbs free energies (*G*, in Hartree) for optimized equilibrium model structures.

Model structure	*G*
CH_3Cl	-500.029526
H_2O	-76.369493
NH_3	-56.496081
Me_2CO	-193.000966
A*	-394.276927
B*	-394.272317
C*	-394.304331
D*	-394.307848
E*	-371.037661
F*	-371.018307
G*	-371.020011
H*	-371.059774
I*	-371.062201
J*	-371.047023
K*	-347.781655
L*	-347.755903
M*	-347.780893
N*	-347.758323
TS_H_2O···CH_3···Cl	-576.287275
TS_H_2O···CH_3···Cl_A*	-970.600090
TS_H_2O···CH_3···Cl_B*	-970.600145
TS_H_2O···CH_3···Cl_C*	-970.638170
TS_H_2O···CH_3···Cl_D*	-970.635717
TS_H_2O···CH_3···Cl_E*	-947.371641
TS_H_2O···CH_3···Cl_F*	-947.343559
TS_H_2O···CH_3···Cl_G*	-947.353740
TS_H_2O···CH_3···Cl_H*	-947.391767
TS_H_2O···CH_3···Cl_I*	-947.399861
TS_H_2O···CH_3···Cl_J*	-947.378971
TS_H_2O···CH_3···Cl_K*	-924.119558
TS_H_2O···CH_3···Cl_L*	-924.096383
TS_H_2O···CH_3···Cl_M*	-924.127193
TS_H_2O···CH_3···Cl_N*	-924.087809
H_2O···NH_3···Me_2CO	-325.830551
H_2O···NH_3···Me_2CO_A*	-720.119952
H_2O···NH_3···Me_2CO_B*	-720.120034
H_2O···NH_3···Me_2CO_C*	-720.157134
H_2O···NH_3···Me_2CO_D*	-720.155868
H_2O···NH_3···Me_2CO_E*	-696.890703
H_2O···NH_3···Me_2CO_F*	-696.866606
H_2O···NH_3···Me_2CO_G*	-696.872361
H_2O···NH_3···Me_2CO_H*	-696.913001
H_2O···NH_3···Me_2CO_I*	-696.920896
H_2O···NH_3···Me_2CO_J*	-696.899278
H_2O···NH_3···Me_2CO_K*	-673.640225
H_2O···NH_3···Me_2CO_L*	-673.615515

$H_2O\cdots NH_3\cdots Me_2CO\_M^*$	-673.647459
$H_2O\cdots NH_3\cdots Me_2CO\_N^*$	-673.610024

Table S3. Calculated values of Gibbs free energies of activation ($\Delta G^{\neq}$, in kJ/mol) for hypothetical transformations.

Transformation	$\Delta G^{\neq}$
$TS\_H_2O\cdots CH_3Cl$	293
$TS\_H_2O\cdots CH_3\cdots Cl\_A^*$	199
$TS\_H_2O\cdots CH_3\cdots Cl\_B^*$	187
$TS\_H_2O\cdots CH_3\cdots Cl\_C^*$	171
$TS\_H_2O\cdots CH_3\cdots Cl\_D^*$	187
$TS\_H_2O\cdots CH_3\cdots Cl\_E^*$	171
$TS\_H_2O\cdots CH_3\cdots Cl\_F^*$	194
$TS\_H_2O\cdots CH_3\cdots Cl\_G^*$	171
$TS\_H_2O\cdots CH_3\cdots Cl\_H^*$	176
$TS\_H_2O\cdots CH_3\cdots Cl\_I^*$	161
$TS\_H_2O\cdots CH_3\cdots Cl\_J^*$	176
$TS\_H_2O\cdots CH_3\cdots Cl\_K^*$	161
$TS\_H_2O\cdots CH_3\cdots Cl\_L^*$	154
$TS\_H_2O\cdots CH_3\cdots Cl\_M^*$	138
$TS\_H_2O\cdots CH_3\cdots Cl\_N^*$	183
$H_2O\cdots NH_3\cdots Me_2CO$	95
$H_2O\cdots NH_3\cdots Me_2CO\_A^*$	62
$H_2O\cdots NH_3\cdots Me_2CO\_B^*$	49
$H_2O\cdots NH_3\cdots Me_2CO\_C^*$	36
$H_2O\cdots NH_3\cdots Me_2CO\_D^*$	49
$H_2O\cdots NH_3\cdots Me_2CO\_E^*$	35
$H_2O\cdots NH_3\cdots Me_2CO\_F^*$	48
$H_2O\cdots NH_3\cdots Me_2CO\_G^*$	37
$H_2O\cdots NH_3\cdots Me_2CO\_H^*$	35
$H_2O\cdots NH_3\cdots Me_2CO\_I^*$	21
$H_2O\cdots NH_3\cdots Me_2CO\_J^*$	38
$H_2O\cdots NH_3\cdots Me_2CO\_K^*$	21
$H_2O\cdots NH_3\cdots Me_2CO\_L^*$	18
$H_2O\cdots NH_3\cdots Me_2CO\_M^*$	0
$H_2O\cdots NH_3\cdots Me_2CO\_N^*$	39

Table S4. Cartesian atomic coordinates for all optimized equilibrium model structures.

Model structure	Atomic charge	X	Y	Z
CH_3Cl				
	6	0.000000	0.000000	-1.127358
	1	0.000000	1.031828	-1.474944
	1	-0.893589	-0.515914	-1.474944
	1	0.893589	-0.515914	-1.474944
	17	0.000000	0.000000	0.658175
H_2O				

	8	0.000000	0.000000	0.118463
	1	0.000000	0.762398	-0.473850
	1	0.000000	-0.762398	-0.473850
NH_3				
	7	0.000000	0.000000	0.117400
	1	0.000000	0.938678	-0.273932
	1	-0.812919	-0.469339	-0.273932
	1	0.812919	-0.469339	-0.273932
Me_2CO				
	6	-0.000001	0.187119	0.000010
	8	-0.000002	1.396142	-0.000001
	6	1.286978	-0.613652	-0.000005
	6	-1.286976	-0.613655	0.000009
	1	2.142184	0.062400	-0.000277
	1	1.328017	-1.262986	0.881097
	1	1.327762	-1.263412	-0.880800
	1	-2.142185	0.062394	0.000394
	1	-1.328047	-1.262862	-0.881190
	1	-1.327722	-1.263544	0.880707
A*				
	7	-2.109169	0.677144	-0.010099
	7	-2.109140	-0.677182	0.009920
	6	-0.838107	-1.123112	0.008297
	6	-0.011082	0.000026	-0.000083
	6	-0.838094	1.123117	-0.008501
	53	2.079151	0.000002	0.000046
	6	-3.349027	-1.443224	-0.027205
	6	-3.349011	1.443187	0.027493
	6	-0.502622	2.575298	-0.011152
	6	-0.502554	-2.575275	0.010883
	1	-3.091415	-2.490857	0.117177
	1	-4.008966	-1.127512	0.782762
	1	-3.842410	-1.321784	-0.994230
	1	-3.091426	2.490835	-0.116842
	1	-3.842096	1.321690	0.994668
	1	-4.009250	1.127579	-0.782271
	1	-0.920164	3.078984	0.865715
	1	0.580978	2.695828	0.011646
	1	-0.880090	3.065395	-0.913834
	1	0.581001	-2.695755	-0.014236
	1	-0.922009	-3.079444	-0.864779
	1	-0.877996	-3.064925	0.914665
B*				
	7	-2.125511	-0.615280	-0.003646
	7	-0.838471	-1.038404	0.005647
	6	-0.047064	0.049716	0.002943
	6	-0.836137	1.197893	-0.001753
	6	-2.153732	0.733250	-0.004176
	53	2.035418	-0.021000	0.002132
	6	-0.506181	-2.458327	-0.020887

	6	-3.237468	-1.557688	0.017866
	6	-3.438582	1.492276	-0.004024
	6	-0.345161	2.610811	-0.004405
	1	0.575465	-2.544655	0.061686
	1	-0.970737	-2.964905	0.826822
	1	-0.833181	-2.902607	-0.963419
	1	-4.156700	-0.979012	-0.050970
	1	-3.177302	-2.232283	-0.838245
	1	-3.239055	-2.123527	0.951995
	1	-3.232587	2.562215	-0.003705
	1	-4.033876	1.264083	0.885156
	1	-4.033539	1.265181	-0.893814
	1	-1.175263	3.318475	-0.009953
	1	0.263612	2.812103	0.881702
	1	0.269844	2.806098	-0.887631
C*				
	6	-2.195990	0.652283	0.001870
	6	-2.170019	-0.713187	-0.000569
	7	-0.830659	-1.086310	0.000248
	6	-0.070422	0.014371	0.003098
	7	-0.874695	1.081948	0.005312
	53	2.010778	0.015244	0.000262
	6	-0.485289	2.491567	-0.007273
	6	-3.284348	-1.703537	-0.002762
	6	-3.332494	1.616371	0.003319
	6	-0.325147	-2.460798	-0.001206
	1	0.595261	2.570892	0.094498
	1	-0.798426	2.944478	-0.949808
	1	-0.966234	3.000674	0.829008
	1	-4.239758	-1.177275	-0.003633
	1	-3.257949	-2.340854	0.886140
	1	-3.255362	-2.339856	-0.892308
	1	-3.292719	2.280873	-0.865248
	1	-3.333340	2.231582	0.908470
	1	-4.278816	1.075657	-0.033579
	1	-1.175738	-3.139058	-0.006602
	1	0.279372	-2.630953	-0.893971
	1	0.272205	-2.635970	0.895353
D*				
	6	-0.038082	0.064224	-0.000005
	6	-0.869899	1.144628	0.000007
	7	-2.159276	0.627430	-0.000002
	6	-2.114121	-0.711837	-0.000013
	7	-0.825536	-1.075538	-0.000019
	53	2.044949	0.012767	0.000001
	6	-0.571464	2.603485	-0.000012
	6	-3.391461	1.420816	0.000025
	6	-3.283665	-1.633375	-0.000015
	6	-0.328339	-2.451527	0.000020
	1	0.509445	2.751934	0.000072

	1	-0.977835	3.094058	0.889684
	1	-0.977696	3.093987	-0.889812
	1	-3.122609	2.475065	0.000159
	1	-3.974359	1.203007	-0.896172
	1	-3.974446	1.202797	0.896112
	1	-4.214557	-1.066095	-0.000043
	1	-3.275377	-2.271248	-0.888574
	1	-3.275400	-2.271220	0.888562
	1	0.276268	-2.618201	-0.893193
	1	-1.176092	-3.134338	0.000031
	1	0.276249	-2.618150	0.893253
E*				
	6	-1.297725	-0.804341	-0.000162
	6	-0.252499	0.095954	-0.000198
	7	-0.831276	1.327218	0.000346
	7	-2.135592	1.260932	0.000693
	7	-2.408749	-0.017550	0.000664
	53	1.800230	-0.231655	-0.000375
	6	-0.177067	2.638427	0.001132
	6	-3.806670	-0.453598	-0.002315
	6	-1.340022	-2.290694	0.002318
	1	-0.965582	3.388614	-0.001792
	1	0.436401	2.726047	0.898620
	1	0.441465	2.724460	-0.892989
	1	-4.424894	0.442073	0.017617
	1	-3.999719	-1.027847	-0.909543
	1	-3.991937	-1.063555	0.882872
	1	-0.325152	-2.687116	-0.053111
	1	-1.903518	-2.667038	-0.856621
	1	-1.806028	-2.666621	0.918245
F*				
	6	0.929663	0.949834	0.005318
	6	0.058598	-0.147484	-0.000545
	7	0.764233	-1.280101	-0.007260
	7	2.014922	-0.931749	-0.008110
	7	2.156947	0.399728	0.004858
	53	-2.025231	-0.136655	-0.000601
	6	0.675666	2.415168	0.008774
	6	3.468972	1.046422	-0.014134
	6	3.123206	-1.883361	0.012775
	1	1.068161	2.880595	0.918127
	1	1.128235	2.897082	-0.862836
	1	-0.400692	2.590535	-0.024913
	1	3.947273	0.882078	-0.981706
	1	3.309482	2.112188	0.141594
	1	4.083165	0.650164	0.795872
	1	3.793921	-1.687542	-0.825455
	1	3.653081	-1.816032	0.965104
	1	2.665298	-2.864994	-0.093494
G*				

	6	-0.248856	0.191464	0.008427
	6	-0.873166	1.444824	-0.000599
	7	-2.196196	1.245502	-0.009540
	7	-2.391843	-0.039075	-0.008208
	7	-1.238407	-0.718270	0.009969
	53	1.782374	-0.235724	0.000259
	6	-1.196212	-2.181110	-0.009950
	6	-3.714932	-0.657615	0.008773
	6	-0.257192	2.800671	-0.000412
	1	-1.459501	-2.541782	-1.006409
	1	-0.180327	-2.483242	0.238796
	1	-1.884192	-2.571099	0.740792
	1	-3.805184	-1.361850	-0.819868
	1	-3.882732	-1.153959	0.966760
	1	-4.419352	0.162712	-0.116448
	1	0.390668	2.930541	-0.871690
	1	-1.043703	3.555635	-0.028288
	1	0.345797	2.949917	0.899621
H*				
	7	0.791905	-1.314165	-0.001948
	7	2.080838	-0.898864	-0.003570
	6	2.177577	0.424142	-0.000989
	7	0.912669	0.888164	0.000006
	6	0.092170	-0.216727	-0.000207
	53	-1.984573	-0.143176	0.000410
	6	3.423090	1.234249	0.002067
	6	3.159450	-1.890604	0.001903
	6	0.491839	2.291230	-0.001346
	1	3.460321	1.873853	0.888588
	1	4.297127	0.582195	0.012275
	1	3.471841	1.864685	-0.890534
	1	3.824835	-1.714494	-0.843984
	1	3.705181	-1.837036	0.944937
	1	2.681338	-2.863087	-0.097621
	1	1.379555	2.921928	-0.002711
	1	-0.100639	2.489216	-0.895994
	1	-0.099811	2.491387	0.893351
I*				
	7	-2.197732	1.255339	-0.002845
	7	-0.849211	1.359465	-0.005528
	6	-0.275361	0.166585	-0.002855
	7	-1.268777	-0.740618	0.000323
	6	-2.448646	-0.027280	-0.000029
	53	1.760156	-0.227673	-0.000055
	6	-0.210834	2.676134	0.004864
	6	-3.807950	-0.628995	0.001155
	6	-1.113975	-2.197196	0.001795
	1	-1.008999	3.405902	-0.114342
	1	0.494092	2.743901	-0.824531
	1	0.301653	2.825268	0.956650

	1	-4.536572	0.182348	-0.002367
	1	-3.967409	-1.240479	0.893797
	1	-3.966192	-1.247220	-0.887028
	1	-0.580981	-2.509395	-0.897805
	1	-0.566014	-2.505267	0.893756
	1	-2.107200	-2.643159	0.011550
J*				
	7	-0.889009	0.855661	-0.002964
	7	-2.160209	0.367248	0.001223
	6	-2.063152	-0.972058	0.002714
	7	-0.783225	-1.345818	0.001830
	6	-0.085169	-0.219582	-0.000829
	53	1.994963	-0.141236	-0.000921
	6	-3.335767	1.230690	-0.009471
	6	-3.228963	-1.895510	0.003706
	6	-0.604357	2.287055	0.009985
	1	-4.210030	0.581509	0.013730
	1	-3.338242	1.871268	0.874190
	1	-3.354199	1.828803	-0.922439
	1	-2.847458	-2.916103	0.022185
	1	-3.857431	-1.736134	0.884732
	1	-3.837421	-1.761357	-0.895525
	1	-1.060845	2.762146	-0.860126
	1	-0.973140	2.730403	0.936936
	1	0.477257	2.401766	-0.042124
K*				
	7	2.343440	0.833857	-0.000066
	7	2.401435	-0.454060	0.000006
	7	1.230884	-1.073845	0.000060
	6	0.363604	-0.082015	0.000023
	7	1.055247	1.087841	-0.000058
	53	-1.698359	-0.269772	-0.000005
	6	0.557181	2.467863	0.000047
	6	3.674609	-1.183100	-0.000004
	1	-0.043250	2.623572	-0.897107
	1	1.426681	3.122501	-0.000150
	1	-0.042824	2.623582	0.897486
	1	3.706128	-1.801783	-0.896415
	1	4.470778	-0.441191	0.000051
	1	3.706117	-1.801794	0.896401
L*				
	7	2.382652	-0.253772	-0.001127
	7	2.079568	-1.513588	-0.002069
	7	0.776566	-1.628663	-0.001105
	6	0.263079	-0.396417	0.000807
	7	1.269735	0.492017	0.001980
	53	-1.763943	0.026582	0.000227
	6	1.292241	1.957031	-0.002706
	6	3.752947	0.260039	0.002335
	1	0.258286	2.294628	0.054497

	1	1.746324	2.309120	-0.930628
	1	1.844303	2.311423	0.869153
	1	4.391732	-0.621989	-0.020139
	1	3.924898	0.831262	0.916132
	1	3.914191	0.870830	-0.887408
M*				
	7	2.667743	0.633802	-0.000171
	7	2.667587	-0.634275	-0.000061
	7	1.388063	-1.054472	0.000164
	6	0.574213	0.000061	0.000123
	7	1.388312	1.054330	-0.000029
	53	-1.492570	0.000082	-0.000020
	6	1.069151	-2.485099	0.000010
	6	1.069748	2.485061	0.000089
	1	0.497760	-2.726283	0.897264
	1	2.022382	-3.011545	0.002291
	1	0.501626	-2.726964	-0.899523
	1	2.023126	3.011247	0.000287
	1	0.500482	2.726796	-0.898369
	1	0.500225	2.726579	0.898440
N*				
	7	-2.096020	0.660565	-0.002713
	7	-2.095994	-0.660571	0.002810
	7	-0.877599	-1.111323	0.003605
	6	-0.125238	0.000052	0.000014
	7	-0.877590	1.111330	-0.003553
	53	1.949177	-0.000002	-0.000007
	6	-3.296039	1.504237	0.002615
	6	-3.296017	-1.504254	-0.002689
	1	-2.934446	2.529605	-0.047343
	1	-3.903964	1.267515	-0.871906
	1	-3.847732	1.335940	0.929206
	1	-2.934433	-2.529615	0.047526
	1	-3.847450	-1.336114	-0.929463
	1	-3.904143	-1.267420	0.871657
TS_$H_2O\cdots CH_3\cdots Cl$				
	6	0.983964	-0.531984	-0.001185
	1	1.051124	-1.138909	0.897669
	1	0.132797	0.180422	0.006582
	1	1.044386	-1.124825	-0.909796
	17	-1.873111	0.097619	0.000375
	8	2.365893	0.245358	-0.000773
	1	2.397885	0.816641	0.792213
	1	2.385763	0.836192	-0.779755
TS_$H_2O\cdots CH_3\cdots Cl$_A*				
	6	-6.115897	0.139184	0.035718
	1	-5.918558	-0.103374	1.070653
	1	-5.956076	-0.652449	-0.683511
	1	-5.795656	1.127810	-0.263977
	17	-3.510815	-0.254535	-0.005365

	8	-7.749619	0.337710	0.063684
	1	-8.214553	-0.472224	0.348397
	1	-8.106264	0.607580	-0.804153
	7	3.750066	-0.589954	-0.008863
	7	3.697705	0.763569	0.020522
	6	2.404544	1.151612	0.012080
	6	1.611258	0.005179	-0.007383
	6	2.491055	-1.076537	-0.016246
	53	-0.513897	-0.081376	-0.011248
	6	4.903281	1.575950	-0.018199
	6	5.013119	-1.307931	0.053009
	6	2.208929	-2.540423	-0.022121
	6	2.010621	2.589406	0.017105
	1	4.602447	2.613520	0.116142
	1	5.575146	1.295714	0.795520
	1	5.407918	1.469517	-0.981676
	1	4.796629	-2.363685	-0.100442
	1	5.483849	-1.175284	1.030354
	1	5.682038	-0.967164	-0.739728
	1	2.641538	-3.026875	-0.901859
	1	2.602475	-3.024443	0.877103
	1	1.128753	-2.690666	-0.045720
	1	0.921882	2.655922	0.006335
	1	2.394596	3.110930	-0.865062
	1	2.375315	3.099564	0.914075
TS_$H_2O\cdots CH_3\cdots Cl$_B*				
	6	-6.051849	-0.012195	-0.033337
	1	-5.838032	-0.617113	-0.903563
	1	-5.765051	1.029503	-0.085640
	1	-5.907306	-0.505317	0.918072
	17	-3.450229	-0.121188	0.074908
	8	-7.707892	0.029908	-0.097726
	1	-8.037950	0.432277	-0.923637
	1	-8.096157	0.514990	0.655263
	7	3.722152	-0.615415	-0.011849
	7	2.426660	-1.022438	-0.015679
	6	1.629902	0.059842	-0.006223
	6	2.442267	1.200152	-0.007184
	6	3.754451	0.735643	-0.013906
	53	-0.491181	-0.007197	0.019590
	6	2.081187	-2.435991	0.019623
	6	4.823195	-1.562970	-0.065084
	6	5.045351	1.484960	-0.025025
	6	1.956265	2.615140	0.001171
	1	0.998268	-2.506023	-0.067332
	1	2.544427	-2.956668	-0.820636
	1	2.397268	-2.879632	0.966645
	1	5.748387	-0.997952	0.035387
	1	4.752783	-2.273625	0.760783
	1	4.829657	-2.093801	-1.020380

	1	4.846456	2.556398	-0.022851
	1	5.632912	1.253671	-0.918735
	1	5.647990	1.253702	0.858690
	1	2.786785	3.323302	-0.006058
	1	1.331943	2.815117	-0.874393
	1	1.350924	2.811035	0.890984
TS_$H_2O\cdots CH_3\cdots Cl$_C*				
	6	-5.875440	0.167300	0.074085
	1	-5.598563	0.208413	1.117398
	1	-5.919739	-0.804467	-0.397114
	1	-5.583198	1.009663	-0.535588
	17	-3.415245	-0.409165	-0.170828
	8	-7.536471	0.547412	0.242035
	1	-8.007250	-0.091817	0.808656
	1	-7.997347	0.581321	-0.616834
	6	3.722682	0.798020	0.033971
	6	3.780169	-0.563788	0.051788
	7	2.464682	-1.014189	0.047233
	6	1.625398	0.030626	0.021337
	7	2.375445	1.140995	0.017133
	53	-0.495765	-0.111251	-0.040226
	6	1.892390	2.516997	-0.021170
	6	4.951253	-1.486251	0.074519
	6	4.797812	1.829912	0.036557
	6	2.046773	-2.414833	0.041689
	1	2.157710	2.973287	-0.977254
	1	0.810057	2.518163	0.095024
	1	2.346398	3.080171	0.795812
	1	5.875245	-0.906814	0.050306
	1	4.953311	-2.154033	-0.792285
	1	4.965972	-2.096697	0.982754
	1	4.765141	2.441377	0.943976
	1	4.714486	2.496290	-0.827729
	1	5.776326	1.349517	-0.006701
	1	1.643597	-2.680627	-0.937796
	1	2.912428	-3.036115	0.263933
	1	1.284780	-2.570349	0.805995
TS_$H_2O\cdots CH_3\cdots Cl$_D*				
	6	6.029472	0.026079	0.149669
	1	5.725124	0.868460	0.753808
	1	5.932336	0.129418	-0.922627
	1	5.818120	-0.947211	0.566903
	17	3.476522	-0.114766	-0.239188
	8	7.685366	0.089604	0.390698
	1	8.074053	0.922686	0.063146
	1	8.147951	-0.651439	-0.044273
	6	-1.622030	0.076455	0.008640
	6	-2.466579	1.148428	0.031685
	7	-3.758269	0.634583	0.079626
	6	-3.709788	-0.704211	0.076487

	7	-2.419709	-1.058665	0.041822
	53	0.495109	0.014684	-0.079936
	6	-2.168517	2.607713	0.009493
	6	-4.985099	1.428106	0.105882
	6	-4.876840	-1.629218	0.104719
	6	-1.914541	-2.429311	0.033582
	1	-1.089640	2.745989	-0.080717
	1	-2.493361	3.102505	0.930509
	1	-2.644772	3.104624	-0.841329
	1	-5.474152	1.403921	-0.870513
	1	-5.658976	1.045506	0.873249
	1	-4.727216	2.456732	0.350903
	1	-5.800634	-1.083489	-0.090653
	1	-4.775964	-2.398926	-0.664576
	1	-4.967613	-2.121243	1.078538
	1	-1.437294	-2.636675	-0.926157
	1	-2.741779	-3.118414	0.196668
	1	-1.181361	-2.542179	0.833288
TS_$H_2O\cdots CH_3\cdots Cl$_E*				
	6	-5.678382	-0.231031	0.118704
	1	-5.396138	-1.229268	-0.182819
	1	-5.689346	0.537688	-0.641387
	1	-5.406233	0.060743	1.122652
	17	-3.192262	0.168583	-0.263817
	8	-7.341766	-0.501602	0.372911
	1	-7.793670	-0.810508	-0.434475
	1	-7.803235	0.298586	0.686307
	6	2.772181	-0.959175	0.028892
	6	1.864795	0.082241	0.020579
	7	2.635458	1.203179	0.070565
	7	3.918758	0.948346	0.109416
	7	3.992067	-0.357469	0.083927
	53	-0.256730	0.086423	-0.066557
	6	2.185307	2.594671	0.081345
	6	5.301222	-1.004555	0.112565
	6	2.586707	-2.434532	-0.013115
	1	3.073595	3.221326	0.131973
	1	1.623267	2.792121	-0.832452
	1	1.547549	2.753574	0.951833
	1	6.052301	-0.219232	0.174712
	1	5.360154	-1.655475	0.986050
	1	5.434436	-1.585651	-0.801256
	1	1.519851	-2.663153	-0.031626
	1	3.026311	-2.913442	0.867089
	1	3.045448	-2.864916	-0.908627
TS_$H_2O\cdots CH_3\cdots Cl$_F*				
	6	-5.868839	-0.204719	0.026885
	1	-5.590662	-0.372384	1.058253
	1	-5.444239	-0.884398	-0.699437
	1	-5.921598	0.835011	-0.263039

	17	-3.344281	0.506373	-0.024585
	8	-7.465687	-0.596402	0.067636
	1	-7.617555	-1.515747	0.358846
	1	-7.899752	-0.472178	-0.798067
	6	2.648897	0.851166	0.003480
	6	1.691145	-0.174897	0.006125
	7	2.328624	-1.351415	0.005457
	7	3.605744	-1.092606	0.007247
	7	3.838917	0.225253	-0.001081
	53	-0.426842	0.028343	-0.001909
	6	2.494249	2.330234	0.004265
	6	5.188050	0.780761	0.026113
	6	4.642987	-2.114121	-0.026335
	1	2.968287	2.781376	0.881126
	1	2.922861	2.774589	-0.899528
	1	1.429582	2.567833	0.028133
	1	5.789395	0.324956	-0.761808
	1	5.103585	1.850569	-0.158610
	1	5.641952	0.611435	1.004814
	1	5.180048	-2.075876	-0.976724
	1	5.328395	-1.980396	0.812725
	1	4.118641	-3.063265	0.066810
TS_$H_2O\cdots CH_3\cdots Cl$_G*				
	6	-5.554849	0.045200	0.151265
	1	-5.284635	-0.234748	1.159057
	1	-5.663476	-0.743649	-0.579501
	1	-5.197528	1.003946	-0.194598
	17	-3.140681	-0.619139	-0.284770
	8	-7.185312	0.476433	0.441920
	1	-7.703543	-0.264177	0.808452
	1	-7.636376	0.784928	-0.365993
	6	1.828732	0.232921	0.009161
	6	2.528176	1.452278	0.015490
	7	3.837617	1.202255	0.087866
	7	3.972555	-0.092666	0.125639
	7	2.780579	-0.710254	0.078704
	53	-0.265440	-0.105549	-0.093629
	6	2.668926	-2.165593	0.108184
	6	5.255563	-0.776652	0.198391
	6	1.973436	2.833448	-0.048938
	1	3.074778	-2.546860	1.046883
	1	1.609527	-2.408236	0.040560
	1	3.198853	-2.592288	-0.745251
	1	5.304991	-1.388770	1.101061
	1	5.407735	-1.389160	-0.692883
	1	6.004188	0.012211	0.241215
	1	1.292408	3.013485	0.787264
	1	2.787351	3.558320	-0.008308
	1	1.412940	2.978042	-0.976665
TS_$H_2O\cdots CH_3\cdots Cl$_H*				

	6	5.672766	0.318890	0.092758
	1	5.240502	1.066669	-0.556919
	1	5.840659	-0.660811	-0.333565
	1	5.356473	0.355403	1.125683
	17	3.292139	-0.673929	-0.146713
	8	7.219857	0.937193	0.246844
	1	7.681930	0.996831	-0.610756
	1	7.772236	0.407492	0.852577
	7	-2.271588	1.405688	-0.038158
	7	-3.599328	1.125998	0.007365
	6	-3.828154	-0.177897	0.066656
	7	-2.617514	-0.762815	0.054927
	6	-1.673659	0.244452	-0.010097
	53	0.428898	-0.087610	-0.060823
	6	-5.148762	-0.856699	0.135623
	6	-4.567566	2.219528	0.005534
	6	-2.337560	-2.196981	0.095425
	1	-5.219490	-1.463471	1.042794
	1	-5.952638	-0.119776	0.153609
	1	-5.293074	-1.506388	-0.732479
	1	-5.317846	2.050690	-0.767692
	1	-5.037841	2.305241	0.986557
	1	-4.005153	3.124344	-0.216589
	1	-3.280952	-2.740214	0.138099
	1	-1.786047	-2.481076	-0.801966
	1	-1.738964	-2.422198	0.979284
TS_$H_2O\cdots CH_3\cdots$Cl_I*				
	6	-5.514565	-0.003386	0.160766
	1	-5.231121	-0.306727	1.157632
	1	-5.620602	-0.764908	-0.598168
	1	-5.240066	0.994473	-0.147337
	17	-3.116271	-0.499469	-0.341819
	8	-7.192034	0.333319	0.507519
	1	-7.665933	-0.449320	0.843947
	1	-7.675226	0.656555	-0.275006
	7	3.861876	1.157689	0.109136
	7	2.521668	1.348820	0.036455
	6	1.852185	0.204197	0.020157
	7	2.789952	-0.762683	0.085499
	6	4.017003	-0.137731	0.139372
	53	-0.251782	-0.061459	-0.100372
	6	1.975588	2.700506	-0.032778
	6	5.326422	-0.838305	0.220430
	6	2.528938	-2.200871	0.093348
	1	1.496625	2.852117	-1.001475
	1	2.814776	3.382712	0.087017
	1	1.250409	2.841900	0.769554
	1	6.114035	-0.085219	0.255074
	1	5.487437	-1.475630	-0.653690
	1	5.388985	-1.454134	1.121974

	1	1.928728	-2.459872	0.966882
	1	1.997472	-2.480775	-0.817584
	1	3.483928	-2.722645	0.136253
TS_$H_2O\cdots CH_3\cdots Cl$_J*				
	6	5.628860	0.336016	0.138565
	1	5.036276	1.201009	0.399381
	1	5.648253	0.044007	-0.902109
	1	5.657713	-0.454869	0.874659
	17	3.301983	-0.711514	-0.207132
	8	7.168502	0.980340	0.372744
	1	7.353607	1.729930	-0.223803
	1	7.871201	0.314659	0.249034
	7	-2.593073	-0.724656	0.078800
	7	-3.802098	-0.093817	0.094457
	6	-3.542577	1.221041	0.007540
	7	-2.233542	1.437583	-0.058000
	6	-1.655293	0.233034	-0.013530
	53	0.444898	-0.124168	-0.084415
	6	-5.066784	-0.807931	0.175186
	6	-4.593233	2.274832	-0.011239
	6	-2.475929	-2.173408	0.159694
	1	-5.858338	-0.059949	0.207322
	1	-5.202556	-1.440092	-0.705021
	1	-5.103378	-1.408126	1.086375
	1	-4.095505	3.239965	-0.101071
	1	-5.269595	2.145297	-0.861126
	1	-5.180737	2.264762	0.911418
	1	-2.880606	-2.530726	1.108754
	1	-2.993169	-2.638592	-0.681733
	1	-1.413769	-2.408644	0.107118
TS_$H_2O\cdots CH_3\cdots Cl$_K*				
	6	5.233419	-0.404266	0.104811
	1	5.313411	0.366438	0.857206
	1	5.302068	-0.114822	-0.933725
	1	4.646851	-1.274976	0.356984
	17	2.995421	0.687247	-0.223437
	8	6.800396	-1.113907	0.348957
	1	7.520843	-0.463647	0.255321
	1	6.980687	-1.847758	-0.266917
	7	-4.091520	0.316267	0.135505
	7	-3.872632	-0.949492	0.031274
	7	-2.596820	-1.301183	-0.048420
	6	-1.946302	-0.150652	0.010760
	7	-2.882997	0.832115	0.124178
	53	0.163555	0.153265	-0.068529
	6	-2.682887	2.278753	0.220412
	6	-4.957909	-1.929335	-0.005164
	1	-2.072180	2.490914	1.098636
	1	-3.665202	2.738047	0.312449
	1	-2.176062	2.623330	-0.681791

	1	-4.805943	-2.631931	0.813475
	1	-5.893451	-1.385453	0.108154
	1	-4.914904	-2.446059	-0.963677
TS_$H_2O\cdots CH_3\cdots Cl$_L*				
	6	-5.162363	-0.239520	0.069601
	1	-4.631732	-1.030322	-0.439308
	1	-5.448344	0.632937	-0.499782
	1	-4.975184	-0.122390	1.126824
	17	-2.967069	0.972883	-0.104189
	8	-6.692029	-1.052574	0.205617
	1	-7.076716	-1.274206	-0.662435
	1	-7.350032	-0.525644	0.695473
	7	3.971692	-0.445930	0.037991
	7	3.602056	-1.687603	-0.031346
	7	2.297190	-1.730192	-0.064158
	6	1.831205	-0.470041	-0.012684
	7	2.891914	0.350369	0.054464
	53	-0.226019	0.103801	-0.046834
	6	2.981735	1.807047	0.121048
	6	5.359784	-0.001982	0.098665
	1	1.961426	2.183831	0.185763
	1	3.460091	2.186504	-0.783713
	1	3.539567	2.098129	1.012435
	1	5.959701	-0.908379	0.031570
	1	5.543056	0.503422	1.048412
	1	5.571471	0.656711	-0.745204
TS_$H_2O\cdots CH_3\cdots Cl$_M*				
	6	5.086552	0.164234	0.090884
	1	4.885736	0.760345	-0.786504
	1	5.291477	-0.889770	-0.027273
	1	4.718912	0.523334	1.040035
	17	2.795523	-0.651142	-0.252344
	8	6.757928	0.748922	0.319377
	1	7.324175	0.574449	-0.454110
	1	7.193107	0.351726	1.095281
	7	-4.305493	-0.256738	0.154195
	7	-4.149511	0.999151	0.094578
	7	-2.825898	1.248337	0.019091
	6	-2.135628	0.107193	0.033364
	7	-3.083343	-0.827626	0.118328
	53	-0.022628	-0.169856	-0.064410
	6	-2.327858	2.618738	-0.068744
	6	-2.934709	-2.280830	0.164333
	1	-1.684837	2.823443	0.788010
	1	-3.199798	3.270423	-0.057024
	1	-1.772397	2.739297	-0.999619
	1	-3.937010	-2.695642	0.255942
	1	-2.460781	-2.622843	-0.756651
	1	-2.327022	-2.552238	1.028134
TS_$H_2O\cdots CH_3\cdots Cl$_N*				

	6	-5.605683	-0.284685	-0.073985
	1	-5.216365	-0.643078	-1.016172
	1	-5.712850	0.785442	0.040250
	1	-5.310687	-0.846015	0.801055
	17	-3.176834	0.541435	0.161036
	8	-7.196888	-0.807137	-0.214572
	1	-7.650267	-0.413567	-0.983897
	1	-7.723974	-0.607742	0.582148
	7	3.749889	-0.846797	-0.003005
	7	3.866393	0.466561	-0.082720
	7	2.690537	1.020953	-0.090505
	6	1.829087	-0.012435	-0.011296
	7	2.494117	-1.182995	0.042898
	53	-0.289600	0.189452	0.040291
	6	4.867371	-1.789638	0.026871
	6	5.132020	1.196171	-0.150700
	1	4.416893	-2.774632	0.131099
	1	5.426032	-1.721639	-0.908191
	1	5.505236	-1.569247	0.884322
	1	4.861332	2.249677	-0.183565
	1	5.668752	0.910514	-1.056936
	1	5.722672	0.981491	0.741412
$H_2O\cdots NH_3\cdots Me_2CO$				
	6	-0.536920	-0.043800	-0.121877
	8	0.178871	0.153214	-1.228121
	6	-0.522934	-1.490063	0.389966
	6	-1.951973	0.511707	-0.234783
	1	-2.509417	0.443072	0.706032
	1	-1.908829	1.553570	-0.565524
	1	-2.483601	-0.058416	-1.000816
	1	0.511769	-1.816358	0.533090
	1	-1.078083	-1.624946	1.325497
	1	-0.973531	-2.121819	-0.379063
	7	0.196829	0.777602	1.030767
	1	1.271820	0.485501	0.826570
	1	-0.135494	0.588692	1.976274
	1	0.103274	1.774049	0.826753
	8	2.299054	0.118820	-0.120771
	1	2.694430	-0.757834	-0.025133
	1	1.377421	0.047934	-0.847745
$H_2O\cdots NH_3\cdots Me_2CO$_A*				
	6	3.971278	0.451257	-0.242056
	8	3.003025	0.113033	0.661242
	6	5.359340	0.446515	0.397351
	6	3.666578	1.768463	-0.940515
	1	4.428459	2.022713	-1.684228
	1	2.688453	1.721136	-1.430769
	1	3.631205	2.561764	-0.189637
	1	5.560083	-0.532758	0.842891
	1	6.153477	0.686888	-0.317555

	1	5.369769	1.189790	1.197102
	7	3.998144	-0.679779	-1.305178
	1	3.839605	-1.645616	-0.613404
	1	4.847109	-0.678045	-1.871217
	1	3.192015	-0.591981	-1.927444
	8	3.343558	-2.232669	0.471508
	1	3.989721	-2.666614	1.046373
	1	3.140460	-1.134679	0.817181
	7	-3.761463	-0.743822	-0.181375
	7	-3.842711	0.606071	-0.096292
	6	-2.600515	1.110896	0.053586
	6	-1.701577	0.045376	0.050317
	6	-2.466023	-1.111301	-0.098545
	53	0.407704	0.145252	0.283475
	6	-5.122543	1.298169	-0.115128
	6	-4.942401	-1.570776	-0.378710
	6	-2.043557	-2.539800	-0.163635
	6	-2.352678	2.573752	0.200055
	1	-4.915780	2.366830	-0.112870
	1	-5.676478	1.047507	-1.021952
	1	-5.709060	1.044411	0.771041
	1	-4.624454	-2.610758	-0.331865
	1	-5.388390	-1.376600	-1.357133
	1	-5.670688	-1.388012	0.413829
	1	-2.319381	-2.994242	-1.120236
	1	-0.959410	-2.595249	-0.057177
	1	-2.493509	-3.123698	0.645190
	1	-1.281707	2.739319	0.323267
	1	-2.862270	2.977740	1.080106
	1	-2.685404	3.126287	-0.684071
$H_2O\cdots NH_3\cdots Me_2CO$_B*				
	6	-3.925129	0.479629	0.133853
	8	-2.929152	-0.072216	-0.629950
	6	-5.276428	0.388565	-0.573258
	6	-3.595227	1.903523	0.556123
	1	-4.384255	2.337314	1.178173
	1	-2.650326	1.929563	1.109211
	1	-3.480221	2.516721	-0.341350
	1	-5.502203	-0.654609	-0.815531
	1	-6.092499	0.803013	0.028065
	1	-5.211893	0.946371	-1.509541
	7	-4.051541	-0.403124	1.398615
	1	-3.882156	-1.506029	0.931010
	1	-4.933160	-0.264553	1.893554
	1	-3.284556	-0.203668	2.044170
	8	-3.353049	-2.311603	0.037301
	1	-3.987065	-2.848872	-0.458847
	1	-3.102303	-1.319113	-0.525491
	7	3.786796	-0.657934	0.130281
	7	2.483268	-1.024736	0.039254

	6	1.726150	0.082462	-0.048690
	6	2.570700	1.196026	0.002945
	6	3.863820	0.690465	0.119188
	53	-0.385904	0.073542	-0.276675
	6	2.099438	-2.428239	-0.026905
	6	4.851010	-1.638456	0.280026
	6	5.173616	1.398589	0.222018
	6	2.137146	2.626469	-0.066754
	1	1.013444	-2.472842	0.032731
	1	2.428204	-2.866784	-0.972152
	1	2.527901	-2.972158	0.816775
	1	5.799079	-1.107068	0.217022
	1	4.781828	-2.136820	1.250092
	1	4.804499	-2.372265	-0.526803
	1	5.010830	2.475879	0.199944
	1	5.831062	1.141876	-0.614306
	1	5.686597	1.155432	1.157501
	1	2.991928	3.304344	-0.039915
	1	1.583554	2.817554	-0.990586
	1	1.481982	2.875899	0.772896
$H_2O\cdots NH_3\cdots Me_2CO$_C*				
	6	3.857734	-0.459215	0.324293
	8	2.871466	-0.161581	-0.589261
	6	5.178781	-0.747422	-0.386352
	6	3.451210	-1.592163	1.254658
	1	4.238020	-1.819666	1.980214
	1	2.534381	-1.336338	1.796186
	1	3.257105	-2.487198	0.657990
	1	5.464927	0.108460	-1.005433
	1	5.989431	-0.969950	0.315230
	1	5.036385	-1.607435	-1.043537
	7	4.092494	0.818196	1.154723
	1	3.967258	1.690589	0.288936
	1	4.986730	0.807674	1.646272
	1	3.349674	0.932853	1.847283
	8	3.467662	2.126112	-0.807165
	1	4.112004	2.404521	-1.474087
	1	3.130313	1.029752	-0.965316
	6	-3.897632	-0.606550	0.055552
	6	-3.823927	0.744270	0.216871
	7	-2.477680	1.080819	0.131910
	6	-1.741709	-0.022066	-0.068467
	7	-2.594507	-1.055557	-0.123865
	53	0.389958	-0.119540	-0.252608
	6	-2.244939	-2.460256	-0.313466
	6	-4.884270	1.768466	0.435715
	6	-5.065830	-1.532038	0.043899
	6	-1.980490	2.446587	0.266514
	1	-2.922264	-2.899401	-1.046704
	1	-1.223847	-2.529498	-0.684010

	1	-2.329934	-2.994955	0.635218
	1	-5.854476	1.282112	0.546286
	1	-4.952630	2.462123	-0.408419
	1	-4.695590	2.350494	1.343088
	1	-4.951524	-2.328777	0.785239
	1	-5.202544	-1.994394	-0.938835
	1	-5.977140	-0.981894	0.282494
	1	-2.573043	3.105662	-0.369199
	1	-2.059674	2.769066	1.307131
	1	-0.940066	2.483651	-0.051059
$H_2O\cdots NH_3\cdots Me_2CO\_D$*				
	6	3.944049	-0.475463	0.137936
	8	2.950059	0.058658	-0.637271
	6	5.306293	-0.356089	-0.544328
	6	3.635860	-1.906638	0.552549
	1	4.419900	-2.324631	1.191642
	1	2.679395	-1.952288	1.084035
	1	3.553521	-2.521101	-0.347569
	1	5.516382	0.692057	-0.779076
	1	6.119543	-0.757035	0.069953
	1	5.268743	-0.911745	-1.483339
	7	4.033409	0.405659	1.409162
	1	3.859724	1.502563	0.941917
	1	4.905328	0.277409	1.923590
	1	3.253592	0.195071	2.035541
	8	3.331568	2.305467	0.035410
	1	3.965219	2.848975	-0.454153
	1	3.101573	1.308382	-0.529583
	6	-1.722996	-0.106332	-0.057663
	6	-2.604987	-1.145621	0.006081
	7	-3.871146	-0.584046	0.131915
	6	-3.770180	0.752028	0.145550
	7	-2.472970	1.057999	0.030365
	53	0.386677	-0.107596	-0.288408
	6	-2.366056	-2.614820	-0.048142
	6	-5.125258	-1.328769	0.239601
	6	-4.895371	1.720035	0.267358
	6	-1.922568	2.410761	-0.022306
	1	-1.294773	-2.794836	-0.152167
	1	-2.865993	-3.074280	-0.906647
	1	-2.706524	-3.114948	0.863917
	1	-4.909082	-2.387513	0.110350
	1	-5.573553	-1.173995	1.222705
	1	-5.815801	-1.013434	-0.544099
	1	-4.773730	2.348527	1.154509
	1	-4.948918	2.367681	-0.612596
	1	-5.844926	1.191932	0.357809
	1	-2.727021	3.131158	0.117230
	1	-1.446946	2.570268	-0.991562
	1	-1.180353	2.529544	0.768225

$H_2O\cdots NH_3\cdots Me_2CO\_E^*$				
	6	3.635460	-0.619124	0.133634
	8	2.669750	-0.021693	-0.642312
	6	4.985376	-0.609786	-0.580781
	6	3.229853	-2.018872	0.570241
	1	3.999790	-2.488663	1.189849
	1	2.290828	-1.990050	1.133180
	1	3.074792	-2.633113	-0.320519
	1	5.264851	0.416636	-0.837711
	1	5.780796	-1.058274	0.023504
	1	4.887877	-1.175710	-1.509260
	7	3.810737	0.270625	1.382339
	1	3.701326	1.388877	0.891338
	1	4.684077	0.087998	1.877710
	1	3.036448	0.122326	2.032930
	8	3.226093	2.195547	-0.000021
	1	3.887294	2.697287	-0.498377
	1	2.916709	1.221153	-0.554153
	6	-2.915226	-0.884943	0.009486
	6	-1.944368	0.095992	-0.030062
	7	-2.635320	1.261012	0.109434
	7	-3.926180	1.085647	0.231261
	7	-4.087149	-0.210584	0.170559
	53	0.169651	-0.025882	-0.280009
	6	-2.099239	2.622327	0.117893
	6	-5.431072	-0.774404	0.275233
	6	-2.831590	-2.366583	-0.094746
	1	-2.936978	3.299096	0.274910
	1	-1.371987	2.712714	0.925394
	1	-1.617501	2.818834	-0.840845
	1	-6.124795	0.055517	0.396780
	1	-5.659684	-1.328604	-0.636207
	1	-5.475866	-1.436025	1.141487
	1	-1.790137	-2.659671	-0.236707
	1	-3.409609	-2.734790	-0.947851
	1	-3.206245	-2.849172	0.813147
$H_2O\cdots NH_3\cdots Me_2CO\_F^*$				
	6	3.833387	0.519999	-0.004944
	8	2.835486	-0.202420	0.595743
	6	5.185736	0.243037	0.650449
	6	3.516810	2.007406	-0.051293
	1	4.313041	2.575808	-0.541961
	1	2.574438	2.184945	-0.579819
	1	3.404541	2.374059	0.972096
	1	5.400476	-0.829700	0.624555
	1	6.004948	0.785518	0.166836
	1	5.129190	0.551577	1.696197
	7	3.950823	-0.014878	-1.452955
	1	3.796168	-1.201757	-1.271350
	1	4.824007	0.254683	-1.906930

	1	3.171929	0.331659	-2.017064
	8	3.285237	-2.207889	-0.598342
	1	3.932206	-2.833496	-0.242284
	1	3.015380	-1.385363	0.185066
	6	-2.722249	-0.909241	0.059398
	6	-1.812983	0.158901	0.044695
	7	-2.494829	1.298745	-0.115721
	7	-3.754204	0.979467	-0.198972
	7	-3.932826	-0.343103	-0.092787
	53	0.299977	0.080661	0.274649
	6	-2.507009	-2.374059	0.203167
	6	-5.254057	-0.960746	-0.159313
	6	-4.833212	1.947148	-0.349815
	1	-2.986348	-2.759189	1.108500
	1	-2.892476	-2.920450	-0.662897
	1	-1.435240	-2.564590	0.278469
	1	-5.683634	-0.815307	-1.152326
	1	-5.125791	-2.025144	0.030574
	1	-5.901026	-0.531173	0.607438
	1	-5.419965	1.717196	-1.241051
	1	-5.463695	1.949150	0.541810
	1	-4.344002	2.912706	-0.462499
$H_2O\cdots NH_3\cdots Me_2CO$_G*				
	6	3.666274	0.375705	-0.129763
	8	2.642050	-0.147953	0.625413
	6	4.994445	0.274323	0.617445
	6	3.370847	1.798299	-0.579670
	1	4.186921	2.210456	-1.180832
	1	2.446345	1.832662	-1.165773
	1	3.236966	2.425968	0.305202
	1	5.197114	-0.768166	0.882194
	1	5.832867	0.665400	0.031600
	1	4.914286	0.848352	1.542572
	7	3.807474	-0.530125	-1.370812
	1	3.594977	-1.635178	-0.883224
	1	4.708139	-0.419563	-1.837831
	1	3.069524	-0.322819	-2.047006
	8	3.038273	-2.401968	-0.003607
	1	3.652857	-2.948676	0.507075
	1	2.794518	-1.403083	0.542745
	6	-1.953606	0.233750	0.032447
	6	-2.772874	1.372544	-0.052612
	7	-4.044519	0.984029	-0.181937
	7	-4.042797	-0.317546	-0.180069
	7	-2.799237	-0.805298	-0.051614
	53	0.159114	0.110331	0.270637
	6	-2.540782	-2.242512	-0.015332
	6	-5.245467	-1.132269	-0.289054
	6	-2.371960	2.807225	-0.010350
	1	-2.878151	-2.699640	-0.947293

	1	-1.465377	-2.375918	0.091603
	1	-3.052288	-2.686081	0.840811
	1	-5.190924	-1.768070	-1.174869
	1	-5.374948	-1.734302	0.612706
	1	-6.067132	-0.425311	-0.386979
	1	-1.711862	3.048716	-0.848057
	1	-3.260097	3.437611	-0.067457
	1	-1.837088	3.029684	0.916951
$H_2O\cdots NH_3\cdots Me_2CO\_H^*$				
	6	-3.773482	-0.477312	0.189817
	8	-2.768233	0.428783	0.442647
	6	-5.102246	0.020908	0.755825
	6	-3.429823	-1.871606	0.692226
	1	-4.238424	-2.581100	0.491966
	1	-2.512279	-2.240640	0.222561
	1	-3.264490	-1.826075	1.771665
	1	-5.341250	1.003931	0.338512
	1	-5.928023	-0.667826	0.549211
	1	-4.996621	0.128384	1.837119
	7	-3.953777	-0.518605	-1.341229
	1	-3.803156	0.667248	-1.626746
	1	-4.842361	-0.934382	-1.622162
	1	-3.198454	-1.056288	-1.771953
	8	-3.289626	1.827959	-1.404908
	1	-3.930199	2.546453	-1.302225
	1	-2.982867	1.371604	-0.379616
	7	2.443191	-1.311977	-0.274948
	7	3.760546	-0.985285	-0.296723
	6	3.955662	0.296970	-0.024609
	7	2.732662	0.818596	0.178710
	6	1.817777	-0.203210	0.018041
	53	-0.293176	0.023275	0.223556
	6	5.256279	1.013539	0.040178
	6	4.758419	-2.010202	-0.595842
	6	2.418731	2.206780	0.513573
	1	5.398752	1.460635	1.027960
	1	6.078858	0.322036	-0.146352
	1	5.294979	1.806756	-0.712253
	1	5.320520	-1.733860	-1.489009
	1	5.427852	-2.138657	0.256121
	1	4.206376	-2.930693	-0.775132
	1	3.341210	2.785968	0.524099
	1	1.737989	2.611211	-0.236749
	1	1.946535	2.243482	1.496675
$H_2O\cdots NH_3\cdots Me_2CO\_I^*$				
	6	-3.478375	0.111404	0.598769
	8	-2.538314	-0.482323	-0.228510
	6	-3.623191	1.606878	0.319281
	6	-3.185578	-0.172857	2.065859
	1	-3.992605	0.184368	2.713053

	1	-3.050024	-1.248491	2.214294
	1	-2.263379	0.333008	2.365898
	1	-3.882190	1.770573	-0.731658
	1	-4.381925	2.079183	0.951382
	1	-2.664273	2.095011	0.512884
	7	-4.807532	-0.533046	0.216184
	1	-4.699384	-0.608617	-1.051010
	1	-5.609782	-0.018708	0.580906
	1	-4.844130	-1.486777	0.582844
	8	-4.015789	-0.734084	-2.074565
	1	-4.108879	-0.009933	-2.710893
	1	-3.118793	-0.589744	-1.385015
	7	4.028625	1.103874	-0.074611
	7	2.690805	1.313616	-0.140363
	6	1.996249	0.186443	-0.049581
	7	2.921838	-0.788660	0.075657
	6	4.161379	-0.186902	0.055476
	53	-0.136221	-0.097259	-0.093962
	6	2.202286	2.680821	-0.268804
	6	5.460188	-0.903276	0.164131
	6	2.641321	-2.218296	0.195210
	1	2.771352	3.169616	-1.058797
	1	2.350945	3.203393	0.677124
	1	1.144531	2.651634	-0.525084
	1	6.261237	-0.166190	0.104287
	1	5.583526	-1.623392	-0.649560
	1	5.540049	-1.432510	1.117890
	1	2.029193	-2.399477	1.080080
	1	2.116841	-2.565682	-0.696376
	1	3.588402	-2.747075	0.292247
$H_2O\cdots NH_3\cdots Me_2CO$_J*				
	6	3.765977	-0.455209	-0.271777
	8	2.767837	0.490936	-0.358432
	6	5.084103	0.105120	-0.803497
	6	3.385704	-1.757536	-0.960626
	1	4.193335	-2.493400	-0.899960
	1	2.483926	-2.187844	-0.513015
	1	3.178593	-1.552729	-2.014092
	1	5.350438	1.016846	-0.259939
	1	5.905024	-0.614742	-0.721041
	1	4.948445	0.364247	-1.855296
	7	3.991313	-0.721095	1.228621
	1	3.865185	0.416871	1.690947
	1	4.882351	-1.181300	1.416839
	1	3.242883	-1.309805	1.600664
	8	3.368466	1.598254	1.655715
	1	4.021056	2.312984	1.635749
	1	3.020619	1.302076	0.588879
	7	-2.726875	0.785247	-0.189065
	7	-3.948782	0.214710	0.011002

	6	-3.719772	-1.073608	0.312834
	7	-2.415477	-1.331043	0.306492
	6	-1.811635	-0.180437	-0.005460
	53	0.301749	0.079822	-0.184618
	6	-5.196333	0.957863	-0.086931
	6	-4.793548	-2.059738	0.611330
	6	-2.579825	2.186698	-0.556644
	1	-6.006838	0.251386	0.088318
	1	-5.230701	1.742085	0.672339
	1	-5.303012	1.386322	-1.085278
	1	-4.319561	-3.022682	0.799122
	1	-5.363802	-1.767389	1.497847
	1	-5.482114	-2.163400	-0.232204
	1	-3.041062	2.369554	-1.529395
	1	-3.025526	2.823421	0.209935
	1	-1.511663	2.389753	-0.618677
$H_2O\cdots NH_3\cdots Me_2CO$_K*				
	6	3.326092	-0.628655	0.290240
	8	2.426989	0.393279	0.025493
	6	3.420642	-1.623095	-0.865876
	6	3.013402	-1.312866	1.613723
	1	3.794006	-2.028707	1.889265
	1	2.912492	-0.562238	2.403545
	1	2.067854	-1.856791	1.535659
	1	3.688289	-1.101149	-1.790130
	1	4.155119	-2.412712	-0.677468
	1	2.443943	-2.091933	-1.010906
	7	4.685077	0.058709	0.384456
	1	4.603023	0.912399	-0.557089
	1	5.460023	-0.603471	0.340427
	1	4.750118	0.571155	1.266728
	8	3.945233	1.676053	-1.276335
	1	4.025342	1.494644	-2.224371
	1	3.028967	1.170550	-0.817981
	7	-4.245147	0.518985	0.144658
	7	-4.094947	-0.706125	-0.224311
	7	-2.838159	-1.110063	-0.351984
	6	-2.124704	-0.041586	-0.033395
	7	-3.009712	0.949424	0.268252
	53	0.021087	0.124217	0.004906
	6	-2.736286	2.327322	0.678455
	6	-5.232931	-1.586530	-0.488860
	1	-2.146371	2.310625	1.595354
	1	-3.695336	2.813931	0.845673
	1	-2.183273	2.827848	-0.117125
	1	-5.194811	-1.885707	-1.536032
	1	-5.143611	-2.457270	0.159882
	1	-6.138209	-1.023356	-0.271906
$H_2O\cdots NH_3\cdots Me_2CO$_L*				
	6	3.485630	-0.351402	-0.344754

	8	2.446183	0.565167	-0.369689
	6	4.746909	0.280727	-0.929557
	6	3.125468	-1.649224	-1.052089
	1	3.969541	-2.345202	-1.054557
	1	2.272242	-2.136981	-0.570057
	1	2.854395	-1.427414	-2.087532
	1	5.002136	1.191494	-0.379086
	1	5.601505	-0.403025	-0.905356
	1	4.546669	0.555822	-1.966839
	7	3.787168	-0.634499	1.130807
	1	3.625974	0.514543	1.636044
	1	4.705779	-1.058196	1.264399
	1	3.087551	-1.268863	1.522593
	8	3.093666	1.642357	1.645815
	1	3.717824	2.382795	1.629846
	1	2.711661	1.371161	0.593211
	7	-4.154674	-0.231805	0.168615
	7	-3.835235	-1.329426	0.780502
	7	-2.532645	-1.432132	0.791997
	6	-2.016043	-0.360616	0.164980
	7	-3.044089	0.404713	-0.233872
	53	0.082165	0.031805	-0.110454
	6	-3.076152	1.679433	-0.946863
	6	-5.524584	0.224429	-0.041908
	1	-3.509380	2.448105	-0.304480
	1	-3.648933	1.569185	-1.869161
	1	-2.044015	1.934751	-1.183526
	1	-6.158011	-0.524626	0.431090
	1	-5.734235	0.276801	-1.111607
	1	-5.665282	1.195773	0.434867
$H_2O\cdots NH_3\cdots Me_2CO$_M*				
	6	3.173781	0.136545	-0.618944
	8	2.232584	-0.268361	0.323456
	6	3.422796	1.641438	-0.549203
	6	2.793230	-0.319798	-2.020929
	1	3.595268	-0.114625	-2.736294
	1	2.578479	-1.393015	-2.018152
	1	1.898142	0.209832	-2.359092
	1	3.742094	1.923876	0.459027
	1	4.178868	1.972585	-1.268045
	1	2.488761	2.165167	-0.768841
	7	4.466822	-0.544163	-0.198535
	1	4.403303	-0.460617	1.103564
	1	5.283281	-0.132633	-0.651450
	1	4.431917	-1.535096	-0.447767
	8	3.769201	-0.419620	2.129510
	1	3.950888	0.357893	2.678850
	1	2.857050	-0.283358	1.476965
	7	-4.365846	0.749412	-0.024203
	7	-4.423411	-0.512366	-0.114135

	7	-3.159977	-0.985648	-0.088807
	6	-2.283949	0.014720	0.020859
	7	-3.063838	1.096880	0.060045
	53	-0.120325	-0.101043	0.119827
	6	-2.906193	-2.422328	-0.168598
	6	-2.677509	2.500273	0.179636
	1	-2.285043	-2.630613	-1.040371
	1	-3.876239	-2.906601	-0.267605
	1	-2.406027	-2.751376	0.743045
	1	-3.598777	3.080185	0.194789
	1	-2.122490	2.642555	1.107685
	1	-2.065729	2.781054	-0.678339
$H_2O\cdots NH_3\cdots Me_2CO\_N$*				
	6	-3.615284	-0.401233	-0.395873
	8	-2.622221	-0.187084	0.533162
	6	-4.860983	-0.981028	0.272401
	6	-3.141775	-1.263859	-1.556783
	1	-3.941225	-1.432764	-2.284615
	1	-2.294300	-0.793550	-2.066259
	1	-2.812374	-2.231520	-1.169163
	1	-5.201380	-0.315926	1.072224
	1	-5.679934	-1.136877	-0.437602
	1	-4.596519	-1.940838	0.720506
	7	-4.025328	0.983627	-0.929525
	1	-3.964118	1.665626	0.109026
	1	-4.927972	0.969750	-1.404895
	1	-3.323178	1.331271	-1.585839
	8	-3.468018	1.914633	1.251099
	1	-4.105147	1.947700	1.979252
	1	-2.983667	0.873751	1.157865
	7	3.895825	0.624667	-0.434269
	7	3.992507	-0.504949	0.243017
	7	2.808856	-0.945467	0.551010
	6	1.963068	-0.033389	0.032646
	7	2.645631	0.950003	-0.585524
	53	-0.166655	-0.125469	0.202583
	6	5.028289	1.404578	-0.934362
	6	5.247965	-1.167274	0.597393
	1	4.591620	2.256434	-1.451872
	1	5.637056	1.739953	-0.092926
	1	5.612876	0.794823	-1.625257
	1	4.962878	-2.061501	1.148095
	1	5.842814	-0.504417	1.227955
	1	5.787108	-1.434355	-0.313000

Table S5. Calculated values of imaginary frequencies (in cm^{-1}) for transition states for hydrolysis of methyl chloride (**TS1**) and coupling of ammonia and acetone (**TS2**) catalyzed by **A***–**N***.

Azolium type	**TS1**	**TS2**
A*	-51.3988	-1205.2608
B*	-117.6285	-1236.7927
C*	-308.7479	-1254.0305
D*	-207.9582	-1230.5528
E*	-291.9048	-1252.8315
F*	-42.8155	-1217.9588
G*	-301.2924	-1253.4887
H*	-188.7565	-1246.9556
I*	-372.2699	-1261.7826
J*	-233.9233	-1250.0144
K*	-355.7278	-1273.9175
L*	-356.3155	-1287.5163
M*	-425.9872	-1240.9418
N*	-215.9592	-1241.8391