Supporting Information

Reestimation of the Taft's Substituent Constant of the Pentafluorophenyl Group

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Cartesian coordinates of **1a** (conformation (**A**))

Optimization at B3LYP/6-31G* level

C	0.11932200	4.88400600	0.00000000
C	-0.36520600	5.41430900	1.20328400
C	1.11428900	3.74263500	0.00000000
C	0.41963700	2.37110200	0.00000000
C	-0.36520600	5.41430900	-1.20328400
C	1.40198600	1.21734600	0.00000000
C	-1.30954900	6.44170400	1.20619900
C	-1.30954900	6.44170400	-1.20619900
C	-0.55098100	-4.04815500	1.20704300
C	-0.97020500	-4.60393600	0.00000000
C	-0.55098100	-4.04815500	-1.20704300
C	-1.78604800	6.95822800	0.00000000
C	0.28040000	-2.93168100	1.19164100
C	0.28040000	-2.93168100	-1.19164100
C	0.72266300	-2.35431600	0.00000000
C	1.60439500	-1.13894800	0.00000000
O	0.74763300	0.02753900	0.00000000
O	2.60977300	1.30965000	0.00000000
F	-0.95138800	-4.58475000	2.36436000
F	-1.76909700	-5.67270600	0.00000000
F	-0.95138800	-4.58475000	-2.36436000
F	0.67044400	-2.41588000	2.36690800
F	0.67044400	-2.41588000	-2.36690800
H	0.00674300	5.02181400	2.14769200
H	1.76899700	3.80756900	0.87597600
H	1.76899700	3.80756900	-0.87597600
H	-0.23633300	2.26253500	0.87307200
H	-0.23633300	2.26253500	-0.87307200
H	0.00674300	5.02181400	-2.14769200
H	-1.66901700	6.84212000	2.15064600
H	-1.66901700	6.84212000	-2.15064600
H	-2.51882700	7.76069400	0.00000000
H	2.24273600	-1.11571400	0.88533600
H	2.24273600	-1.11571400	-0.88533600

Heat of formation (MP2/6-31G**) -1262.5873857 Hartrees

Cartesian coordinates of **1a** (conformation (**B**))

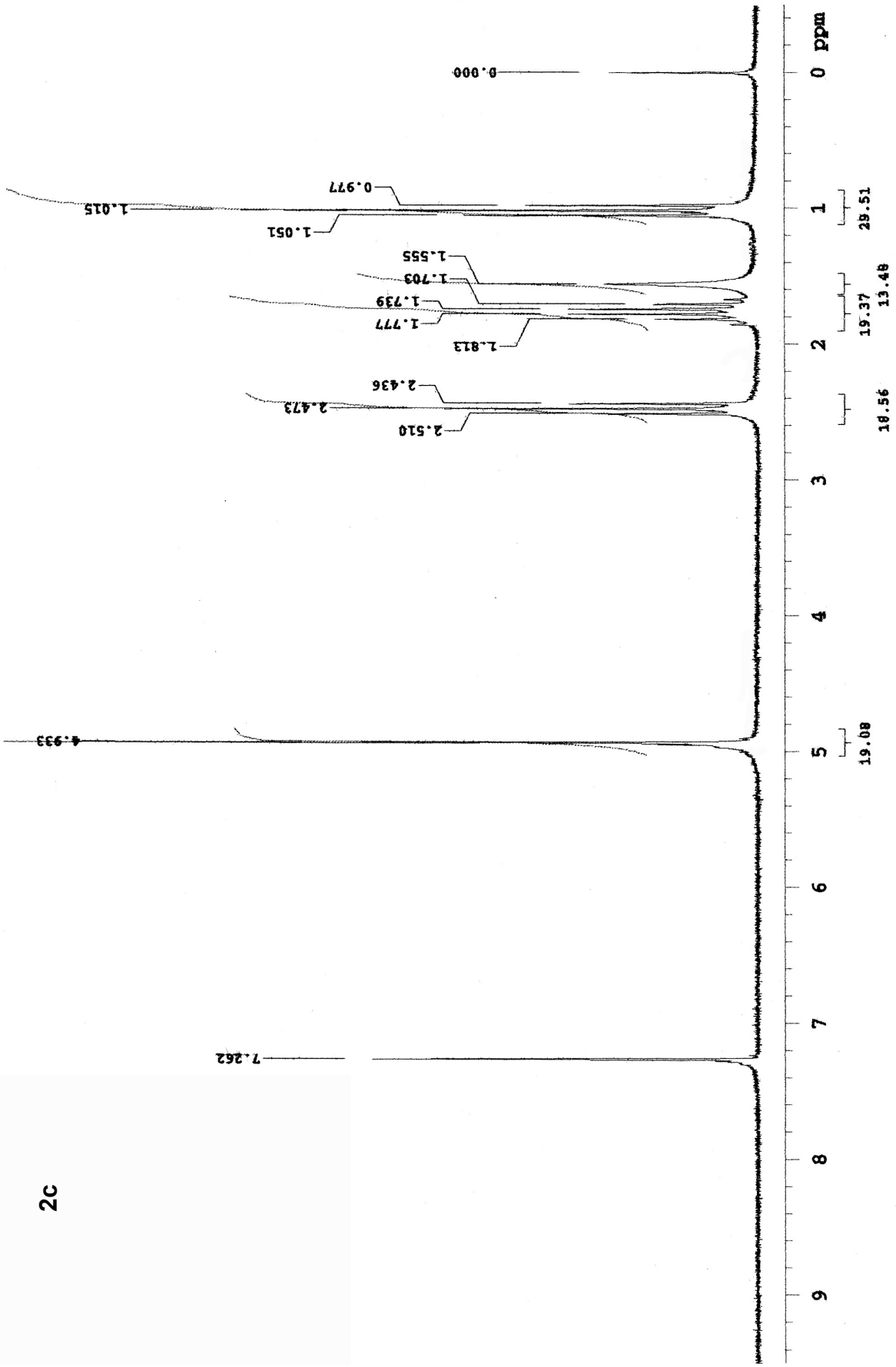
Optimization at B3LYP/6-31G* level

C	-2.40744700	1.34224200	-0.22587800
C	-2.10688100	1.35184900	-1.59508000
C	-3.42569600	0.37502900	0.34521500
C	-2.77806500	-0.92076700	0.88019200
C	-1.71407800	2.22330300	0.61697600
C	-2.31210100	-1.82809800	-0.25339600
C	-1.13983700	2.21978200	-2.10639400
C	-0.74441200	3.08957800	0.10985600
C	2.59720000	-0.66209500	-0.70626500
C	2.66772700	0.51720400	0.03399300
C	1.80391600	0.71737200	1.10643600
C	-0.45470800	3.08996400	-1.25665300
C	1.65056300	-1.62431500	-0.36991200
C	0.87163600	-0.26643500	1.42395900
C	0.76172800	-1.45055200	0.69549000
C	-0.28011600	-2.50481700	0.99245200
O	-2.91670300	-1.92337200	-1.29413400
O	-1.22326900	-2.63752700	-0.08408600
F	3.43603600	-0.85860400	-1.72780700
F	3.56590200	1.45112800	-0.28359600
F	1.86560200	1.84914900	1.81576500
F	1.60922300	-2.75441500	-1.08640300
F	0.05745700	-0.03929000	2.47345600
H	-2.63014400	0.66883300	-2.25835800
H	-4.16551100	0.10521400	-0.41327600
H	-3.96139300	0.85095400	1.17493300
H	-1.98267400	-0.66696200	1.58057900
H	-3.52415600	-1.50064000	1.44289500
H	-1.93713800	2.23186600	1.68209400
H	-0.92342900	2.21594000	-3.17159900
H	-0.21666100	3.76204300	0.78073700
H	0.29584000	3.76701300	-1.65599600
H	0.19122300	-3.48830100	1.04874700
H	-0.77074400	-2.30595400	1.94632300

Heat of formation (MP2/6-31G**) -1262.5807456 Hartrees

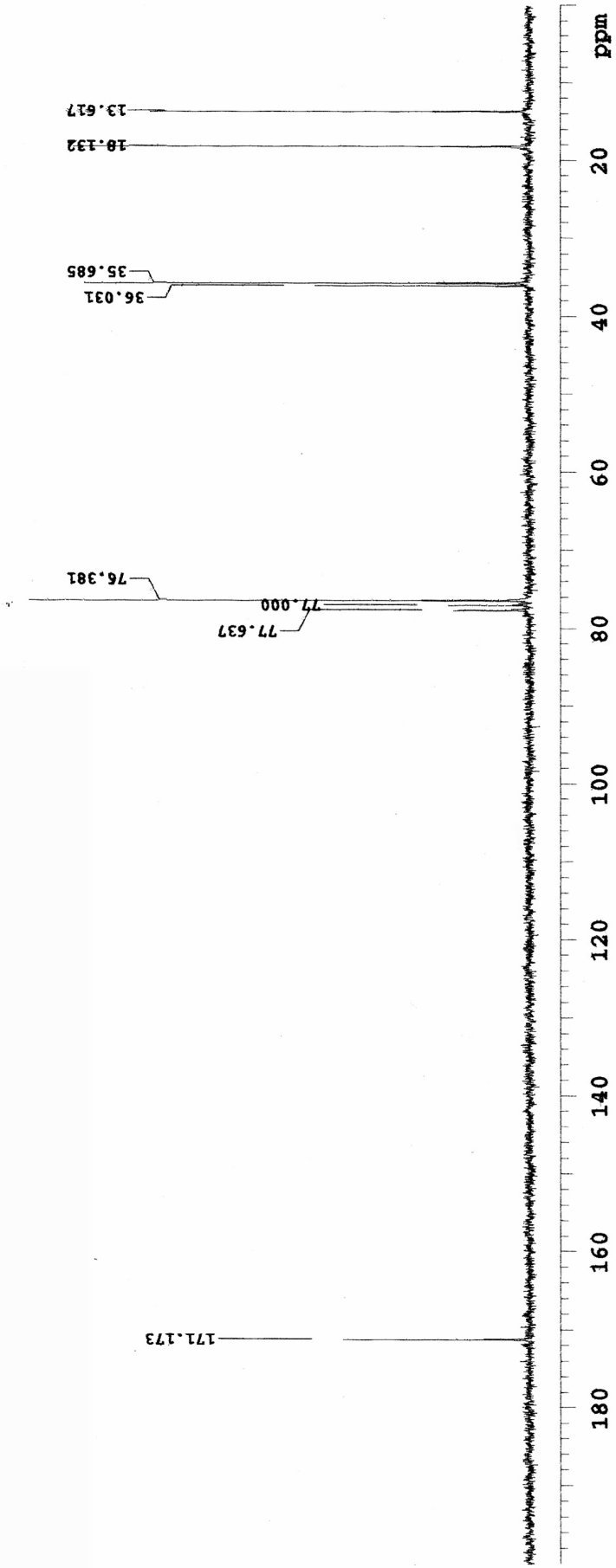
^{1}H NMR

2c


0.000
0.977
1.015
1.051
1.555
1.703
1.739
1.777
1.813
2.436
2.473
2.510
4.933
7.262
ppm
0
1
2
3
4
5
6
7
8
9
29.51
13.48
19.37
10.56
19.08

^{13}C NMR

2c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76.381
77.000
77.637
36.031
35.685
18.132
13.617
ppm
180
160
140
120
100
80
60
40
20

General Experimental Methods. All reactions were carried out under a nitrogen atmosphere with dry and freshly distilled solvents under anhydrous conditions, unless otherwise noted. Tetrahydrofuran (THF) was distilled from sodium, and methylene chloride (CH_2Cl_2) was distilled from calcium hydride. Reactions were monitored by thin-layer chromatography with precoated silica gel plates (Merck 60 F_{254}, plate length 40mm). As a usual workup procedure, the reaction mixture was extracted with ethyl acetate (EtOAc). The organic layer was dried over $MgSO_4$, filtrated with suction, and then concentrated in vacuo. Preparative column chromatography was carried out by using silica gel (Fuji Silysia BW-127 ZH, 100-270 mesh). All synthetic and commercially available esters were purified by distillation before IR analysis. ^{1}H NMR and ^{13}C NMR spectra were measured at 200 MHz (or 300 MHz) and 50 MHz (or 75 MHz), respectively, and chemical shifts are given relative to tetramethylsilane (TMS). ^{19}F NMR spectra were measured at 188 MHz, and chemical shifts are given relative to CCl_3F using C_6F_6 as secondary reference (–162.9 ppm).