Supporting Information

HUSY zeolite-promoted reactions of trifluoromethylated propargyl alcohols with arenes: synthesis of CF_3-indenes and DFT study of intermediate carbocations

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1. Copies of ^{1}H, ^{13}C, ^{19}F NMR spectra of compounds 1, 2

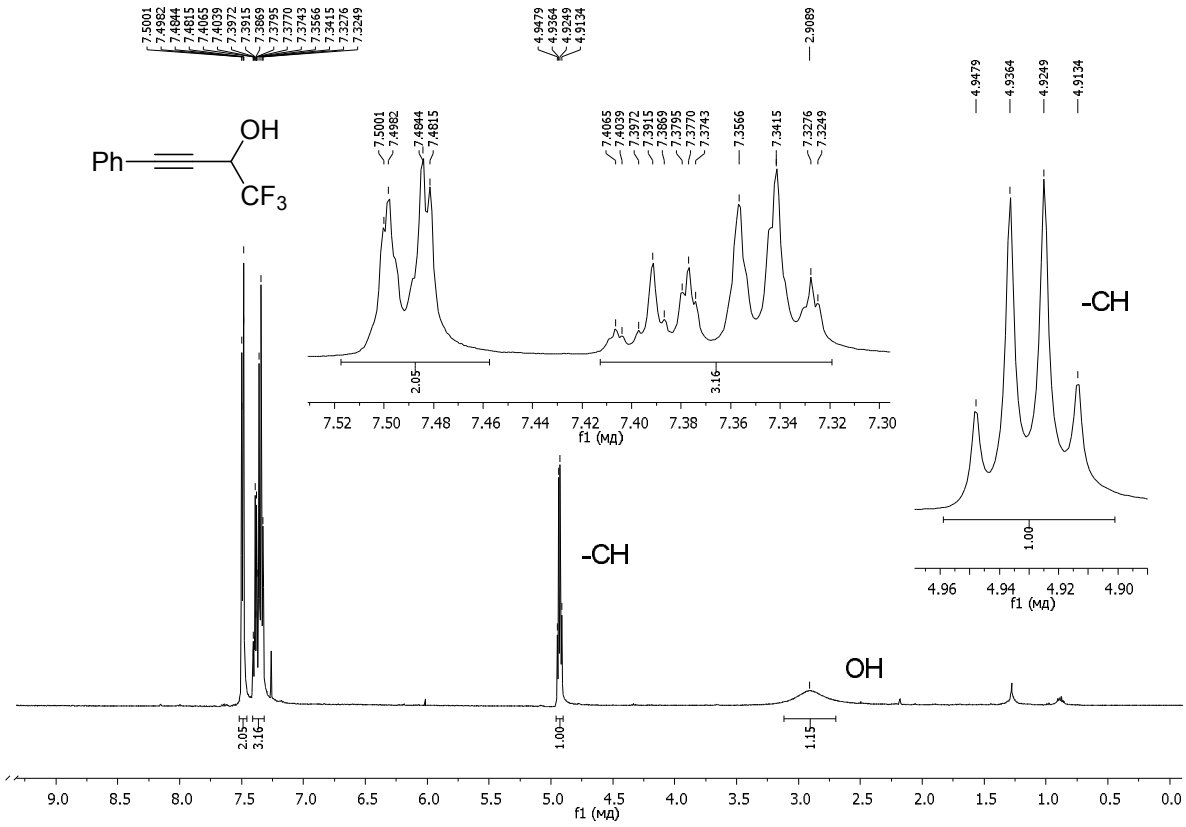


Figure S1. ^{1}H NMR spectrum of compound **1a** (500 MHz, $CDCl_3$).

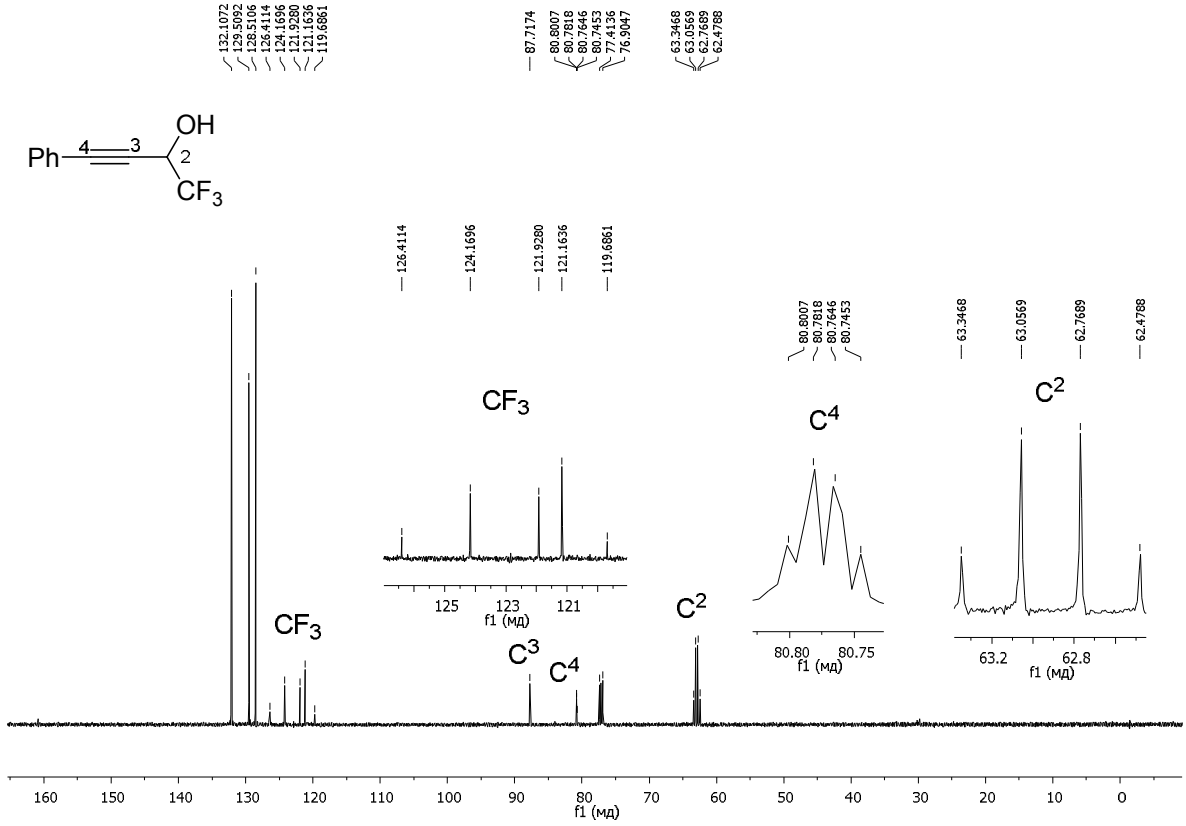


Figure S2. ^{13}C NMR spectrum of compound **1a** (125 MHz, $CDCl_3$).

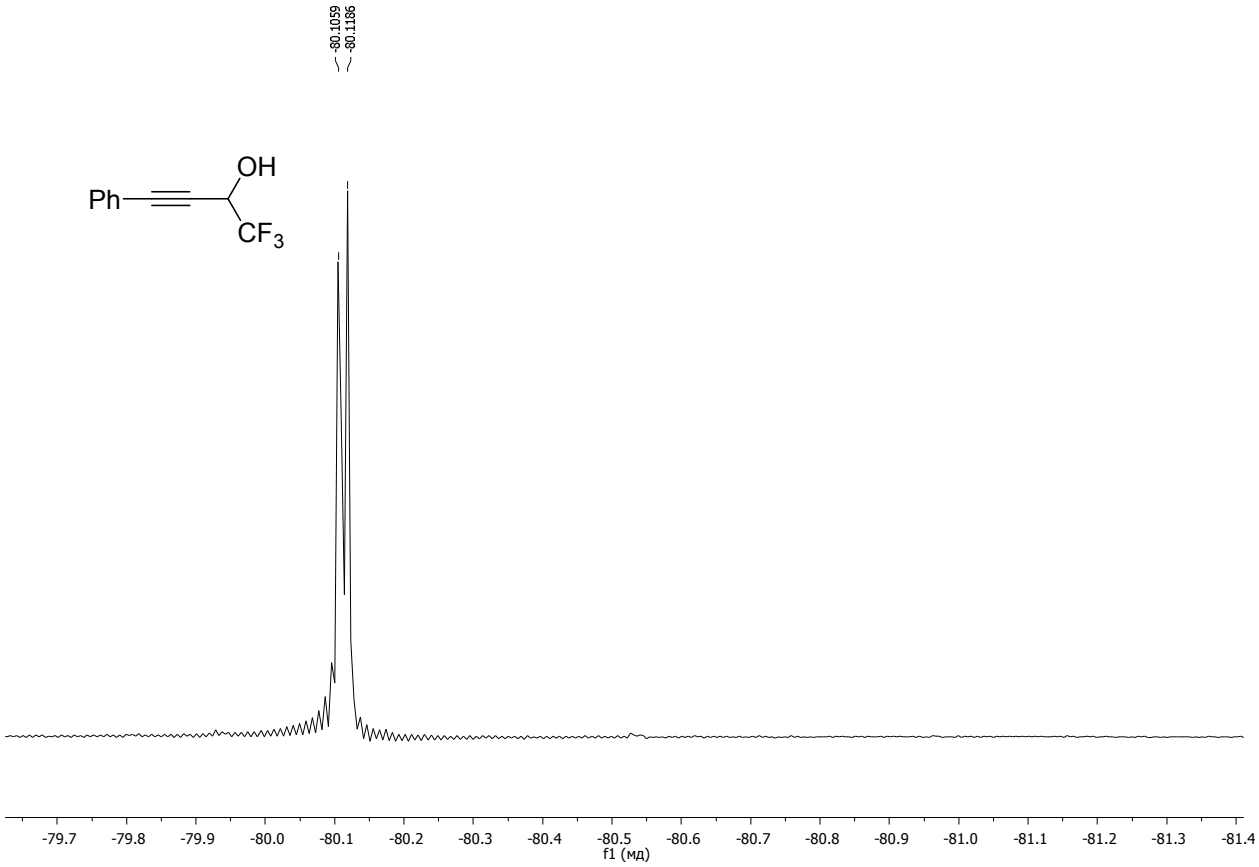


Figure S3. ^{19}F NMR spectrum of compound **1a** (470 MHz, $CDCl_3$).

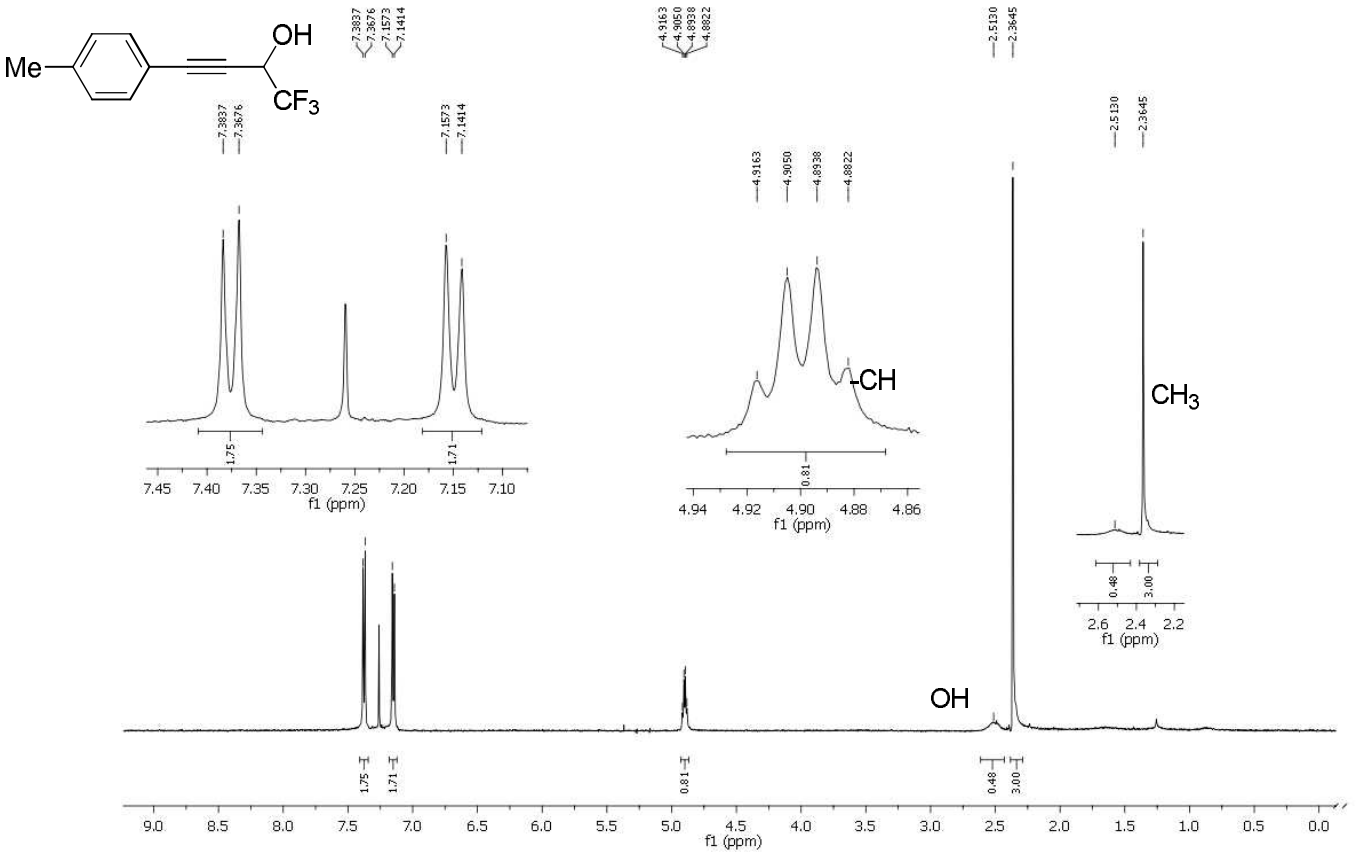


Figure S4. ^{1}H NMR spectrum of compound **1b** (500 MHz, $CDCl_3$).

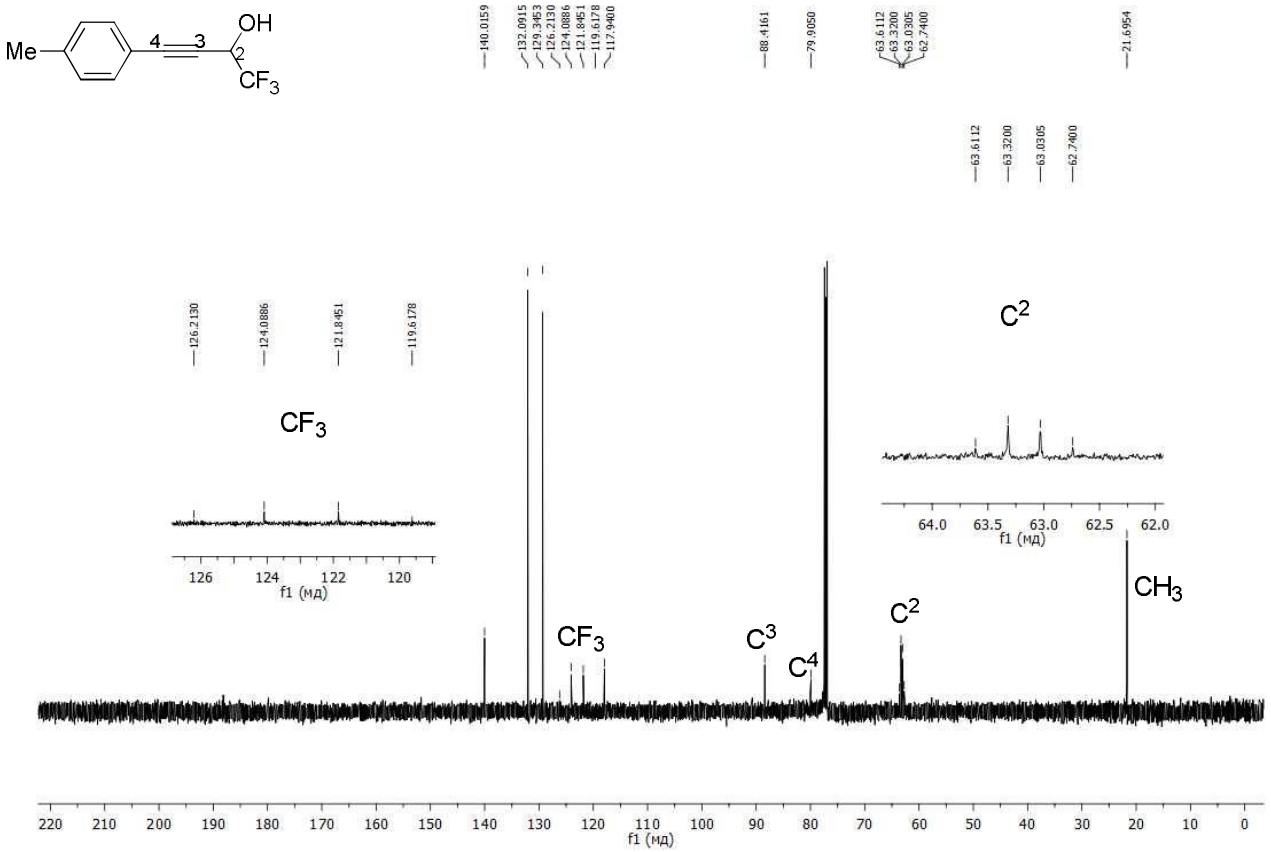


Figure S5. ^{13}C NMR spectrum of compound **1b** (125 MHz, $CDCl_3$).

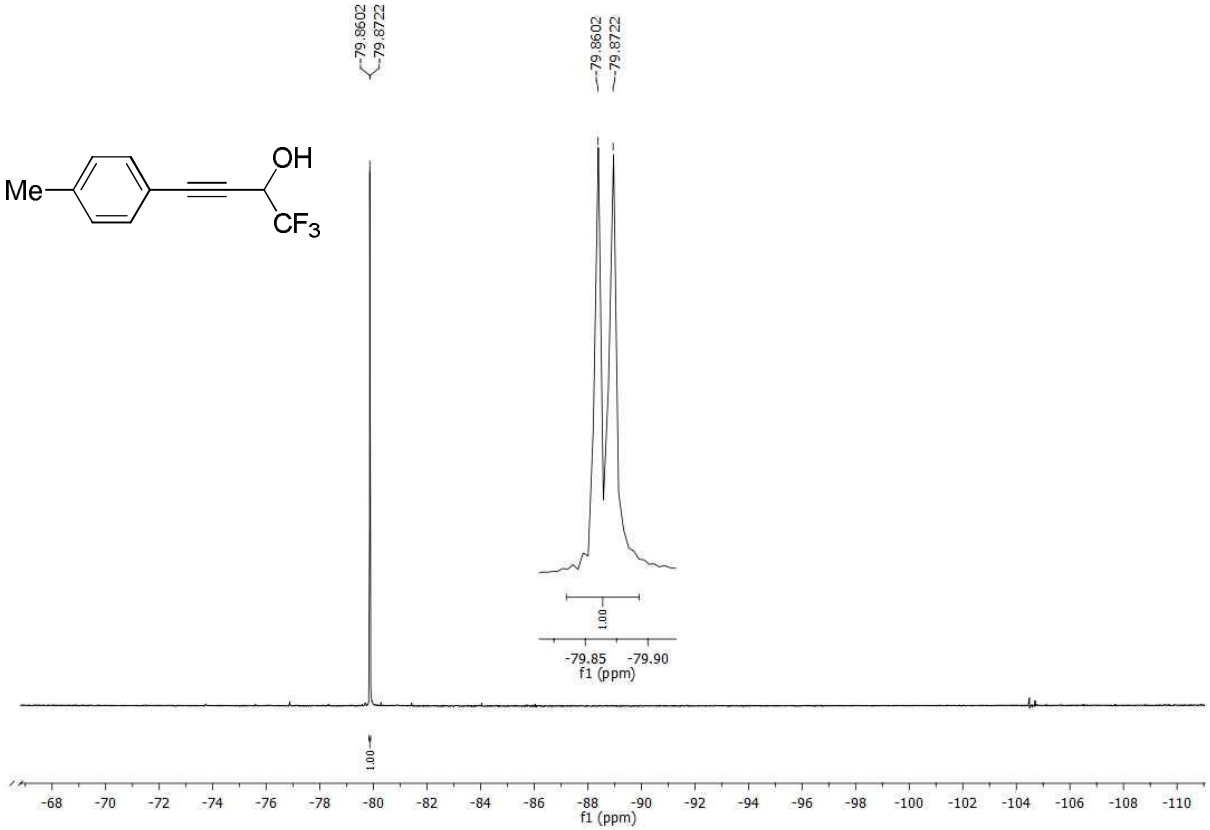


Figure S6. ^{19}F NMR spectrum of compound **1b** (470 MHz, $CDCl_3$).

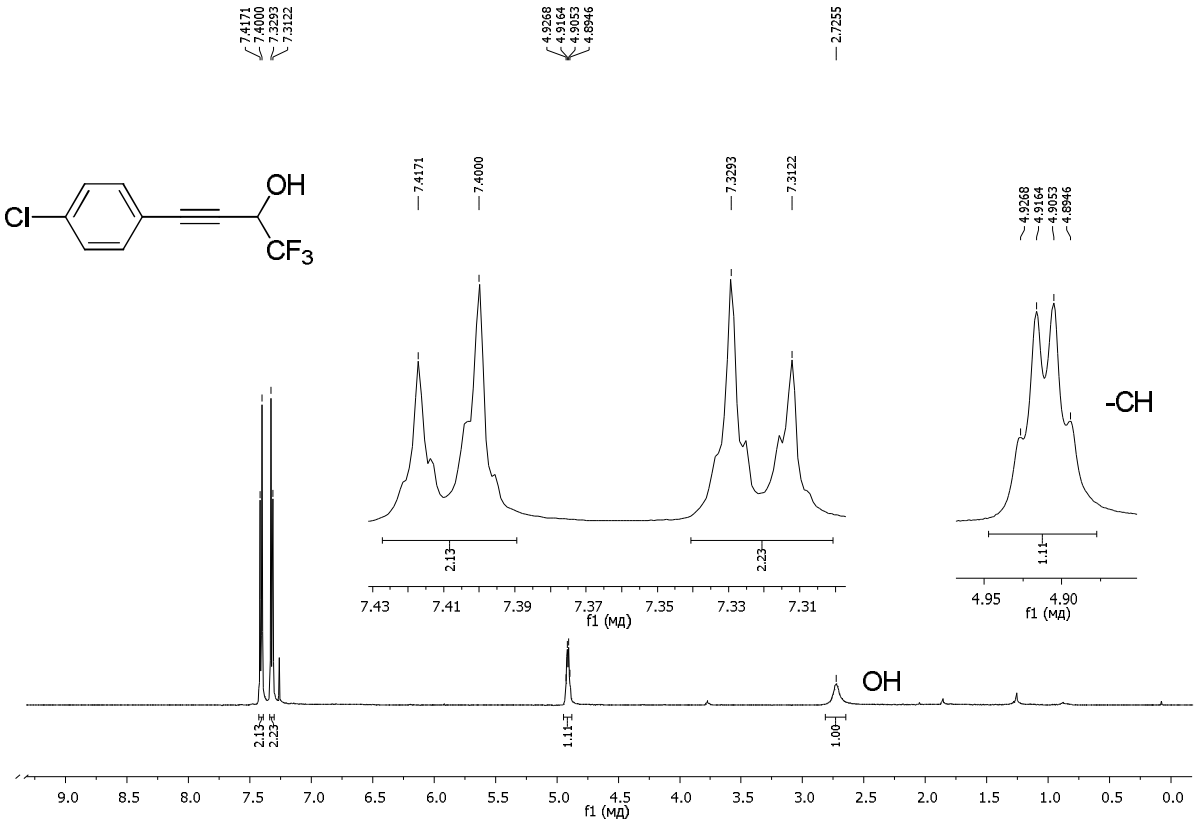


Figure S7. ^{1}H NMR spectrum of compound **1c** (500 MHz, $CDCl_3$).

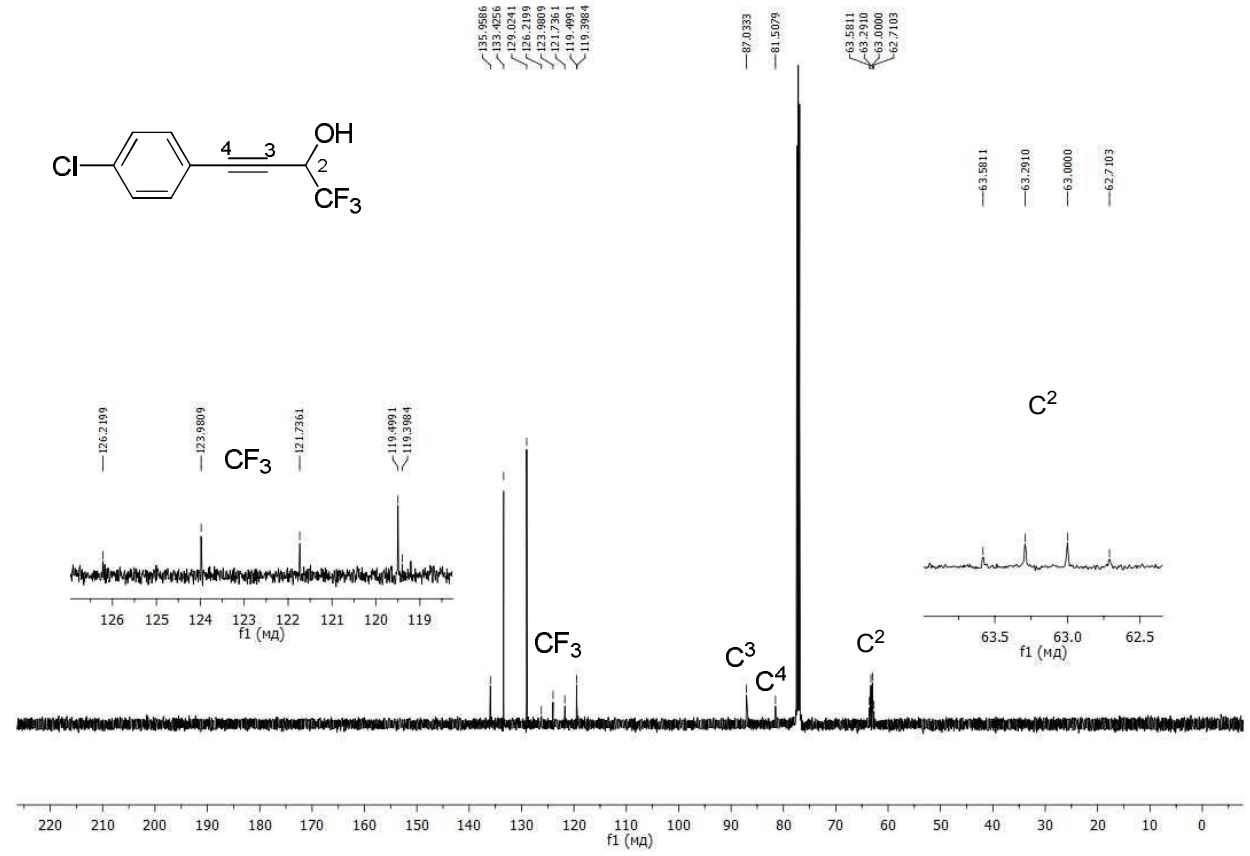


Figure S8. ^{13}C NMR spectrum of compound **1c** (125 MHz, $CDCl_3$).

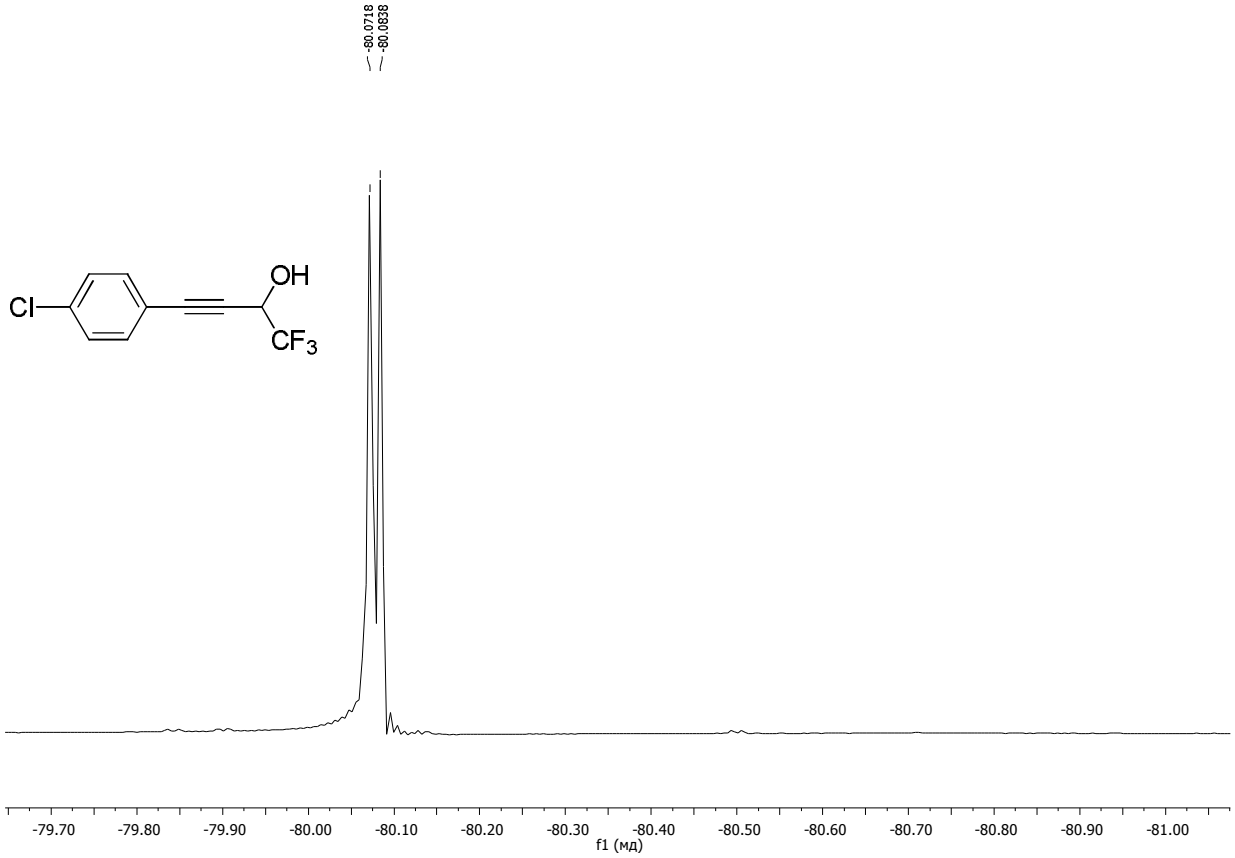


Figure S9. ^{19}F NMR spectrum of compound **1c** (470 MHz, $CDCl_3$).

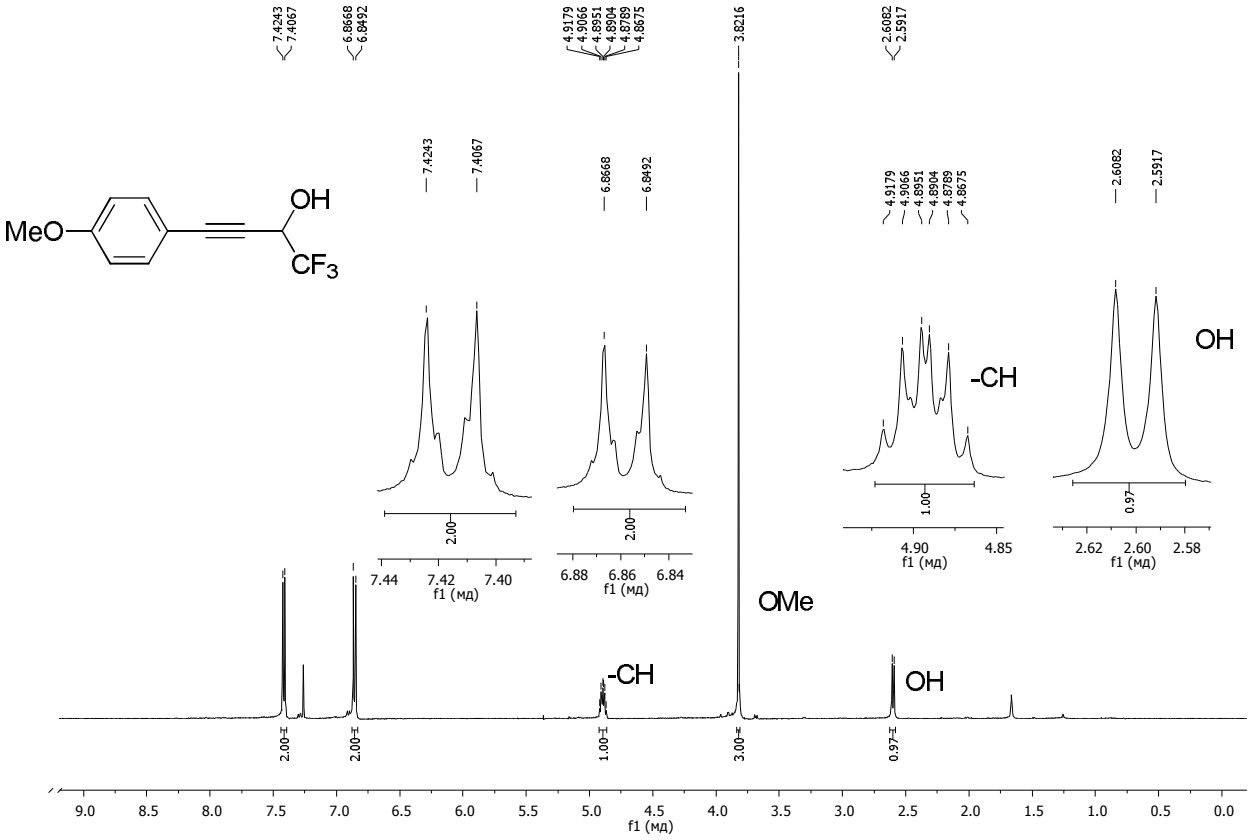


Figure S10. ^{1}H NMR spectrum of compound **1d** (500 MHz, $CDCl_3$).

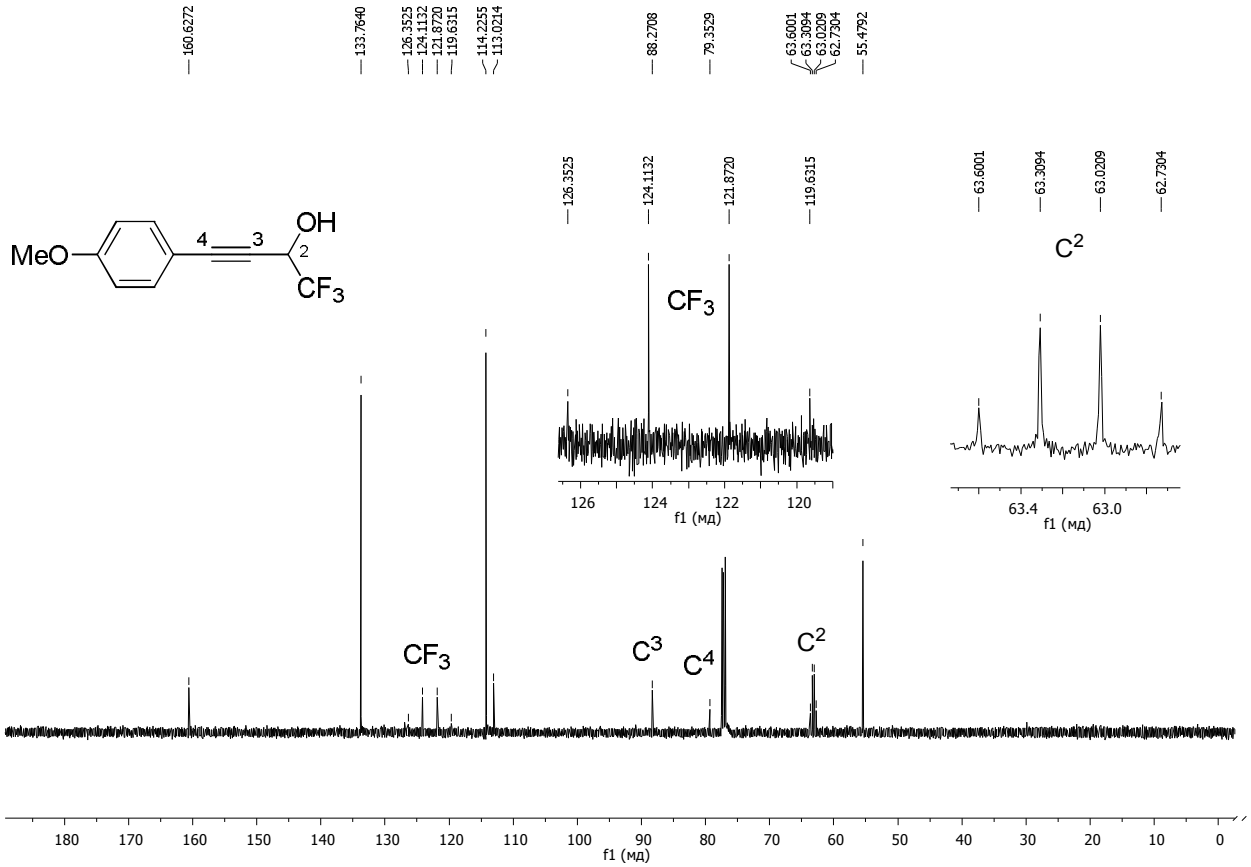


Figure S11. ^{13}C NMR spectrum of compound **1d** (125 MHz, $CDCl_3$).

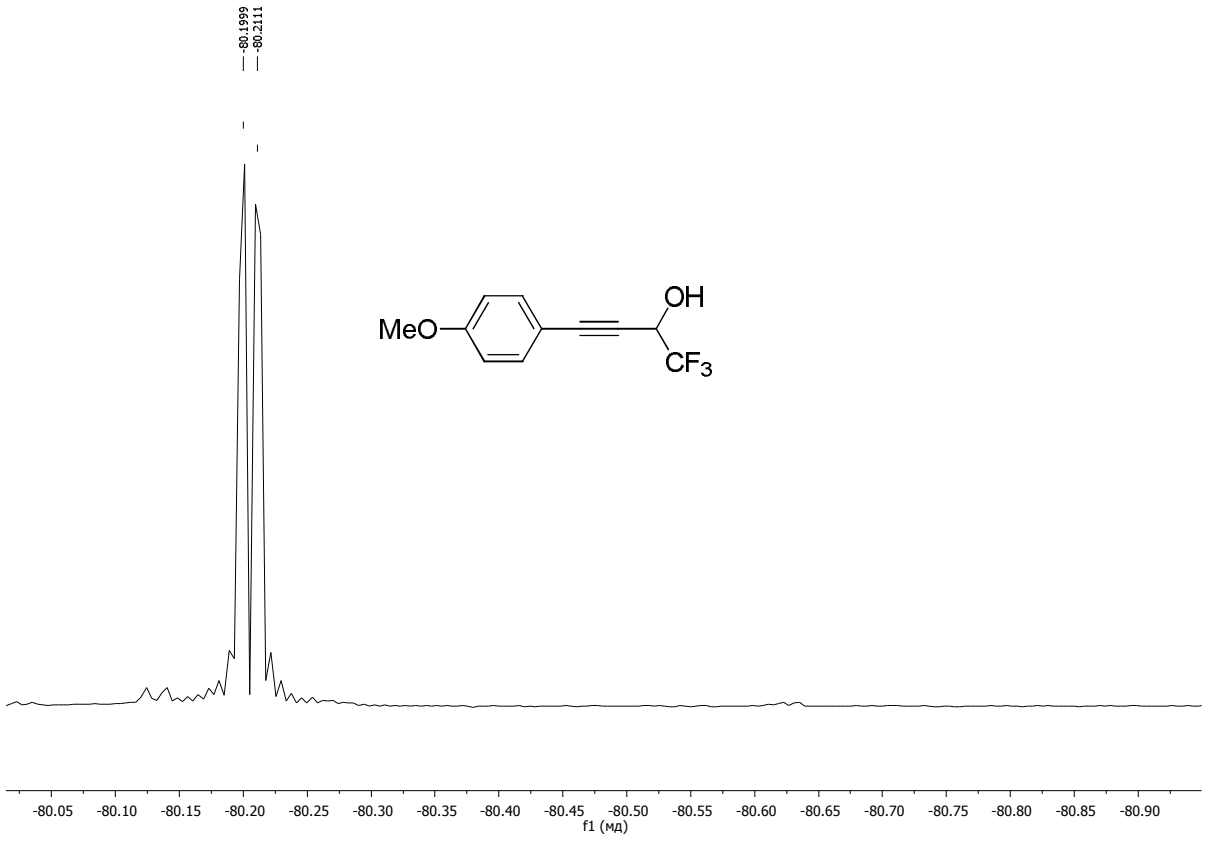


Figure S12. ^{19}F NMR spectrum of compound **1d** (470 MHz, $CDCl_3$).

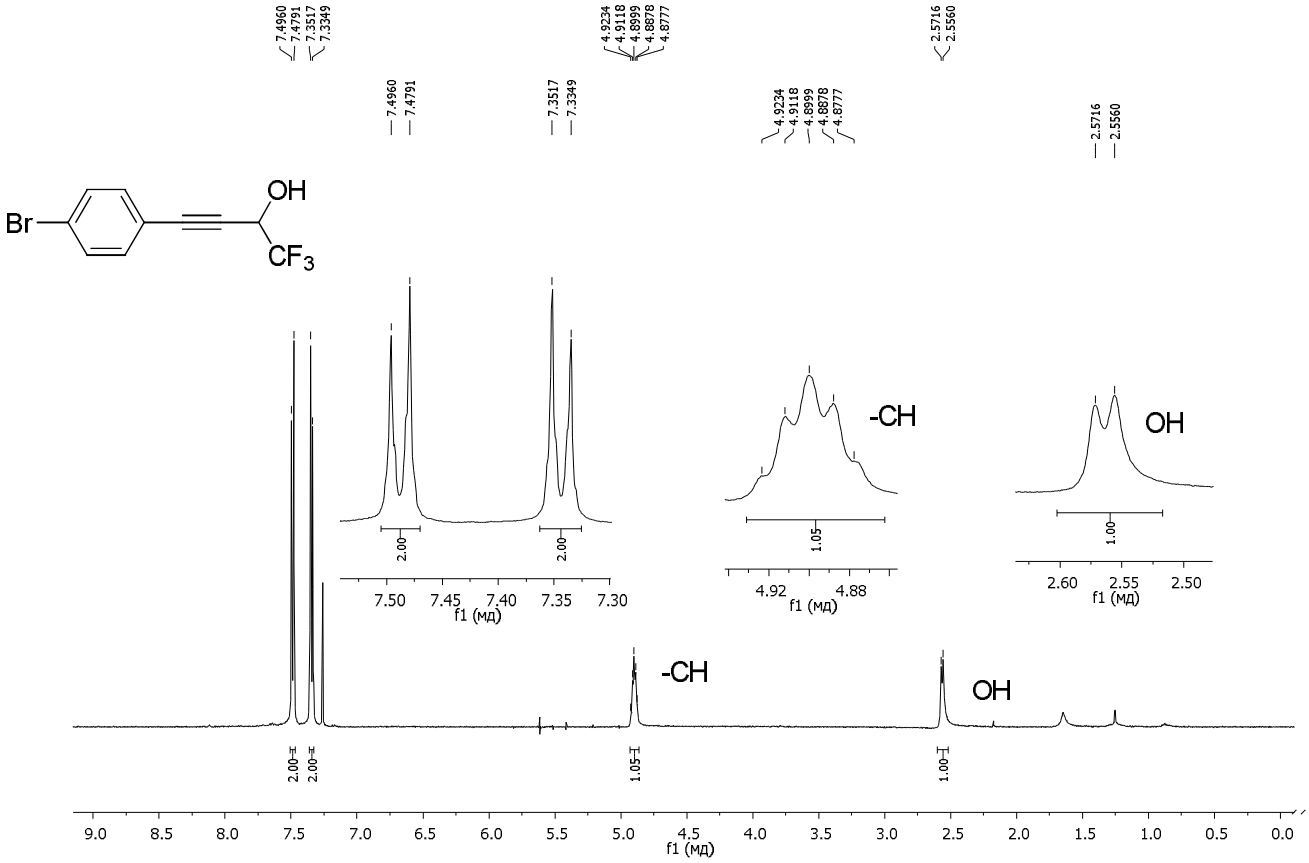


Figure S13. ^{1}H NMR spectrum of compound **1e** (500 MHz, $CDCl_3$).

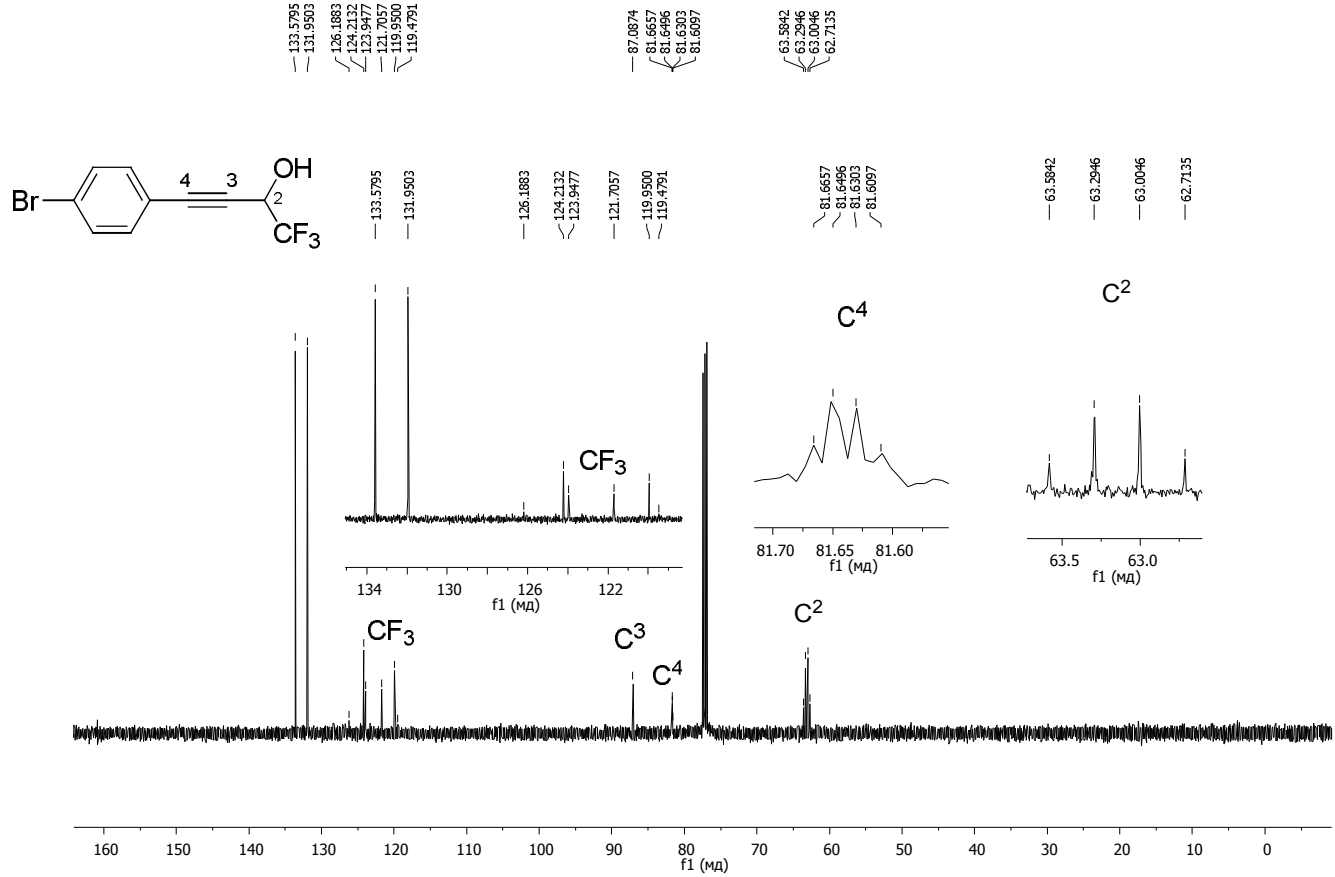


Figure S14. ^{13}C NMR spectrum of compound **1e** (125 MHz, $CDCl_3$).

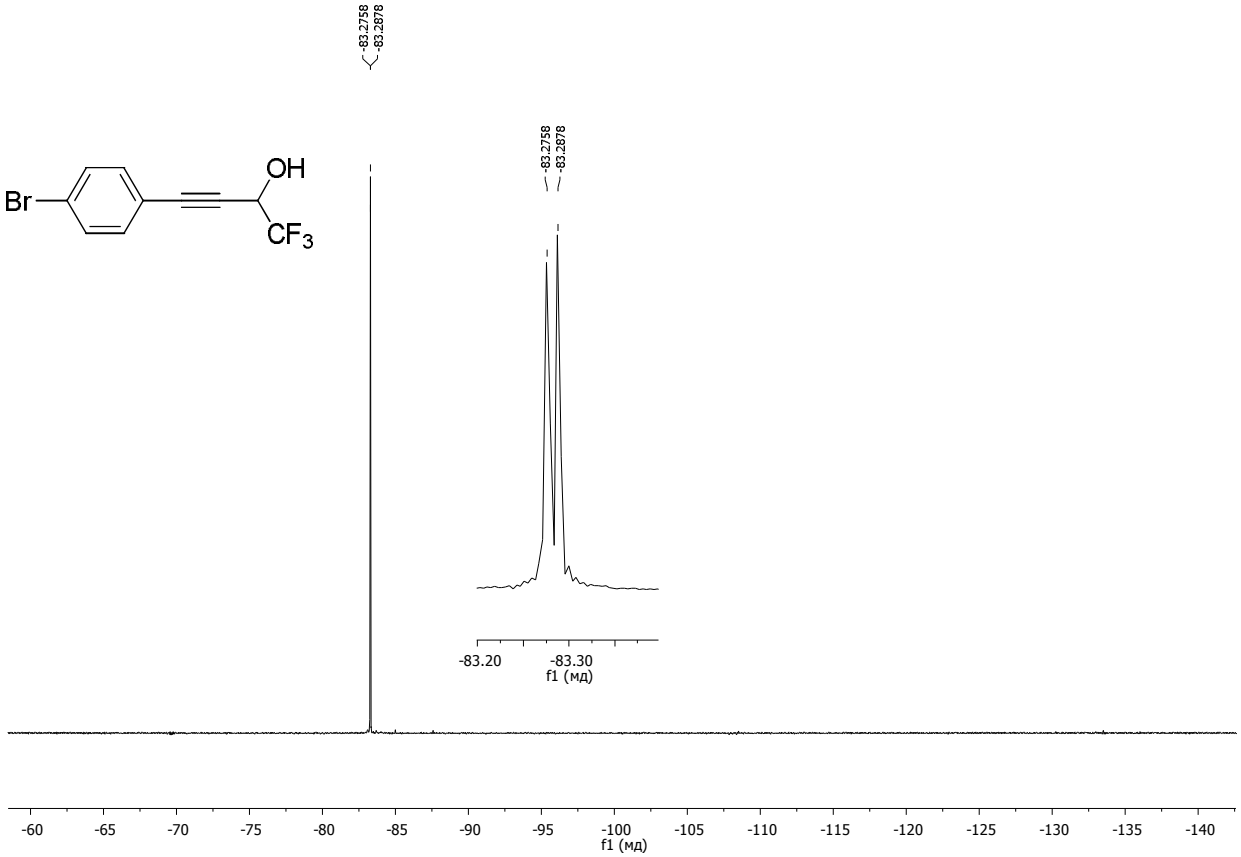


Figure S15. ^{19}F NMR spectrum of compound **1e** (470 MHz, $CDCl_3$).

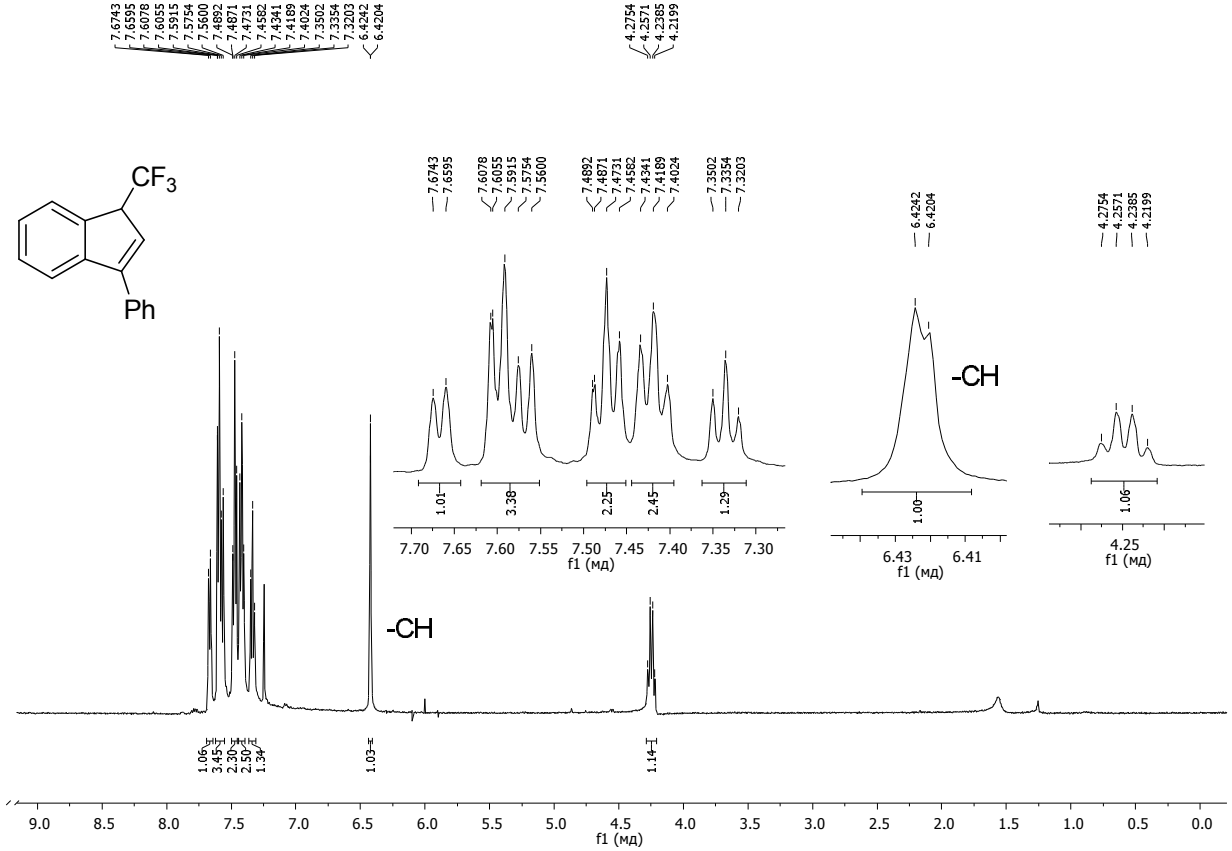


Figure S16. ^{1}H NMR spectrum of compound **2a** (500 MHz, $CDCl_3$).

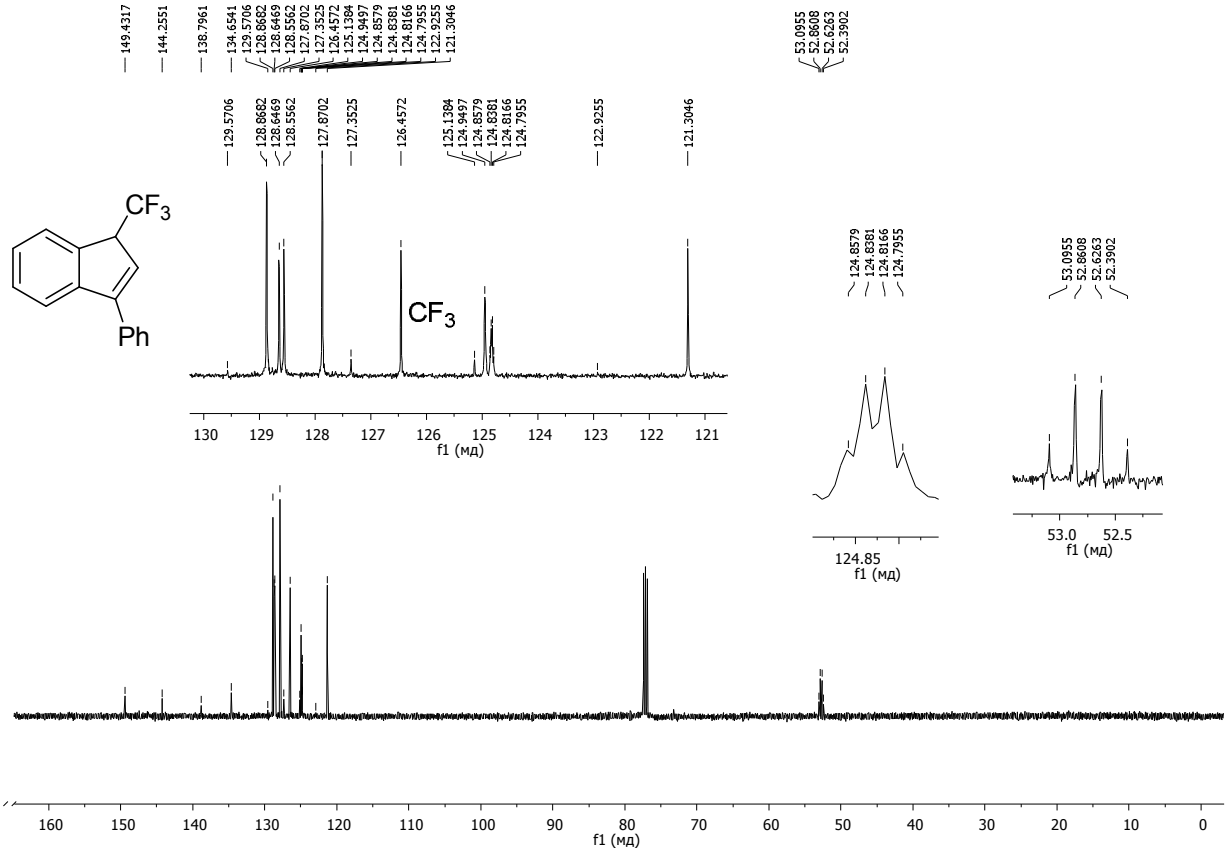


Figure S17. ^{13}C NMR spectrum of compound **2a** (125 MHz, $CDCl_3$).

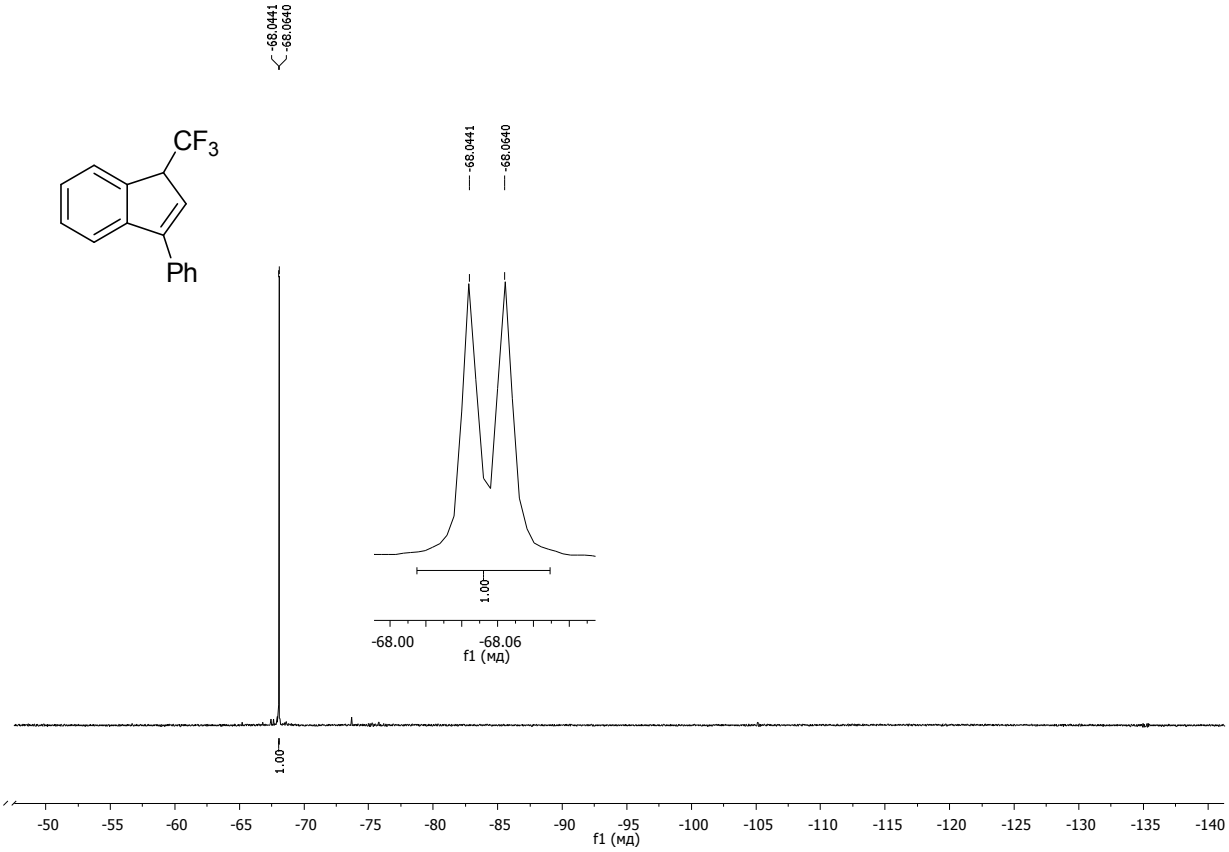


Figure S18. ^{19}F NMR spectrum of compound **2a** (470 MHz, $CDCl_3$).

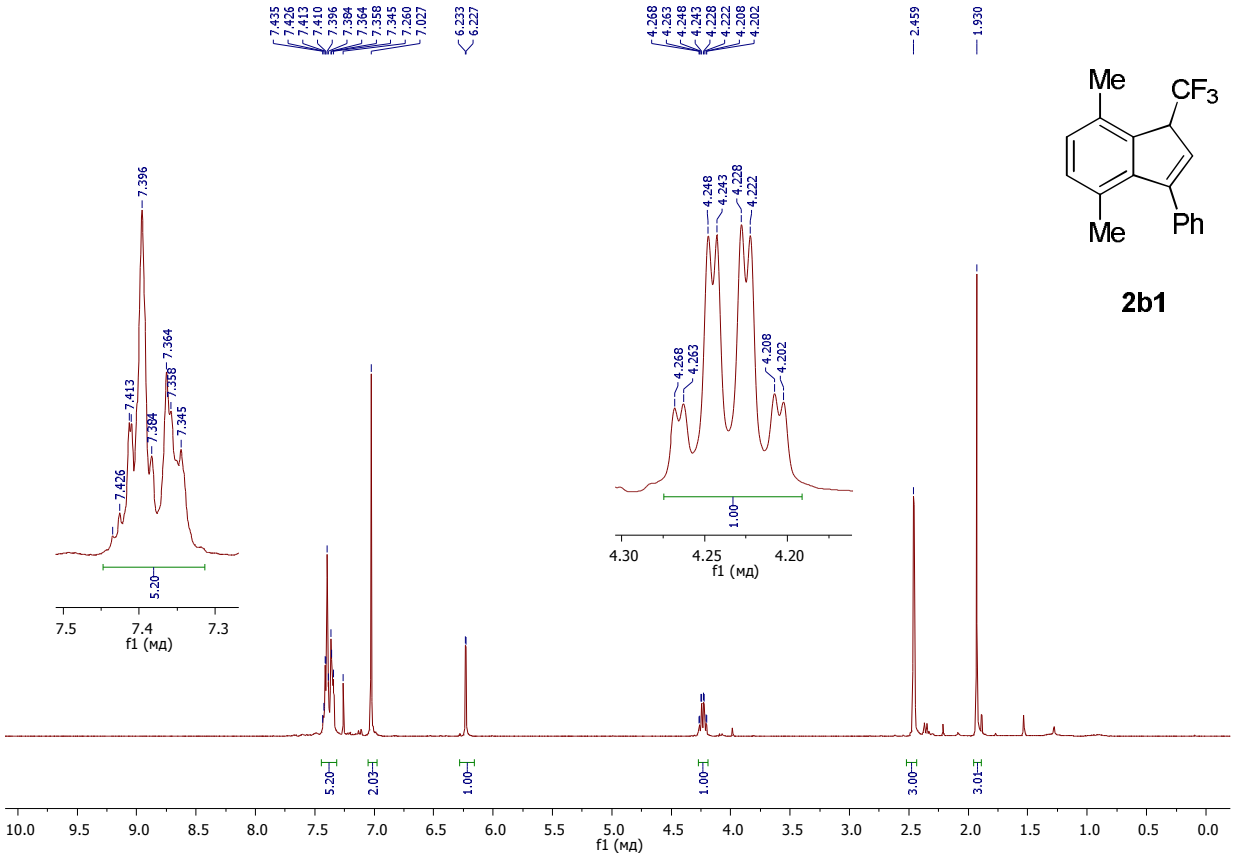


Figure S19. ^{1}H NMR spectrum of mixture of isomers **2b1** (500 MHz, $CDCl_3$).

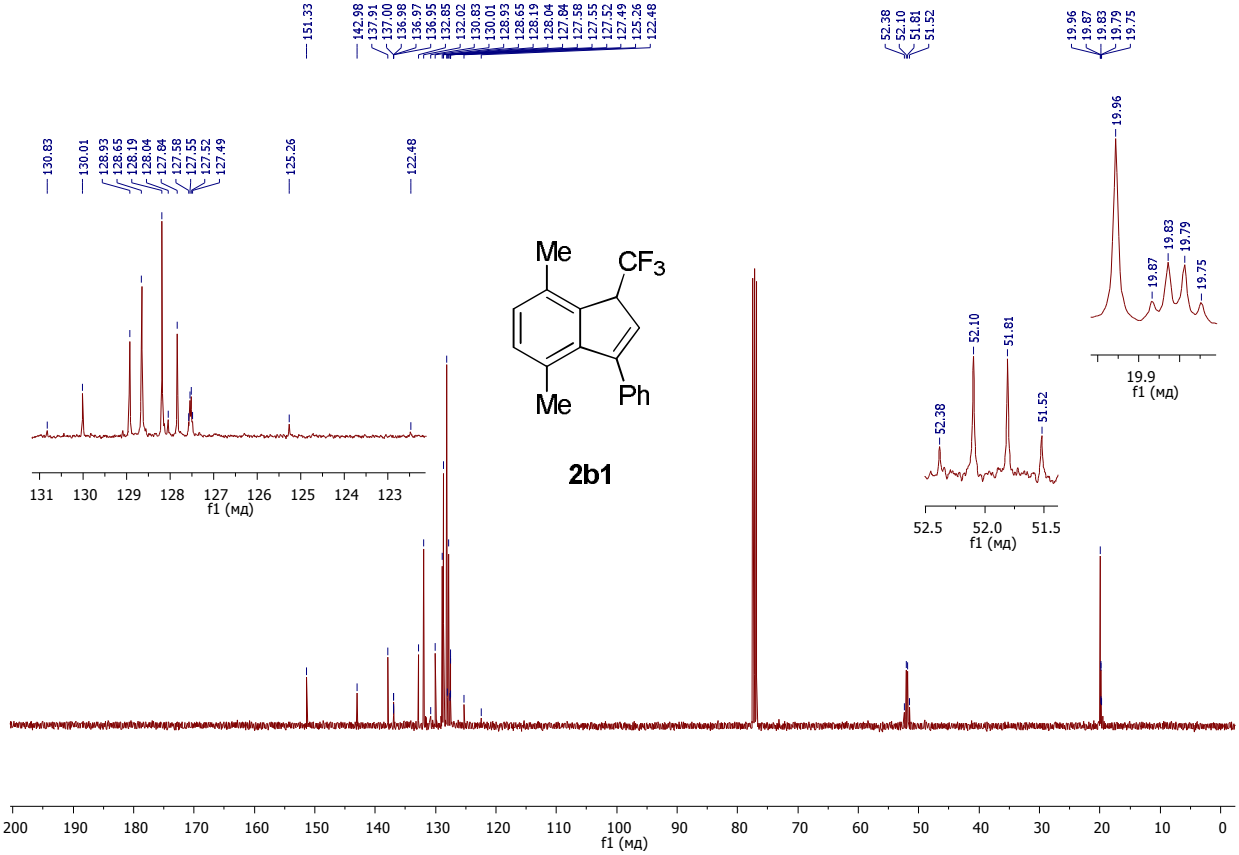


Figure S20. ^{13}C NMR spectrum of mixture of isomers **2b1** (125 MHz, $CDCl_3$).

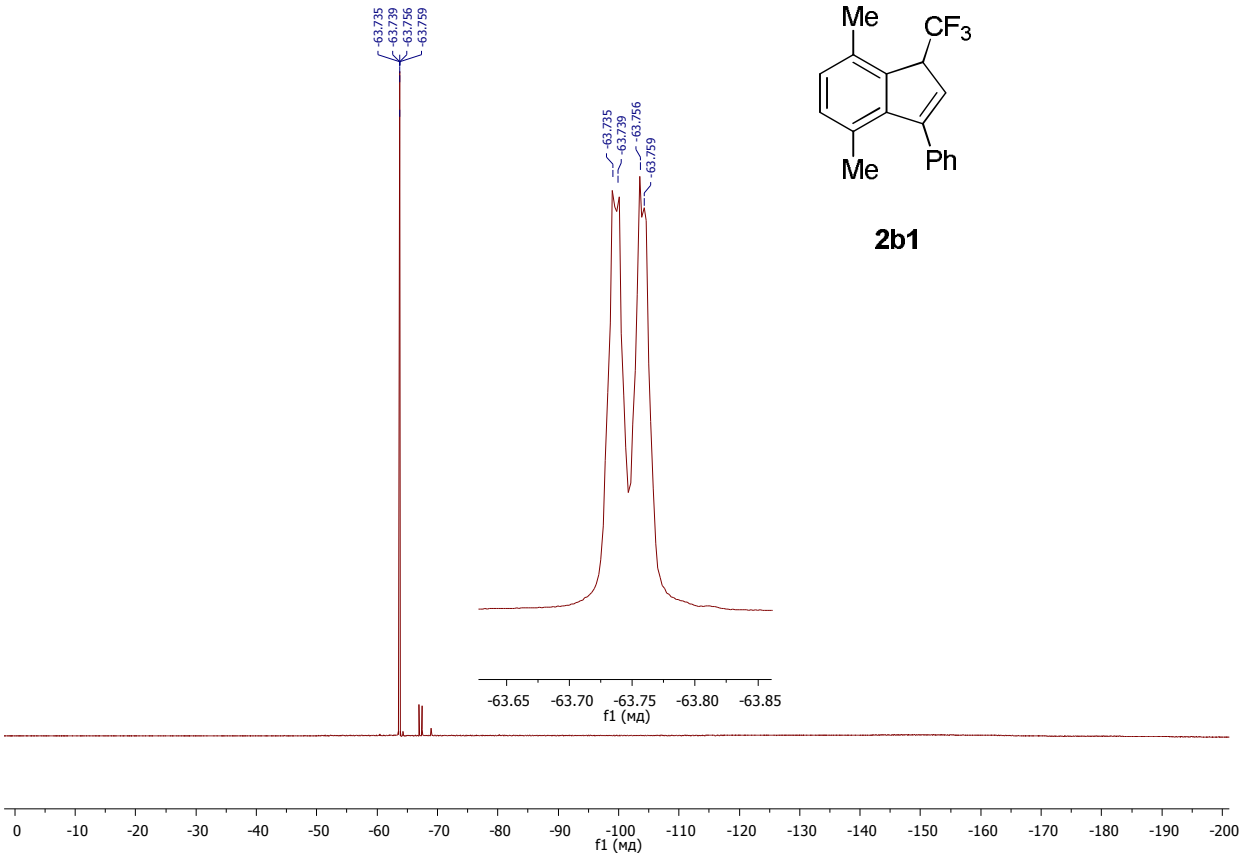


Figure S21. ^{19}F NMR spectrum of mixture of isomers **2b1** (470 MHz, $CDCl_3$).

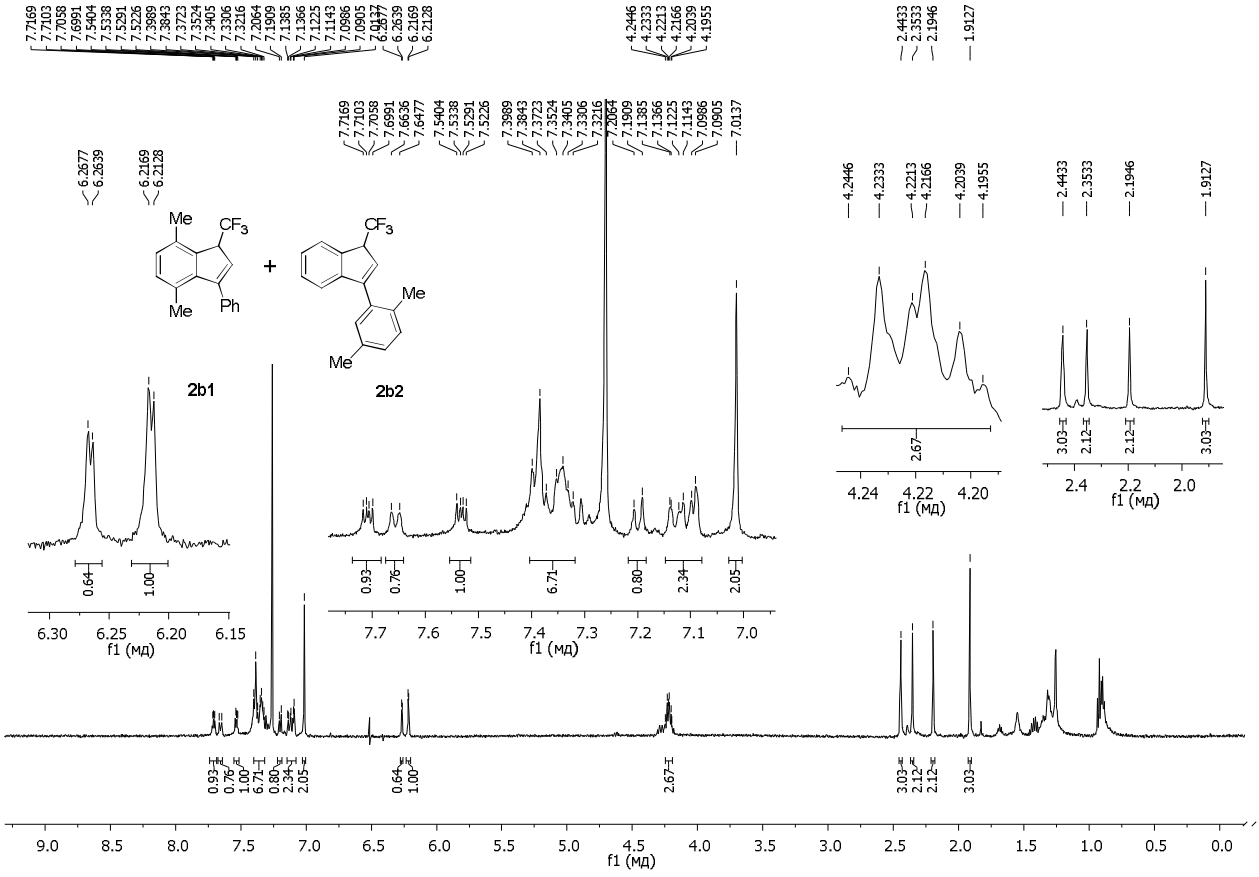


Figure S22. ^{1}H NMR spectrum of mixture of isomers **2b1, 2b2** (500 MHz, $CDCl_3$).

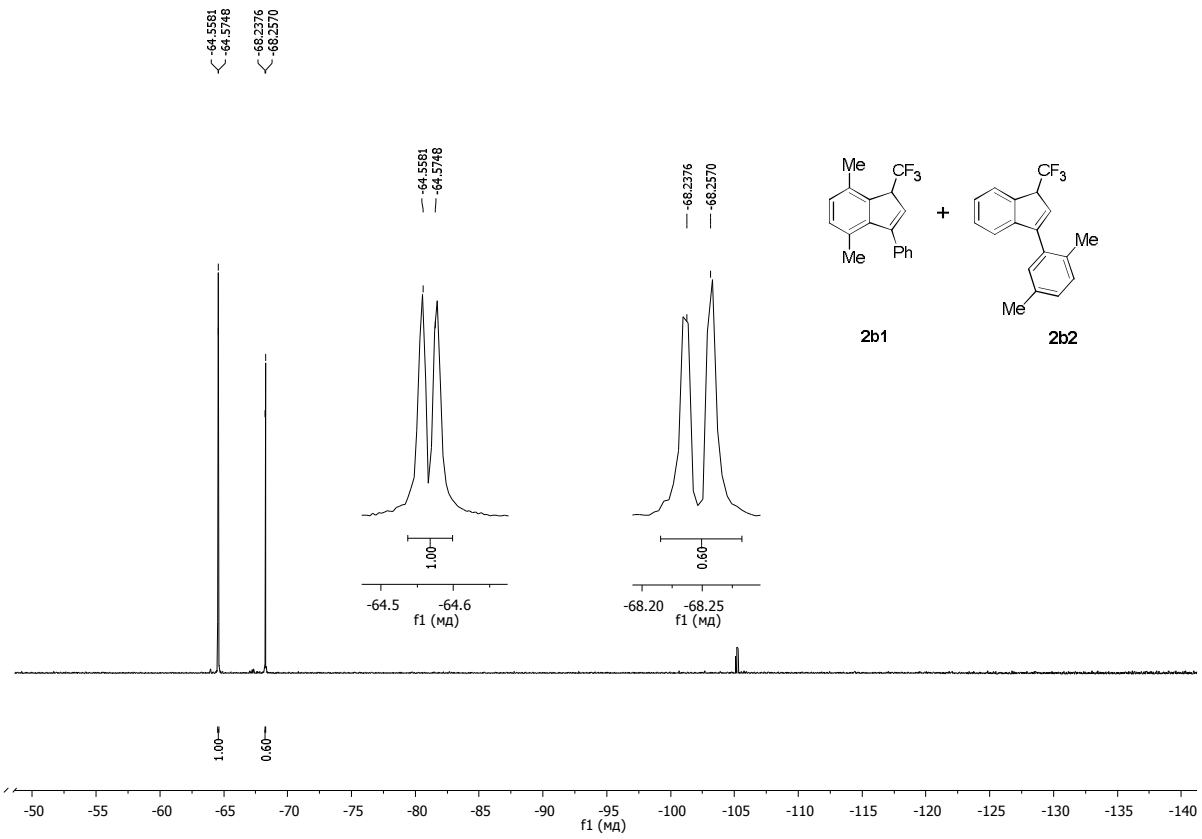


Figure S23. ^{19}F NMR spectrum of mixture of isomers **2b1, 2b2** (470 MHz, $CDCl_3$).

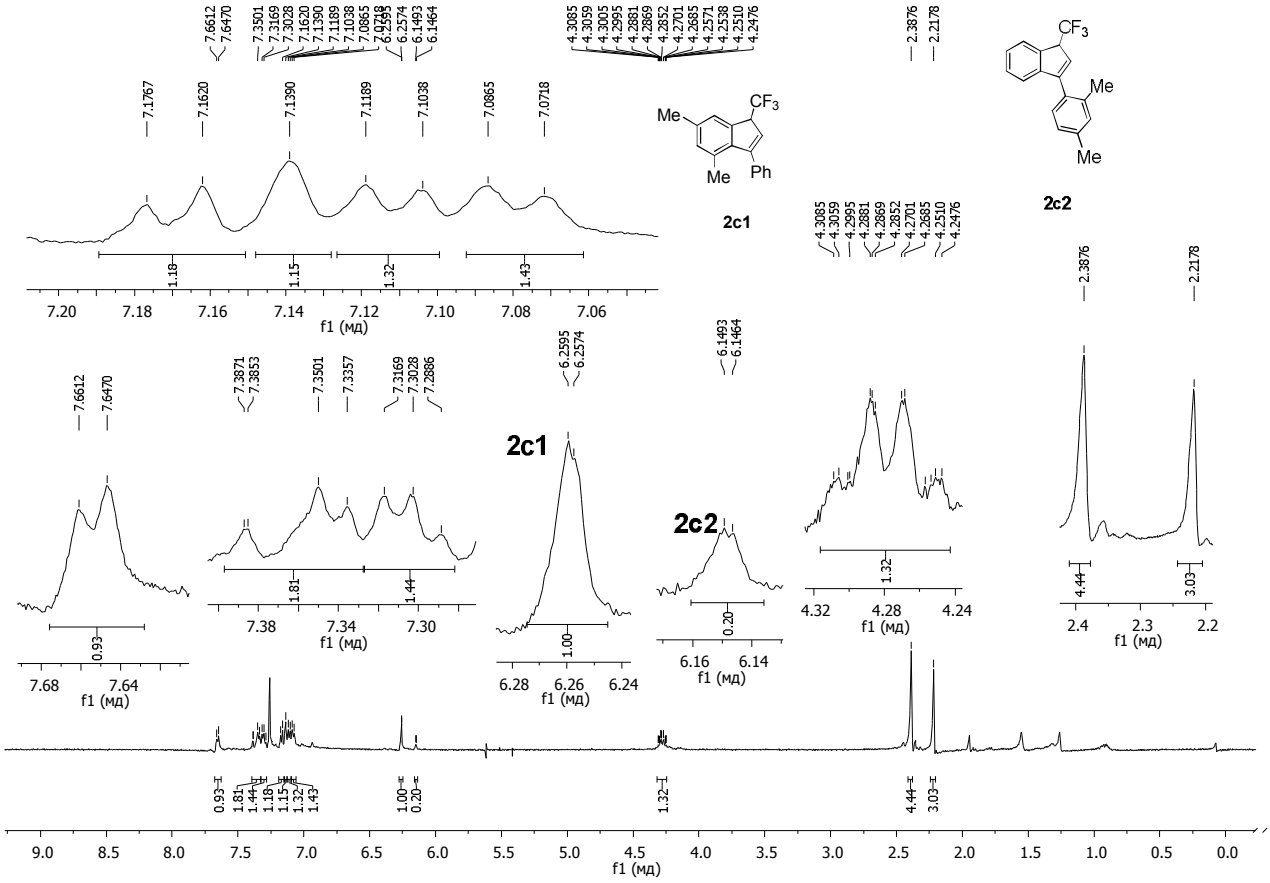


Figure S24. ^{1}H NMR spectrum of mixture of isomers **2c1, 2c2** (500 MHz, $CDCl_3$).

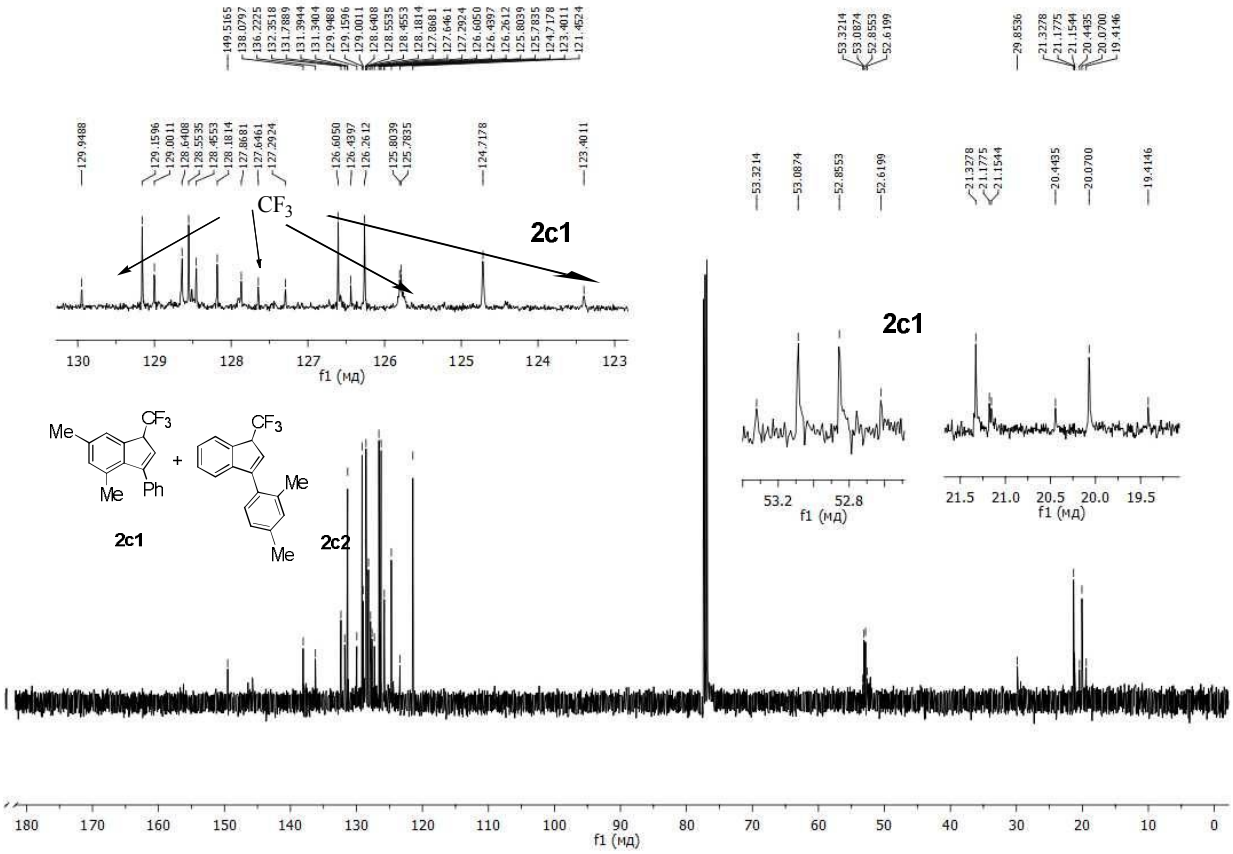


Figure S25. ^{13}C NMR spectrum of mixture of isomers **2c1, 2c2** (125 MHz, $CDCl_3$).

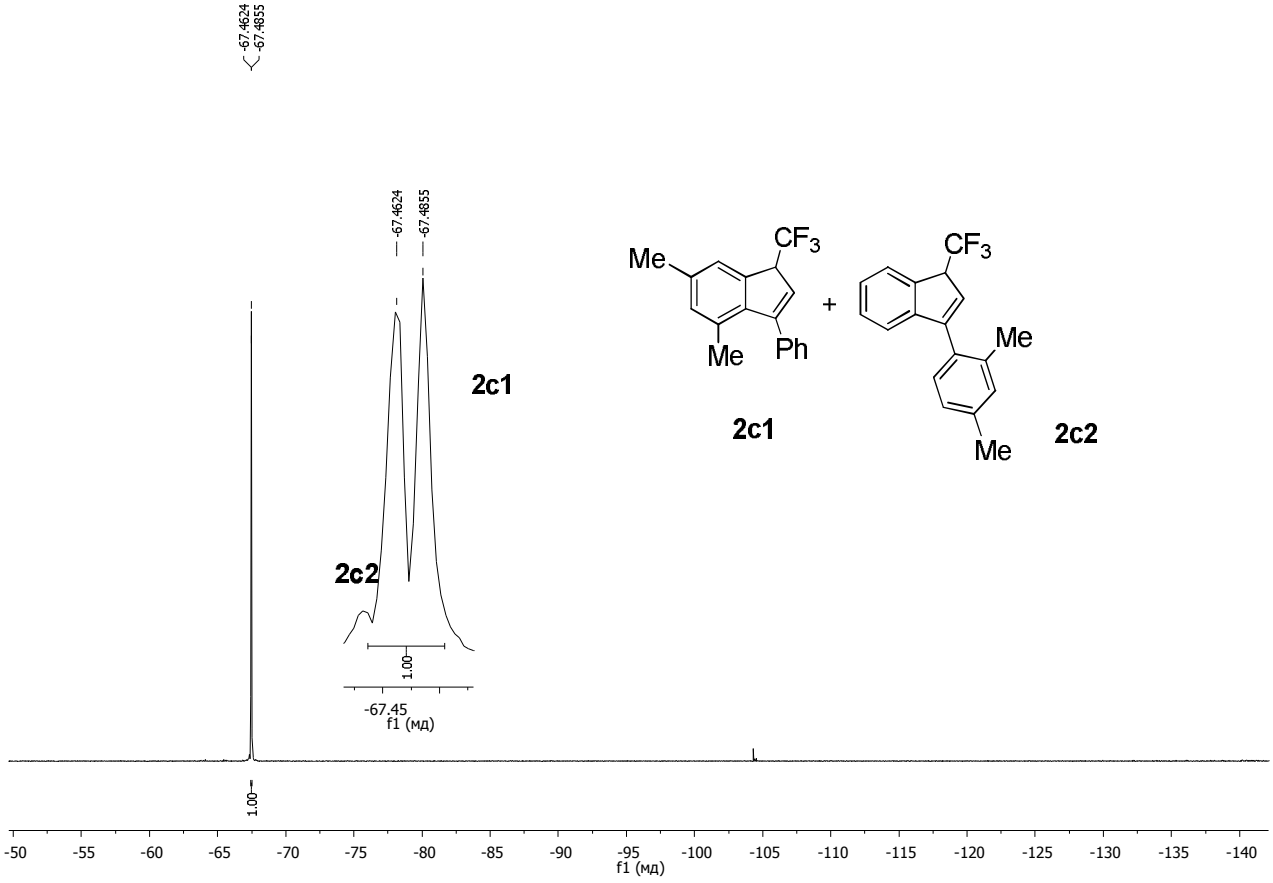


Figure S26. ^{19}F NMR spectrum of mixture of isomers **2c1, 2c2** (470 MHz, $CDCl_3$).

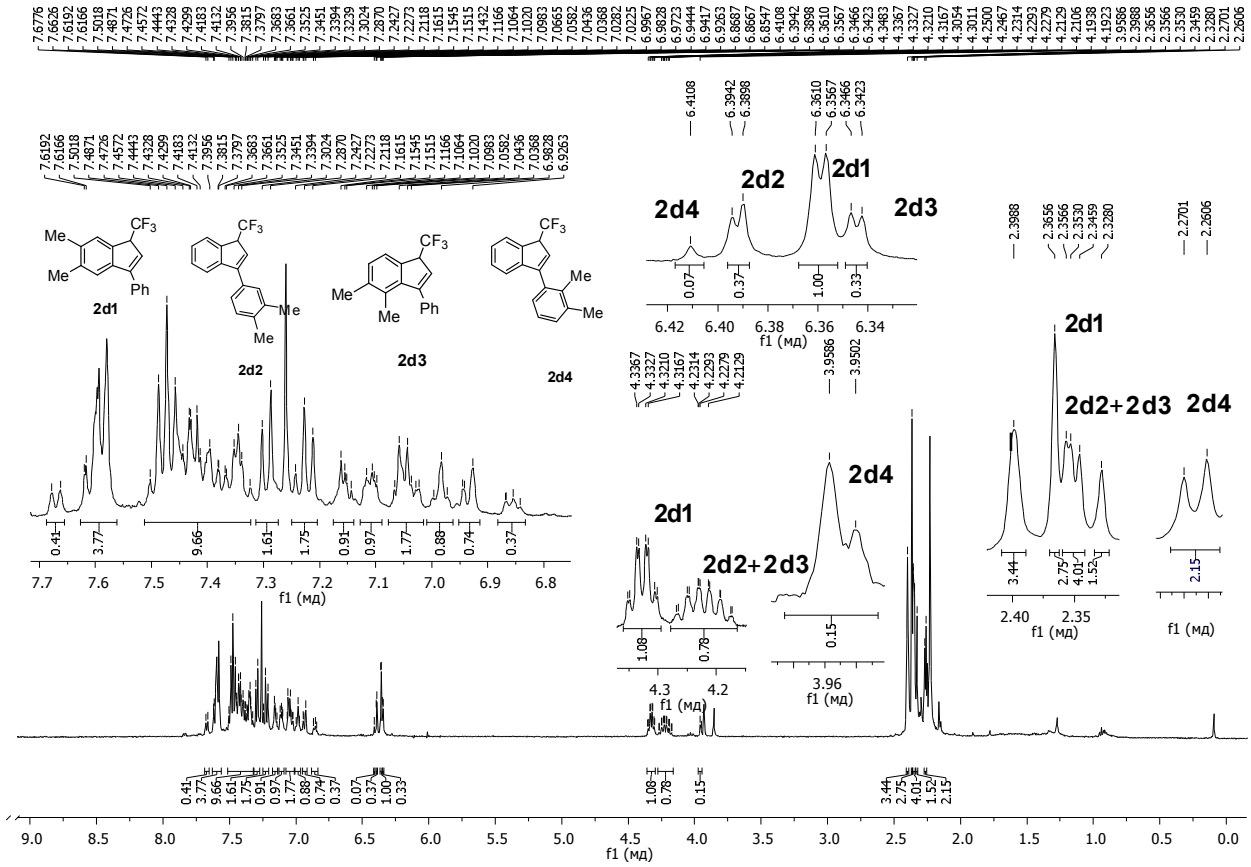


Figure S27. ^{1}H NMR spectrum of mixture of isomers **2d1, 2d2, 2d3, 2d4** (500 MHz, $CDCl_3$).

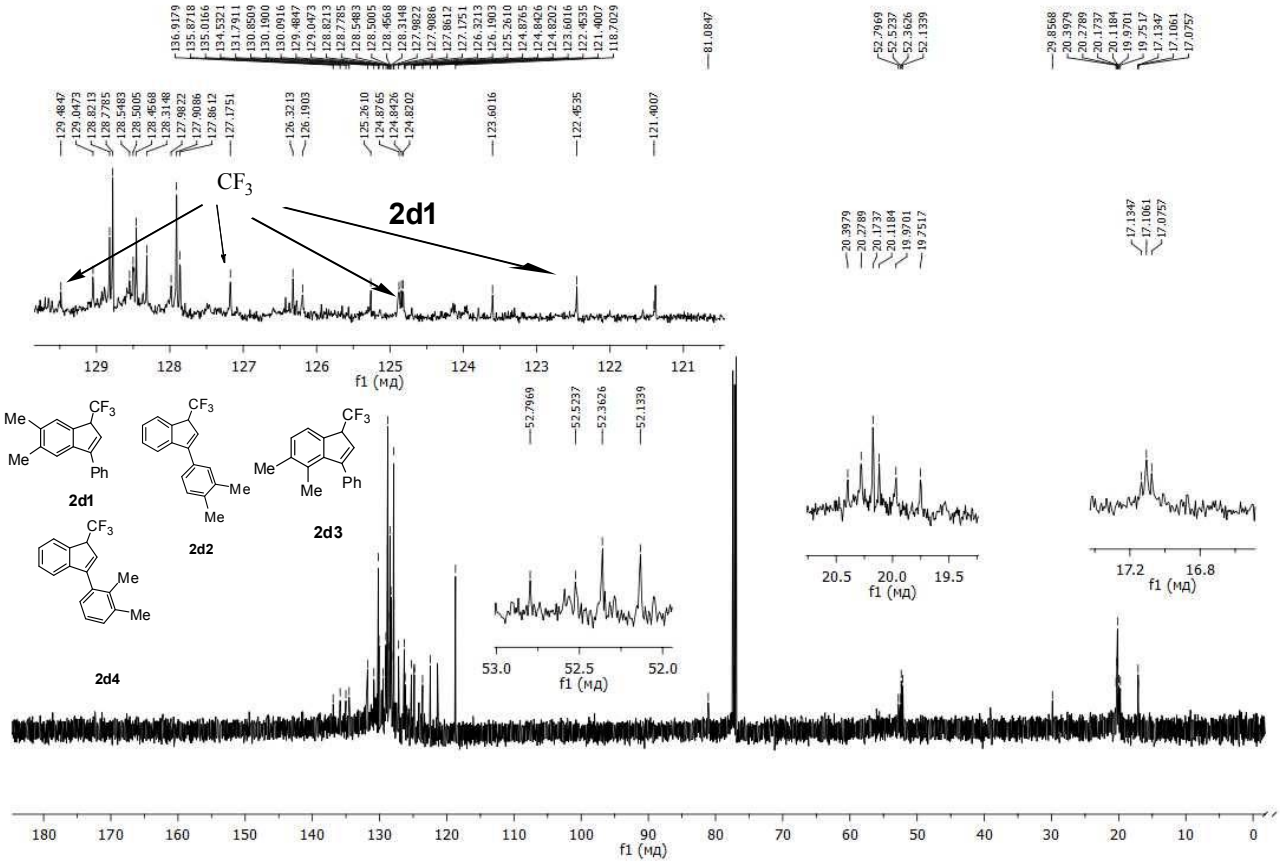


Figure S28. ^{13}C NMR spectrum of mixture of isomers **2d1, 2d2, 2d3, 2d4** (125 MHz, $CDCl_3$).

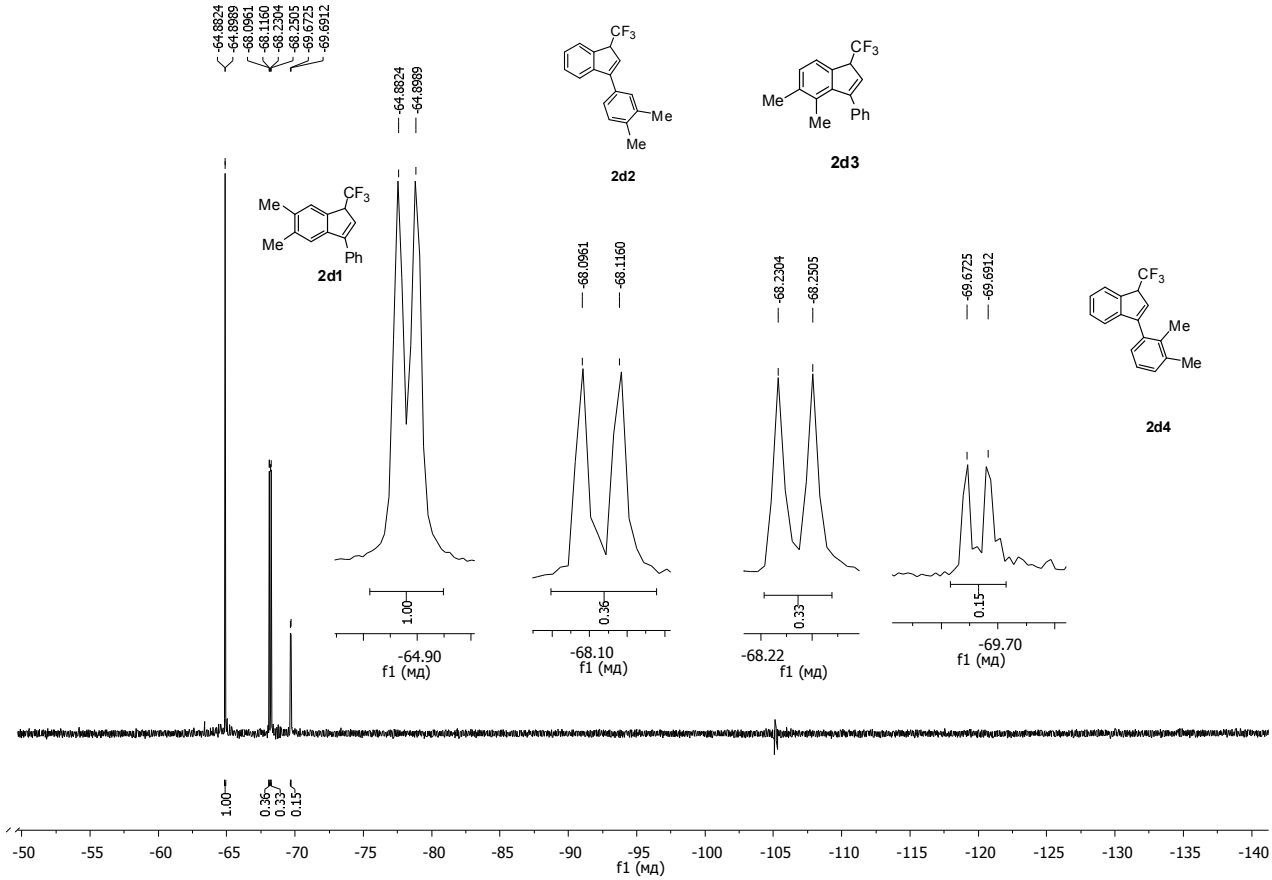


Figure S29. ^{19}F NMR spectrum of mixture of isomers **2d1, 2d2, 2d3, 2d4** (470 MHz, $CDCl_3$).

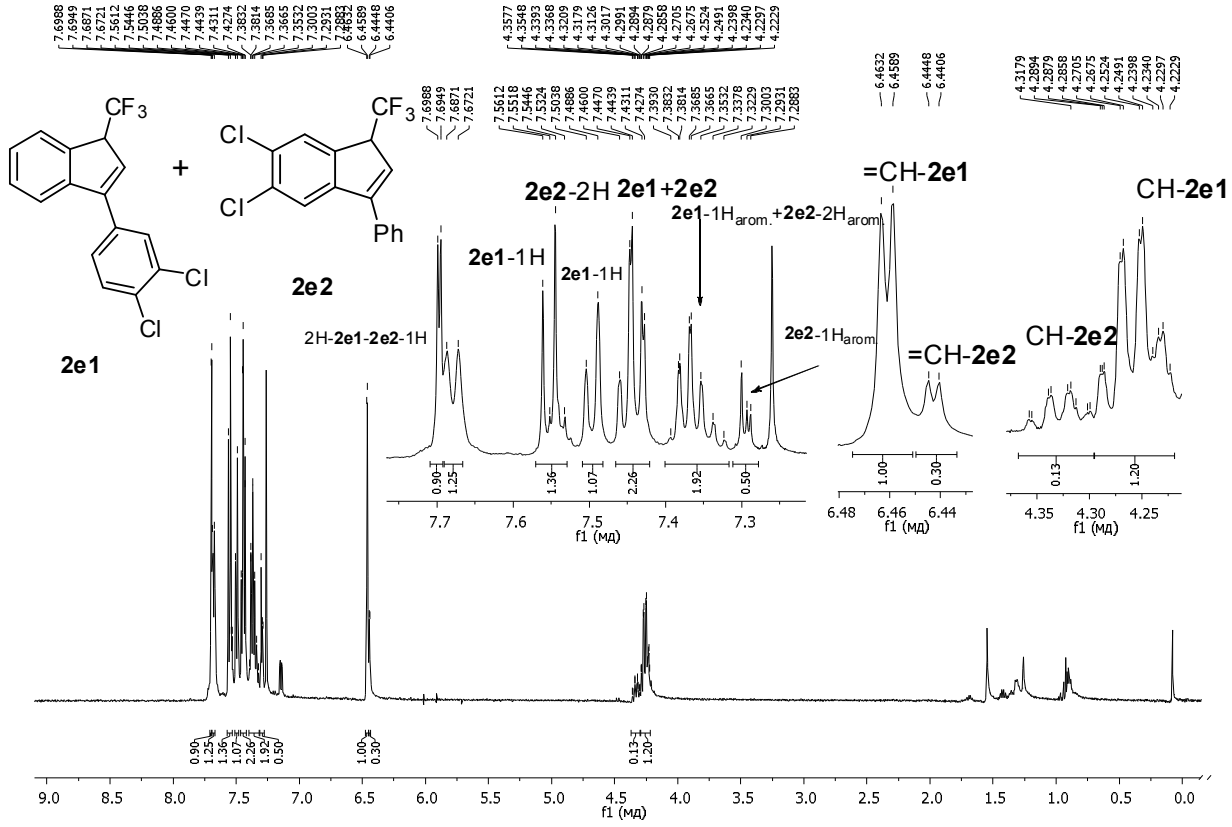


Figure S30. ^{1}H NMR spectrum of mixture of isomers **2e1, 2e2** (500 MHz, $CDCl_3$).

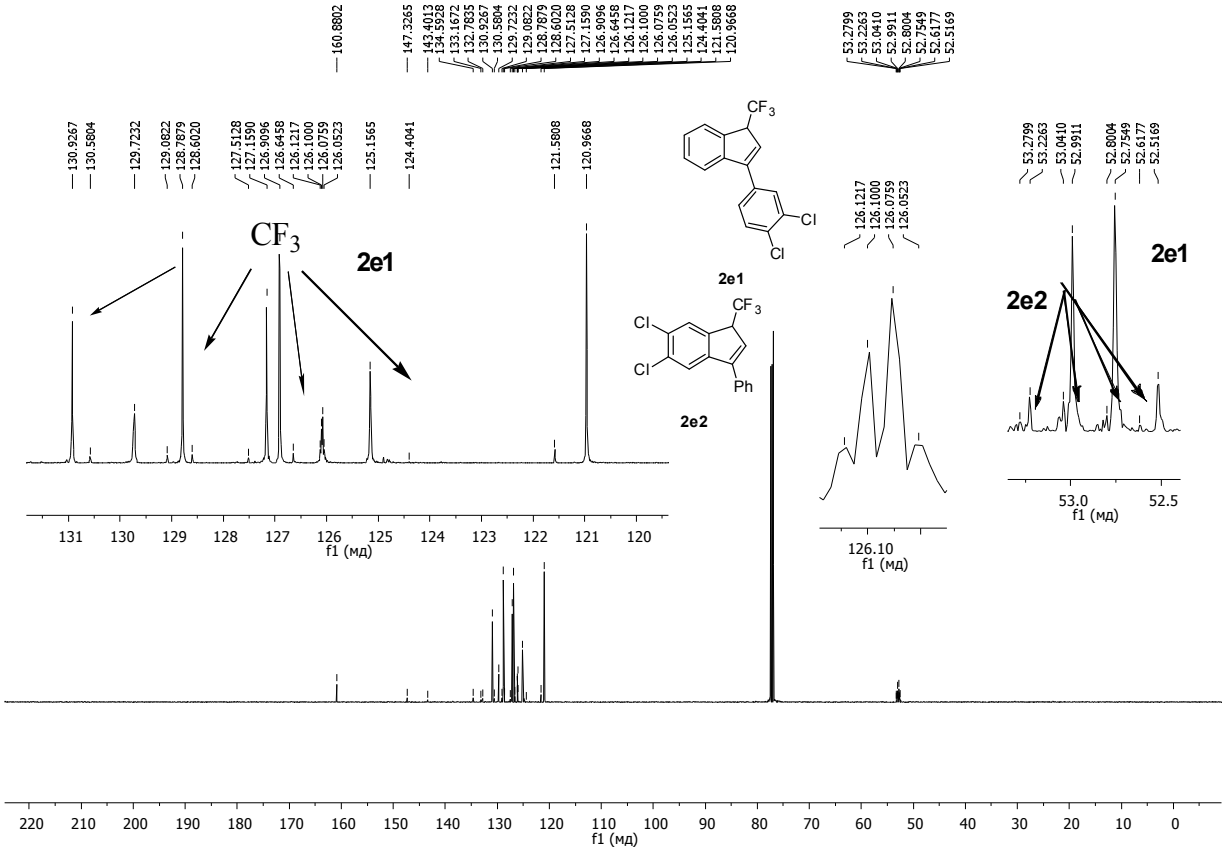


Figure S31. ^{13}C NMR spectrum of mixture of isomers **2e1, 2e2** (125 MHz, $CDCl_3$).

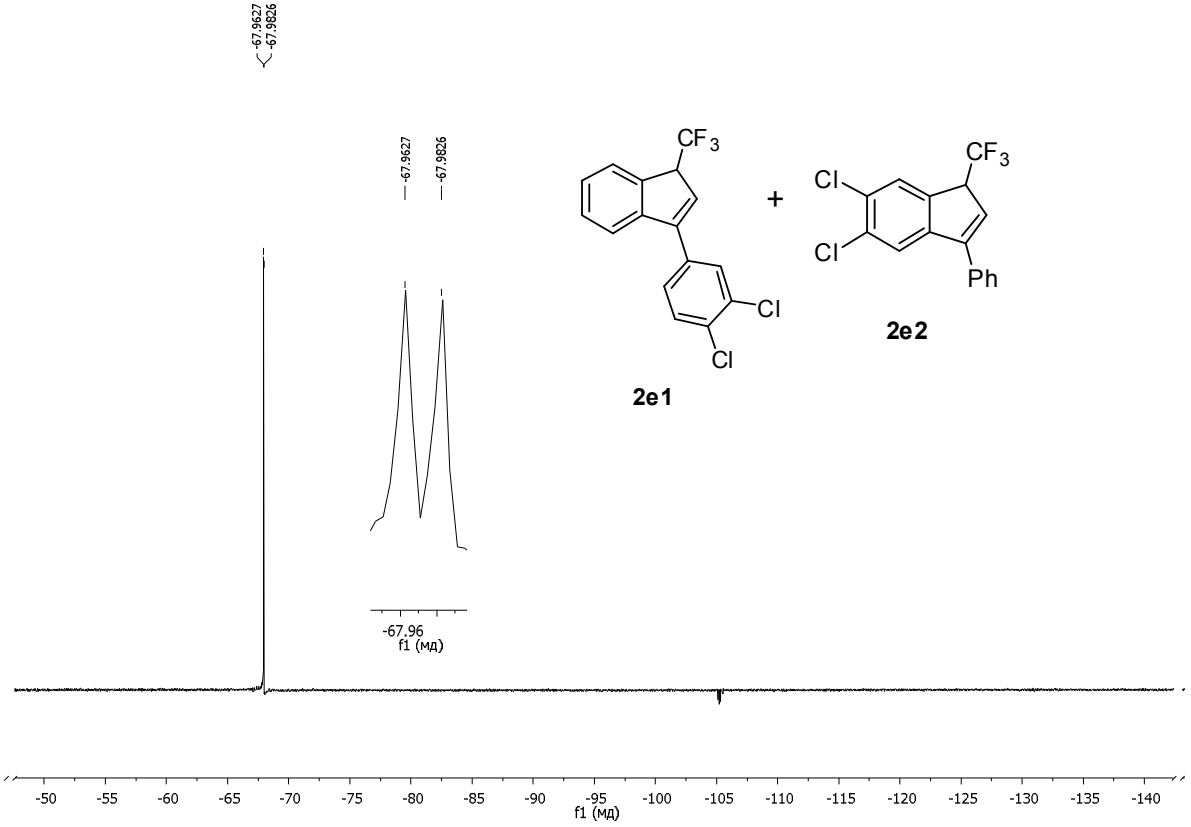


Figure S32. ^{19}F NMR spectrum of mixture of isomers **2e1, 2e2** (470 MHz, $CDCl_3$).

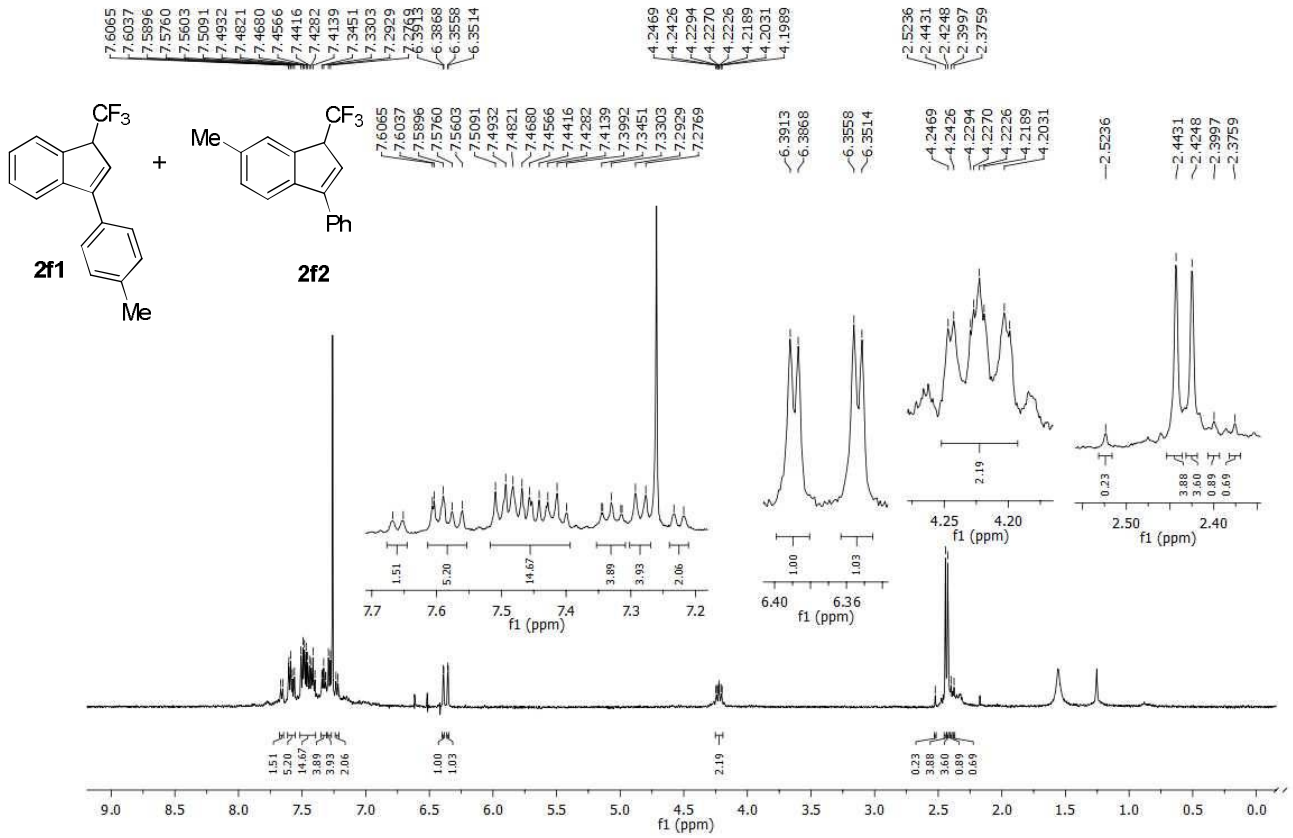


Figure S33. ^{1}H NMR spectrum of mixture of isomers **2f1, 2f2** (500 MHz, $CDCl_3$).

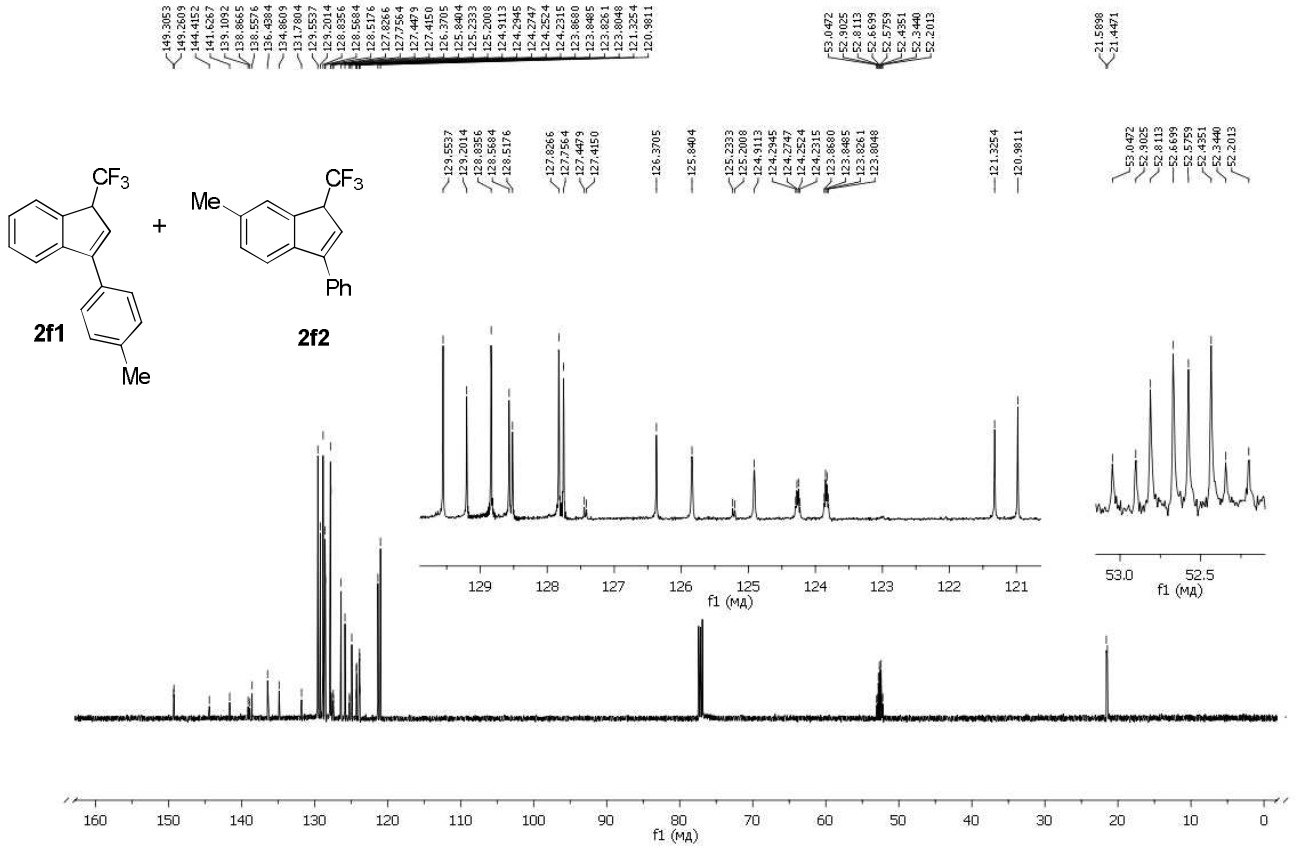


Figure S34. ^{13}C NMR spectrum of mixture of isomers **2f1, 2f2** (125 MHz, $CDCl_3$).

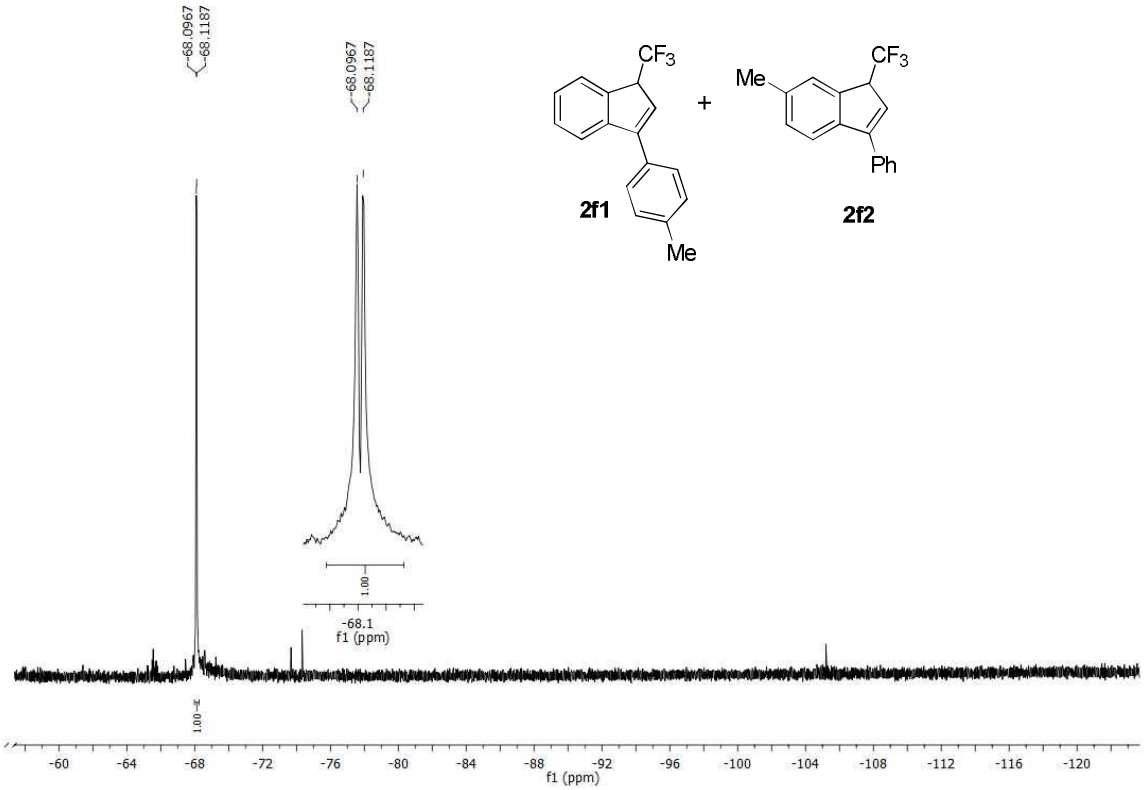


Figure S35. ^{19}F NMR spectrum of mixture of isomers **2f1, 2f2** (470 MHz, $CDCl_3$).

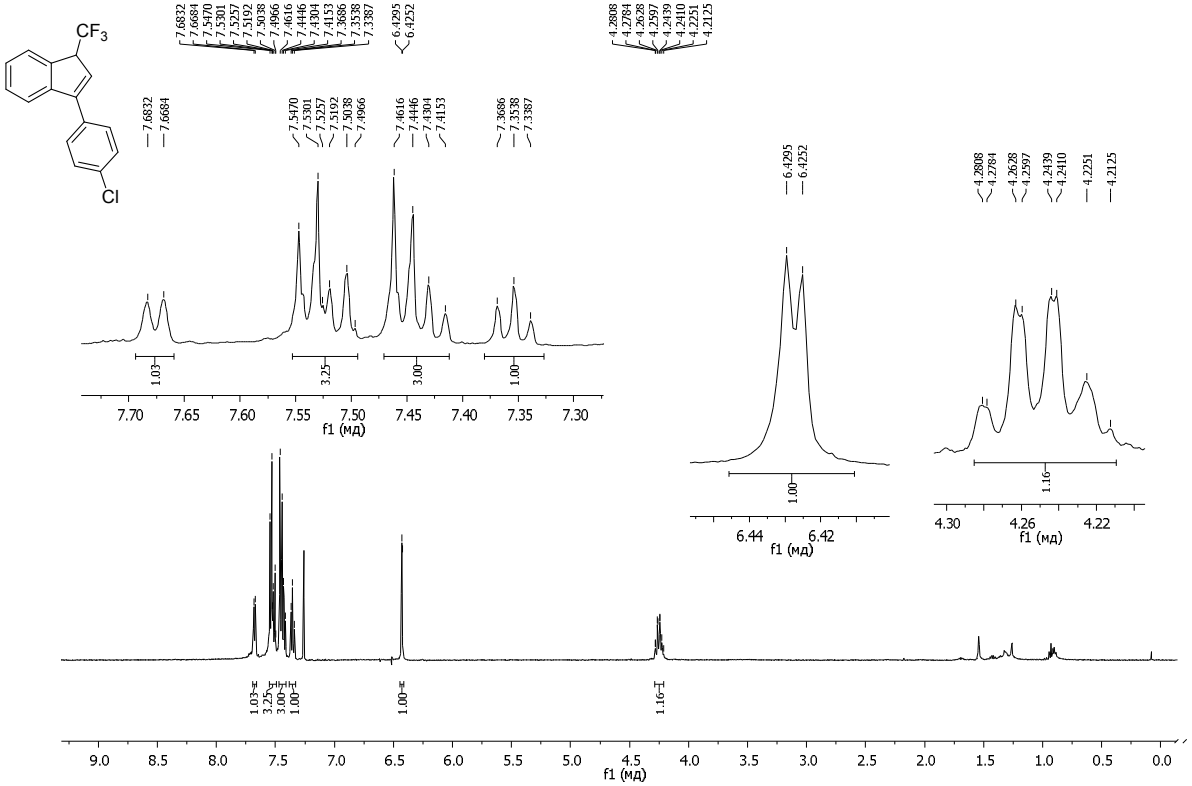


Figure S36. ^{1}H NMR spectrum of compound **2g** (500 MHz, $CDCl_3$).

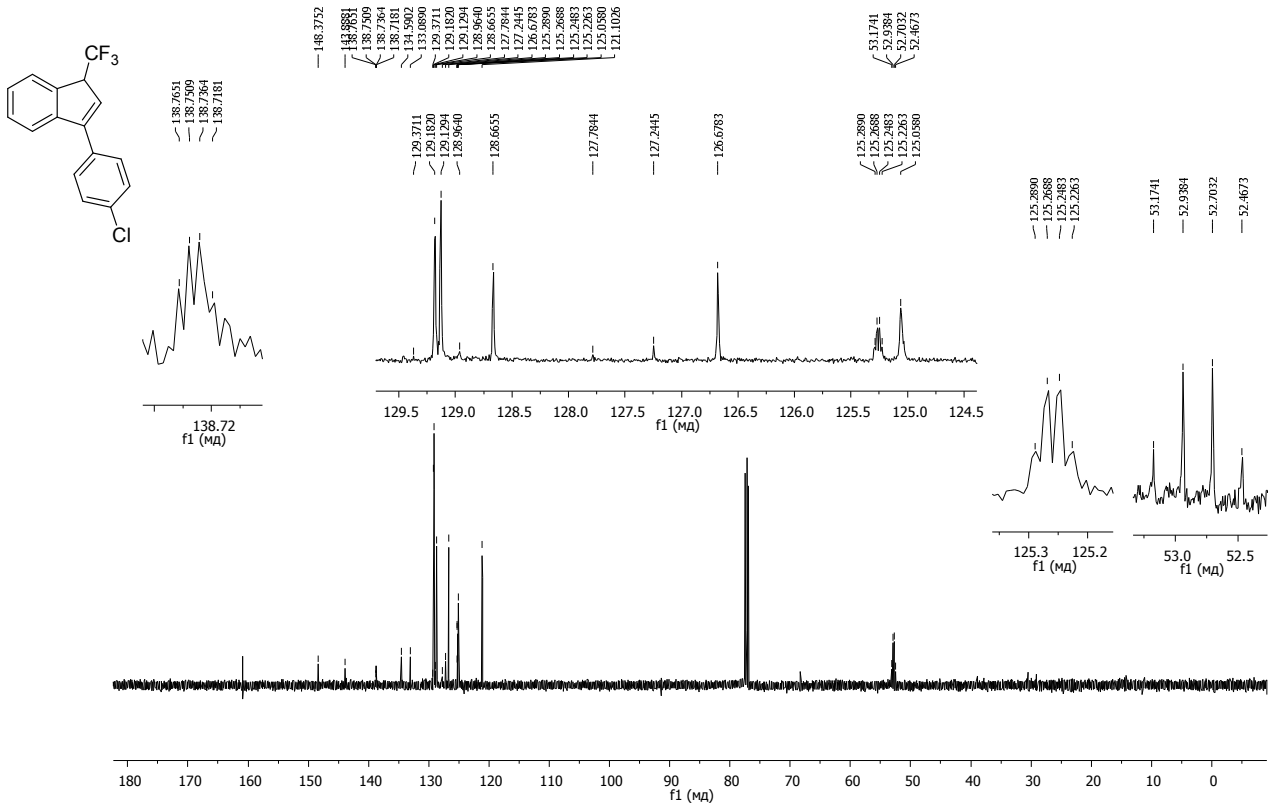


Figure S37. ^{13}C NMR spectrum of compound **2g** (125 MHz, $CDCl_3$).

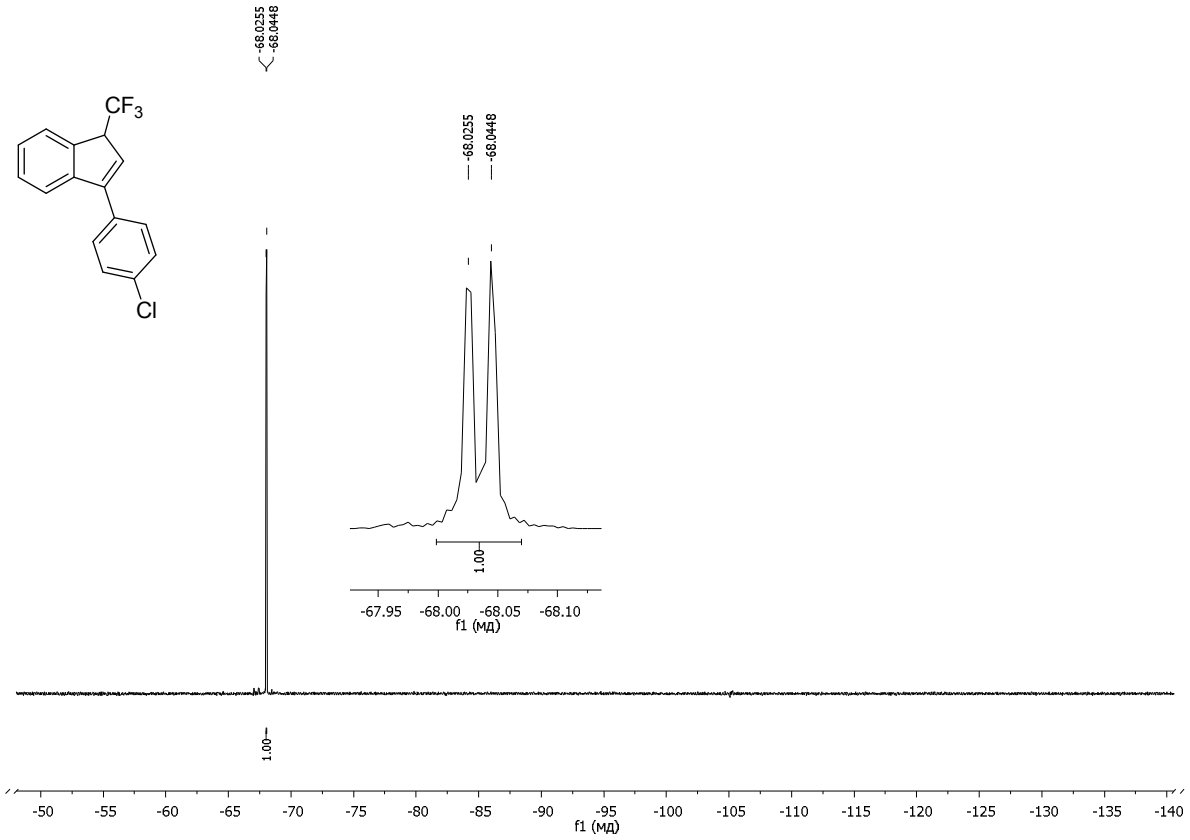


Figure S38. ^{19}F NMR spectrum of compound **2g** (470 MHz, $CDCl_3$).

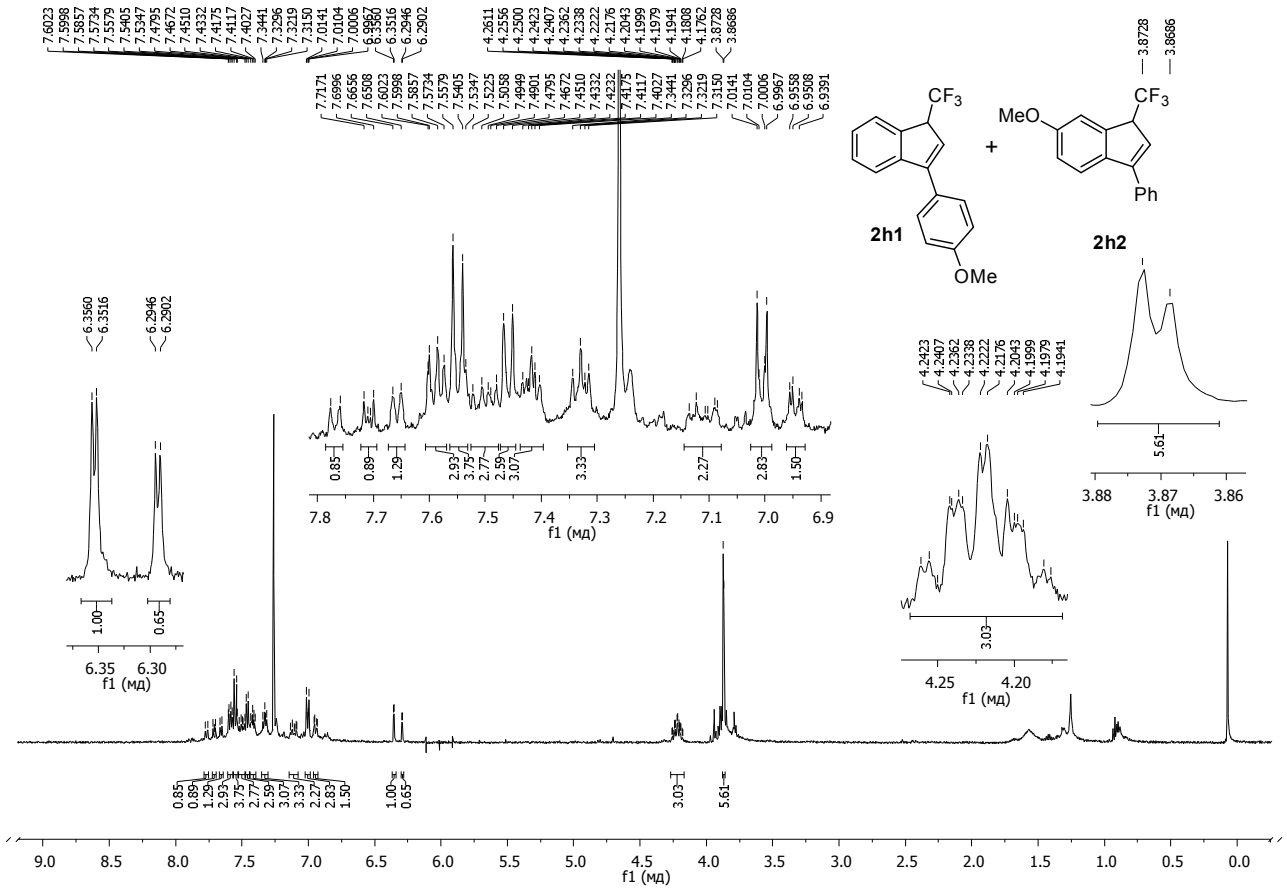


Figure S39. ^{1}H NMR spectrum of mixture of isomers **2h1, 2h2** (500 MHz, $CDCl_3$).

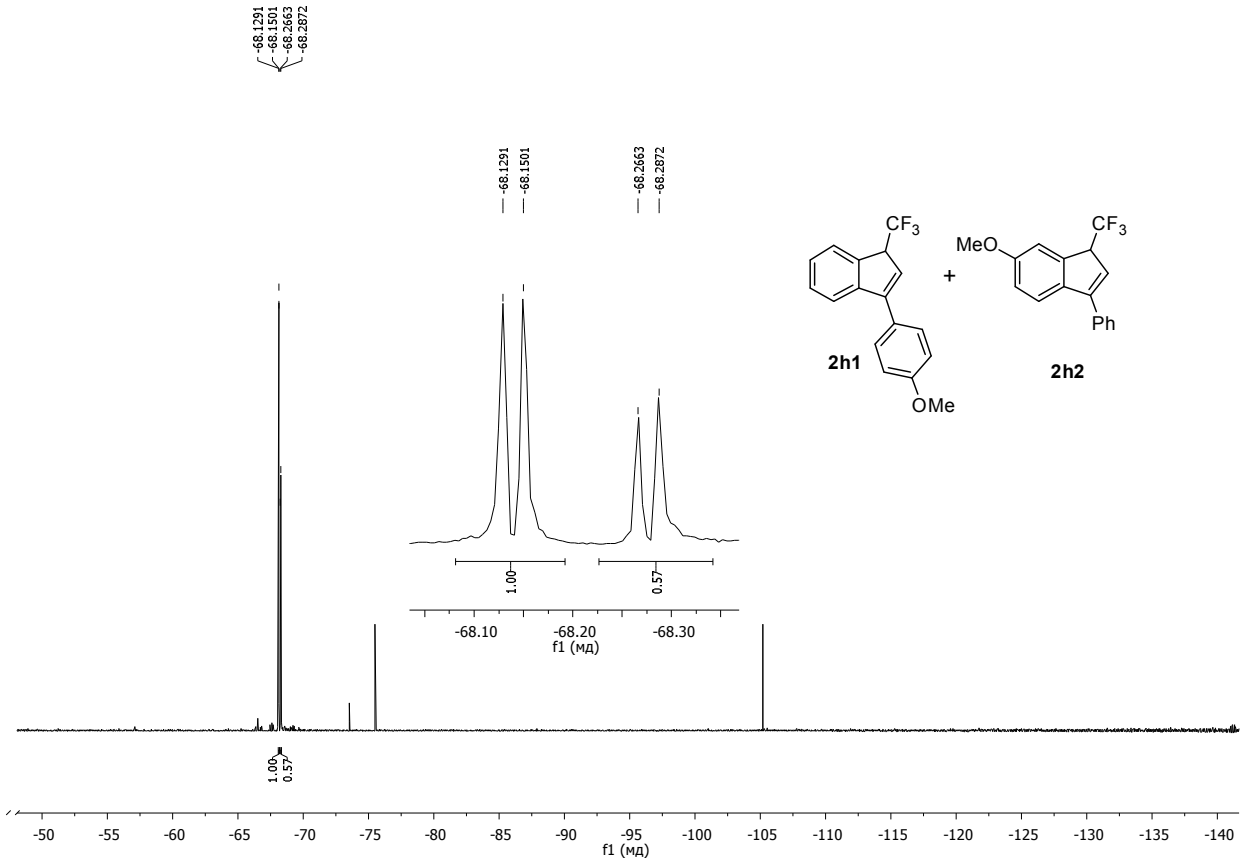


Figure S40. ^{19}F NMR spectrum of mixture of isomers **2h1, 2h2** (470 MHz, $CDCl_3$).

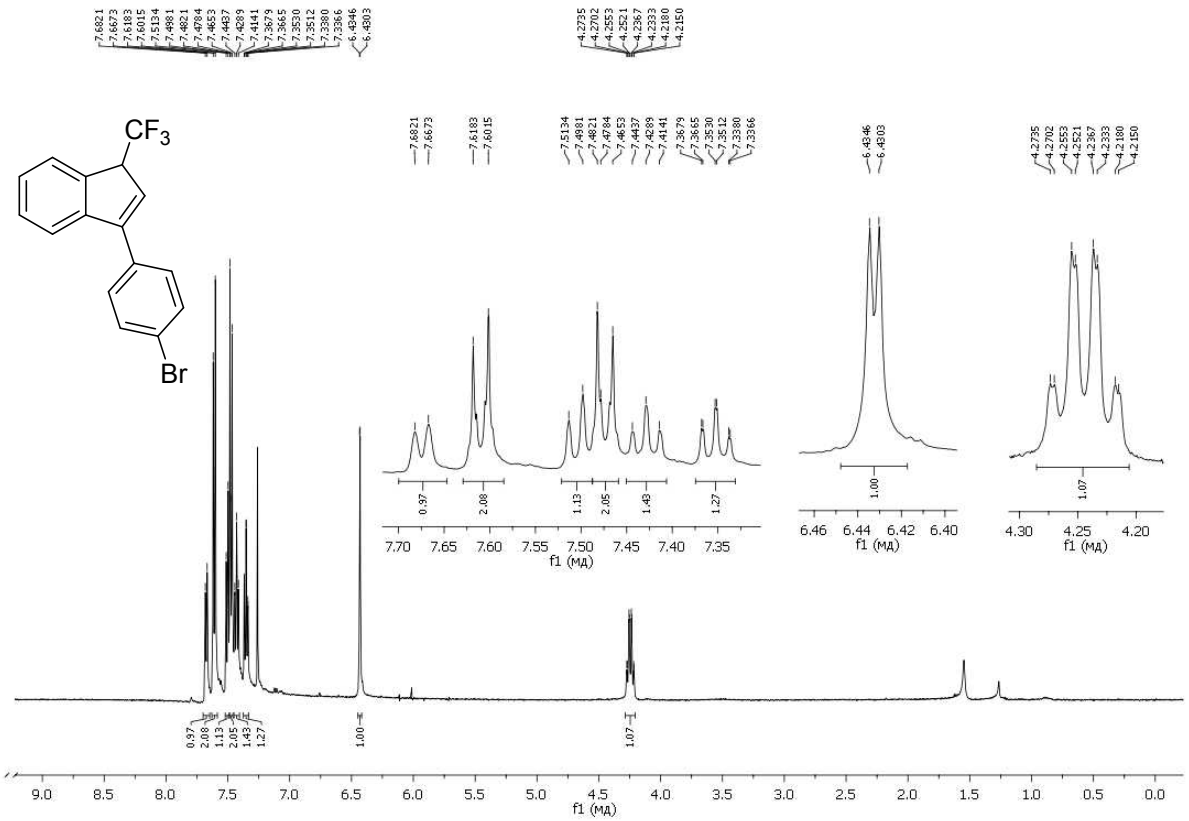


Figure S41. ^{1}H NMR spectrum of compound **2i** (500 MHz, $CDCl_3$).

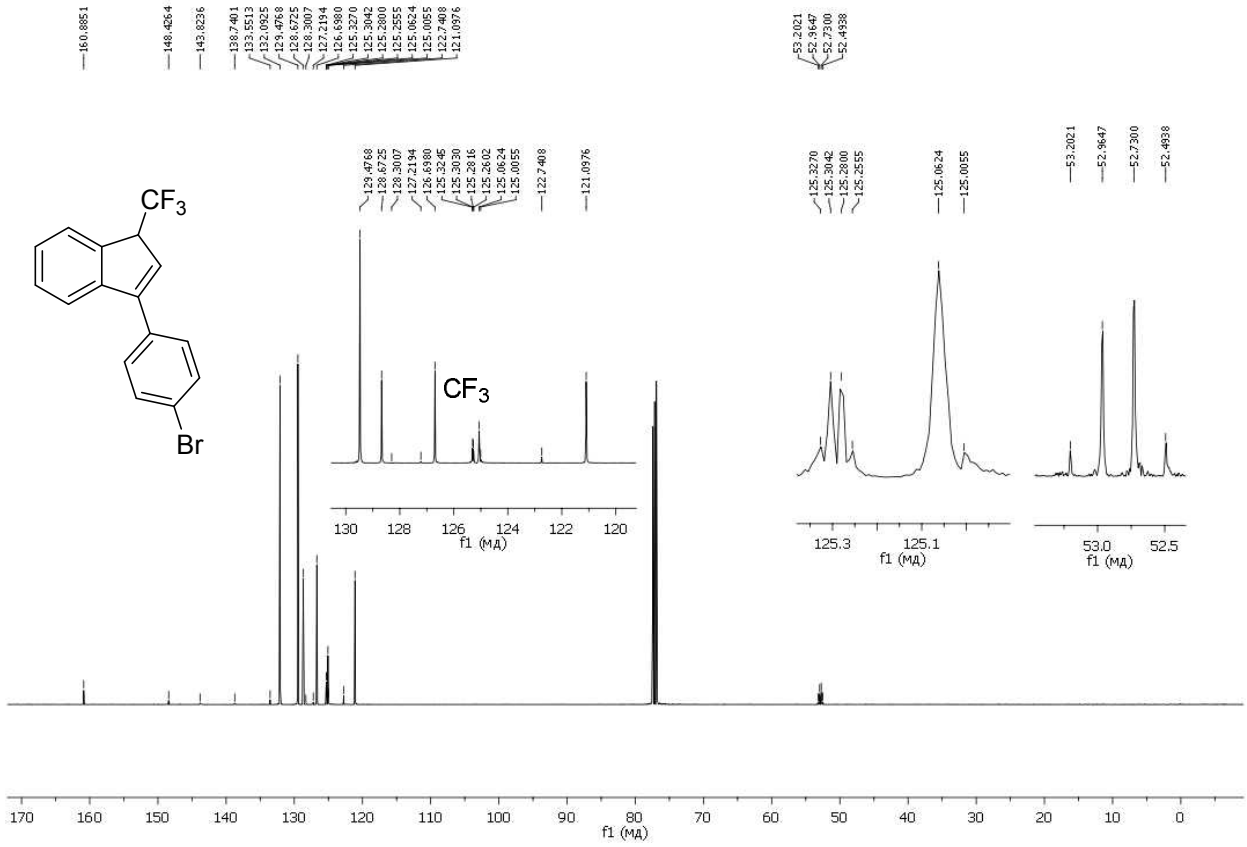


Figure S42. ^{13}C NMR spectrum of compound **2i** (125 MHz, $CDCl_3$).

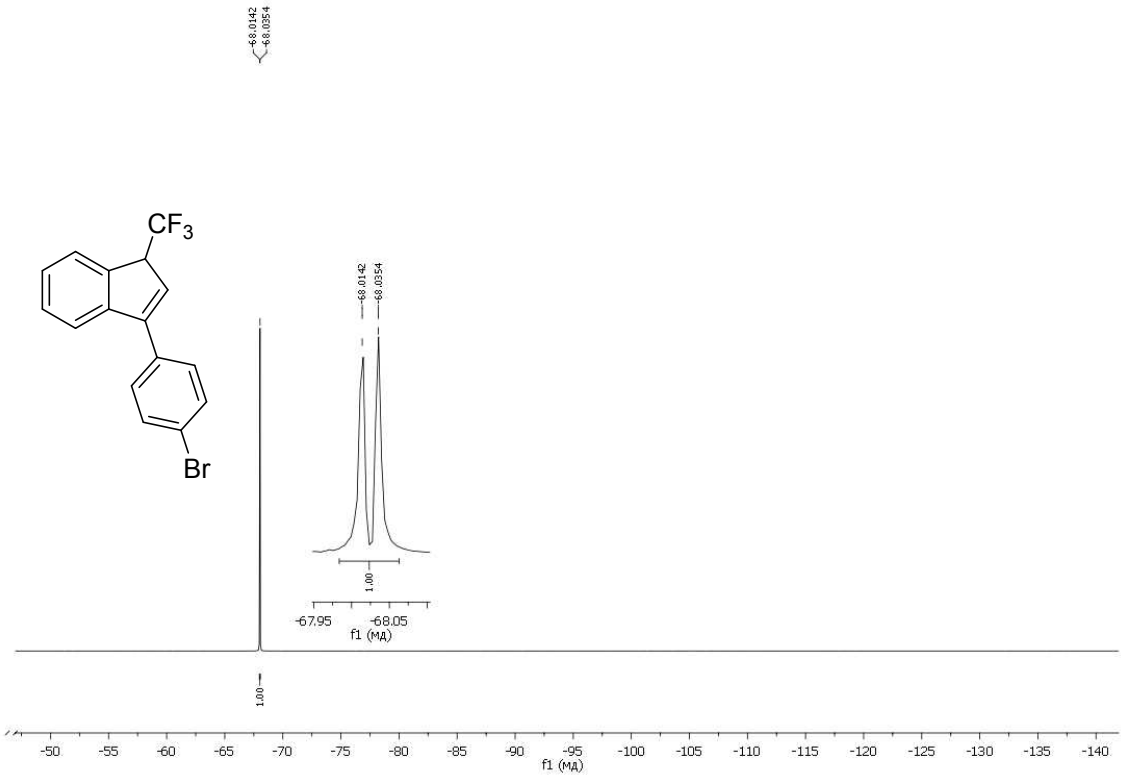


Figure S43. ^{19}F NMR spectrum of compound **2i** (470 MHz, $CDCl_3$).

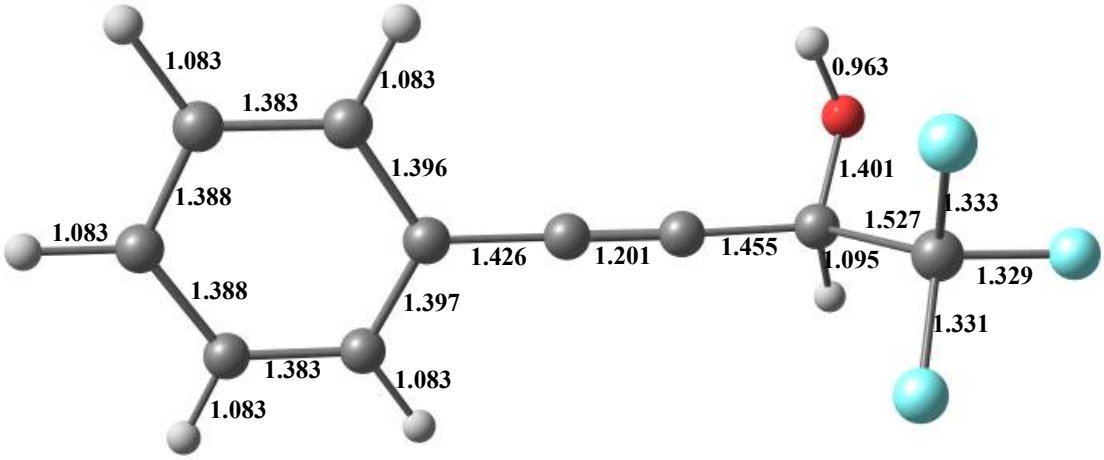
2. Data of DFT calculations of alcohols 1 and cations A, B

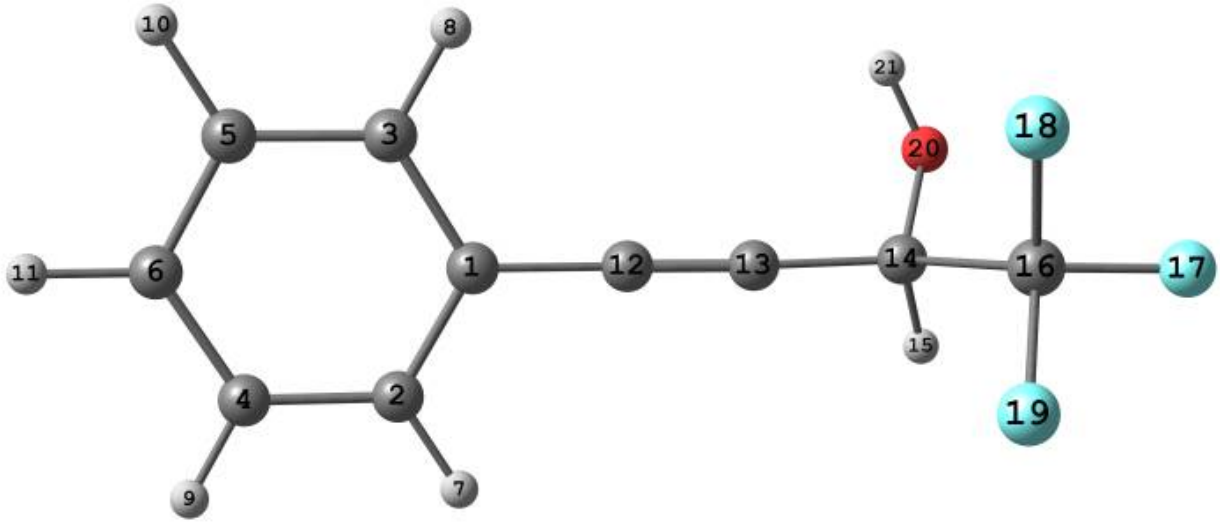
1a

Energy **E= -759.791015103 h, G^{298}= -759.68191 h, μ=4.05 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.942561	-0.017048	-0.185572
2	C	2.704726	1.079039	-0.596204
3	C	2.567198	-1.082408	0.466258
4	C	4.066658	1.105161	-0.356609
5	C	3.930234	-1.049829	0.699071
6	C	4.681860	0.042525	0.289610
7	H	2.218347	1.904547	-1.101701
8	H	1.974373	-1.931519	0.784297
9	H	4.651661	1.958886	-0.675879
10	H	4.408866	-1.879913	1.203961
11	H	5.748731	0.065819	0.474936
12	C	0.538687	-0.046833	-0.431502
13	C	-0.643387	-0.065660	-0.642849
14	C	-2.075746	-0.136350	-0.891481
15	H	-2.358166	0.569232	-1.680057
16	C	-2.850742	0.301241	0.349326
17	F	-4.159274	0.300453	0.115886
18	F	-2.625373	-0.517172	1.377322
19	F	-2.504017	1.531441	0.720542
20	O	-2.515841	-1.403162	-1.297343
21	H	-2.091406	-2.073290	-0.750859





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.14969	1.99891	4.13433	0.01646	6.14969
C	2	-0.16256	1.99905	4.14553	0.01798	6.16256
C	3	-0.16289	1.99905	4.14587	0.01798	6.16289
C	4	-0.20224	1.99912	4.18345	0.01968	6.20224

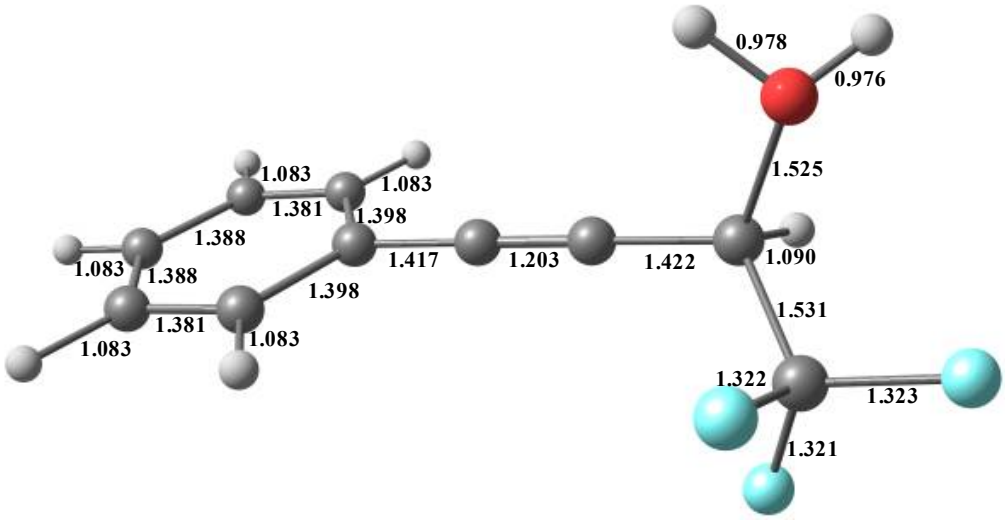
C	5	-0.20206	1.99912	4.18328	0.01966	6.20206
C	6	-0.18793	1.99912	4.16897	0.01984	6.18793
H	7	0.21847	0.00000	0.77996	0.00157	0.78153
H	8	0.21841	0.00000	0.78000	0.00159	0.78159
H	9	0.21676	0.00000	0.78162	0.00162	0.78324
H	10	0.21676	0.00000	0.78163	0.00161	0.78324
H	11	0.21484	0.00000	0.78365	0.00151	0.78516
C	12	0.04828	1.99837	3.93796	0.01539	5.95172
C	13	-0.05500	1.99832	4.04264	0.01404	6.05500
C	14	-0.00627	1.99893	3.97623	0.03111	6.00627
H	15	0.23445	0.00000	0.76299	0.00256	0.76555
C	16	1.11234	1.99930	2.83052	0.05784	4.88766
F	17	-0.36751	1.99991	7.35622	0.01138	9.36751
F	18	-0.37446	1.99991	7.36281	0.01175	9.37446
F	19	-0.36898	1.99991	7.35805	0.01103	9.36898
O	20	-0.74072	1.99978	6.71889	0.02204	8.74072
H	21	0.50000	0.00000	0.49697	0.00302	0.50000
* Total *		0.00000	27.98877	73.71157	0.29965	102.00000

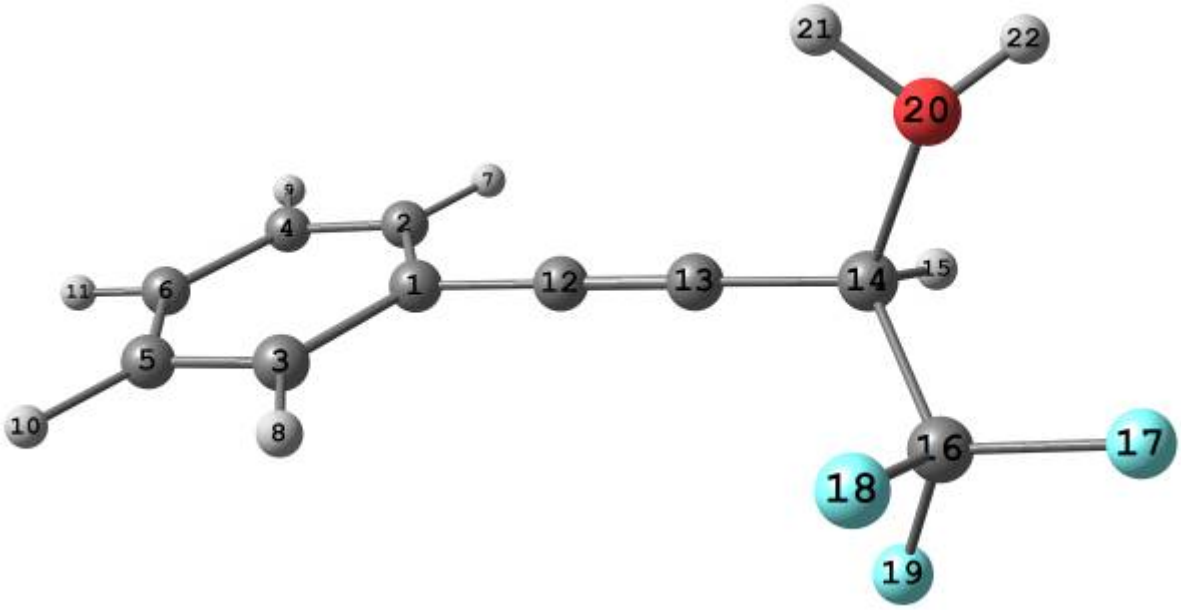
Aa

Energy **E=-760.167202886 h, G^{298}=-760.049324 h, μ=10.54 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.973397	0.163678	0.039451
2	C	2.868963	1.105592	0.553873
3	C	2.452457	-1.024958	-0.518973
4	C	4.226893	0.856388	0.507725
5	C	3.812243	-1.264131	-0.559068
6	C	4.697869	-0.326000	-0.046616
7	H	2.487743	2.023251	0.984437
8	H	1.750225	-1.747959	-0.914853
9	H	4.921961	1.584652	0.905768
10	H	4.185049	-2.184474	-0.990324
11	H	5.763369	-0.517433	-0.079612
12	C	0.578415	0.409676	0.086143
13	C	-0.605995	0.615226	0.128519
14	C	-2.008946	0.841506	0.169556
15	H	-2.326803	1.517340	0.964126
16	C	-2.837434	-0.443484	0.239169
17	F	-4.129733	-0.161429	0.201231
18	F	-2.554830	-1.252030	-0.767848
19	F	-2.564511	-1.056535	1.376884
20	O	-2.471497	1.496835	-1.127319
21	H	-1.729489	1.662190	-1.741887
22	H	-2.985591	2.316733	-1.000193





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.18152	1.99890	4.16426	0.01836	6.18152
C	2	-0.13830	1.99905	4.12143	0.01782	6.13830

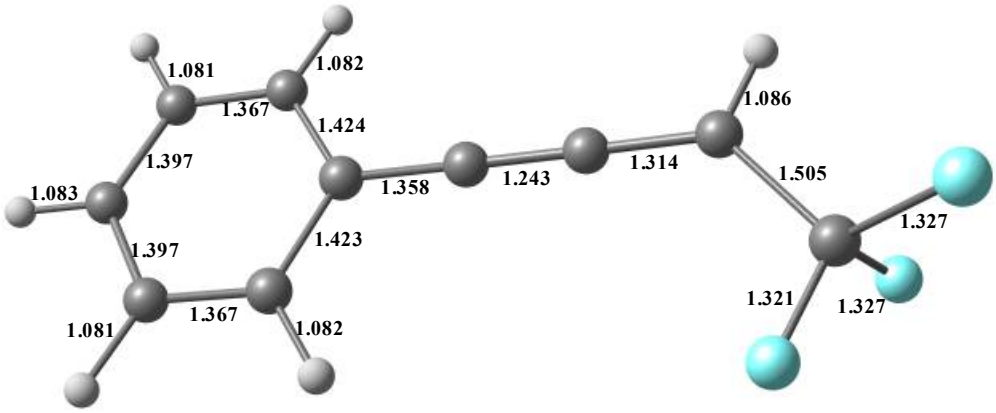
C	3	-0.13798	1.99905	4.12114	0.01780	6.13798
C	4	-0.20348	1.99912	4.18470	0.01967	6.20348
C	5	-0.20355	1.99912	4.18475	0.01969	6.20355
C	6	-0.16135	1.99913	4.14256	0.01967	6.16135
H	7	0.22335	0.00000	0.77507	0.00157	0.77665
H	8	0.22345	0.00000	0.77494	0.00161	0.77655
H	9	0.22121	0.00000	0.77718	0.00161	0.77879
H	10	0.22123	0.00000	0.77716	0.00160	0.77877
H	11	0.21833	0.00000	0.78019	0.00148	0.78167
C	12	0.17231	1.99840	3.81349	0.01581	5.82769
C	13	-0.14506	1.99837	4.13312	0.01357	6.14506
C	14	0.03299	1.99863	3.94511	0.02327	5.96701
H	15	0.27718	0.00000	0.71972	0.00311	0.72282
C	16	1.11088	1.99933	2.83036	0.05942	4.88912
F	17	-0.35166	1.99990	7.34249	0.00927	9.35166
F	18	-0.35093	1.99990	7.34166	0.00936	9.35093
F	19	-0.34597	1.99990	7.33657	0.00950	9.34597
O	20	-0.66001	1.99973	6.64752	0.01276	8.66001
H	21	0.58888	0.00000	0.40812	0.00300	0.41112
H	22	0.59006	0.00000	0.40705	0.00289	0.40994
* Total *		1.00006	27.98852	73.72859	0.28283	101.99994

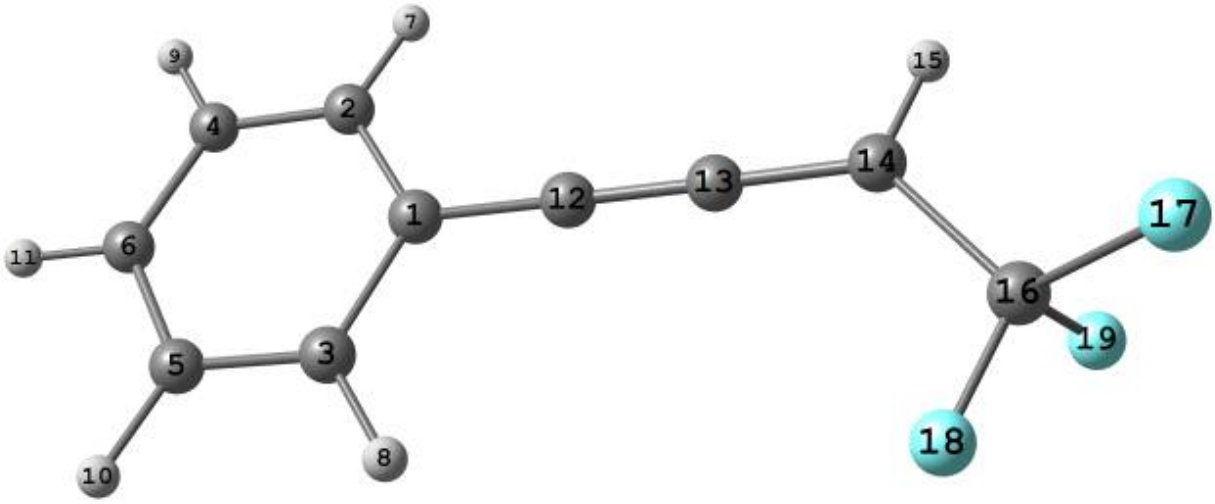
Ba

Energy **E= -683.724917402 h, G^{298}= -683.633517 h, μ=9.04 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.754124	0.190269	-0.000030
2	C	-2.684772	1.267594	-0.000006
3	C	-2.212348	-1.157076	-0.000027
4	C	-4.024254	0.993817	0.000021
5	C	-3.556627	-1.405711	0.000003
6	C	-4.454602	-0.335158	0.000032
7	H	-2.310595	2.282610	-0.000023
8	H	-1.484632	-1.957625	-0.000042
9	H	-4.748775	1.796161	0.000037
10	H	-3.926967	-2.421236	0.000004
11	H	-5.517766	-0.542358	0.000066
12	C	-0.421689	0.453489	-0.000030
13	C	0.796008	0.703596	-0.000035
14	C	2.080503	0.979941	-0.000018
15	H	2.443790	2.003286	-0.000023
16	C	3.142682	-0.086057	-0.000006
17	F	3.908465	0.053395	1.075120
18	F	2.636250	-1.305690	-0.000103
19	F	3.908650	0.053510	-1.074955





Summary of Natural Population Analysis:

Natural Population

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.18344	1.99893	4.16596	0.01854	6.18344
C	2	-0.03933	1.99906	4.02350	0.01677	6.03933
C	3	-0.02871	1.99889	4.01104	0.01879	6.02871
C	4	-0.21758	1.99911	4.19878	0.01969	6.21758
C	5	-0.22379	1.99913	4.20399	0.02067	6.22379

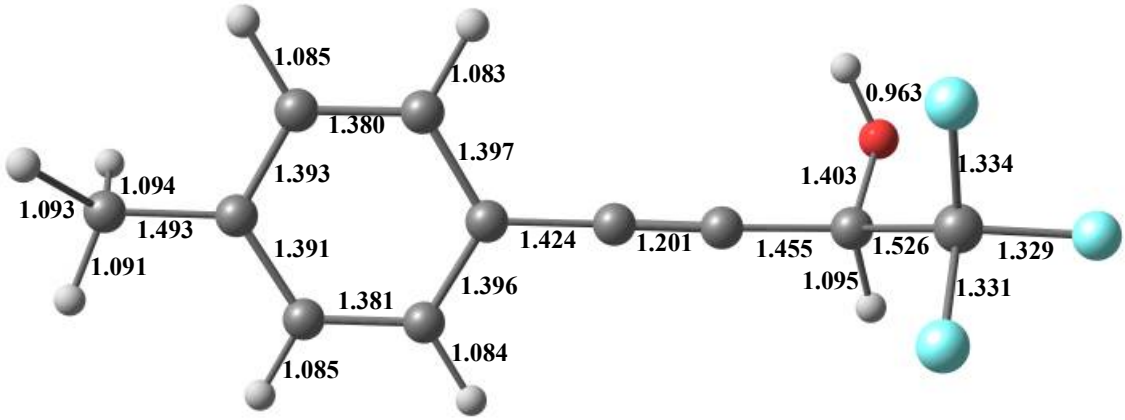
C	6	-0.01264	1.99916	3.99560	0.01788	6.01264
H	7	0.24095	0.00000	0.75767	0.00138	0.75905
H	8	0.24001	0.00000	0.75866	0.00133	0.75999
H	9	0.24080	0.00000	0.75764	0.00157	0.75920
H	10	0.24073	0.00000	0.75776	0.00151	0.75927
H	11	0.23298	0.00000	0.76570	0.00132	0.76702
C	12	0.28710	1.99860	3.69820	0.01610	5.71290
C	13	-0.02078	1.99853	4.01106	0.01119	6.02078
C	14	-0.07150	1.99874	4.05346	0.01930	6.07150
H	15	0.27189	0.00000	0.72593	0.00218	0.72811
C	16	1.08476	1.99938	2.86009	0.05577	4.91524
F	17	-0.34668	1.99991	7.33603	0.01074	9.34668
F	18	-0.34802	1.99991	7.33723	0.01089	9.34802
F	19	-0.34666	1.99991	7.33602	0.01074	9.34666
* Total *		1.00007	25.98926	65.75431	0.25635	91.99993

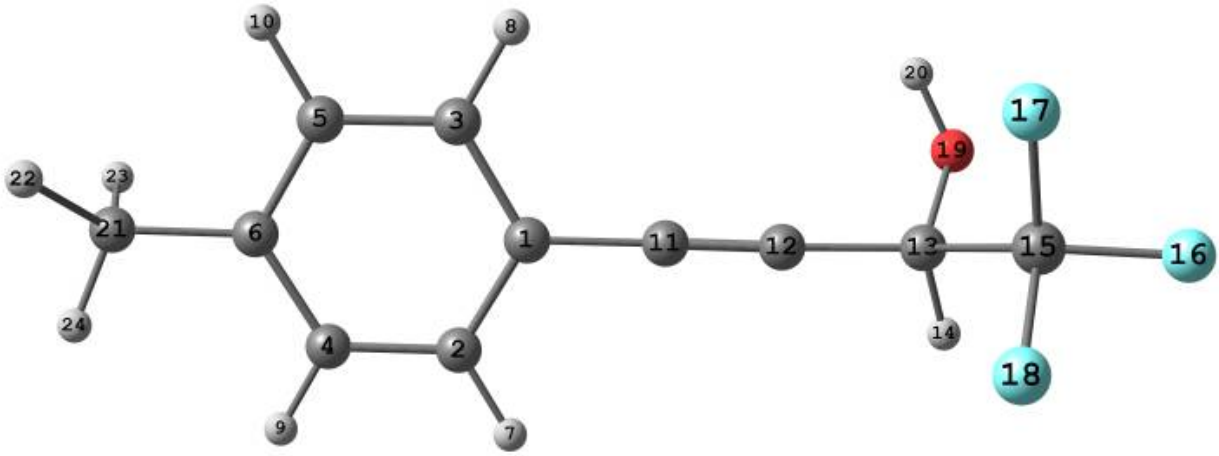
1b

Energy **E= -799.087927602 h, G^{298}= -798.954054 h, μ=4.88 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.471654	0.003623	0.254657
2	C	-2.245377	1.096588	0.650563
3	C	-2.102378	-1.085411	-0.352096
4	C	-3.610774	1.093779	0.444114
5	C	-3.468326	-1.075744	-0.547940
6	C	-4.246652	0.010371	-0.153793
7	H	-1.763190	1.945731	1.120159
8	H	-1.511575	-1.937851	-0.665090
9	H	-4.202041	1.949385	0.753915
10	H	-3.946591	-1.928153	-1.020128
11	C	-0.064012	0.000768	0.472279
12	C	1.122118	0.006873	0.661028
13	C	2.559784	-0.025524	0.884483
14	H	2.850307	0.769373	1.579354
15	C	3.309881	0.260528	-0.413512
16	F	4.622212	0.293531	-0.203479
17	F	3.072600	-0.683815	-1.326013
18	F	2.951592	1.432368	-0.933623
19	O	3.019626	-1.233701	1.429282
20	H	2.599522	-1.966337	0.966024
21	C	-5.724806	-0.001975	-0.359874
22	H	-5.978051	-0.251517	-1.393275
23	H	-6.197910	-0.757559	0.274382
24	H	-6.171930	0.964516	-0.121016





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.16568	1.99890	4.14789	0.01889	6.16568
C	2	-0.15195	1.99905	4.13473	0.01818	6.15195
C	3	-0.15276	1.99905	4.13570	0.01801	6.15276
C	4	-0.21022	1.99900	4.19208	0.01914	6.21022
C	5	-0.20671	1.99900	4.18854	0.01917	6.20671

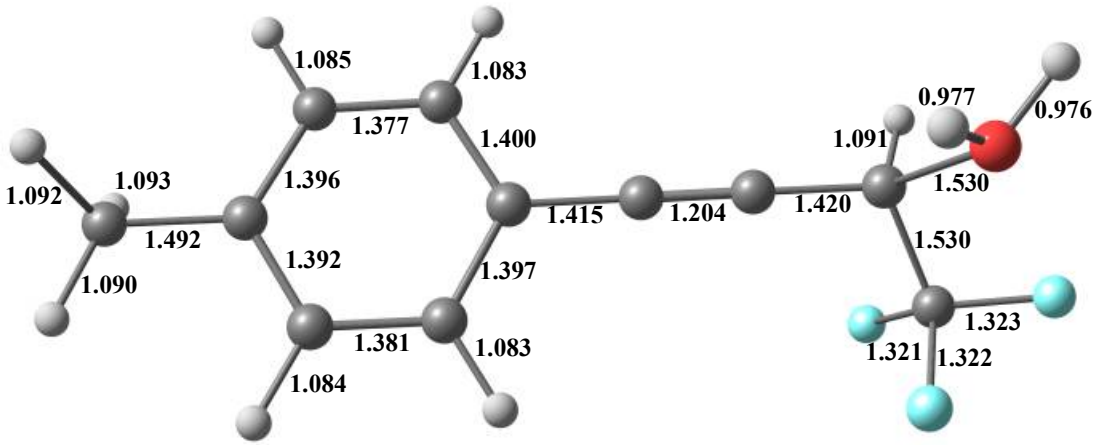
C	6	-0.00332	1.99900	3.98680	0.01752	6.00332
H	7	0.21740	0.00000	0.78090	0.00170	0.78260
H	8	0.21741	0.00000	0.78087	0.00172	0.78259
H	9	0.21327	0.00000	0.78483	0.00189	0.78673
H	10	0.21321	0.00000	0.78502	0.00178	0.78679
C	11	0.05037	1.99837	3.93490	0.01635	5.94963
C	12	-0.07262	1.99833	4.05950	0.01479	6.07262
C	13	0.01366	1.99869	3.95742	0.03023	5.98634
H	14	0.23262	0.00000	0.76424	0.00314	0.76738
C	15	1.10919	1.99931	2.83366	0.05784	4.89081
F	16	-0.36783	1.99991	7.35663	0.01129	9.36783
F	17	-0.37550	1.99991	7.36382	0.01177	9.37550
F	18	-0.36893	1.99991	7.35793	0.01110	9.36893
O	19	-0.74356	1.99978	6.72085	0.02293	8.74356
H	20	0.49967	0.00000	0.49725	0.00308	0.50033
C	21	-0.60118	1.99925	4.58994	0.01199	6.60118
H	22	0.21936	0.00000	0.77914	0.00151	0.78064
H	23	0.22219	0.00000	0.77628	0.00153	0.77781
H	24	0.21197	0.00000	0.78661	0.00143	0.78803
* Total *		0.00004	29.98747	79.69552	0.31698	109.99996

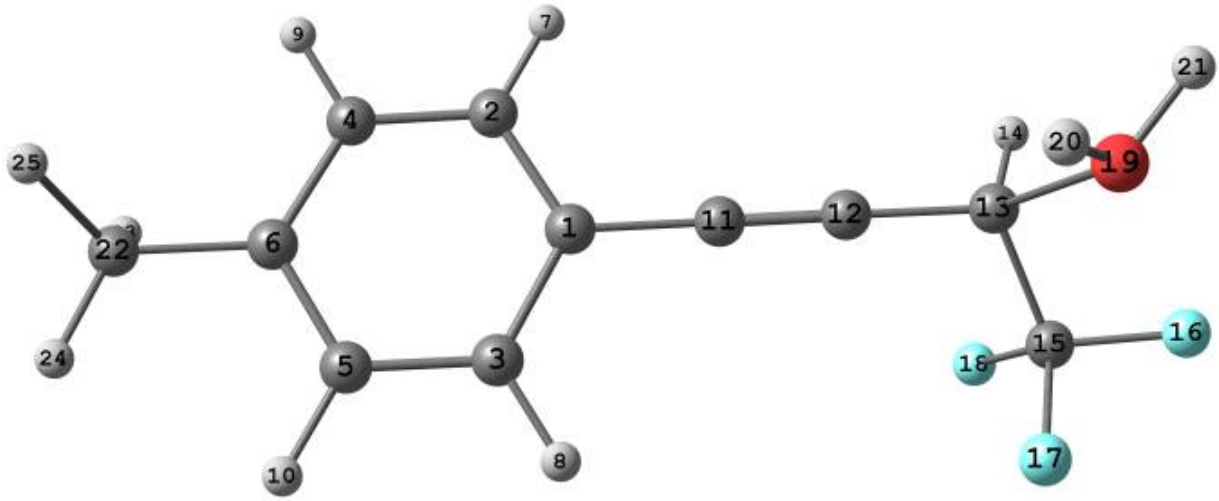
Ab

Energy **E= -799.464966852 h, G^{298}= -799.324269 h, μ=11.11 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.505552	0.240047	0.040134
2	C	2.375490	1.204387	0.562258
3	C	2.030756	-0.929367	-0.514644
4	C	3.736139	0.993616	0.526271
5	C	3.397174	-1.125627	-0.542185
6	C	4.270116	-0.173094	-0.023195
7	H	1.968602	2.111936	0.991301
8	H	1.358545	-1.675577	-0.919963
9	H	4.407116	1.743626	0.930929
10	H	3.799301	-2.035187	-0.973993
11	C	0.106684	0.446356	0.078770
12	C	-1.083628	0.622578	0.118312
13	C	-2.489121	0.818247	0.165232
14	H	-2.818732	1.490450	0.958201
15	C	-3.294215	-0.480936	0.238784
16	F	-4.591554	-0.222044	0.203763
17	F	-3.000112	-1.286414	-0.767829
18	F	-3.008375	-1.088181	1.376609
19	O	-2.976501	1.464488	-1.132784
20	H	-2.242688	1.627646	-1.757477
21	H	-3.486708	2.285909	-1.001305
22	C	5.747286	-0.383527	-0.042714
23	H	6.141938	-0.449119	0.974480
24	H	6.017021	-1.297782	-0.571005
25	H	6.254587	0.455867	-0.523921





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.19484	1.99890	4.17758	0.01836	6.19484
C	2	-0.12896	1.99905	4.11222	0.01769	6.12896
C	3	-0.12641	1.99905	4.10957	0.01779	6.12641

C	4	-0.20852	1.99900	4.19031	0.01921	6.20852
C	5	-0.21271	1.99900	4.19460	0.01910	6.21271
C	6	0.02506	1.99901	3.95867	0.01726	5.97494
H	7	0.22244	0.00000	0.77592	0.00164	0.77756
H	8	0.22268	0.00000	0.77566	0.00166	0.77732
H	9	0.21784	0.00000	0.78040	0.00176	0.78216
H	10	0.21789	0.00000	0.78023	0.00188	0.78211
C	11	0.17454	1.99841	3.81119	0.01586	5.82546
C	12	-0.15344	1.99837	4.14135	0.01372	6.15344
C	13	0.03227	1.99862	3.94581	0.02329	5.96773
H	14	0.27630	0.00000	0.72057	0.00313	0.72370
C	15	1.11069	1.99933	2.83059	0.05939	4.88931
F	16	-0.35201	1.99990	7.34285	0.00926	9.35201
F	17	-0.35143	1.99990	7.34218	0.00935	9.35143
F	18	-0.34633	1.99990	7.33692	0.00950	9.34633
O	19	-0.66184	1.99974	6.64930	0.01280	8.66184
H	20	0.58772	0.00000	0.40927	0.00301	0.41228
H	21	0.58896	0.00000	0.40813	0.00291	0.41104
C	22	-0.60484	1.99925	4.59349	0.01209	6.60484
H	23	0.22649	0.00000	0.77202	0.00150	0.77351
H	24	0.21425	0.00000	0.78432	0.00142	0.78575
H	25	0.22420	0.00000	0.77431	0.00149	0.77580

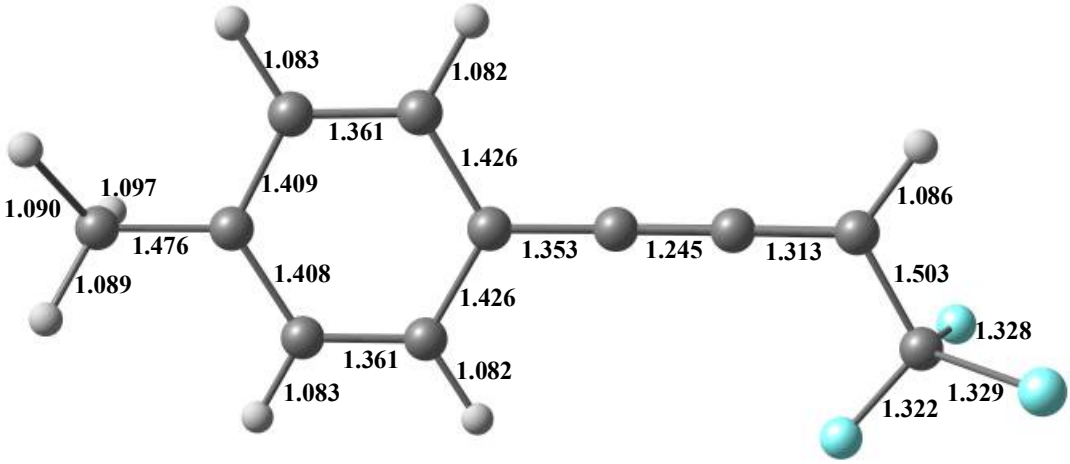
* Total *	1.00004	29.98744	79.71746	0.29506	109.99996

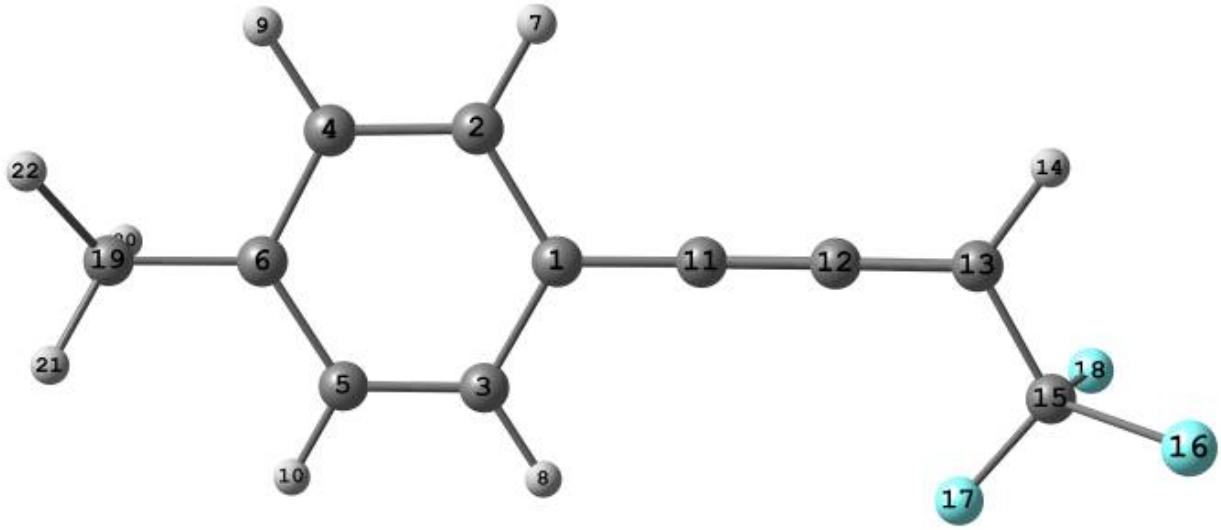
Bb

Energy **E= -723.028617163 h, G^{298}= -722.912242 h, μ=9.22 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.247230	-0.309040	0.001469
2	C	-2.174963	-1.392418	0.000060
3	C	-1.729296	1.033322	-0.001797
4	C	-3.510895	-1.132349	-0.005553
5	C	-3.070212	1.266187	-0.010639
6	C	-3.984070	0.194411	-0.011721
7	H	-1.795260	-2.405529	0.001358
8	H	-1.013325	1.844648	-0.002176
9	H	-4.226580	-1.944709	-0.010035
10	H	-3.449543	2.280093	-0.020406
11	C	0.083884	-0.549987	0.001558
12	C	1.310079	-0.764348	-0.000195
13	C	2.605338	-0.980894	-0.003852
14	H	3.021740	-1.983356	-0.013753
15	C	3.606947	0.139814	0.001901
16	F	4.340525	0.090412	-1.104892
17	F	3.035752	1.329993	0.069819
18	F	4.422942	0.005584	1.041375
19	C	-5.436308	0.460333	0.006101
20	H	-5.772330	0.500377	1.049301
21	H	-5.678393	1.421463	-0.446136
22	H	-5.998920	-0.337072	-0.478859





Summary of Natural Population Analysis:

Natural Population

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.17647	1.99893	4.15930	0.01825	6.17647
C	2	-0.03870	1.99905	4.02277	0.01688	6.03870
C	3	-0.02652	1.99889	4.00867	0.01895	6.02652
C	4	-0.22254	1.99898	4.20383	0.01973	6.22254

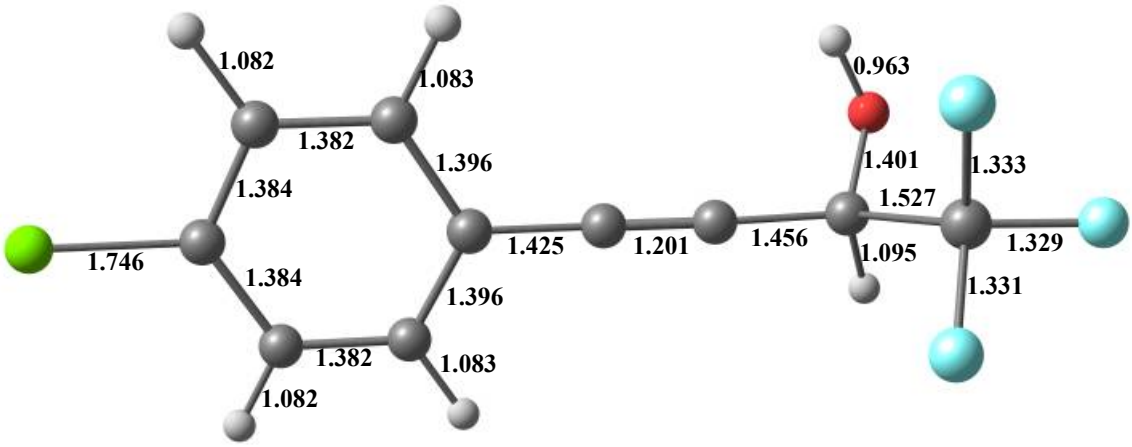
C	5	-0.22963	1.99900	4.20985	0.02079	6.22963
C	6	0.18290	1.99906	3.80190	0.01614	5.81710
H	7	0.24085	0.00000	0.75774	0.00141	0.75915
H	8	0.23988	0.00000	0.75876	0.00136	0.76012
H	9	0.23807	0.00000	0.76014	0.00179	0.76193
H	10	0.23809	0.00000	0.76016	0.00174	0.76191
C	11	0.25789	1.99860	3.72732	0.01619	5.74211
C	12	-0.01344	1.99854	4.00361	0.01128	6.01344
C	13	-0.10138	1.99874	4.08333	0.01932	6.10138
H	14	0.26902	0.00000	0.72880	0.00218	0.73098
C	15	1.08614	1.99936	2.85876	0.05573	4.91386
F	16	-0.34974	1.99991	7.33912	0.01070	9.34974
F	17	-0.35053	1.99991	7.33977	0.01086	9.35053
F	18	-0.34981	1.99991	7.33921	0.01069	9.34981
C	19	-0.62960	1.99922	4.61612	0.01425	6.62960
H	20	0.26407	0.00000	0.73449	0.00144	0.73593
H	21	0.23509	0.00000	0.76334	0.00157	0.76491
H	22	0.23639	0.00000	0.76205	0.00156	0.76361
* Total *		1.00004	27.98810	71.73906	0.27281	99.99996

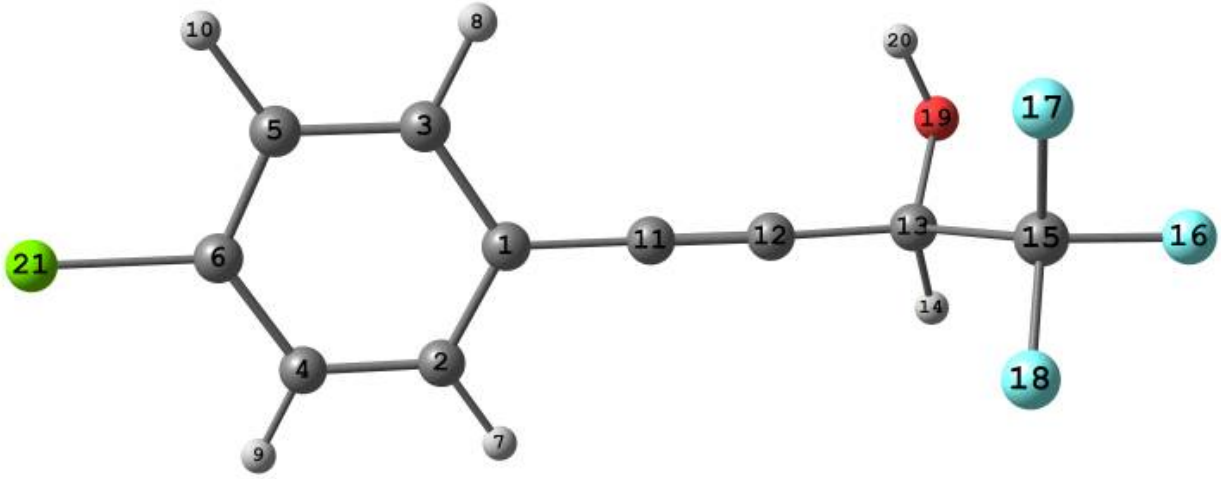
1c

Energy **E= -1219.38701302 h, G^{298}= -1219,289542 h, μ=2.06 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.061992	0.017212	-0.305288
2	C	-1.823278	-1.071491	-0.735490
3	C	-1.698714	1.092852	0.316301
4	C	-3.192048	-1.087461	-0.548973
5	C	-3.067587	1.084287	0.503055
6	C	-3.799029	-0.007596	0.068312
7	H	-1.333800	-1.908040	-1.218424
8	H	-1.112718	1.939301	0.651979
9	H	-3.785170	-1.930064	-0.879215
10	H	-3.565179	1.916279	0.983616
11	C	0.349295	0.028318	-0.500148
12	C	1.538169	0.030293	-0.667777
13	C	2.979035	0.076619	-0.869175
14	H	3.281437	-0.680873	-1.600108
15	C	3.707607	-0.284869	0.423087
16	F	5.022449	-0.312341	0.232062
17	F	3.459338	0.603430	1.385766
18	F	3.333987	-1.483363	0.864410
19	O	3.444225	1.311124	-1.340231
20	H	3.013686	2.018628	-0.848518
21	Cl	-5.528398	-0.022514	0.305232





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.14780	1.99891	4.13274	0.01616	6.14780
C	2	-0.14189	1.99905	4.12531	0.01753	6.14189
C	3	-0.14225	1.99905	4.12569	0.01751	6.14225
C	4	-0.22572	1.99891	4.20505	0.02175	6.22572
C	5	-0.22548	1.99892	4.20483	0.02173	6.22548

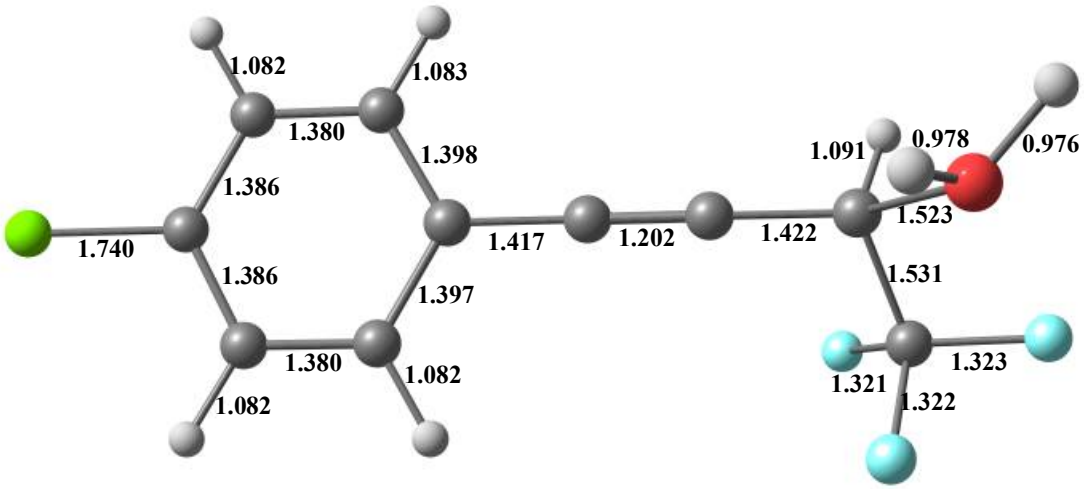
C	6	-0.02658	1.99851	3.99993	0.02814	6.02658
H	7	0.22549	0.00000	0.77292	0.00159	0.77451
H	8	0.22544	0.00000	0.77295	0.00161	0.77456
H	9	0.23229	0.00000	0.76567	0.00203	0.76771
H	10	0.23222	0.00000	0.76575	0.00203	0.76778
C	11	0.04432	1.99836	3.94195	0.01536	5.95568
C	12	-0.04662	1.99831	4.03424	0.01407	6.04662
C	13	-0.00708	1.99893	3.97705	0.03110	6.00708
H	14	0.23536	0.00000	0.76210	0.00254	0.76464
C	15	1.11239	1.99930	2.83047	0.05784	4.88761
F	16	-0.36709	1.99991	7.35579	0.01139	9.36709
F	17	-0.37436	1.99991	7.36270	0.01175	9.37436
F	18	-0.36854	1.99991	7.35761	0.01103	9.36854
O	19	-0.74009	1.99978	6.71826	0.02205	8.74009
H	20	0.50019	0.00000	0.49679	0.00302	0.49981
Cl	21	0.00582	9.99959	6.97694	0.01765	16.99418
* Total *		0.00000	37.98734	79.68478	0.32788	118.00000

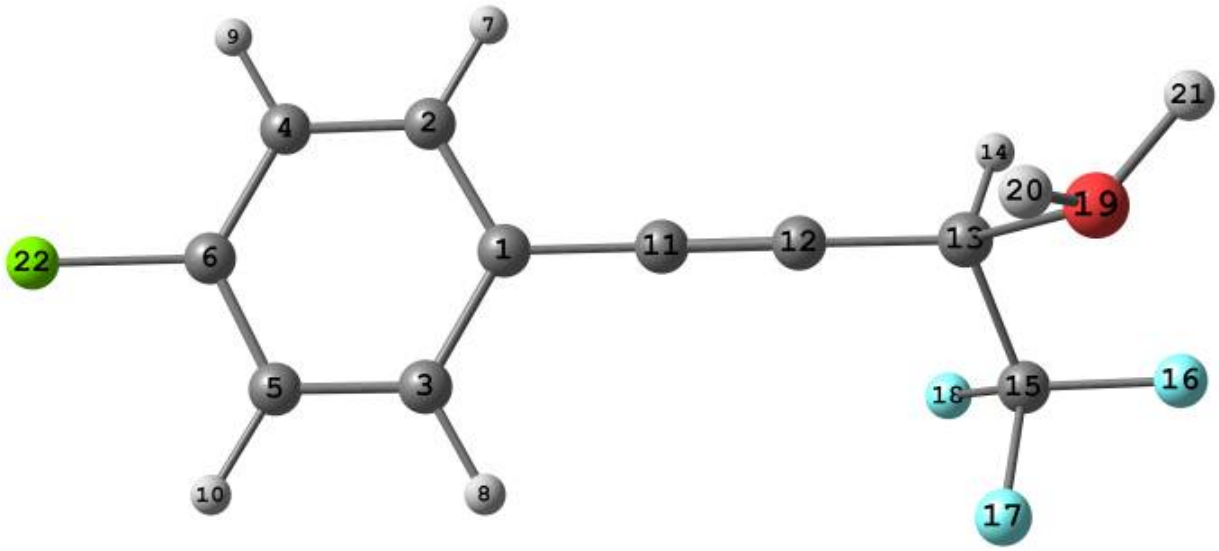
Ac

Energy **E= -1219.76264667 h, G^{298}= -1219.65356 h, μ=14.83 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.099713	0.286935	0.045824
2	C	1.950076	1.272262	0.554938
3	C	1.638540	-0.884882	-0.492119
4	C	3.317270	1.090271	0.528058
5	C	3.005218	-1.070873	-0.519061
6	C	3.828617	-0.080846	-0.007651
7	H	1.530360	2.179142	0.971435
8	H	0.977858	-1.646427	-0.886244
9	H	3.984774	1.846176	0.919438
10	H	3.433102	-1.974736	-0.931631
11	C	-0.304172	0.472755	0.081598
12	C	-1.495669	0.630431	0.118947
13	C	-2.906162	0.806288	0.164217
14	H	-3.243370	1.467844	0.963041
15	C	-3.691492	-0.505868	0.233590
16	F	-4.991723	-0.264444	0.202619
17	F	-3.387518	-1.300935	-0.778226
18	F	-3.393266	-1.114267	1.367220
19	O	-3.399624	1.451440	-1.124486
20	H	-2.675919	1.606223	-1.763160
21	H	-3.904413	2.275787	-0.989693
22	Cl	5.552678	-0.314562	-0.038932





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.18032	1.99890	4.16324	0.01818	6.18032
C	2	-0.11913	1.99905	4.10267	0.01741	6.11913
C	3	-0.11903	1.99905	4.10259	0.01739	6.11903
C	4	-0.22661	1.99891	4.20576	0.02194	6.22661
C	5	-0.22670	1.99891	4.20584	0.02195	6.22670

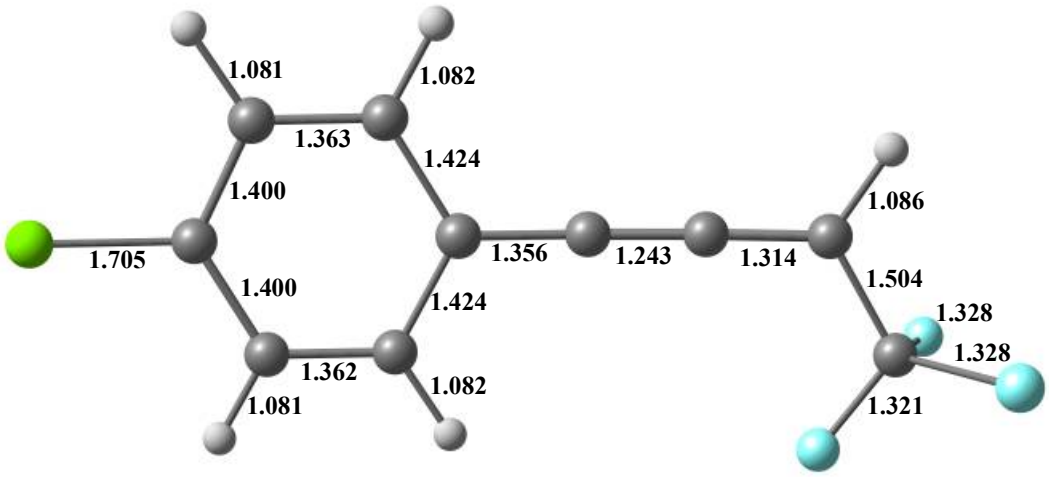
C	6	-0.00892	1.99853	3.98183	0.02856	6.00892
H	7	0.23015	0.00000	0.76825	0.00160	0.76985
H	8	0.23031	0.00000	0.76806	0.00164	0.76969
H	9	0.23619	0.00000	0.76179	0.00202	0.76381
H	10	0.23618	0.00000	0.76180	0.00202	0.76382
C	11	0.16778	1.99840	3.81795	0.01587	5.83222
C	12	-0.13726	1.99836	4.12537	0.01353	6.13726
C	13	0.03213	1.99863	3.94597	0.02327	5.96787
H	14	0.27808	0.00000	0.71880	0.00311	0.72192
C	15	1.11103	1.99933	2.83018	0.05945	4.88897
F	16	-0.35102	1.99990	7.34185	0.00927	9.35102
F	17	-0.35101	1.99990	7.34174	0.00937	9.35101
F	18	-0.34567	1.99990	7.33626	0.00950	9.34567
O	19	-0.65906	1.99973	6.64658	0.01274	8.65906
H	20	0.58901	0.00000	0.40801	0.00298	0.41099
H	21	0.59061	0.00000	0.40652	0.00288	0.40939
Cl	22	0.02332	9.99958	6.95945	0.01765	16.97668
* Total *		1.00005	37.98709	79.70052	0.31234	117.99995

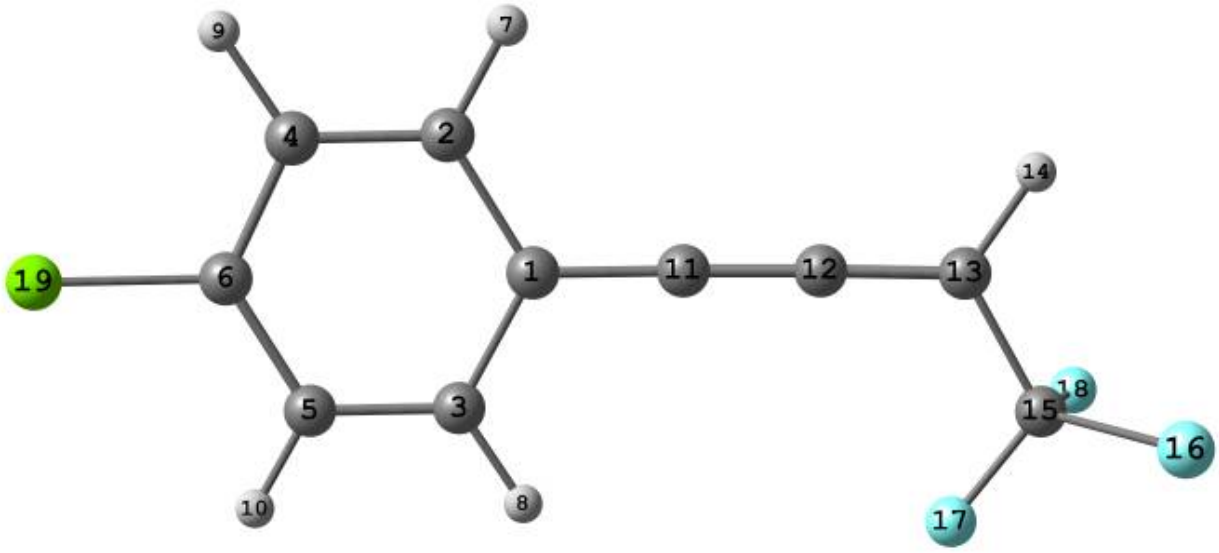
Bc

Energy **E= -1143.32127734 h, G^{298}= -1143.238982 h, μ=5.34 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-0.822448	0.378984	0.000004
2	C	-1.736739	1.470831	-0.000059
3	C	-1.311141	-0.958949	0.000075
4	C	-3.078083	1.230526	-0.000050
5	C	-2.653831	-1.190182	0.000086
6	C	-3.527169	-0.095790	0.000026
7	H	-1.349718	2.480902	-0.000113
8	H	-0.602687	-1.776540	0.000122
9	H	-3.795483	2.038867	-0.000096
10	H	-3.053264	-2.194391	0.000144
11	C	0.514439	0.605814	0.000016
12	C	1.742970	0.796829	0.000067
13	C	3.044706	0.976748	0.000153
14	H	3.491267	1.966292	0.000139
15	C	4.009761	-0.177341	-0.000048
16	F	4.785838	-0.108721	1.075022
17	F	3.397785	-1.348221	-0.000397
18	F	4.786061	-0.108186	-1.074921
19	Cl	-5.206592	-0.391400	0.000051





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.17842	1.99894	4.16130	0.01818	6.17842
C	2	-0.03308	1.99905	4.01731	0.01672	6.03308
C	3	-0.02104	1.99889	4.00320	0.01895	6.02104
C	4	-0.23413	1.99891	4.21243	0.02278	6.23413

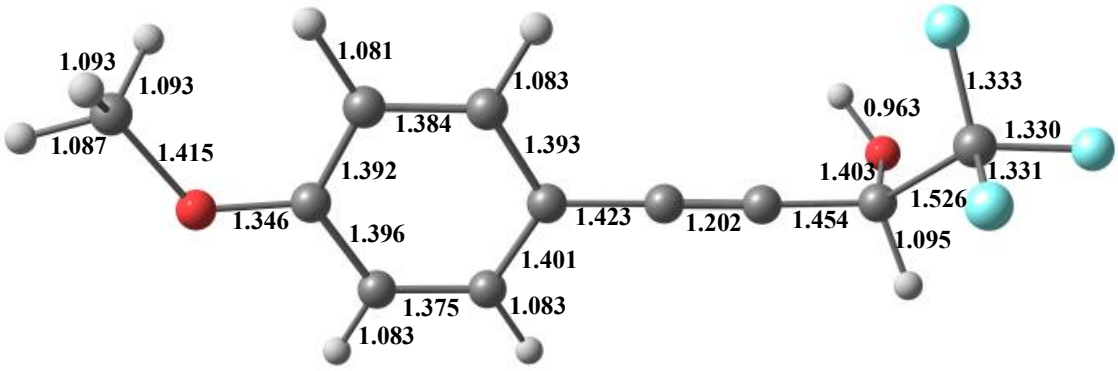
C	5	-0.24095	1.99894	4.21843	0.02358	6.24095
C	6	0.08483	1.99866	3.88601	0.03049	5.91517
H	7	0.24709	0.00000	0.75150	0.00141	0.75291
H	8	0.24602	0.00000	0.75262	0.00136	0.75398
H	9	0.25343	0.00000	0.74458	0.00199	0.74657
H	10	0.25345	0.00000	0.74464	0.00191	0.74655
C	11	0.26776	1.99860	3.71738	0.01627	5.73224
C	12	-0.01327	1.99854	4.00352	0.01121	6.01327
C	13	-0.08527	1.99874	4.06710	0.01943	6.08527
H	14	0.27109	0.00000	0.72675	0.00216	0.72891
C	15	1.08554	1.99937	2.85929	0.05580	4.91446
F	16	-0.34795	1.99991	7.33732	0.01072	9.34795
F	17	-0.34923	1.99991	7.33841	0.01091	9.34923
F	18	-0.34795	1.99991	7.33732	0.01072	9.34795
Cl	19	0.14212	9.99950	6.84020	0.01818	16.85788
* Total *		1.00005	35.98786	71.71931	0.29279	107.99995

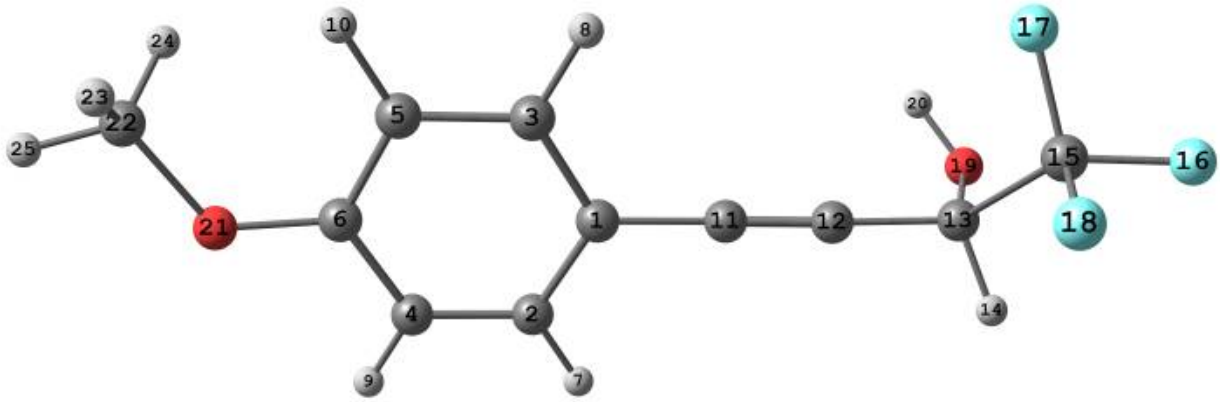
1d

Energy **E= -874.29165152 h, G^{298}= -874.15655 h, μ=5.47 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-1.043916	0.425427	-0.018456
2	C	-1.855807	1.475719	-0.465952
3	C	-1.651944	-0.760950	0.387001
4	C	-3.223042	1.337397	-0.503401
5	C	-3.027420	-0.909139	0.352503
6	C	-3.820891	0.144100	-0.093893
7	H	-1.396554	2.403429	-0.785563
8	H	-1.035314	-1.580990	0.735067
9	H	-3.857566	2.144475	-0.848606
10	H	-3.468475	-1.842190	0.674285
11	C	0.371118	0.567926	0.019887
12	C	1.566511	0.691937	0.046272
13	C	3.011207	0.836923	0.121456
14	H	3.355762	1.581576	-0.604418
15	C	3.695887	-0.468166	-0.275892
16	F	5.018239	-0.327704	-0.273962
17	F	3.396039	-1.454902	0.569041
18	F	3.330150	-0.849589	-1.497564
19	O	3.480321	1.244963	1.379495
20	H	2.983618	0.782679	2.062750
21	O	-5.164793	0.104372	-0.166035
22	C	-5.819453	-1.082735	0.240117
23	H	-5.516786	-1.933173	-0.376599
24	H	-5.618393	-1.305735	1.291347
25	H	-6.883868	-0.905623	0.108570





Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.19065	1.99890	4.17272	0.01903	6.19065
C	2	-0.14029	1.99906	4.12373	0.01750	6.14029
C	3	-0.13169	1.99907	4.11452	0.01810	6.13169
C	4	-0.25099	1.99902	4.23177	0.02020	6.25099
C	5	-0.29625	1.99901	4.27941	0.01783	6.29625
C	6	0.36421	1.99875	3.61495	0.02209	5.63579
H	7	0.21954	0.00000	0.77882	0.00163	0.78046
H	8	0.21912	0.00000	0.77920	0.00168	0.78088

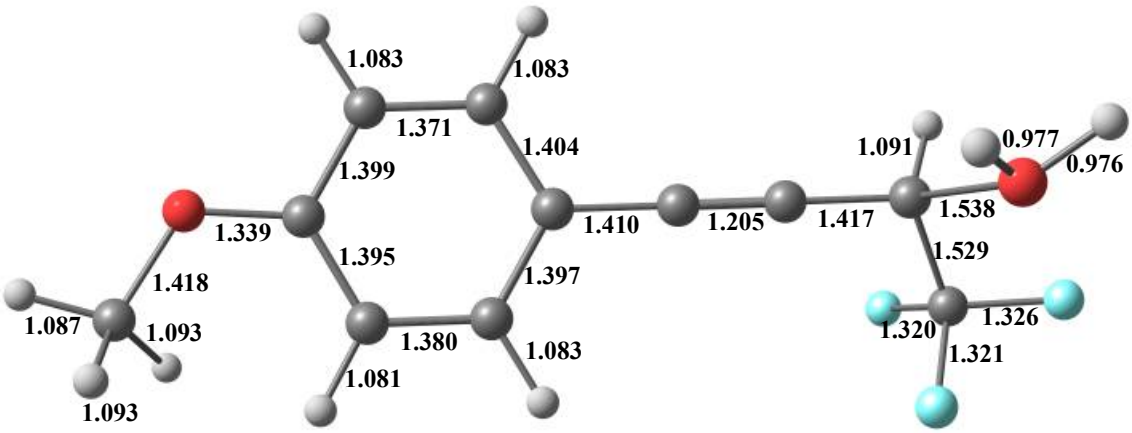
H	9	0.22475	0.00000	0.77321	0.00204	0.77525
H	10	0.22692	0.00000	0.77104	0.00205	0.77308
C	11	0.05198	1.99838	3.93335	0.01628	5.94802
C	12	-0.08224	1.99834	4.06899	0.01490	6.08224
C	13	0.01302	1.99869	3.95792	0.03038	5.98698
H	14	0.23126	0.00000	0.76554	0.00320	0.76874
C	15	1.10952	1.99931	2.83326	0.05791	4.89048
F	16	-0.36861	1.99991	7.35743	0.01127	9.36861
F	17	-0.37480	1.99991	7.36308	0.01181	9.37480
F	18	-0.36960	1.99991	7.35853	0.01116	9.36960
O	19	-0.74556	1.99978	6.72286	0.02291	8.74556
H	20	0.49987	0.00000	0.49704	0.00309	0.50013
O	21	-0.56259	1.99970	6.53600	0.02689	8.56259
C	22	-0.20375	1.99920	4.19078	0.01377	6.20375
H	23	0.17950	0.00000	0.81840	0.00210	0.82050
H	24	0.17946	0.00000	0.81844	0.00210	0.82054
H	25	0.19789	0.00000	0.80094	0.00116	0.80211
* Total *		0.00004	31.98694	85.66193	0.35109	117.99996

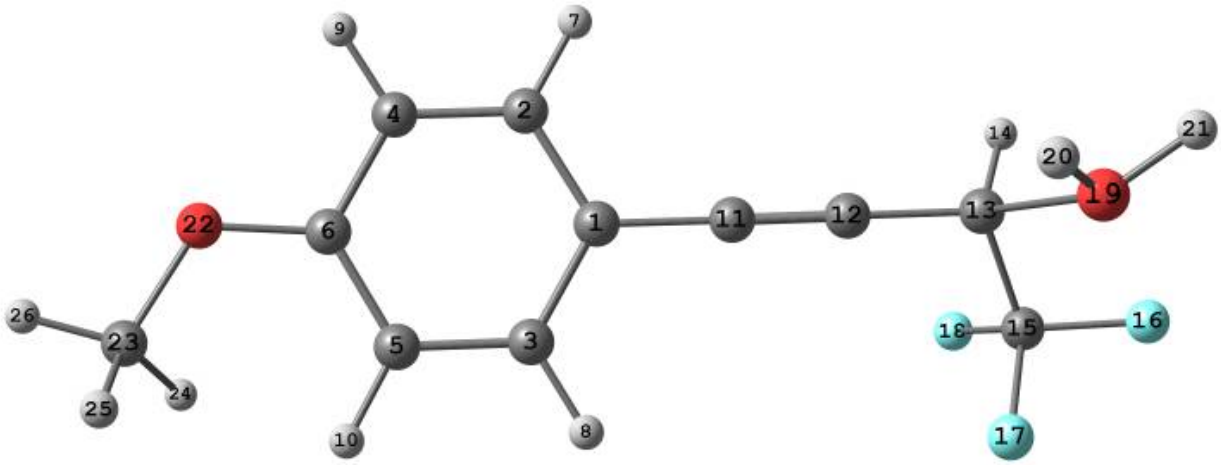
Ad

Energy **E= -874.669518254 h, G^{298}= -874.522358 h, μ=11.41 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.082067	0.401359	0.078029
2	C	1.892459	1.459400	0.518997
3	C	1.686858	-0.779963	-0.357053
4	C	3.257708	1.332612	0.519781
5	C	3.060071	-0.914974	-0.355449
6	C	3.854010	0.144988	0.083068
7	H	1.430313	2.377932	0.858968
8	H	1.066669	-1.599889	-0.697850
9	H	3.896158	2.139904	0.855882
10	H	3.504252	-1.839588	-0.695675
11	C	-0.322233	0.530091	0.077993
12	C	-1.522097	0.645677	0.083240
13	C	-2.932645	0.775666	0.107528
14	H	-3.303122	1.481807	0.852306
15	C	-3.678697	-0.551939	0.242161
16	F	-4.985389	-0.352572	0.143286
17	F	-3.314986	-1.409227	-0.695210
18	F	-3.412913	-1.068405	1.427998
19	O	-3.423124	1.311106	-1.247845
20	H	-2.691421	1.710706	-1.756868
21	H	-4.167162	1.940345	-1.187905
22	O	5.192202	0.116970	0.121580
23	C	5.855919	-1.060308	-0.308265
24	H	5.578709	-1.916533	0.311265
25	H	5.632585	-1.276967	-1.355631
26	H	6.919461	-0.866148	-0.199228





Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.21890	1.99890	4.20146	0.01854	6.21890
C	2	-0.11932	1.99906	4.10304	0.01722	6.11932
C	3	-0.10670	1.99907	4.08987	0.01776	6.10670
C	4	-0.25123	1.99902	4.23201	0.02020	6.25123
C	5	-0.29705	1.99901	4.28027	0.01777	6.29705
C	6	0.38956	1.99878	3.58961	0.02206	5.61044
H	7	0.22448	0.00000	0.77394	0.00158	0.77552

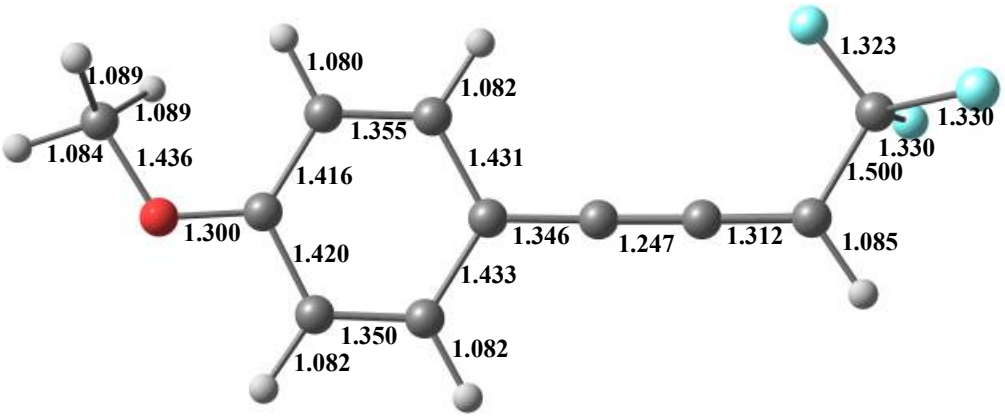
H	8	0.22444	0.00000	0.77394	0.00162	0.77556
H	9	0.22923	0.00000	0.76875	0.00202	0.77077
H	10	0.23113	0.00000	0.76685	0.00202	0.76887
C	11	0.17640	1.99843	3.80938	0.01580	5.82360
C	12	-0.16284	1.99838	4.15026	0.01419	6.16284
C	13	0.03180	1.99862	3.94675	0.02283	5.96820
H	14	0.27479	0.00000	0.72210	0.00311	0.72521
C	15	1.10979	1.99932	2.83146	0.05944	4.89021
F	16	-0.35486	1.99991	7.34570	0.00926	9.35486
F	17	-0.35016	1.99990	7.34095	0.00931	9.35016
F	18	-0.34567	1.99990	7.33628	0.00949	9.34567
O	19	-0.66614	1.99974	6.65347	0.01293	8.66614
H	20	0.58667	0.00000	0.41021	0.00312	0.41333
H	21	0.58571	0.00000	0.41125	0.00304	0.41429
O	22	-0.55183	1.99969	6.52533	0.02681	8.55183
C	23	-0.20553	1.99920	4.19280	0.01353	6.20553
H	24	0.18290	0.00000	0.81511	0.00200	0.81710
H	25	0.18275	0.00000	0.81525	0.00200	0.81725
H	26	0.20062	0.00000	0.79824	0.00114	0.79938
* Total *		1.00004	31.98693	85.68424	0.32878	117.99996

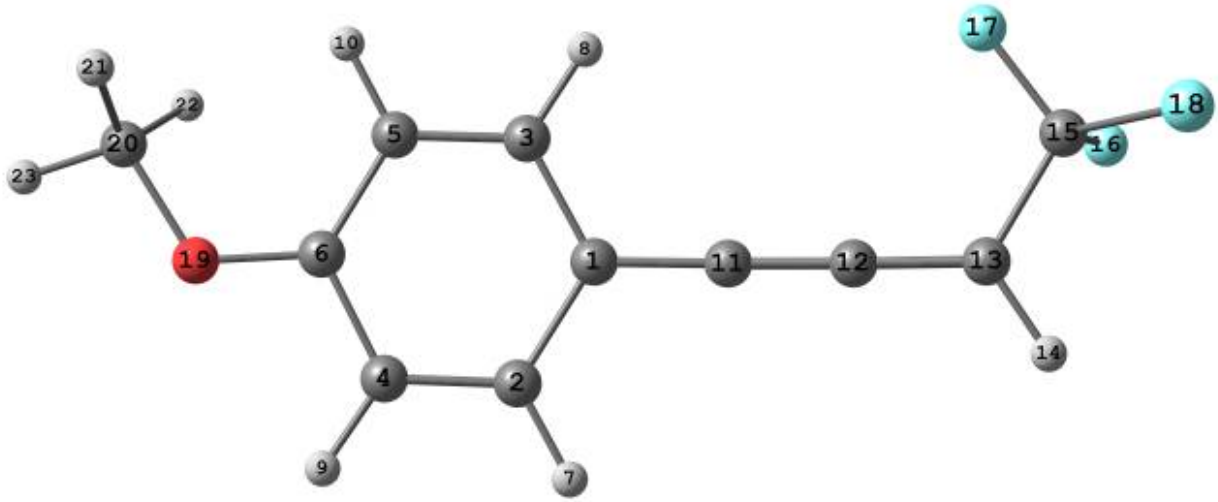
Bd

Energy **E= -798.241975319 h, G^{298}= -798.121258 h, μ=9.52 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-0.798223	0.516172	0.000084
2	C	-1.681619	1.644551	-0.000006
3	C	-1.351260	-0.803812	0.000124
4	C	-3.018472	1.455127	-0.000056
5	C	-2.693166	-0.992677	0.000081
6	C	-3.546803	0.137191	-0.000007
7	H	-1.256076	2.639176	-0.000039
8	H	-0.673795	-1.647558	0.000193
9	H	-3.716655	2.281169	-0.000127
10	H	-3.104815	-1.991074	0.000114
11	C	0.537861	0.679760	0.000141
12	C	1.777573	0.813316	0.000242
13	C	3.084159	0.936212	0.000333
14	H	3.573932	1.904759	-0.000030
15	C	3.997851	-0.253118	-0.000070
16	F	4.782539	-0.224483	1.073997
17	F	3.340117	-1.401515	-0.000135
18	F	4.782115	-0.224115	-1.074439
19	O	-4.844630	0.061584	-0.000044
20	C	-5.502754	-1.214322	0.000021
21	H	-5.237570	-1.773440	-0.896666
22	H	-5.237633	-1.773319	0.896801
23	H	-6.564164	-0.991768	-0.000032





Summary of Natural Population Analysis:

Natural Population

Natural ----------

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.16420	1.99890	4.14728	0.01802	6.16420
C	2	-0.06174	1.99905	4.04571	0.01697	6.06174
C	3	-0.03165	1.99907	4.01512	0.01747	6.03165
C	4	-0.24122	1.99901	4.22173	0.02049	6.24122
C	5	-0.28815	1.99901	4.27134	0.01780	6.28815

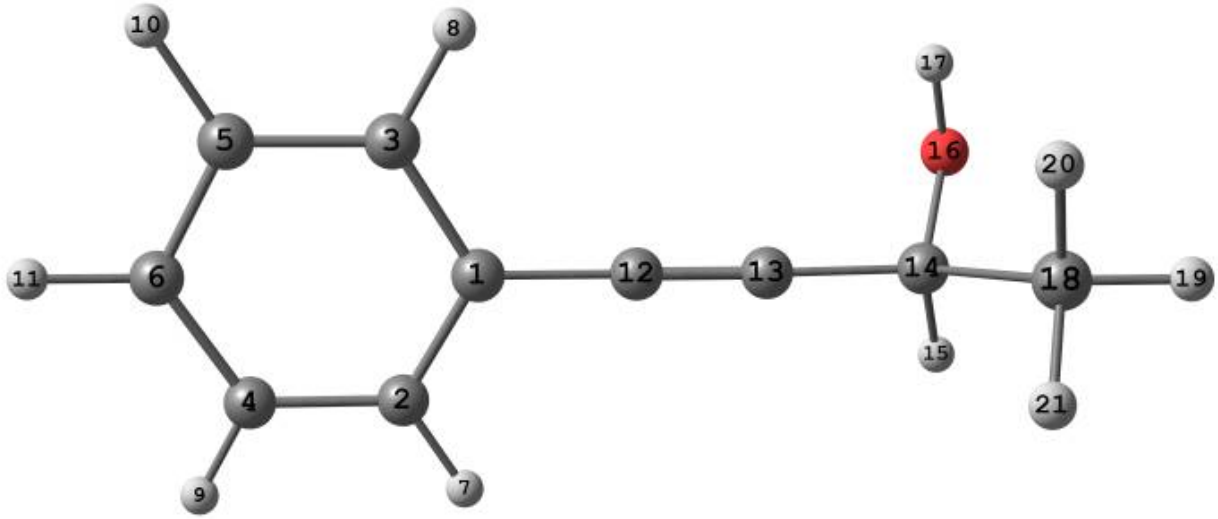
C	6	0.51768	1.99892	3.46107	0.02233	5.48232
H	7	0.24256	0.00000	0.75598	0.00146	0.75744
H	8	0.24274	0.00000	0.75576	0.00150	0.75726
H	9	0.24868	0.00000	0.74940	0.00192	0.75132
H	10	0.24935	0.00000	0.74874	0.00191	0.75065
C	11	0.21241	1.99859	3.77217	0.01683	5.78759
C	12	-0.00057	1.99855	3.99059	0.01143	6.00057
C	13	-0.14427	1.99873	4.12619	0.01935	6.14427
H	14	0.26523	0.00000	0.73254	0.00223	0.73477
C	15	1.08815	1.99935	2.85680	0.05571	4.91185
F	16	-0.35419	1.99991	7.34362	0.01066	9.35419
F	17	-0.35376	1.99991	7.34304	0.01081	9.35376
F	18	-0.35418	1.99991	7.34361	0.01066	9.35418
O	19	-0.47808	1.99966	6.45176	0.02666	8.47808
C	20	-0.21394	1.99917	4.20245	0.01232	6.21394
H	21	0.20205	0.00000	0.79636	0.00159	0.79795
H	22	0.20205	0.00000	0.79636	0.00159	0.79795
H	23	0.21508	0.00000	0.78389	0.00103	0.78492
* Total *		1.00003	29.98773	77.71150	0.30074	107.99997

1f

Energy **E= -462.043585527 h, G^{298}= -461.912149 h, μ=2.44 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-0.993625	-0.072542	-0.045374
2	C	-1.792193	-1.208710	-0.198857
3	C	-1.605119	1.165139	0.168455
4	C	-3.170673	-1.105775	-0.137532
5	C	-2.984262	1.261040	0.225500
6	C	-3.770174	0.127618	0.073697
7	H	-1.319982	-2.169727	-0.364929
8	H	-0.987523	2.047174	0.288511
9	H	-3.780775	-1.992898	-0.256251
10	H	-3.448632	2.225823	0.390166
11	H	-4.849441	0.205657	0.120152
12	C	0.428577	-0.174250	-0.104857
13	C	1.627117	-0.260929	-0.158504
14	C	3.088112	-0.333601	-0.197826
15	H	3.376899	-1.281830	-0.662057
16	O	3.632786	0.667220	-1.048146
17	H	3.401660	1.527998	-0.685073
18	C	3.681760	-0.261245	1.196106
19	H	4.768041	-0.339065	1.139370
20	H	3.418978	0.688556	1.668429
21	H	3.301367	-1.069913	1.821998



Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.13714	1.99891	4.12142	0.01681	6.13714
C	2	-0.17131	1.99905	4.15414	0.01812	6.17131
C	3	-0.17139	1.99905	4.15425	0.01810	6.17139
C	4	-0.20262	1.99912	4.18378	0.01972	6.20262
C	5	-0.20250	1.99912	4.18366	0.01972	6.20250
C	6	-0.19746	1.99912	4.17832	0.02002	6.19746
H	7	0.21611	0.00000	0.78230	0.00160	0.78389
H	8	0.21606	0.00000	0.78233	0.00161	0.78394
H	9	0.21503	0.00000	0.78334	0.00163	0.78497
H	10	0.21499	0.00000	0.78339	0.00162	0.78501
H	11	0.21343	0.00000	0.78504	0.00153	0.78657
C	12	-0.01418	1.99839	4.00062	0.01517	6.01418
C	13	-0.01266	1.99837	4.00077	0.01351	6.01266
C	14	0.06158	1.99903	3.91504	0.02434	5.93842
H	15	0.20568	0.00000	0.79186	0.00246	0.79432
O	16	-0.76331	1.99979	6.74923	0.01429	8.76331
H	17	0.48336	0.00000	0.51206	0.00458	0.51664
C	18	-0.58506	1.99929	4.57477	0.01101	6.58506
H	19	0.21197	0.00000	0.78642	0.00161	0.78803

H	20	0.20374	0.00000	0.79442	0.00185	0.79626
H	21	0.21569	0.00000	0.78285	0.00145	0.78431

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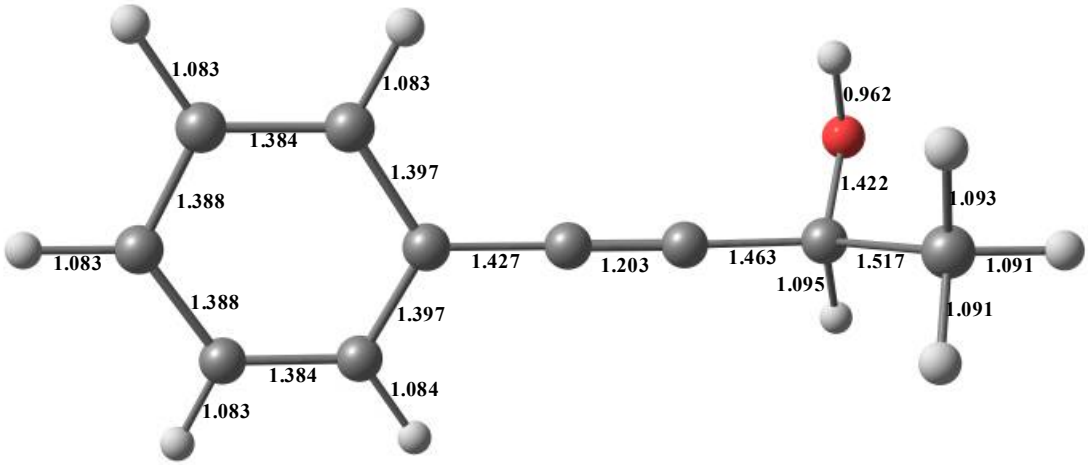
* Total *	0.00000	21.98923	55.80001	0.21075	78.00000

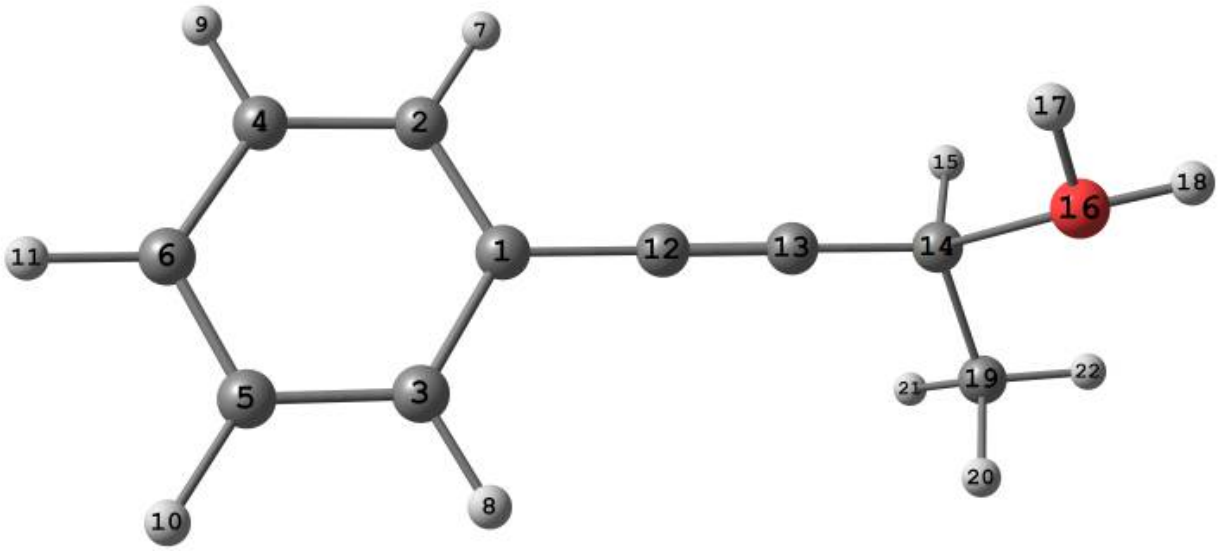


Af

Energy **E= -462.439153132 h, G^{298}= -462.293685 h, μ=14.27 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	1.045855	-0.046949	-0.060428
2	C	1.826010	-1.173223	-0.335555
3	C	1.665126	1.156155	0.288676
4	C	3.203975	-1.092520	-0.263026
5	C	3.043734	1.226988	0.360437
6	C	3.813160	0.105319	0.084180
7	H	1.340254	-2.103173	-0.604911
8	H	1.055226	2.025643	0.500845
9	H	3.806210	-1.966268	-0.477964
10	H	3.521316	2.160383	0.631087
11	H	4.893071	0.165096	0.140069
12	C	-0.371185	-0.125247	-0.139502
13	C	-1.569463	-0.194219	-0.210193
14	C	-2.994021	-0.269550	-0.332694
15	H	-3.309801	-1.142039	-0.905601
16	O	-3.526851	-0.557874	1.110921
17	H	-3.018942	-1.268085	1.543704
18	H	-4.469772	-0.804973	1.115268
19	C	-3.677911	0.993509	-0.756429
20	H	-3.381790	1.824294	-0.117315
21	H	-3.371000	1.211149	-1.779691
22	H	-4.761645	0.879397	-0.745659



Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.16774	1.99890	4.15123	0.01761	6.16774
C	2	-0.14708	1.99905	4.13040	0.01763	6.14708
C	3	-0.14702	1.99905	4.13035	0.01762	6.14702
C	4	-0.20375	1.99912	4.18505	0.01958	6.20375
C	5	-0.20371	1.99912	4.18500	0.01959	6.20371
C	6	-0.17201	1.99913	4.15319	0.01969	6.17201
H	7	0.22076	0.00000	0.77770	0.00155	0.77924
H	8	0.22093	0.00000	0.77753	0.00155	0.77907
H	9	0.21918	0.00000	0.77922	0.00160	0.78082
H	10	0.21913	0.00000	0.77927	0.00160	0.78087
H	11	0.21682	0.00000	0.78170	0.00149	0.78318
C	12	0.11294	1.99840	3.87470	0.01396	5.88706
C	13	-0.09492	1.99836	4.08362	0.01294	6.09492
C	14	0.09768	1.99896	3.88798	0.01539	5.90232
H	15	0.24762	0.00000	0.75037	0.00201	0.75238
O	16	-0.67016	1.99975	6.65888	0.01153	8.67016
H	17	0.57234	0.00000	0.42463	0.00302	0.42766
H	18	0.57095	0.00000	0.42613	0.00292	0.42905

C	19	-0.60439	1.99925	4.59120	0.01394	6.60439
H	20	0.23083	0.00000	0.76747	0.00170	0.76917
H	21	0.25081	0.00000	0.74802	0.00117	0.74919
H	22	0.23088	0.00000	0.76776	0.00136	0.76912

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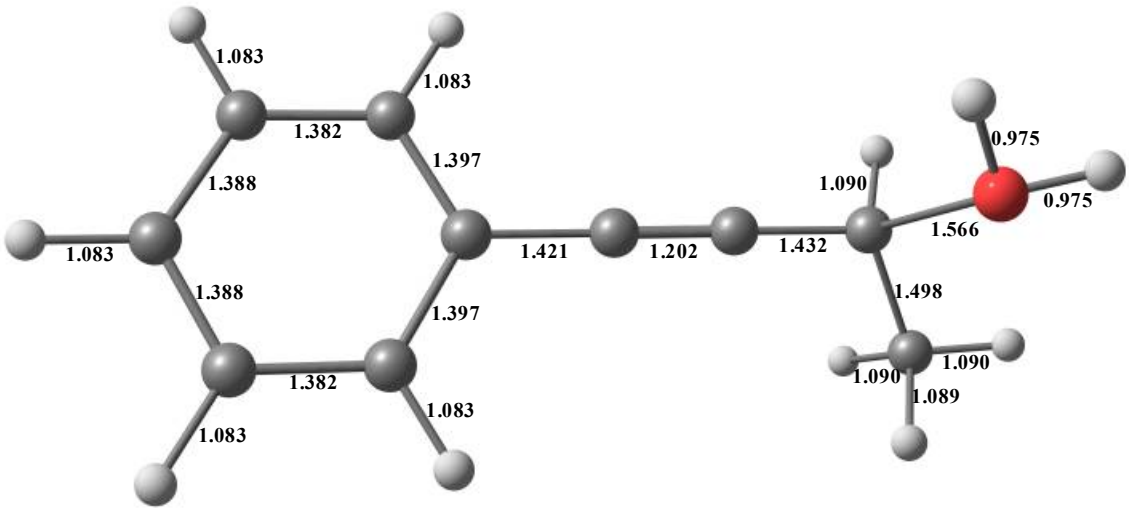
* Total *	1.00008	21.98907	55.81141	0.19944	77.99992

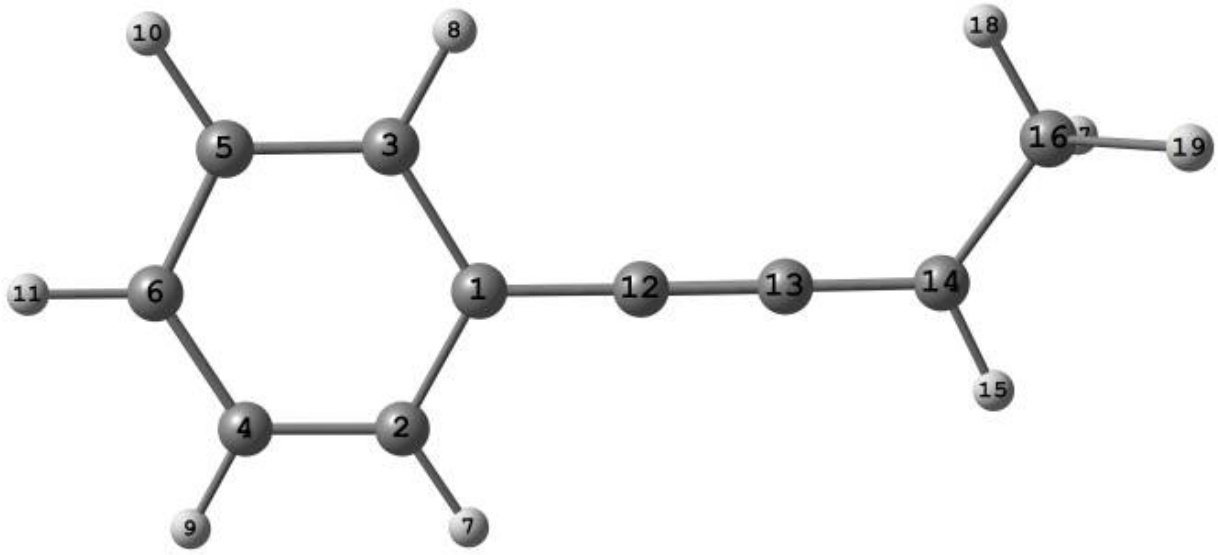


Bf

Energy **E= -386.004290112 h, G^{298}= -385.886781 h, μ=4.85 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	0.542049	-0.106663	-0.000098
2	C	1.381672	-1.242637	-0.000018
3	C	1.101488	1.190836	-0.000053
4	C	2.744410	-1.075689	0.000051
5	C	2.466308	1.338858	0.000038
6	C	3.281673	0.209701	0.000112
7	H	0.934042	-2.228022	-0.000074
8	H	0.441313	2.048272	-0.000178
9	H	3.399031	-1.936544	0.000053
10	H	2.908178	2.326078	0.000059
11	H	4.357610	0.333202	0.000216
12	C	-0.828498	-0.260230	-0.000304
13	C	-2.053098	-0.387328	0.000042
14	C	-3.382111	-0.520355	0.000116
15	H	-3.785210	-1.531409	0.000090
16	C	-4.326540	0.592953	0.000020
17	H	-4.987565	0.493748	0.868392
18	H	-3.842659	1.565197	-0.000744
19	H	-4.988862	0.492817	-0.867250



Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.19681	1.99890	4.17874	0.01917	6.19681
C	2	-0.09626	1.99910	4.06783	0.02933	6.09626
C	3	-0.10119	1.99910	4.06693	0.03516	6.10119
C	4	-0.63419	1.99886	4.55506	0.08027	6.63419
C	5	-0.54217	1.99894	4.47649	0.06674	6.54217
C	6	0.68696	1.99900	3.01422	0.29983	5.31304
H	7	0.23080	0.00000	0.76707	0.00213	0.76920
H	8	0.23110	0.00000	0.76663	0.00227	0.76890
H	9	0.22726	0.00000	0.76847	0.00428	0.77274
H	10	0.22622	0.00000	0.76968	0.00410	0.77378
H	11	0.20326	0.00000	0.79208	0.00466	0.79674
C	12	0.26925	1.99859	3.71739	0.01476	5.73075
C	13	-0.09702	1.99873	4.08640	0.01188	6.09702
C	14	0.13396	1.99886	3.85457	0.01261	5.86604
H	15	0.24568	0.00000	0.75268	0.00165	0.75432
C	16	-0.65057	1.99927	4.63842	0.01288	6.65057
H	17	0.27235	0.00000	0.72621	0.00144	0.72765
H	18	0.23556	0.00000	0.76306	0.00138	0.76444

H	19	0.27229	0.00000	0.72627	0.00144	0.72771

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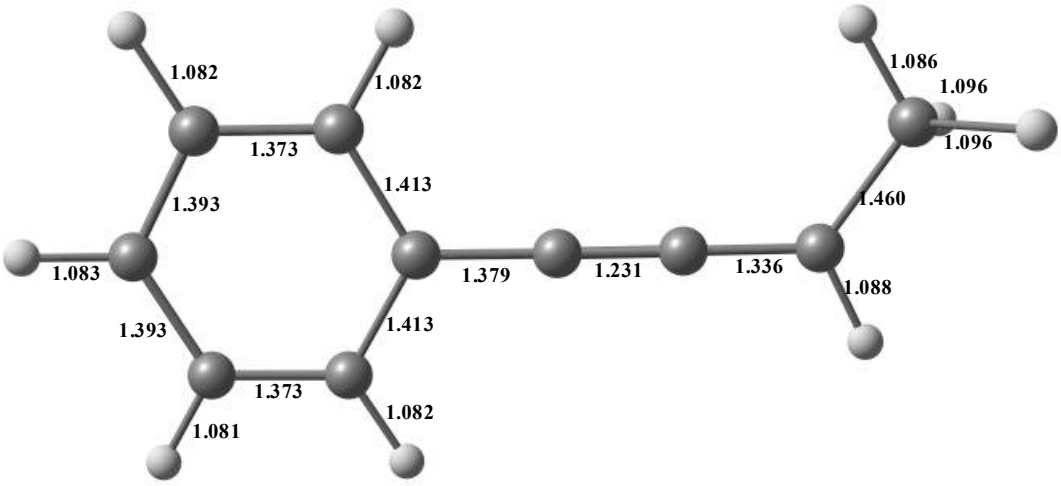
* Total *	0.91648	19.98935	47.48820	0.60597	68.08352

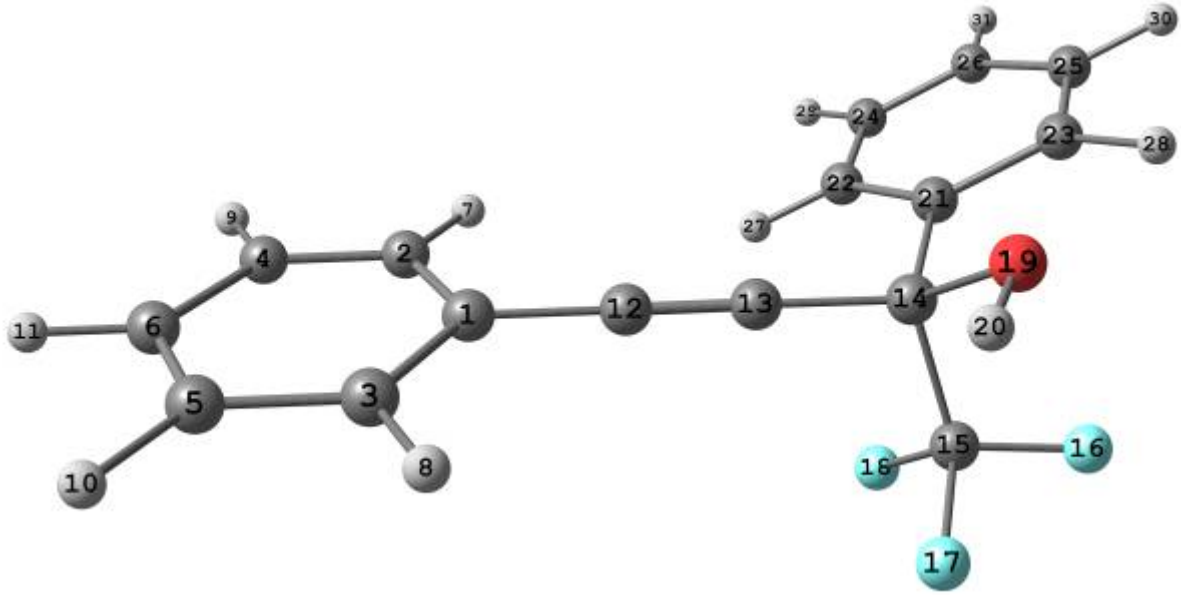


1g

Energy **E= -990.722304933 h, G^{298}= -990.542521 h, μ=4.85 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.872601	0.154854	0.179481
2	C	-3.272720	1.387054	-0.342496
3	C	-3.839335	-0.767057	0.586197
4	C	-4.618010	1.687405	-0.456016
5	C	-5.182582	-0.457617	0.471595
6	C	-5.574223	0.767572	-0.048990
7	H	-2.519310	2.099836	-0.656928
8	H	-3.526025	-1.722356	0.989643
9	H	-4.922776	2.643662	-0.863058
10	H	-5.928105	-1.176269	0.788946
11	H	-6.627028	1.006265	-0.137583
12	C	-1.485890	-0.156318	0.288503
13	C	-0.313853	-0.404938	0.368108
14	C	1.108221	-0.729834	0.473181
15	C	1.444853	-1.746898	-0.642415
16	F	2.725681	-2.095191	-0.611763
17	F	0.725911	-2.861846	-0.493691
18	F	1.183639	-1.256275	-1.850060
19	O	1.412690	-1.346878	1.701925
20	H	0.737089	-2.004384	1.898320
21	C	1.993338	0.496194	0.313509
22	C	1.603151	1.552341	-0.499720
23	C	3.222596	0.546133	0.959697
24	C	2.435873	2.646749	-0.668978
25	C	4.050631	1.644454	0.793036
26	C	3.661416	2.695304	-0.023296
27	H	0.639190	1.528378	-0.995238
28	H	3.527020	-0.270691	1.600871
29	H	2.121324	3.466930	-1.302620
30	H	5.004594	1.677968	1.305188
31	H	4.310226	3.553119	-0.151691



Summary of Natural Population Analysis:

			Natural Population			
		Natural	----------			
Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	-0.15711	1.99889	4.13193	0.02629	6.15711
C	2	-0.16244	1.99905	4.14405	0.01934	6.16244
C	3	-0.16319	1.99905	4.14460	0.01955	6.16319
C	4	-0.20260	1.99912	4.18317	0.02031	6.20260
C	5	-0.20206	1.99912	4.18311	0.01984	6.20206
C	6	-0.18789	1.99912	4.16852	0.02025	6.18789
H	7	0.21729	0.00000	0.78047	0.00224	0.78271
H	8	0.21802	0.00000	0.78010	0.00188	0.78198
H	9	0.21687	0.00000	0.78148	0.00164	0.78313
H	10	0.21678	0.00000	0.78158	0.00164	0.78322
H	11	0.21482	0.00000	0.78363	0.00155	0.78518
C	12	0.03866	1.99839	3.92395	0.03900	5.96134
C	13	-0.24804	1.99848	4.06590	0.18365	6.24804
C	14	-0.68929	1.99873	3.39757	1.29299	6.68929
C	15	0.99219	1.78050	2.17714	1.05017	5.00781
F	16	-0.39520	1.99686	6.32737	1.07096	9.39520
F	17	-0.40757	1.99683	7.01040	0.40034	9.40757
F	18	-0.37829	1.99663	5.98795	1.39371	9.37829

O	19	-0.87501	1.99807	5.54685	1.33009	8.87501
H	20	0.47919	0.00000	0.48380	0.03701	0.52081
C	21	-0.25538	1.97536	3.64545	0.63457	6.25538
C	22	-0.21688	1.98901	3.15195	1.07592	6.21688
C	23	-0.20551	1.98839	3.08370	1.13342	6.20551
C	24	-0.20154	1.98684	3.85492	0.35978	6.20154
C	25	-0.20218	1.98706	3.87058	0.34454	6.20218
C	26	-0.19617	1.98957	3.33236	0.87424	6.19617
H	27	0.21363	0.00000	0.51533	0.27104	0.78637
H	28	0.22500	0.00000	0.74873	0.02626	0.77500
H	29	0.21451	0.00000	0.78020	0.00530	0.78549
H	30	0.21401	0.00000	0.78218	0.00382	0.78599
H	31	0.21363	0.00000	0.77703	0.00934	0.78637

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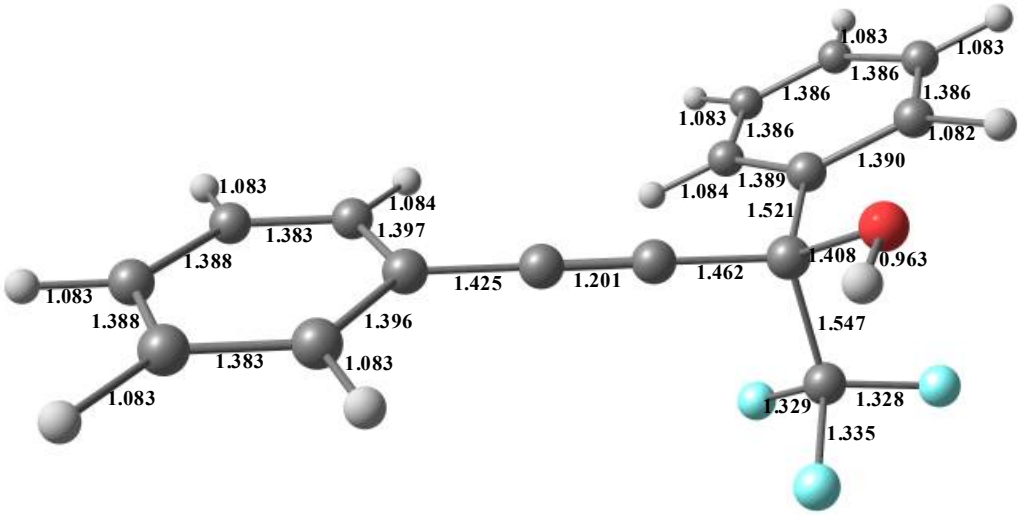
* Total *	-1.67174	39.67507	92.32599	11.67068	143.67174



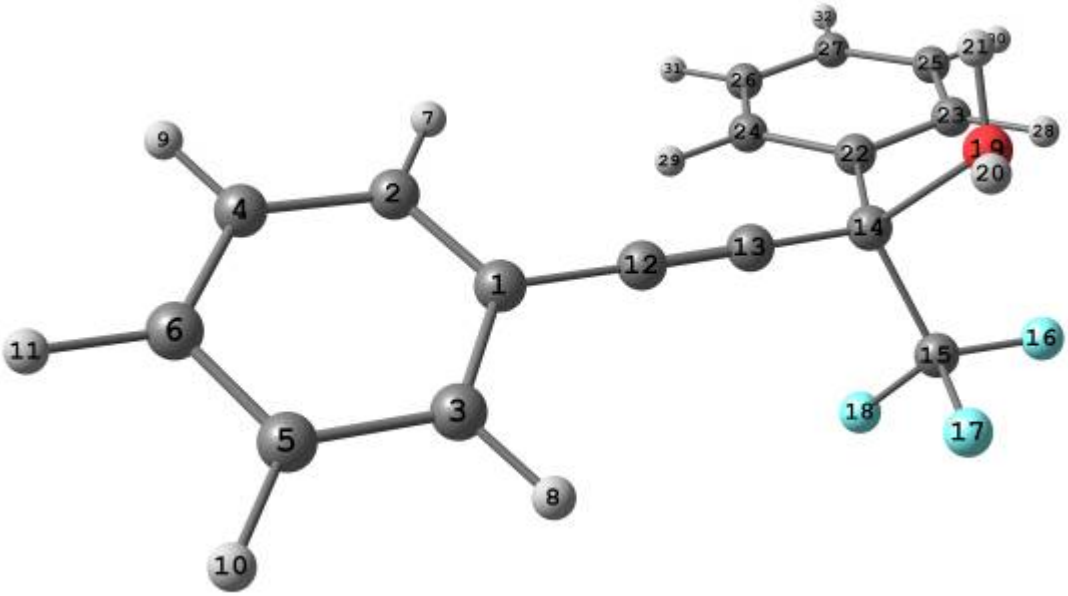
Ag

Energy **E= -991.099709705 h, G^{298}= -990.907838 h, μ=7.38 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	-2.890865	0.160655	0.095356
2	C	-3.332019	1.486111	0.149511
3	C	-3.814197	-0.879258	-0.042492
4	C	-4.683004	1.762643	0.066841
5	C	-5.163159	-0.591124	-0.121219
6	C	-5.597084	0.726360	-0.067197
7	H	-2.606687	2.283764	0.255956
8	H	-3.462527	-1.902493	-0.084729
9	H	-5.026125	2.788529	0.107702
10	H	-5.880585	-1.394974	-0.226430
11	H	-6.655533	0.947295	-0.129703
12	C	-1.504337	-0.120017	0.180592
13	C	-0.322346	-0.332113	0.249379
14	C	1.076194	-0.598058	0.359736
15	C	1.448977	-1.853666	-0.463383
16	F	2.705588	-2.218635	-0.294921
17	F	0.676559	-2.875134	-0.114296
18	F	1.250576	-1.580453	-1.739610
19	O	1.362696	-1.126689	1.829228
20	H	0.610940	-1.643821	2.180822
21	H	1.528796	-0.375081	2.431939
22	C	1.993186	0.567631	0.156971
23	C	3.343602	0.483647	0.501099
24	C	1.487963	1.744144	-0.388656
25	C	4.170375	1.572939	0.301716
26	C	2.327365	2.822912	-0.600156
27	C	3.665848	2.740005	-0.252689
28	H	3.752138	-0.420946	0.932475
29	H	0.440293	1.812611	-0.653078
30	H	5.214258	1.508142	0.579681

31	H	1.930307	3.733210	-1.030407
32	H	4.319654	3.588404	-0.411055



Summary of Natural Population Analysis:

Natural Population

Atom	No	Charge	Core	Valence	Rydberg	Total
C	1	0.76240	1.99894	2.55487	0.68380	5.23760
C	2	-0.61980	1.99871	4.54094	0.08015	6.61980
C	3	-0.46056	1.99880	4.39645	0.06530	6.46056
C	4	-0.21453	1.99914	4.19440	0.02099	6.21453
C	5	-0.21292	1.99915	4.19325	0.02052	6.21292
C	6	-0.16100	1.99913	4.14287	0.01900	6.16100
H	7	0.20972	0.00000	0.78127	0.00900	0.79028
H	8	0.20544	0.00000	0.78229	0.01227	0.79456
H	9	0.22060	0.00000	0.77797	0.00143	0.77940
H	10	0.22099	0.00000	0.77756	0.00145	0.77901
H	11	0.21818	0.00000	0.78026	0.00156	0.78182
C	12	0.08862	1.99848	3.86435	0.04855	5.91138
C	13	-0.15257	1.99841	4.12571	0.02845	6.15257
C	14	0.18088	1.99863	3.79033	0.03015	5.81912

C	15	1.12412	1.99913	2.81713	0.05963	4.87588
F	16	-0.34549	1.99990	7.33722	0.00837	9.34549
F	17	-0.35676	1.99990	7.34706	0.00980	9.35676
F	18	-0.34270	1.99990	7.33454	0.00826	9.34270
O	19	-0.67601	1.99975	6.66342	0.01284	8.67601
H	20	0.57882	0.00000	0.41839	0.00279	0.42118
H	21	0.57937	0.00000	0.41782	0.00281	0.42063
C	22	-0.13968	1.99889	4.11726	0.02354	6.13968
C	23	-0.17632	1.99901	4.15889	0.01841	6.17632
C	24	-0.15329	1.99900	4.13655	0.01774	6.15329
C	25	-0.18720	1.99912	4.16867	0.01941	6.18720
C	26	-0.18951	1.99912	4.17117	0.01922	6.18951
C	27	-0.15494	1.99913	4.13694	0.01887	6.15494
H	28	0.23098	0.00000	0.76721	0.00181	0.76902
H	29	0.23012	0.00000	0.76644	0.00344	0.76988
H	30	0.22464	0.00000	0.77382	0.00155	0.77536
H	31	0.22402	0.00000	0.77444	0.00154	0.77598
H	32	0.22170	0.00000	0.77689	0.00141	0.77830

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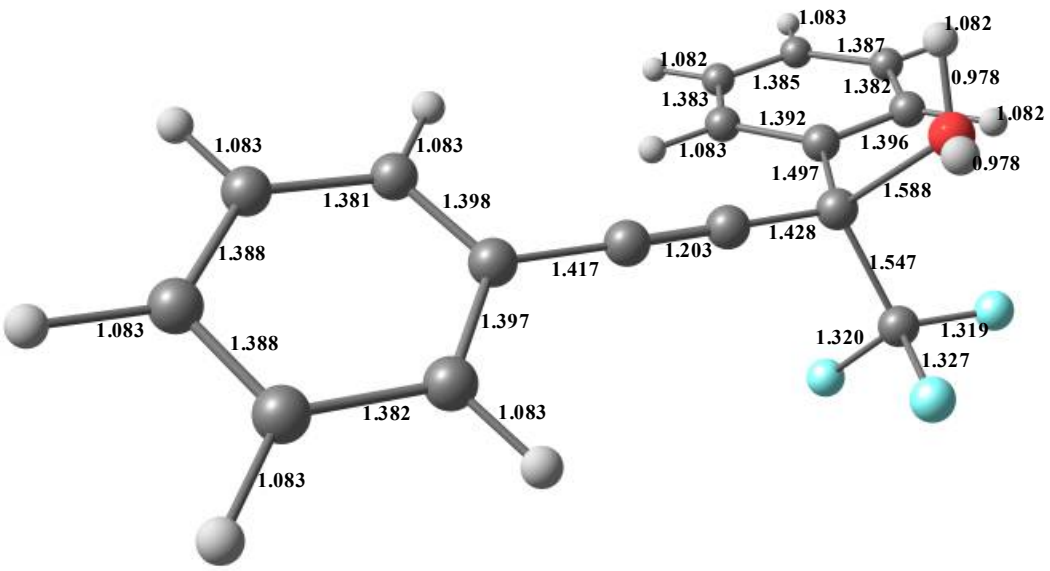
* Total *	0.97734	39.98224	100.78637	1.25406	142.02266

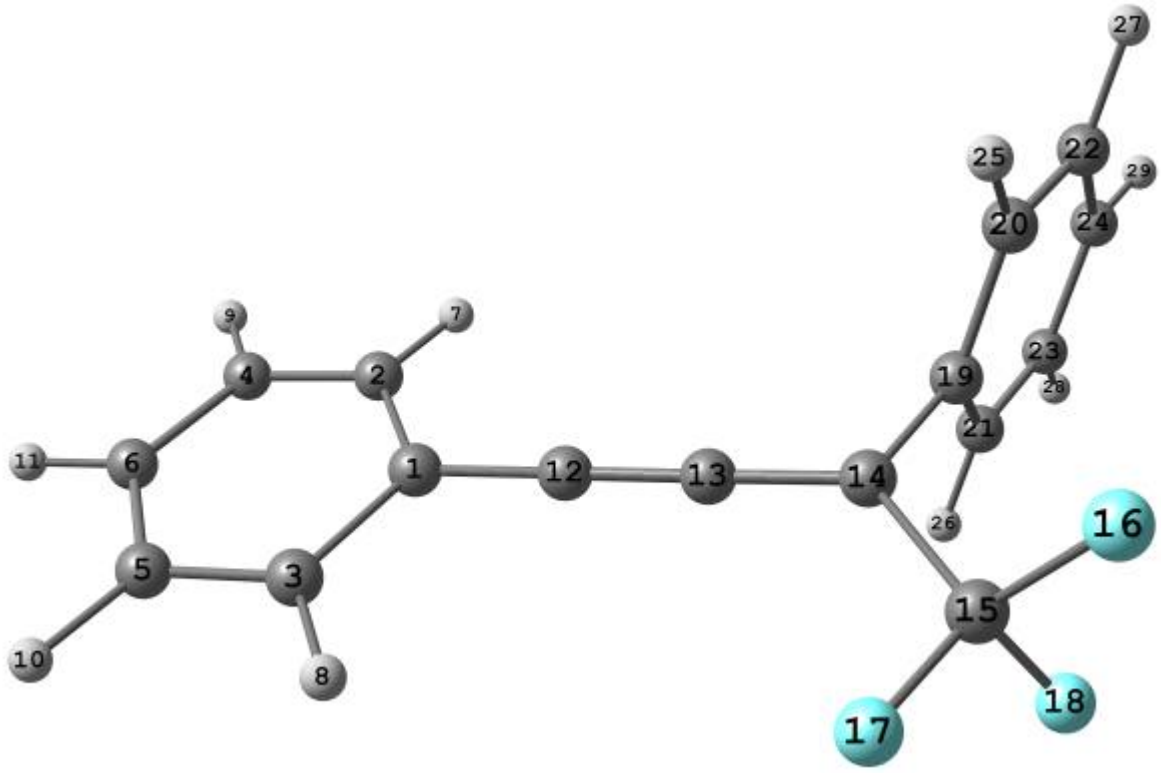


Bg

Energy **E= -914.660481734 h, G^{298}= -914.493623 -990.542521 h, μ=11.29 D**

Cartesian coordinates, Å

N	atom	x	y	z
1	C	2.832328	-0.227685	-0.000018
2	C	3.270082	-1.579433	-0.001462
3	C	3.777259	0.833854	0.000752
4	C	4.611694	-1.848806	-0.002141
5	C	5.113911	0.540648	0.000089
6	C	5.525860	-0.793215	-0.001360
7	H	2.531265	-2.369858	-0.002055
8	H	3.419112	1.854663	0.001845
9	H	4.965338	-2.870377	-0.003285
10	H	5.849303	1.333161	0.000665
11	H	6.585772	-1.016306	-0.001904
12	C	1.499341	0.054267	0.000503
13	C	0.286083	0.312193	0.000650
14	C	-1.011927	0.567659	-0.000070
15	C	-1.491812	2.009364	0.000705
16	F	-2.239224	2.223463	1.075992
17	F	-0.495170	2.874466	0.001524
18	F	-2.239019	2.225381	-1.074330
19	C	-2.040114	-0.487462	-0.000413
20	C	-2.518178	-0.981284	1.209103
21	C	-2.525333	-0.974628	-1.209797
22	C	-3.490836	-1.966469	1.201411
23	C	-3.497703	-1.960084	-1.201708
24	C	-3.980905	-2.454005	-0.000054
25	H	-2.127559	-0.599131	2.144593
26	H	-2.140143	-0.587743	-2.145544
27	H	-3.863821	-2.354919	2.140668
28	H	-3.875951	-2.343675	-2.140858
29	H	-4.741091	-3.225083	0.000067



Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.17995	1.99890	4.16225	0.01880	6.17995
C	2	-0.04684	1.99906	4.03046	0.01733	6.04684
C	3	-0.04624	1.99906	4.02979	0.01739	6.04624
C	4	-0.21628	1.99911	4.19757	0.01960	6.21628
C	5	-0.21671	1.99911	4.19790	0.01970	6.21671
C	6	-0.02572	1.99916	4.00815	0.01841	6.02572
H	7	0.23943	0.00000	0.75907	0.00150	0.76057
H	8	0.23938	0.00000	0.75912	0.00151	0.76062
H	9	0.23913	0.00000	0.75935	0.00153	0.76087
H	10	0.23917	0.00000	0.75929	0.00154	0.76083
H	11	0.23182	0.00000	0.76685	0.00132	0.76818
C	12	0.25842	1.99863	3.72396	0.01900	5.74158
C	13	-0.01105	1.99852	2.98807	1.02446	6.01105
C	14	0.08018	1.99876	3.88676	0.03430	5.91982

C	15	1.10194	1.99921	2.84121	0.05764	4.89806
F	16	-0.34623	1.99991	7.33794	0.00838	9.34623
F	17	-0.34659	1.99990	7.33765	0.00904	9.34659
F	18	-0.34618	1.99991	7.33794	0.00833	9.34618
C	19	-0.13366	1.99890	4.11063	0.02413	6.13366
C	20	-0.16218	1.99885	4.14409	0.01924	6.16218
C	21	-0.17148	1.99899	4.15451	0.01798	6.17148
C	22	-0.19236	1.99913	4.17303	0.02020	6.19236
C	23	-0.18732	1.99911	4.16860	0.01961	6.18732
C	24	-0.17884	1.99912	4.16065	0.01907	6.17884
H	25	0.22559	0.00000	0.77270	0.00171	0.77441
H	26	0.22638	0.00000	0.77187	0.00175	0.77362
H	27	0.22247	0.00000	0.77598	0.00155	0.77753
H	28	0.22245	0.00000	0.77593	0.00161	0.77755
H	29	0.21940	0.00000	0.77913	0.00148	0.78060

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* Total *	0.93812	37.98334	92.67044	1.40810	132.06188