

Fast-Track Computational Access to Reaction Mechanisms Provides Comprehensive Insights into Aminolysis Postpolymerization Modification Reactions

*Kiho Matsubara^a, Li-Chieh Chou^a, Hideki Amii^a, and Ryohei Kakuchi^{*a}*

^a. Division of Molecular Science, Faculty of Science and Technology, Gunma University, 1-5-1 Tenjin, Kiryu, Gunma 376-8515, Japan

SUPPORTING INFORMATION

The noncatalytic concerted mechanism for PFP ester aminolysis

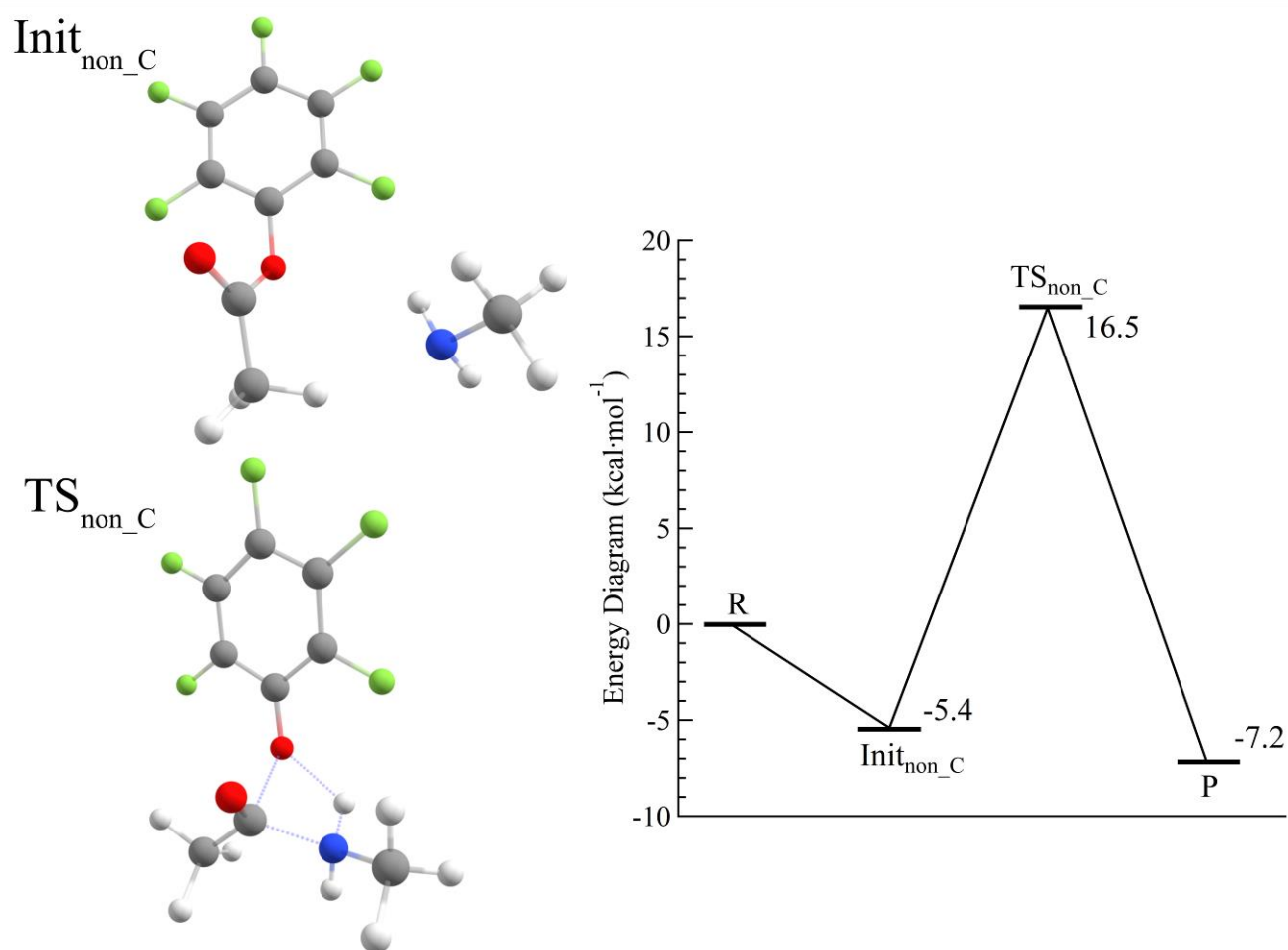


Figure S1. Energy diagram of the noncatalytic concerted mechanism for the aminolysis of pentafluorophenyl acetate by methylamine calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level of theory in the gas phase. The color code is as follows: O, red; N, blue; C, gray; F, green; H, white.

Energy diagram of the noncatalytic stepwise mechanism for PFP ester aminolysis

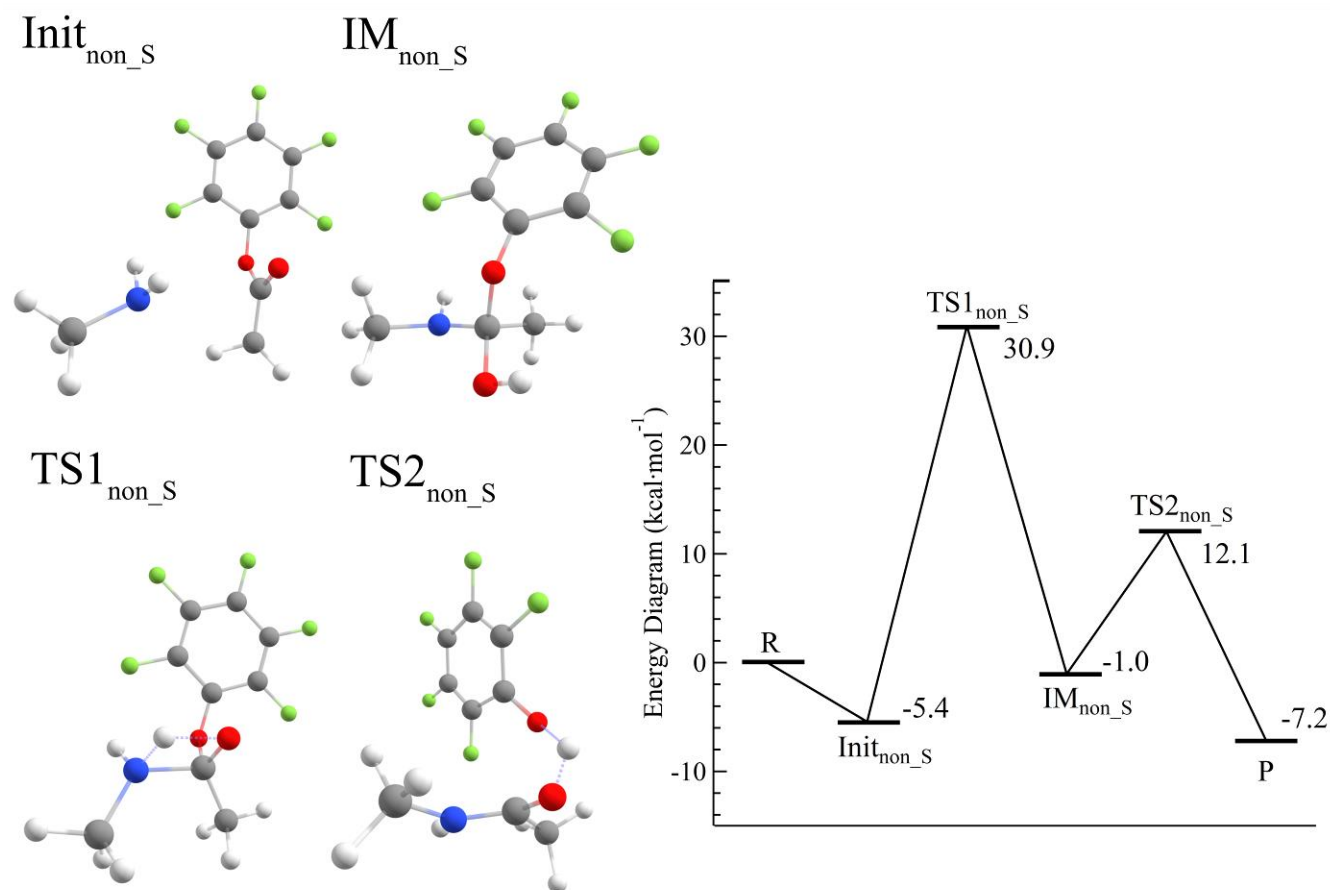


Figure S2. Energy diagram of the noncatalytic stepwise mechanism for the aminolysis of pentafluorophenyl acetate by methylamine calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level of theory in the gas phase. The color code is as follows: O, red; N, blue; C, gray; F, green; H, white.

The noncatalytic concerted mechanism for 4-NO₂-Ph ester aminolysis

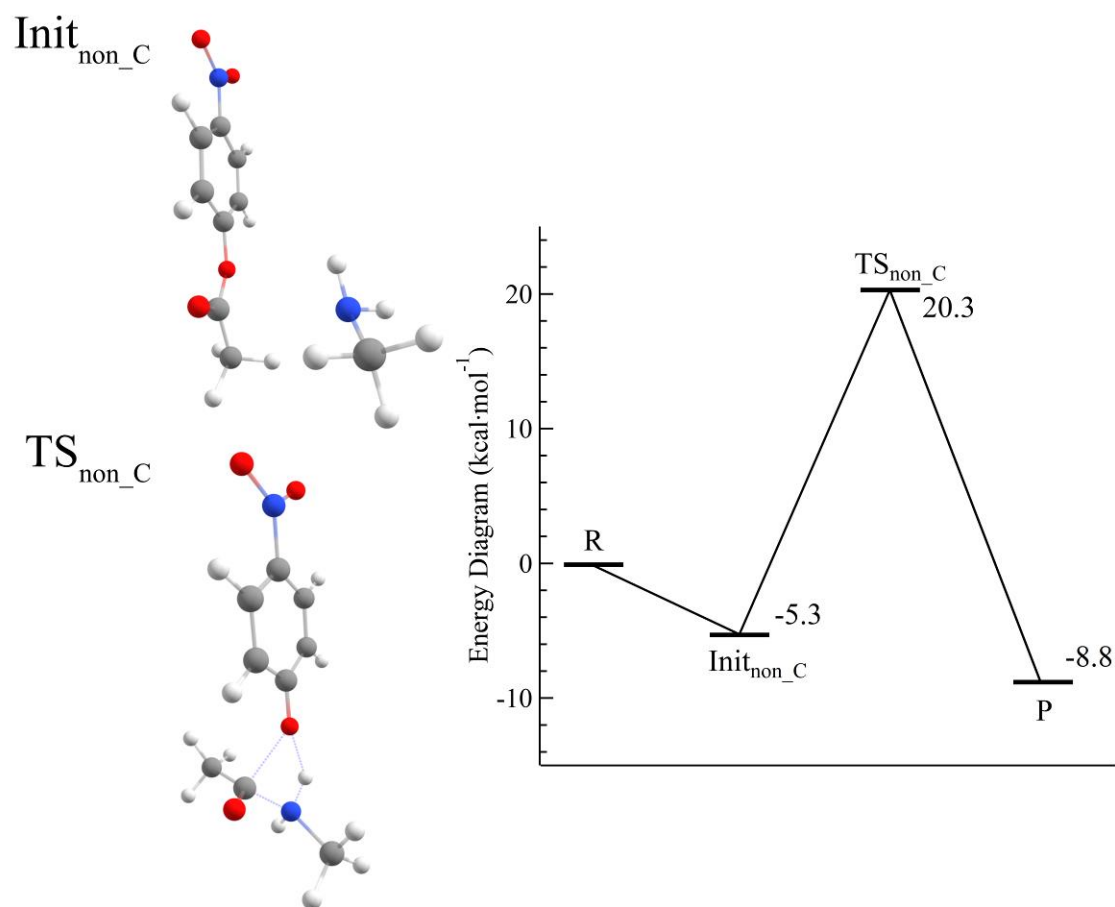


Figure S3. Energy diagram of the noncatalytic concerted mechanism for the aminolysis of 4-nitrophenyl acetate by methylamine calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level of theory in the gas phase. The color code is as follows: O, red; N, blue; C, gray; H, white.

The noncatalytic stepwise mechanism for 4-NO₂-Ph ester aminolysis

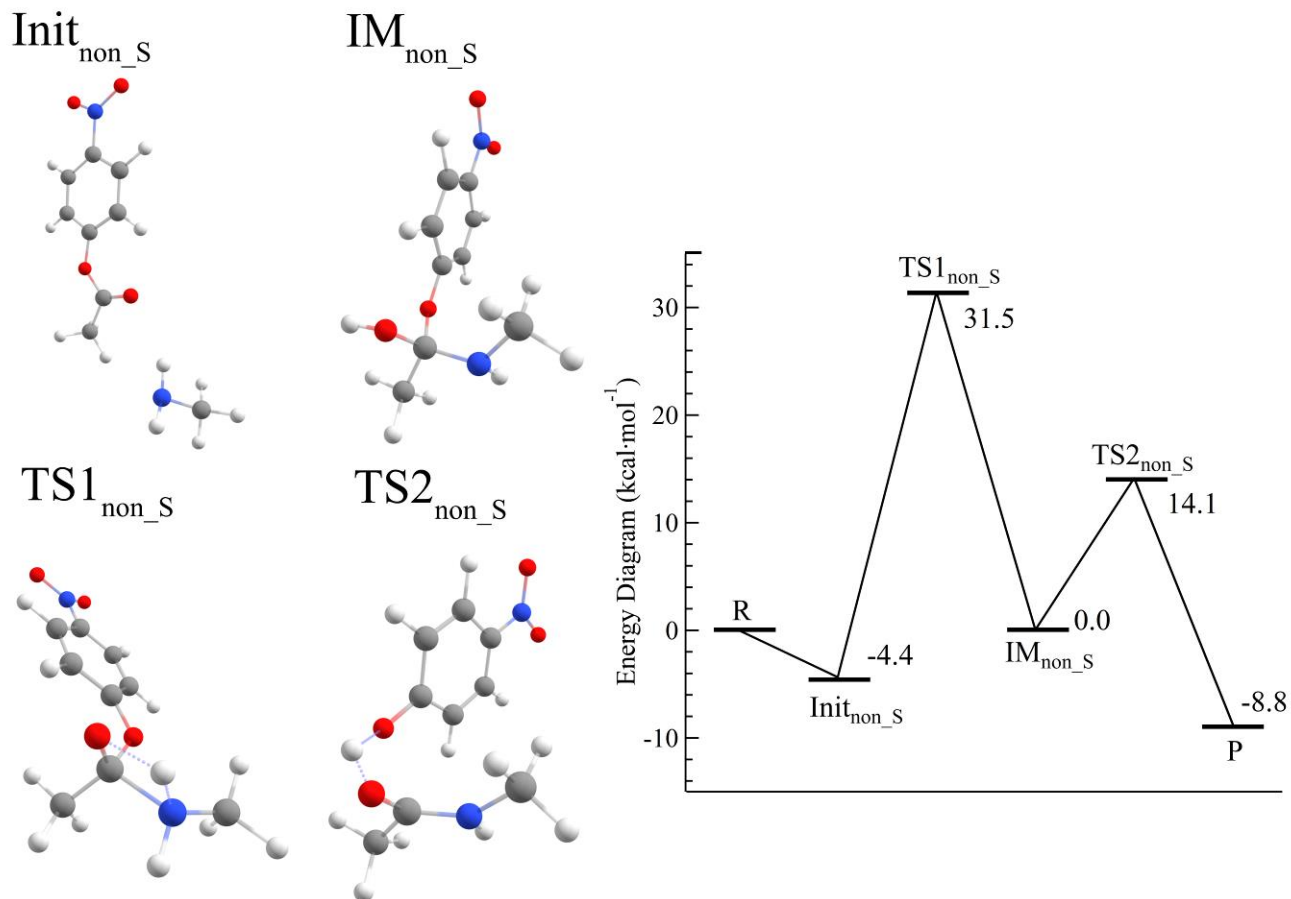


Figure S4. Energy diagram of the noncatalytic stepwise mechanism for the aminolysis of 4-nitrophenyl acetate by methylamine calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level of theory in the gas phase. The color code is as follows: O, red; N, blue; C, gray; H, white.

The noncatalytic concerted mechanism for HFIP ester aminolysis

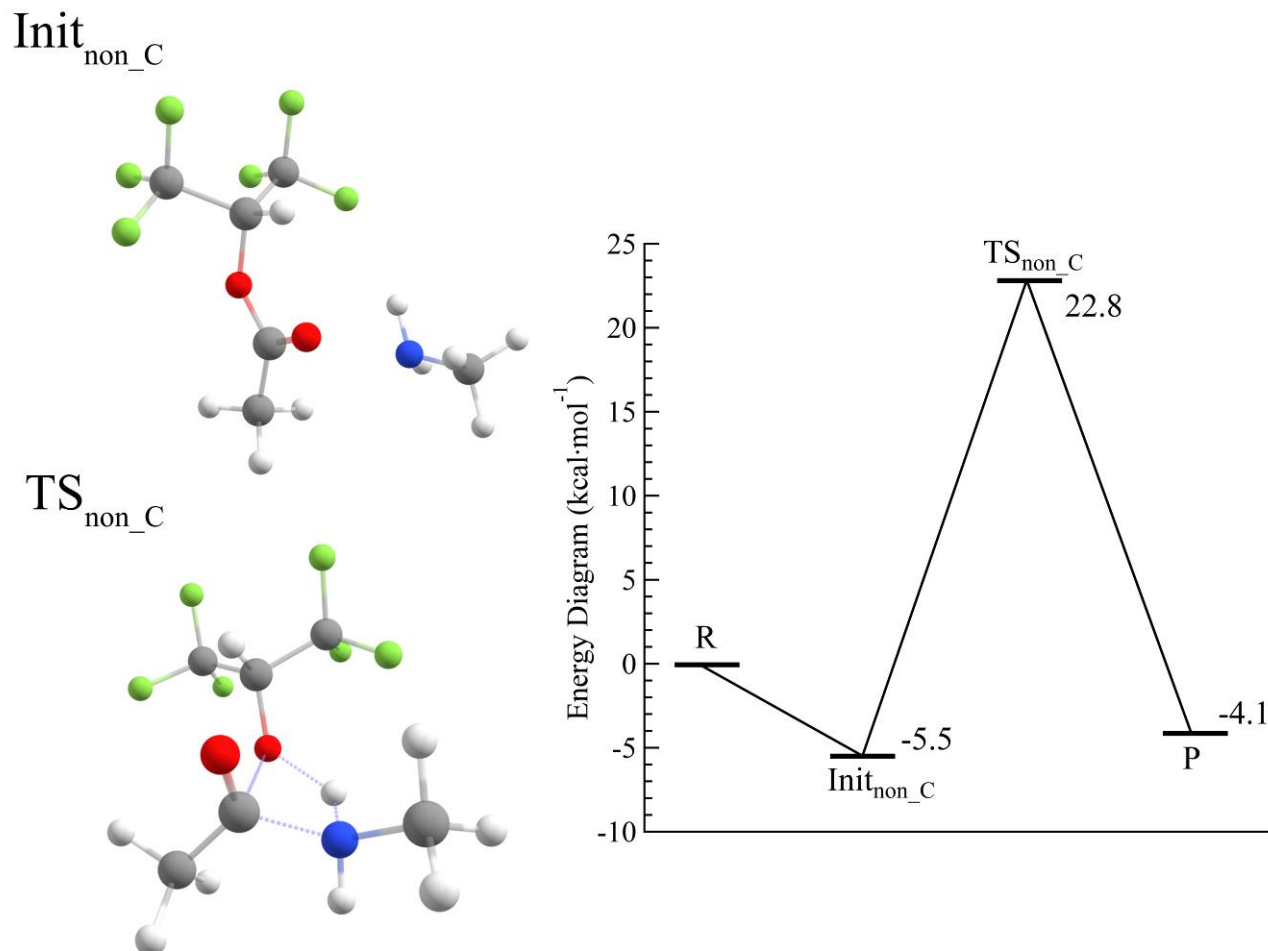


Figure S5. Energy diagram of the noncatalytic concerted mechanism for the aminolysis of hexafluoroisopropyl acetate by methylamine calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level of theory in the gas phase. The color code is as follows: O, red; N, blue; C, gray; F, green; H, white.

The noncatalytic stepwise mechanism for HFIP ester aminolysis

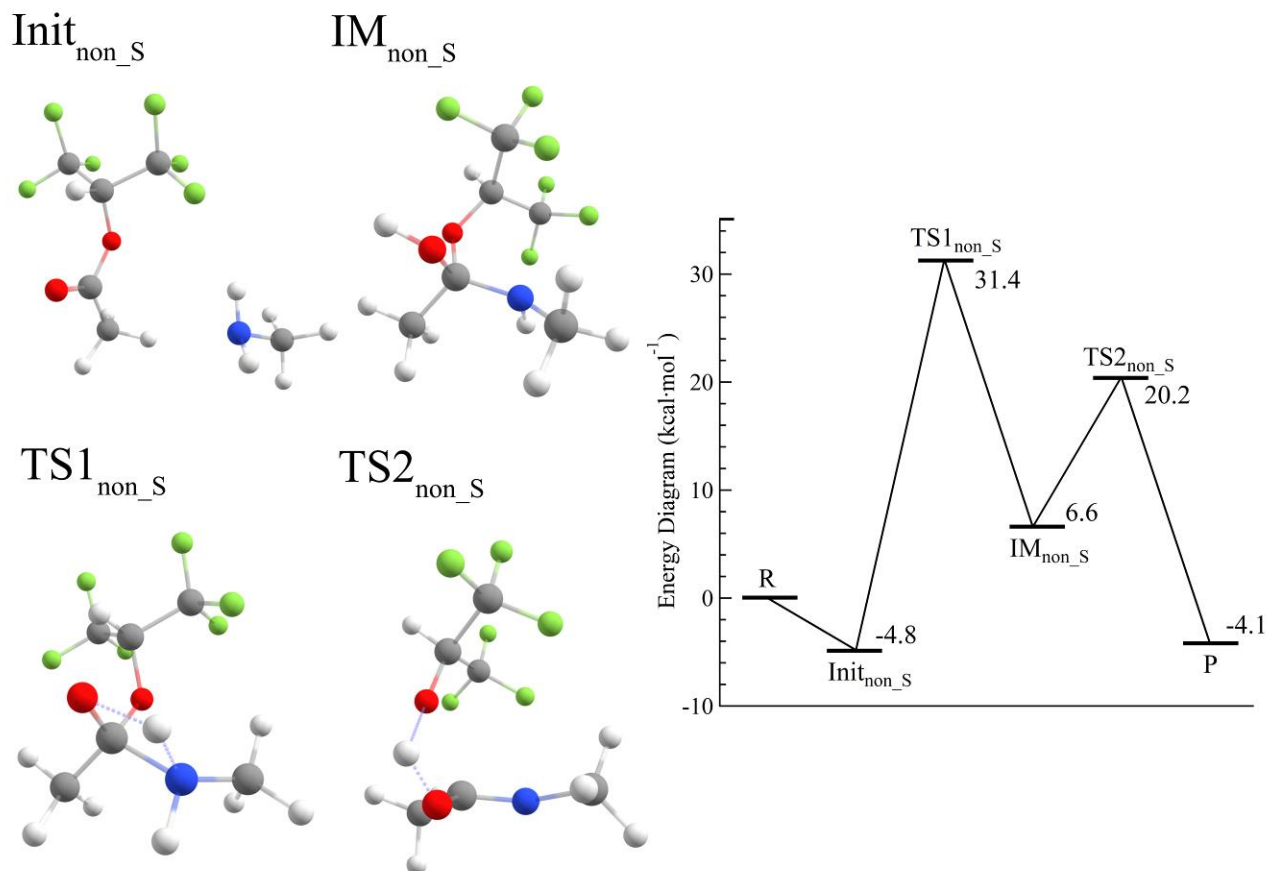


Figure S6. Energy diagram of the noncatalytic stepwise mechanism for the aminolysis of hexafluoroisopropyl acetate by methylamine calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level of theory in the gas phase. The color code is as follows: O, red; N, blue; C, gray; F, green; H, white.

The noncatalytic concerted mechanism for 4-CF₃-Ph ester aminolysis

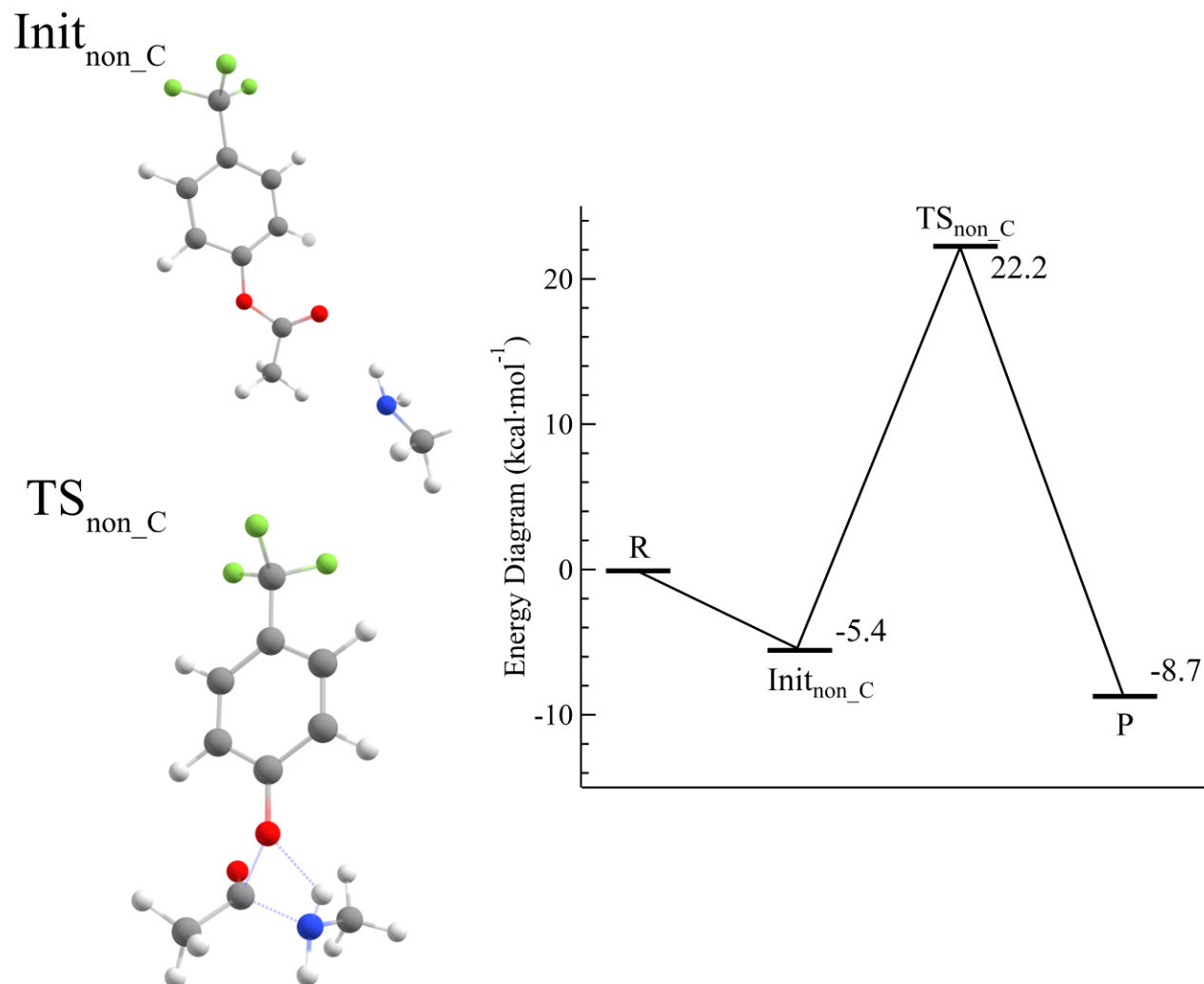


Figure S7. Energy diagram of the non-catalytic concerted mechanism for the aminolysis of 4-trifluoromethyl phenyl acetate by methylamine calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level of theory in the gas phase. The color code is as follows: O, red; N, blue; C, gray; F, green; H, white.

The noncatalytic stepwise mechanism for 4-CF₃-Ph ester aminolysis

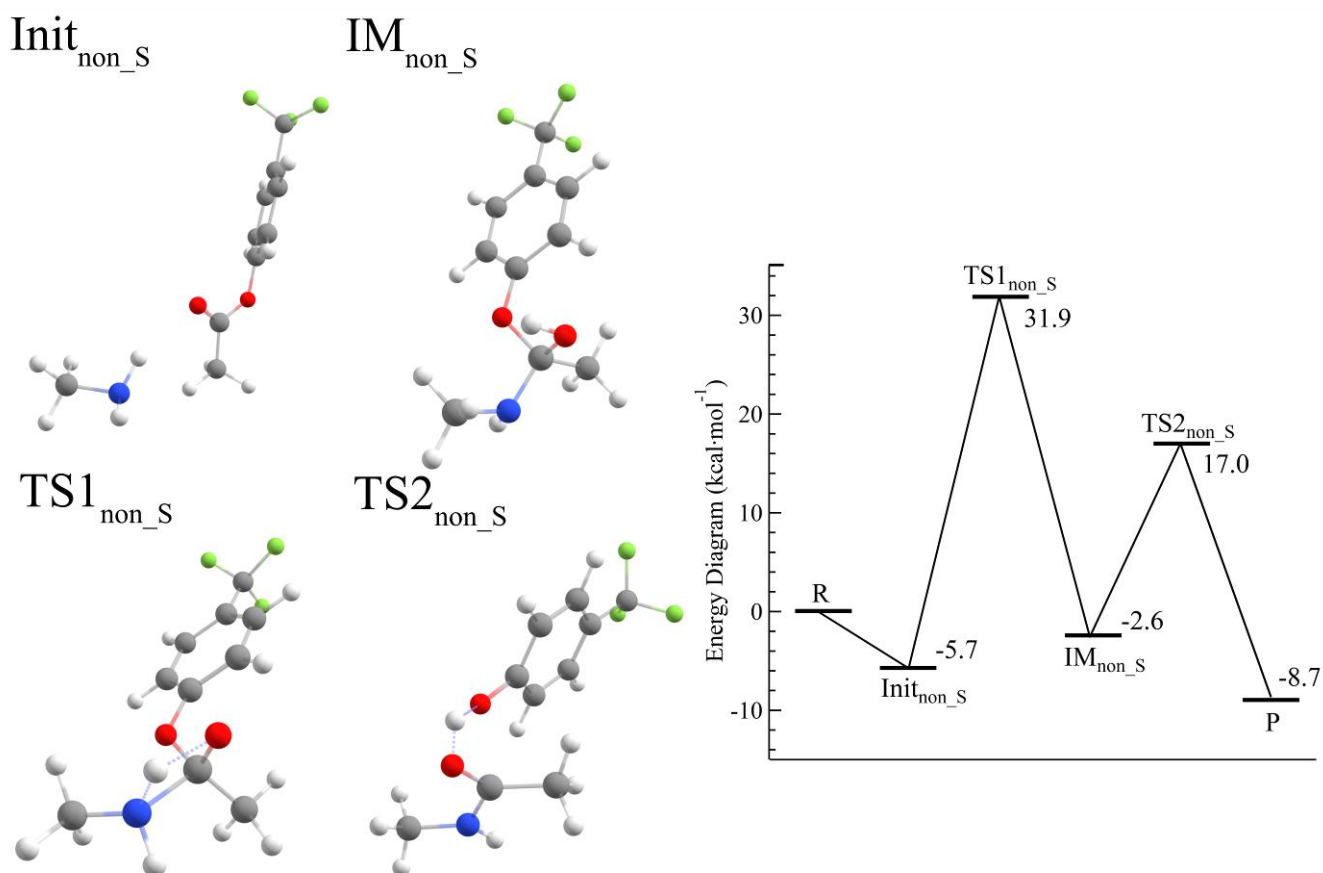


Figure S8. Energy diagram of the noncatalytic stepwise mechanism for the aminolysis of 4-trifluoromethyl phenyl acetate by methylamine calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level of theory in the gas phase. The color code is as follows: O, red; N, blue; C, gray; F, green; H, white.

The noncatalytic concerted mechanism for Ph ester aminolysis

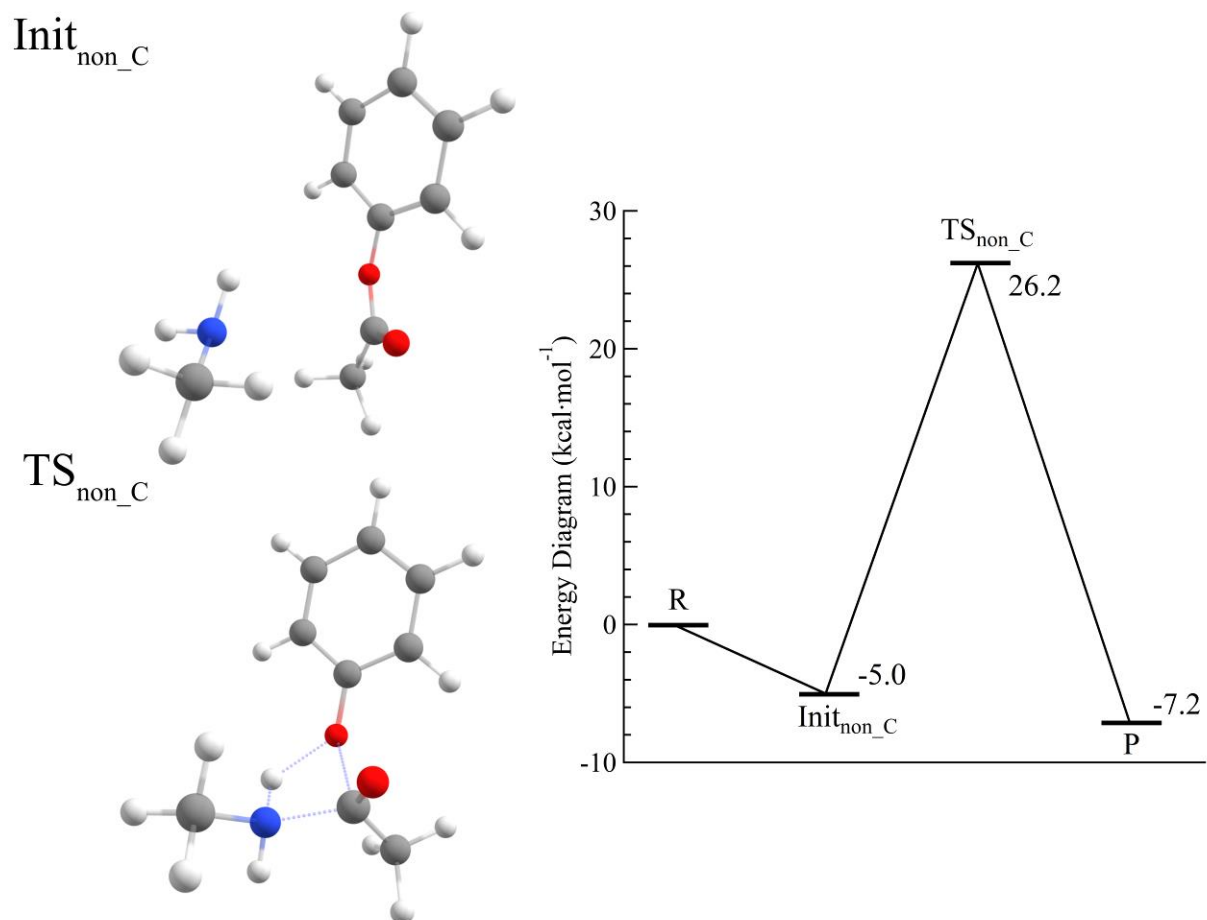


Figure S9. Energy diagram of the noncatalytic concerted mechanism for the aminolysis of phenyl acetate by methylamine calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level of theory in the gas phase. The color code is as follows: O, red; N, blue; C, gray; H, white.

The noncatalytic stepwise mechanism for Ph ester aminolysis

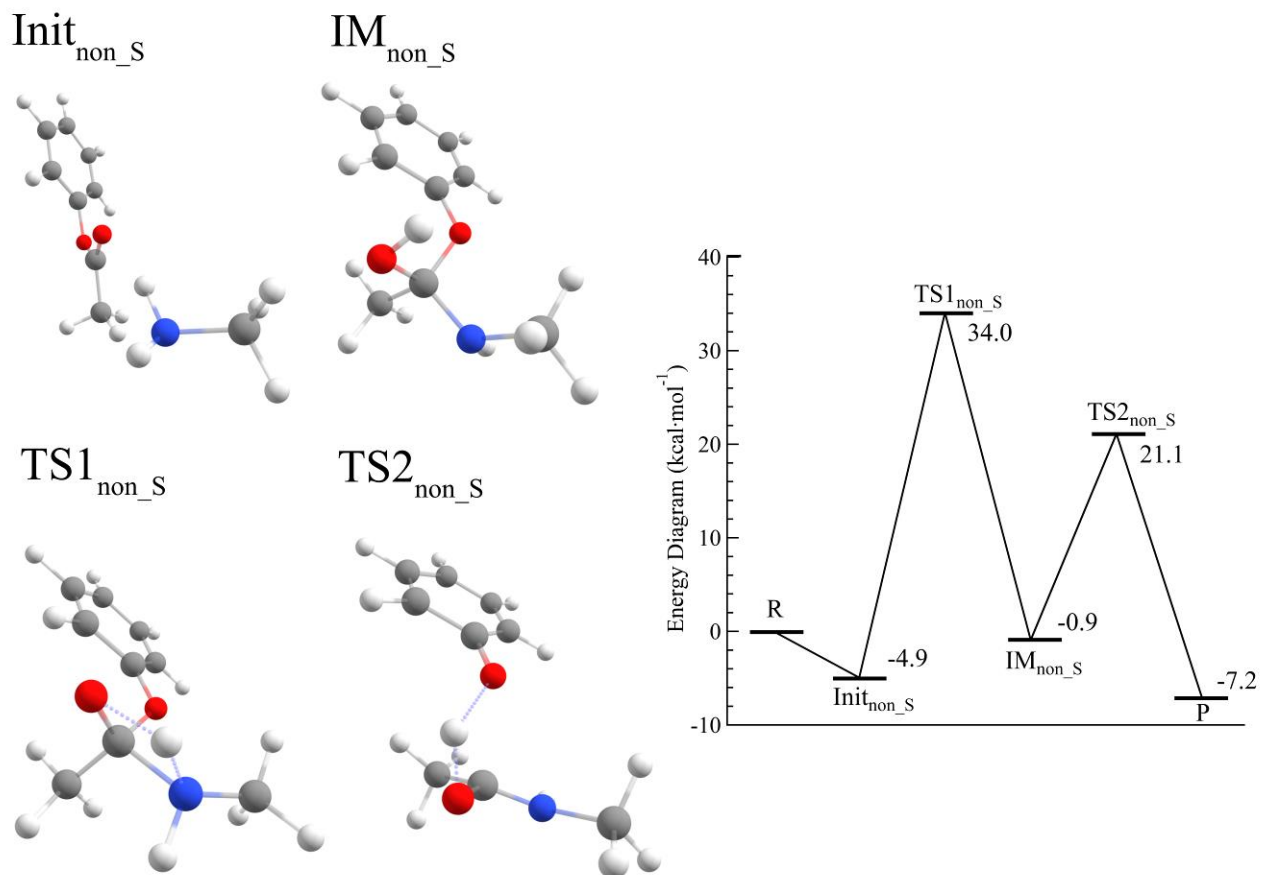


Figure S10. Energy diagram of the noncatalytic stepwise mechanism for the aminolysis of phenyl acetate by methylamine calculated at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/def2-SVP level of theory in the gas phase. The color code is as follows: O, red; N, blue; C, gray; H, white.

The optimized structure coordinates

<N-hydroxysuccinimide acetate amionolysis>

<N-hydroxysuccinimide acetate >

C	-0.156588400210	-1.028825470416	1.129785100991
N	-0.433645869045	0.006765729312	0.229476485611
C	-0.292116767660	1.314777470545	0.707271862249
C	0.061024078969	1.171796260390	2.183287770555
C	0.144620946227	-0.341848403571	2.457152521271
O	-0.167780363081	-2.199670083647	0.862061227420
O	-0.430467973339	2.310067986109	0.049096476322
O	-0.743823917807	-0.245219522589	-1.074318220638
C	0.376791656199	-0.324765108614	-1.908063230857
O	1.489432185071	-0.193284790271	-1.499125925637
C	-0.083846179759	-0.579978255462	-3.313017184720
H	-0.707905569499	1.686387965840	2.780096893960
H	1.009790071584	1.701347686357	2.359798995325
H	1.138675254240	-0.671704947507	2.795639664554
H	-0.581323092723	-0.694065160636	3.206384291248
H	-0.732152414445	-1.468568625003	-3.341351515869
H	-0.680215745282	0.277015511100	-3.663389269915
H	0.789532110559	-0.720228221937	-3.960785951870

<N-hydroxysuccinimide>

C	-0.132012046915	-0.680756039155	1.128011789156
N	-0.007828097306	-1.071069202672	-0.206602080989
C	0.114164363011	-0.061489856390	-1.141359760713
C	0.071462592487	1.251436605421	-0.381803878070
C	-0.087673408426	0.848986218004	1.098037188796
O	0.228510580653	-0.291257577621	-2.327204550870
O	-0.247954157566	-1.414275213003	2.072160109958
O	-0.003790909082	-2.376210569359	-0.602678948443
H	0.995446758269	1.813617639150	-0.588644912729
H	-0.763298899098	1.858552451070	-0.765464923427
H	0.746634232227	1.184555049001	1.733002214062
H	-1.011834028631	1.232344745076	1.557099022737
H	0.098173030377	-2.294434219523	-1.574551289468

<methylamine>

C	-0.077392370521	0.000000012958	0.559376119580
N	-0.217669301297	0.000000001613	-0.890832807941
H	0.249156708570	0.813940294833	-1.292344447234
H	0.249156696337	-0.813940301136	-1.292344431882
H	0.963592759391	-0.000000005696	0.951256530574
H	-0.583422260773	0.884109130648	0.982444523861
H	-0.583422241707	-0.884109133220	0.982444503042

<N-methylacetamide>

C	-1.717580242697	-0.002373596440	0.828218488364
C	-0.662956718456	-0.037498831278	-0.269196738663

N	0.634086545827	0.014361357959	0.168634305004
O	-0.965112626475	-0.096460892719	-1.448557724775
C	1.765105108789	0.009296002375	-0.734376785664
H	-1.307639236821	-0.054659270850	1.848371440661
H	-2.302539668446	0.925289417036	0.725279440229
H	-2.412938564483	-0.840615478613	0.672408606632
H	0.807865859106	0.060632901983	1.164495659910
H	1.368887493657	-0.031127688603	-1.757989520267
H	2.377727207860	0.921318772287	-0.626038060779
H	2.415094842140	-0.868162693136	-0.571249100652

The noncatalytic concerted mechanism for N-hydroxysuccinimide acetate amionolysis (Figure1)

<Init _{non_C} >			
C	0.647633661877	-1.832364732677	2.024413429143
N	-0.094005735505	-1.029703703262	1.142928947198
C	-0.440731726128	0.238833770230	1.598617896882
C	0.054649539824	0.315051550174	3.036753794315
C	0.778830742582	-1.017192488034	3.305696830266
O	1.067930220008	-2.927220560776	1.770943912207
O	-1.021051047310	1.080495600635	0.958617486275
O	-0.389972004425	-1.445696684578	-0.120308659206
C	0.604093416878	-1.118418284114	-1.062663815321
O	1.602478765513	-0.546233563542	-0.745288185384
C	0.145898401642	-1.538556765821	-2.420610826143
H	-0.810932135951	0.485692516447	3.695844161031
H	0.706080340318	1.197266573121	3.129761222423
H	1.851073028612	-0.893522023132	3.522060945410
H	0.348077353939	-1.594672834311	4.138015619888
H	-0.491554243386	-0.708059503158	-2.781589899154
H	1.015725408907	-1.651745963915	-3.079884902556
H	-0.445332362959	-2.463048423018	-2.377348123596
C	-0.291728729545	2.545048537704	-2.414211459757
N	-1.258081592366	1.474012089538	-2.193940166432
H	-1.393192310300	1.329283938874	-1.190246539998
H	-2.168927326349	1.730243312921	-2.576016746518
H	-0.561692104451	3.527425929228	-1.972288503498
H	0.682387913037	2.251603187087	-1.990389556932
H	-0.138006888172	2.701822157783	-3.495356511451

<TS _{non_C} >			
C	0.161914015557	-1.654623295863	1.734328096349
N	-0.461298177989	-0.612752910319	1.037457482128
C	-0.339674068550	0.630338143978	1.628523533277
C	0.334468222011	0.439346647387	2.977266187444
C	0.698289947558	-1.054256546930	3.031242392100
O	0.249354131115	-2.794416737636	1.347669032384
O	-0.728713932500	1.667979089469	1.118978777885
O	-1.031878871281	-0.781360437037	-0.146693103774
C	0.400904261563	-0.216516728291	-1.713259392040
O	1.419626016946	0.156754585329	-1.206528510157
C	0.161170880421	-1.483507098921	-2.483330533324

H	-0.363483221813	0.749283028800	3.771995918236
H	1.205536449480	1.109965710836	3.041482184989
H	1.783545081876	-1.235699501199	3.078655916882
H	0.249830232059	-1.587677426775	3.884192284640
H	-0.905389294626	-1.735378635709	-2.545886756789
H	0.584761218809	-1.378586804167	-3.499046051570
H	0.681286072461	-2.297997709919	-1.963201616178
C	-0.283691656927	2.259790336659	-1.885647983240
N	-0.722957427570	0.851445728000	-1.899141309739
H	-1.234966381869	0.531940353896	-0.989599517512
H	-1.309826212463	0.629171008794	-2.707461460153
H	-1.171390041126	2.906240081212	-1.885825341681
H	0.279494699516	2.429246806632	-0.962672953713
H	0.343088057346	2.471272311772	-2.763497276445

The noncatalytic stepwise mechanism for N-hydroxysuccinimide acetate amionolysis (Figure 2)

< Init_{non_S} >

C	-0.427076093046	0.169716443017	1.630734344892
N	-0.787149894289	1.155309566576	0.716437909034
C	-1.063570124139	2.427811865597	1.240903190174
C	-0.943211532085	2.279507901659	2.753317158020
C	-0.536810687613	0.815637600695	3.005539009303
O	-0.102421774006	-0.958128785630	1.352987729235
O	-1.334854044580	3.398217671931	0.589604833223
O	-0.803134093624	0.913712337583	-0.623963052710
C	0.433097257609	1.160114785958	-1.252022649346
O	1.375068911536	1.567686718522	-0.642500587339
N	0.899358755702	-2.266138138758	-1.405799976071
H	-1.906020720117	2.554647255703	3.210962727578
H	-0.198900453479	3.007323600025	3.110732844891
H	0.434653956138	0.710975248060	3.512409793841
H	-1.270721875003	0.250353469278	3.600808622738
C	0.716283008620	-3.671868394393	-1.745450087437
C	0.333499931303	0.763154419845	-2.688186995313
H	1.876217323327	-2.087565125811	-1.166833171515
H	0.370787413378	-2.019050185519	-0.565412143790
H	-0.654632520730	1.006348152574	-3.101918584112
H	1.135138738783	1.248143105487	-3.258912806314
H	0.467863634001	-0.337081170086	-2.701308310609
H	-0.340378521559	-3.859479811091	-1.999227748091
H	0.994867767290	-4.394805548058	-0.949622251313
H	1.307689534366	-3.926051525660	-2.641062209243

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C	-0.613899418988	-0.120025925946	1.835216463118
N	-0.853082842699	0.661329988820	0.720554604933
C	-0.847217681013	2.049858728067	0.931614365603
C	-0.635824008133	2.239268345399	2.430271417618
C	-0.569905361849	0.821609593087	3.028020483188
O	-0.469959527774	-1.325299835424	1.820973043138
O	-0.988281925362	2.881634038693	0.077816441865

O	-0.970827565296	0.129290945247	-0.514592798708
C	0.364180218355	-0.119232879166	-1.173328345374
O	1.392206801910	0.430222494965	-0.560130138429
N	0.714987028345	-1.603286071904	-0.851709459860
H	-1.449467727491	2.859331426321	2.835611348792
H	0.299664470567	2.803798464059	2.567072693578
H	0.347537877054	0.621035673737	3.601199182386
H	-1.419363296045	0.587774164285	3.689737363921
C	0.901981913345	-2.611100398186	-1.894470363245
C	0.101580395610	0.201627353931	-2.631254926240
H	1.606345302470	-0.866335493975	-0.377902637100
H	0.088873676930	-1.915874322090	-0.095875418229
H	-0.084267053124	1.283006162381	-2.692665679418
H	0.985544334395	-0.037593320495	-3.239148290489
H	-0.778730589622	-0.331104206865	-3.021119371134
H	-0.032173418580	-2.806159938757	-2.446456398405
H	1.238279899846	-3.551255809933	-1.432443809224
H	1.671818497151	-2.282519176253	-2.606989772285

< IM_{non_S} >

C	-0.283264546299	1.676843913668	0.967667250676
N	-0.620548202910	0.742444674722	-0.003321711895
C	-1.924191055300	0.230400179854	0.088465565626
C	-2.558490818851	0.887447601982	1.309635523734
C	-1.489747200167	1.836937764842	1.876646154614
O	0.798746925581	2.219550602494	1.059860630312
O	-2.408743077751	-0.574912485180	-0.663083997965
O	0.165091207131	0.521656692330	-1.081405048207
C	1.399541583425	-0.424255959385	-0.872496838121
O	1.845110315218	-0.248364443473	0.412271303948
C	2.324472470921	0.131691712731	-1.948233708250
H	-2.861295030637	0.098131746464	2.015043905847
H	-3.479639403615	1.399571570354	0.991329482701
H	-1.792814270872	2.895760326126	1.872975797819
H	-1.186582851216	1.597994339338	2.907849081814
H	3.272497070028	-0.423293899846	-1.925098603662
H	1.869135376948	0.035051592090	-2.945353697157
H	2.511864104117	1.198090776717	-1.761368531663
C	0.323819902874	-2.545554395853	-0.129753298025
N	1.103478186733	-1.775891128404	-1.088214288929
H	1.904639690034	0.710694742522	0.590836018270
H	0.839794659562	-1.948300151665	-2.052959774745
H	0.504158745058	-3.619635874725	-0.296261268610
H	0.666636907071	-2.304735498724	0.885449649767
H	-0.764008051860	-2.361836314820	-0.196966346355

< TS_{2non_S} >

C	-0.454295007747	1.804854840984	1.631119973049
N	-0.275507144985	1.174265634910	0.392286073350
C	-1.422047769447	0.611342627291	-0.135129322928
C	-2.576014575574	0.947285307479	0.800152425037
C	-1.938274423001	1.709710919671	1.971272769507
O	0.428286104563	2.309482695521	2.282010560953

O	-1.476624316407	-0.050752593098	-1.160983312270
O	0.897234073993	1.141535194712	-0.233257927400
C	1.678931884475	-0.732584588482	-1.080451249852
O	2.634139593367	-0.499632114321	-0.193620217278
C	1.725783835300	-0.106915164179	-2.439429615303
H	-3.084235242991	0.016619868846	1.099084532367
H	-3.317198128883	1.542645106793	0.242434548871
H	-2.337502678067	2.727579537785	2.105192092945
H	-2.049810876641	1.198227397299	2.940650812359
H	2.114179268085	0.913430768078	-2.353680524088
H	2.402189032225	-0.703306441231	-3.077814308420
H	0.722111011763	-0.072852419713	-2.883069531497
C	0.781089452061	-2.527538197311	0.351213571393
N	0.886351290166	-1.771840643919	-0.886236512514
H	2.283189887645	0.386502185192	0.169356683648
H	0.112239618341	-1.851479280541	-1.542326960515
H	0.871077930087	-3.605452625698	0.144739842779
H	1.587917747963	-2.220271686442	1.026046603232
H	-0.193210566285	-2.340856329626	0.830438992572

<The PFP ester amionolysis>

< pentafluorophenyl acetate >

C	1.512513656176	1.147753689147	0.017602191220
C	2.096375516955	-0.119927176742	0.098629869209
C	1.312508132841	-1.265244493612	-0.073920437917
C	-0.058129246451	-1.138099238802	-0.308186327827
C	-0.649567004413	0.126387581944	-0.396345885909
C	0.138739896484	1.266305202187	-0.209464446692
F	-0.416826923590	2.472202126644	-0.263275960090
F	2.259979424127	2.234913749525	0.178081186577
F	3.399495795267	-0.237208033924	0.323579065247
F	1.871252210620	-2.468796117691	-0.001659381202
F	-0.804810474885	-2.226620169732	-0.461919929531
O	-1.985917664206	0.259557802322	-0.672257817910
C	-2.881662310133	0.030498733863	0.361577673557
C	-4.288194562974	0.203430648258	-0.135358309485
O	-2.526142096615	-0.258250715573	1.465587148054
H	-4.412185386707	1.210075215807	-0.563310233701
H	-4.486682330059	-0.520081774477	-0.941385446424
H	-4.990805197695	0.050398944686	0.692194878457

<pentafluorophenol>

C	-0.852293701028	0.000000682080	-0.868673492046
C	-1.431572906412	-0.000000858557	0.400351218153
C	-0.609334533269	0.000000172541	1.530685933120
C	0.780878348112	-0.000000209475	1.372520002237
C	1.350574517883	-0.000000034402	0.096387057212
C	0.537638991735	-0.000000306871	-1.047326928894
O	1.104278304250	-0.000000190535	-2.270569316658
F	2.674508488785	0.000000371228	-0.033103528536
F	1.566103958451	0.000000227510	2.444727953611
F	-1.144032898472	0.000000613649	2.748935859609
F	-2.754173290760	-0.000001826135	0.533078004036
F	-1.625061098778	0.000003040706	-1.968151611333
H	0.402485829502	-0.000001681738	-2.938861150510

The noncatalytic concerted mechanism for PFP ester amionolysis (Figure S1)

< Init_{non_C} >

C	0.301042394148	0.030295577396	1.659746502402
C	0.094729225200	-0.171310682153	3.026519690485
C	-0.961421424926	0.480290931428	3.669929998697
C	-1.787390181891	1.351481602559	2.952439976620
C	-1.562911229004	1.557527122931	1.589327498105
C	-0.507997436200	0.910951377154	0.934202820297
O	-0.241279562319	1.142335819286	-0.386075607833
F	-2.346197970955	2.390204521428	0.913569635119
F	-2.784327686889	1.976812293087	3.569562750509
F	-1.169942209384	0.284664961636	4.966439343964
F	0.883977997309	-0.993797699441	3.710253145034

F	1.299708903509	-0.612370390622	1.049335079384
H	2.038034094900	-0.535774493744	-1.207778581479
C	-0.653570826690	0.968608627009	-2.709627435383
C	-1.132779856531	0.629731022137	-1.334210290242
N	2.025910892961	-0.992026185940	-2.120582824302
O	-2.089881653135	-0.010166892944	-1.013314367209
C	1.887503555712	-2.436127902804	-1.961278027193
H	0.261208668966	0.370048455004	-2.887236365973
H	-1.429063768023	0.716053860744	-3.442697353365
H	-0.384060129971	2.033176663535	-2.772408951443
H	2.912479968488	-0.761384719485	-2.570184601353
H	1.844515479494	-2.920481322095	-2.950751290391
H	2.695973685734	-2.930257440770	-1.383281793433
H	0.936614709466	-2.661849190354	-1.452285376958

< TS_{non_C} >

C	0.375776120801	-0.225103139994	1.748633125313
C	-0.117148077275	-0.382556462504	3.042762564885
C	-1.119819459874	0.472723860536	3.506992342515
C	-1.578724985617	1.505797848445	2.682331462902
C	-1.077499345314	1.645538558839	1.388695925318
C	-0.038604232139	0.820769115843	0.893461480982
O	0.471775255921	0.981317424066	-0.302231257785
F	-1.555888447659	2.621621280364	0.609213758051
F	-2.527921291448	2.330490166214	3.129860806378
F	-1.611619295524	0.328099567733	4.739843312209
F	0.335355214598	-1.364007271413	3.826285534699
F	1.334380271341	-1.065791908017	1.307678659482
H	1.676547947516	-0.068481780066	-1.095682081816
C	-0.675424218409	0.825009057385	-2.626273345436
C	-0.254347300399	-0.252454363560	-1.665629630064
N	1.329460750498	-0.651059881515	-1.888639784068
O	-0.924254920817	-1.116638609723	-1.180907254430
C	1.619518232202	-2.087018888836	-1.728697951487
H	0.106497845307	1.581368169614	-2.771522037519
H	-0.950080791454	0.365916495135	-3.592424990067
H	-1.561429700785	1.320075865724	-2.207471313843
H	1.690302753132	-0.269924973391	-2.767236128408
H	1.203550516218	-2.648200686426	-2.576245986245
H	2.706017088067	-2.242068162978	-1.671186397935
H	1.143580071112	-2.425421281474	-0.801610813632

The noncatalytic stepwise mechanism for PFP ester amionolysis (Figure S2)

< Init_{non_S} >

C	0.351189212081	-2.240927580181	1.601261862239
C	0.179733396967	-2.254050254909	2.986968297084
C	0.353110172107	-1.075583783608	3.719909956103
C	0.695973028478	0.110571481163	3.064981938351
C	0.856209782306	0.115741009373	1.676543048731
C	0.699508985828	-1.059912457785	0.935507336733
O	0.913892760333	-1.054723254094	-0.415900095622

F	1.164270899450	1.257969823687	1.060682808104
F	0.859509191528	1.230245031310	3.762333201428
F	0.196595636465	-1.084435537938	5.038412940512
F	-0.144061018824	-3.381077806848	3.611617086245
F	0.189703295452	-3.361745464203	0.907493120687
H	-1.509859585754	1.584568912383	-1.337719201675
C	0.218722720568	-1.131663929652	-2.682892489875
C	-0.199437706453	-1.150196052652	-1.245929591124
N	-0.635754123231	1.982748855020	-1.683618089450
O	-1.311606133555	-1.191669294237	-0.805666391375
C	-0.881292163930	3.225790353462	-2.404912962790
H	0.281384138684	-0.065001934388	-2.958794471676
H	1.198508679461	-1.605729938806	-2.826352875620
H	-0.553482685652	-1.615614124642	-3.294431745761
H	-0.057592523983	2.148428550706	-0.859193184618
H	0.071733030753	3.635879827886	-2.778091015385
H	-1.510094322516	3.026843013163	-3.288556832146
H	-1.379047053957	4.028215568351	-1.820567221086

<TSI_{non S}>

C	0.558162217699	-1.840252620029	1.251734621703
C	0.353083545383	-2.246630992462	2.572100973030
C	0.242063992009	-1.291143153927	3.587348735646
C	0.361118889851	0.067520797879	3.281776594210
C	0.558714821686	0.456510518970	1.956197586977
C	0.694715038755	-0.483165213898	0.925731927876
O	0.946421274862	-0.083958592278	-0.340571942990
F	0.635608338888	1.762941524400	1.662774386878
F	0.250847016321	0.980216324764	4.245271294334
F	0.046379851564	-1.675362711583	4.845817201971
F	0.243260747376	-3.539525427117	2.867477450947
F	0.662444389845	-2.760007902116	0.296930856654
H	-1.483085869339	0.922639200908	-0.734467564894
C	0.270736231300	-0.595132352157	-2.577143357193
C	-0.220824118028	-0.006799912367	-1.269361836069
N	-0.555665445368	1.529959446224	-1.287928787416
O	-1.361758618073	-0.415303497986	-0.765441715756
C	-0.806842352515	2.230395678362	-2.549132499574
H	1.217342125724	-0.140930383505	-2.905575627782
H	0.437517331215	-1.667818073938	-2.405579292858
H	-0.493806554780	-0.486144226160	-3.358971897924
H	0.095170629734	2.035754703607	-0.679825968520
H	0.100904210477	2.296470547230	-3.170284056270
H	-1.588033558944	1.700995146989	-3.112825784045
H	-1.164474135645	3.248771170192	-2.336051298934

<IM_{non S}>

C	-1.226064404653	1.154818468131	0.255673595717
C	-1.474704912397	2.520280882416	0.091098283670
C	-0.464151171958	3.450412764657	0.348256608894
C	0.789034959474	3.008635473663	0.783895396154
C	1.023971655937	1.642645658303	0.944790837261
C	0.023576481640	0.683200158287	0.698065973815

O	0.268065093827	-0.616236582698	0.930637009239
F	2.229723698697	1.234361526531	1.345392889795
F	1.756189020169	3.890150973308	1.022936953170
F	-0.695445176949	4.749451418517	0.185801819480
F	-2.669210988805	2.938064678468	-0.320355615948
F	-2.214215157049	0.290700167253	0.003476524256
H	1.845237556495	-2.147879904397	1.155087231271
C	1.530822924825	-0.860652366713	-1.203496120164
C	0.634731362064	-1.589379431844	-0.207405730524
N	-0.494195614867	-2.143939333860	-0.826594203636
O	1.297884855986	-2.582314619548	0.486096283381
C	-1.445035558399	-2.886259047766	-0.009306652839
H	0.986072873319	-0.085204007686	-1.763729495079
H	2.373471463330	-0.386633683655	-0.681074438794
H	1.919799260904	-1.600348425544	-1.916347643663
H	-0.941280438744	-1.486302546858	-1.457500073125
H	-2.205836180914	-3.333209586711	-0.666456381675
H	-0.920099598871	-3.699309716177	0.509262024346
H	-1.951693893604	-2.258460754356	0.745589789281

<TS_{2non_S}>

C	-0.367454180330	1.486980187176	-0.510512415043
C	-1.083121204569	2.637520045406	-0.181831500709
C	-0.813769029928	3.312022886707	1.011033037267
C	0.219797841374	2.845217444755	1.831042378487
C	0.919256270659	1.686554205566	1.497521710215
C	0.707117562140	0.991534788352	0.274712259422
O	1.410213720026	-0.041084412772	-0.073530444691
F	1.883589420743	1.251466634725	2.320175866163
F	0.496868020882	3.489026346352	2.967520426426
F	-1.502820267058	4.410077752389	1.341956564944
F	-2.056199118044	3.072917924461	-0.987872072531
F	-0.674135215267	0.848694451692	-1.667201232332
H	1.852258614731	-1.569924541865	0.494305923794
C	1.161164984822	-1.773068014955	-2.125054350895
C	0.602718205557	-1.947252788816	-0.747018675142
N	-0.707656054837	-2.020301734650	-0.585435662111
O	1.369995602638	-2.410059233038	0.229658527626
C	-1.388778394997	-2.287563206696	0.674220950492
H	0.545513659549	-1.088515611082	-2.722216199672
H	2.176447165331	-1.368991623824	-2.053673663350
H	1.198691881442	-2.763479375331	-2.612403073897
H	-1.272339583900	-1.686626575963	-1.361620796481
H	-2.115914052125	-3.103603191204	0.542461784341
H	-0.643737208880	-2.584242516032	1.420414216794
H	-1.917708639963	-1.387299841353	1.023346440886

<The 4-NO₂-Ph ester aminolysis>

<4-nitrophenyl acetate>

C	-1.955293464628	0.525486280218	0.990808039509
C	-0.579653102472	0.581271201039	1.190120803207
C	0.296896273445	0.164036417580	0.176870121470
C	-0.196532972337	-0.312533445312	-1.047256513728
C	-1.576044118339	-0.366712305290	-1.246326683085
C	-2.437770060913	0.048949848143	-0.230611686117
N	-3.895041497982	-0.013259248387	-0.452878041469
O	-4.285000833482	-0.435149432330	-1.530236956020
O	-4.620865448441	0.362024302137	0.454773666196
O	1.634870907296	0.322576880268	0.467885204874
C	2.640405459776	-0.453438363342	-0.056623032320
C	3.970003660939	0.035408230258	0.453833052916
O	2.458761667204	-1.375869474500	-0.800621984480
H	-2.660320337934	0.841562128276	1.759422178877
H	-0.159455885935	0.950806214906	2.127461025183
H	0.483880167827	-0.644496079173	-1.827706292247
H	-1.996706560626	-0.728771726716	-2.184447997673
H	4.117502205298	1.086972516863	0.161166779649
H	3.988364432437	-0.001330334179	1.554092845478
H	4.771999508866	-0.587533600457	0.040275489781

<4-nitrophenol>

C	-0.051520331704	0.000006206936	1.654735604142
O	-0.109292833129	-0.000018237806	3.002947022161
C	-1.270594700131	-0.001691535168	0.951463145467
C	-1.271994512719	-0.001807973664	-0.437885794919
C	-0.052884566192	-0.000136067049	-1.125332205317
C	1.165870908594	0.001606454453	-0.443683873207
C	1.164927737028	0.001634167258	0.948580096162
N	-0.053640936310	-0.000220427958	-2.595351437700
O	-1.136897820423	-0.002898987778	-3.161271103950
O	1.029199146548	0.002417840508	-3.162814215200
H	0.783742083637	0.001346763001	3.374169915391
H	-2.203340904162	-0.002899516775	1.518692629789
H	-2.202041338977	-0.003190139573	-1.006388312886
H	2.095321292269	0.002930194717	-1.013033136011
H	2.113146755674	0.002921248898	1.495171666078

The noncatalytic concerted mechanism for 4-NO₂-Ph ester aminolysis (Figure S3)

<Init_{non_C}>

C	-0.395467135473	-1.084942300064	-0.171140655336
O	0.971837713776	-1.183334733523	-0.090265062053
C	-0.922552272782	-1.511302562141	-1.403440413550
C	-2.293027315364	-1.482481932702	-1.629591754665
C	-3.133309478963	-1.022406616176	-0.611623877188
C	-2.625588268298	-0.599006936913	0.616121689711
C	-1.249099712646	-0.627698962542	0.847884485105
N	-4.589157222725	-0.986614110396	-0.842561095262

O	-4.998170441844	-1.375235640072	-1.926078557029
O	-5.296119749734	-0.570269836907	0.061929486461
H	0.921656365166	2.036477471436	-0.391521974962
H	-0.231035141524	-1.863307882710	-2.171207305439
H	-2.725269575115	-1.807959578982	-2.575614964718
H	-3.315794924181	-0.251076624185	1.384852774307
H	-0.839287988407	-0.303065354947	1.799976629129
C	3.210530414143	-0.901446428199	0.565538167157
C	1.765542967987	-0.694349842703	0.919081267315
N	1.936959695672	2.142841208356	-0.375835138228
O	1.344203497222	-0.174550534519	1.916824701866
C	2.333635260951	2.993861653404	0.743851424797
H	3.470666632847	-0.119444143604	-0.165734841803
H	3.829050755280	-0.781681865468	1.463505010673
H	3.371887991751	-1.885746306792	0.103707611463
H	2.183998213101	2.580511056694	-1.264364220082
H	2.074616484074	2.492429175757	1.689681157985
H	3.428004371311	3.127720816374	0.738218888613
H	1.876834811504	4.005218087272	0.758823046256

< TS_{non_C} >

C	-0.560106391814	-0.103345930163	-0.479797133413
O	0.622664282773	0.456610232620	-0.492400457336
C	-1.273737480833	-0.296036350628	-1.698209714417
C	-2.527281203442	-0.887975028163	-1.713205647253
C	-3.105495945221	-1.314239335587	-0.508762185819
C	-2.432277862768	-1.140728165037	0.707949075391
C	-1.180658833451	-0.541256642460	0.726395694613
N	-4.422087753027	-1.939879256937	-0.522068416548
O	-4.990512943454	-2.063504092804	-1.601949895989
O	-4.894442656357	-2.311515442941	0.547098218527
H	2.028788585722	1.387853589539	-0.784807762156
H	-0.803281254388	0.038504816055	-2.626276293403
H	-3.077373341817	-1.036630237936	-2.642918063499
H	-2.914151587211	-1.476998371133	1.626596218281
H	-0.662062363898	-0.381924170679	1.673634422898
C	2.581382990553	-0.970484911037	0.561652926063
C	2.044586003404	0.373401656540	0.973864007468
N	2.641856406931	1.545944292808	0.045935165828
O	1.664487036579	0.706188934608	2.056986980454
C	2.426059822992	2.891566993134	0.614319525610
H	2.748565918954	-1.047435938625	-0.519817413070
H	3.521162166195	-1.161100657586	1.109581485370
H	1.852587959123	-1.735701969116	0.861576483349
H	3.625102923152	1.369369306060	-0.181177098898
H	1.346195825755	3.031482291620	0.740239259726
H	2.909691392367	2.958989856107	1.596715178898
H	2.830338303179	3.648844531739	-0.071154560673

The noncatalytic stepwise mechanism for 4-NO₂-Ph ester aminolysis (Figure S4)

< Init_{non_S} >

C	-2.768664485455	2.603808091231	-1.248349241070
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C	-1.494609236508	2.503487326928	-0.702747206004
C	-0.916432477654	1.242209429133	-0.478649508709
C	-1.616188817148	0.067887393070	-0.801156683427
C	-2.896197491927	0.172991028187	-1.348457674038
C	-3.457891517528	1.430386359641	-1.566246229206
N	-4.811362923398	1.526375466332	-2.145396610125
O	-5.387513947387	0.483655833515	-2.412859813308
O	-5.271604398767	2.644088940575	-2.320631504675
O	0.344450072861	1.303718626741	0.073031212061
C	1.170608323180	0.248286125720	0.353810813788
N	3.508919464922	-2.471676874582	1.165469268722
O	0.887475212696	-0.902272501005	0.135333336219
C	2.454100997549	0.744460684874	0.959150336787
C	3.513605381962	-3.427534030335	2.265418971005
H	-3.239630364544	3.569198841438	-1.432315270781
H	-0.921833327436	3.394303578825	-0.438389279734
H	-1.164361642525	-0.904395959840	-0.628133713822
H	-3.468625500529	-0.716783420541	-1.611012182777
H	4.113561976305	-2.791897940995	0.408272874911
H	2.572874115868	-2.373638471344	0.766786014877
H	2.232289762068	1.325824367456	1.868211255433
H	3.098944542651	-0.115530398338	1.192854696620
H	2.953374325229	1.428705363200	0.254565422957
H	2.848693946654	-3.071222449574	3.069525172948
H	4.525297651771	-3.500019829880	2.698787744058
H	3.191776543343	-4.458809787133	2.006757885830

< TS1_{non_s} >

C	-2.767801730184	1.104004082922	0.276615140192
C	-1.577998709445	0.665238331518	0.842164102363
C	-0.548775960284	0.141883833904	0.032215627641
C	-0.730514715637	0.058696522503	-1.363501211782
C	-1.923491833066	0.505173606241	-1.927554605371
C	-2.930573393034	1.023592131923	-1.110439038104
N	-4.185208717333	1.489039647708	-1.715303523943
O	-4.296458767758	1.408473846545	-2.930368458843
O	-5.046764098756	1.931258910099	-0.967740467011
O	0.565655654741	-0.254729774403	0.692369958492
C	1.797637405511	-0.605540565516	-0.011121746218
N	2.514722756808	-1.532117312093	1.031565509050
O	1.702705971223	-1.503677013055	-0.970939821892
C	2.564323651925	0.679660598828	-0.305944492824
C	2.072499585381	-1.672690223972	2.425797607624
H	-3.574341023027	1.512581681927	0.885283503303
H	-1.415413170155	0.720376563176	1.920499953315
H	0.049068207830	-0.386861319935	-1.979604171843
H	-2.091181809796	0.449174323453	-3.003293237297
H	3.522163825090	-1.360537057604	0.975101211264
H	2.180589014060	-2.225679226721	0.072958292917
H	2.005628874963	1.262059904234	-1.053593630454
H	2.692947384776	1.302039041471	0.592872936199
H	3.543929423262	0.432733659148	-0.742750985854
H	1.018805402220	-1.973215459416	2.442314765913

H	2.177020297774	-0.724294845536	2.975276918208
H	2.680826472914	-2.446643887350	2.917119864957

< IM_{non_S} >

C	0.360541132584	-1.451048059270	-2.462984294344
C	0.352345617149	-0.165742453869	-1.935486246888
C	0.538219012154	0.051693125092	-0.553635155172
C	0.740092152232	-1.057742948154	0.295668417850
C	0.740462395702	-2.346823910771	-0.231040760780
C	0.550162903363	-2.536468889556	-1.601800215112
N	0.554081854349	-3.899926565059	-2.149196467064
O	0.718644851362	-4.826423619358	-1.368238234712
O	0.391860093255	-4.028332224774	-3.354339420784
O	0.572396462100	1.346191547565	-0.159930348511
C	0.018835044925	1.884637310649	1.115787589108
N	-1.382346021499	1.742606883033	1.245027902075
O	0.621037798719	1.250322254588	2.200070613359
C	0.401846060776	3.359834521118	1.023728111371
C	-2.014158009725	0.480990870326	1.601213448812
H	0.217154204886	-1.634093960732	-3.527942857811
H	0.205345173542	0.704668770987	-2.578054510811
H	0.892488849077	-0.902692939142	1.361674461759
H	0.893876177988	-3.217255926158	0.407129478057
H	-1.869763031327	2.248453359631	0.512598196941
H	1.572124003088	1.419416559311	2.153876730195
H	-0.103853480797	3.841055731294	0.173575005916
H	0.110977163035	3.865318262442	1.954243226717
H	1.486231266396	3.460499671216	0.864565484246
H	-1.488161654502	0.038348737627	2.457595122014
H	-2.044158755163	-0.267678328972	0.787642124667
H	-3.050180047150	0.682440710167	1.917239334168

< TS_{non_S} >

C	-0.043977336036	-1.221734620454	-2.110677089810
C	0.317062857470	-0.085593697121	-1.400904610173
C	1.078026061156	-0.168621713175	-0.193458101185
C	1.467050112535	-1.473159979549	0.239819551908
C	1.115319694649	-2.607836754346	-0.474213042619
C	0.350934872584	-2.483289503295	-1.644577402865
N	-0.030853862143	-3.676987141296	-2.388829026823
O	0.343604869245	-4.764649228574	-1.964378215274
O	-0.710468820043	-3.531947811795	-3.399845617338
O	1.387814199833	0.895984354448	0.485730925086
C	-0.126670741949	2.131969703354	1.312656774049
N	-1.334958791673	1.646371729419	1.063394292511
O	0.437139155859	1.804938560614	2.472241847823
C	0.324174013595	3.370662894937	0.599455102444
C	-1.948174516861	0.514979005423	1.748227241072
H	-0.621207105815	-1.161149325262	-3.034022716387
H	0.046164883455	0.905188917522	-1.776188092331
H	2.062819201434	-1.552148576598	1.152875740455
H	1.413086617152	-3.604281654350	-0.145977973336
H	-1.796997966969	1.986965047008	0.226035119411

H	1.254881525660	1.329821154110	2.149130686339
H	-0.071605320707	3.422489878896	-0.424519183784
H	-0.027941561741	4.248576259824	1.169300417797
H	1.418924319914	3.385001857885	0.559321295439
H	-2.961269085004	0.784413349029	2.084591275910
H	-1.336402280347	0.258021110413	2.619729732064
H	-2.006474995256	-0.353983817073	1.075081069616

<The HFIP ester aminolysis>

<hexafluoroisopropyl acetate>

C	0.054253271052	-0.110510150198	0.884346801560
C	0.961550987965	0.960872435577	1.506191752515
F	0.844879207065	0.965156972570	2.838745439953
F	0.589074946718	2.164675468965	1.050083138249
F	2.248474716244	0.780575522992	1.198679631160
C	0.404679741845	-1.555270933579	1.265102019416
F	0.359403346762	-1.719396967266	2.592432912817
F	1.617620146016	-1.913180547005	0.838376347781
F	-0.490828182335	-2.383374132888	0.710272894192
O	0.136573940940	0.003309588790	-0.518330375215
C	-1.011682066360	0.347500119622	-1.195533095801
C	-0.732377767036	0.443445211231	-2.667675477657
O	-2.059463837768	0.534082679811	-0.643742856566
H	-0.974279451731	0.085250761265	1.225351780256
H	-1.655855821400	0.695768762604	-3.201886539637
H	-0.326272106144	-0.511822191067	-3.034113867421
H	0.034248928166	1.212917418575	-2.848300505604

< hexafluoroisopropanol >

C	-0.350539160944	-0.000000283980	-0.434650859369
C	0.354780467946	1.291365149179	0.018359635094
F	0.314653917226	1.403981092481	1.358902267074
F	-0.273866498682	2.350784910368	-0.498652159875
F	1.633104532128	1.337320464907	-0.366948106410
C	0.354781453602	-1.291365640463	0.018358551127
F	1.633103237013	-1.337321848585	-0.366957048165
F	0.314663015380	-1.403980248934	1.358901462091
F	-0.273869222300	-2.350785791980	-0.498648026635
O	-1.677461384314	0.000000124207	-0.011237965546
H	-0.341945691083	-0.000000232909	-1.535970517630
H	-1.687404655972	0.000002305709	0.958542778244

The noncatalytic concerted mechanism for HFIP ester aminolysis (Figure S5)

< Init_{non_C} >

C	-0.552360277010	1.146641079330	-2.048843061087
C	-0.913190984600	0.703680435509	-0.666574479775
N	1.078857079040	-1.790404330339	-1.821321997542
O	-1.792793254143	-0.051446540413	-0.352980489342
C	0.071994010003	-2.846322269659	-1.897706688872
H	0.189947335894	0.410061265653	-2.409022768420
H	-1.441134639126	1.101403153705	-2.691238978229
H	-0.107577088166	2.150348104875	-2.049141500267
H	1.910974906251	-2.045255283950	-2.354253698628
H	-0.822673409293	-2.540711134780	-1.332325606885
H	-0.243505911225	-2.984377641450	-2.945005825215
H	0.393284547122	-3.837503612458	-1.515036531918
C	-0.240054624983	0.880363822847	1.608019813205

C	1.047010422108	0.226149697465	2.125447698703
F	2.113139560480	1.015856049874	2.001645150353
F	1.287392937529	-0.898422088633	1.423620694495
F	0.919825580715	-0.114517665998	3.412889441526
C	-0.678163543827	2.125258304505	2.396124928736
F	-1.069197254658	1.780475460423	3.629277976794
F	0.296486890689	3.033050064623	2.505688111869
F	-1.714245409963	2.700876624545	1.774877792084
O	-0.041411264946	1.239776493339	0.262328351039
H	-1.051484549834	0.139644801887	1.688743086876
H	1.387487504909	-1.662081416091	-0.857042469941

< TS_{non_C} >

C	-0.688710550363	1.119121361715	-2.190233191021
C	-0.743338268312	-0.101096975179	-1.314683320242
N	0.501867661155	-1.051831596020	-1.507322385233
O	-1.707716380716	-0.583472294412	-0.786841584600
C	0.235045427399	-2.488527875994	-1.322351019038
H	0.335829497786	1.492130937064	-2.315798869061
H	-1.131723494284	0.882325720890	-3.174123343649
H	-1.290489747103	1.903599401797	-1.713574150051
H	1.005193769130	-0.848088395527	-2.374297607331
H	-0.334411986151	-2.612292548416	-0.394868491133
H	-0.354356358578	-2.881972928039	-2.162570577444
H	1.189211060143	-3.027631575390	-1.246519270989
C	-0.048578053611	0.622746690808	1.360428299975
C	0.687709885072	-0.329078483385	2.323620986425
F	1.888958548725	0.124375339217	2.702040040781
F	0.893083288651	-1.513771114395	1.694188350374
F	-0.020552043795	-0.592562377051	3.430624492854
C	-0.172152745634	2.050372981718	1.922833363535
F	-0.722027207849	2.065665818493	3.151916666006
F	1.007931990123	2.675489784316	1.996892911035
F	-0.967241071745	2.780220213083	1.118196010157
O	0.542723740306	0.652544302337	0.137448862309
H	-1.093126221620	0.225117539100	1.320269612314
H	0.986869261267	-0.563383926728	-0.655275785971

The noncatalytic stepwise mechanism for HFIP ester aminolysis (Figure S6)

< Init_{non_S} >

C	-0.503742601523	1.111527565903	1.659118851675
C	0.138742815211	-0.128599688090	2.294306576428
F	-0.236479977490	-1.223132886080	1.603024573701
F	-0.269473862600	-0.282973275313	3.558156265631
F	1.471530899614	-0.081374764045	2.285175448467
C	-0.146533772203	2.438851340005	2.344800840057
F	-0.587372571837	2.448310131205	3.609061802641
F	1.169280118997	2.667884237860	2.358561267700
F	-0.736907896815	3.445673897230	1.689170012983
O	-0.092209193842	1.174405791207	0.315797670607
C	-1.082947491754	1.163103333002	-0.650500894235
C	-0.474332357278	1.139045946335	-2.016058826206

O	-2.248539564600	1.127372911623	-0.367428509829
N	0.232918763254	-2.171249719663	-1.692842432644
C	1.352851602121	-2.971128134140	-2.178173645299
H	-1.597662717289	0.993909742770	1.720080799829
H	-1.228744997757	1.419422625699	-2.761459922890
H	-0.135888618879	0.097915059234	-2.193626936956
H	0.402368359868	1.799748202249	-2.068874585396
H	0.275424054713	-2.070058906033	-0.677824244262
H	-0.653707952786	-2.636103903935	-1.892637279597
H	2.301405599307	-2.458743864762	-1.949477096761
H	1.296562938427	-3.065091759179	-3.275045825884
H	1.420936466186	-3.997001046679	-1.760059304690

< TS1_{non_S} >

C	-0.168189914030	0.594421763960	1.326938786167
C	0.382199922029	-0.443376284717	2.314758730927
F	0.003182088994	-1.675227262703	1.919887728665
F	-0.090500278738	-0.251862371768	3.551973508230
F	1.719712582256	-0.438862096634	2.374567051922
C	0.180222258239	2.043315946776	1.697013068813
F	-0.318202946696	2.372212153725	2.897570555654
F	1.499613624129	2.263430279944	1.724664357566
F	-0.353691861025	2.877445504358	0.789329051503
O	0.324375181528	0.323879564757	0.050906539496
C	-0.671716680030	0.015276298340	-0.975831810508
C	-0.561281169263	1.084125203240	-2.051276705758
O	-1.874830782253	-0.293418808140	-0.521196661395
N	-0.296883979734	-1.418069954481	-1.478271088318
C	1.011936268858	-2.040205918225	-1.233896899414
H	-1.268159637985	0.493102046546	1.337389354125
H	-1.216903129368	0.836394803048	-2.900344665004
H	0.476317066793	1.209483844195	-2.396599446130
H	-0.899556974991	2.037262501308	-1.621673020722
H	-1.350733897260	-1.495484683383	-0.823698733384
H	-0.552512168321	-1.480373193347	-2.467275125117
H	1.205229770798	-2.079597000267	-0.157491394006
H	1.818960352042	-1.469864603428	-1.720842332920
H	1.001414304031	-3.064007733104	-1.636600850390

< IM_{non_S} >

C	0.358831916972	1.701613510872	1.850825871692
C	-0.123347676834	0.869599124174	0.658599856673
N	0.738730752925	0.906985773674	-0.482630028358
O	-1.389462877344	1.270503555469	0.235253261515
C	0.448644707003	1.792342265925	-1.599927909915
H	1.356544888305	1.368737210430	2.174442318368
H	0.400487457879	2.761813870462	1.560473936981
H	-0.327098219211	1.591063556335	2.705399039791
H	1.712184294959	0.943631897740	-0.196265808127
H	1.222157029575	1.637424065520	-2.367596803691
H	-0.521397222960	1.535476357016	-2.042883574635
H	0.431133278774	2.870110337742	-1.339068904002
C	-0.265149259897	-1.613629156600	0.401768727252

C	-1.478478219381	-1.701953025968	-0.551327894488
F	-1.430815876528	-0.906999253746	-1.617683932530
F	-2.601093214085	-1.419720815804	0.130774133651
F	-1.581166383762	-2.968762922173	-0.996838066000
C	1.067302270837	-2.047726868726	-0.281540945889
F	1.173782592396	-3.388671120366	-0.196889641893
F	1.172763980074	-1.737602339790	-1.575831548506
F	2.116055858874	-1.523930850854	0.367140533874
O	-0.190634250727	-0.474409544321	1.202633659210
H	-0.453252733474	-2.426921405765	1.119983407996
H	-2.009629794190	1.088022026795	0.954067615991

< TS_{non_S} >

C	1.347637642296	1.246303734500	1.220516753876
C	0.063507169610	1.531741640217	0.504387303121
N	0.103807437730	1.922306023175	-0.762773351146
O	-1.026050277353	1.812262393193	1.200589589066
C	-1.086022967817	2.183161451105	-1.561469344555
H	2.058894496587	0.704700531368	0.583794033623
H	1.792182754936	2.206751953532	1.537034495543
H	1.135457615782	0.644604939005	2.110498328701
H	0.955728812850	1.697840067429	-1.267793642375
H	-1.472013794330	1.243070743536	-1.986707592224
H	-1.855739558561	2.627465686062	-0.919928439857
H	-0.835654662622	2.882767750113	-2.371402674988
C	-0.544690131897	-1.681511872369	0.223139231095
C	-0.032764572383	-1.715074217198	-1.235228022612
F	1.060468190399	-0.934360529071	-1.408152177946
F	-0.979341738920	-1.235283949617	-2.065395391788
F	0.286785757993	-2.943910953500	-1.663751023357
C	0.430418896488	-2.410510299316	1.180686408611
F	0.511925298126	-3.728492570585	0.929749273054
F	1.684141970876	-1.912744197097	1.114339065825
F	0.014556538132	-2.265402555892	2.446883472474
O	-0.797685388156	-0.415586376554	0.608119530493
H	-1.451141070390	-2.334221611135	0.209352865593
H	-1.364407419377	0.874123219098	1.373511309773

<The 4-CF₃-Ph ester aminolysis>

<4-trifluoromethylphenyl acetate >

C	0.602884083132	-0.214803854125	-1.453662683896
C	-0.782327405897	-0.155007122534	-1.343439709039
C	-1.378542566869	0.013252652195	-0.085495323358
C	-0.570690446907	0.125676812013	1.049272322352
C	0.823157975344	0.068860237521	0.953505173308
C	1.406530729944	-0.105499468235	-0.308619237981
C	-2.881180732033	0.021609223642	0.037112990883
F	-3.387335364227	-1.228149703343	0.043209074325
F	-3.462647914786	0.666877299844	-0.992082360970
F	-3.291177589810	0.615064322839	1.171613623798
O	2.762052015274	-0.186632765280	-0.569539450171
C	3.771937469272	-0.088705914832	0.345534695857
C	5.099472674196	-0.235648498951	-0.353877213779
O	3.616550142659	0.085908619528	1.523826086542
H	1.088048768404	-0.343895495568	-2.423073689952
H	-1.403461470449	-0.233304936528	-2.238246255665
H	-1.030859049801	0.266257488408	2.029149352339
H	1.445661182825	0.160907330943	1.838838309174
H	5.201004163333	0.531459935268	-1.137225455158
H	5.155485759640	-1.217218998244	-0.850227481695
H	5.909540201858	-0.137991145463	0.378717823585

<4-trifluoromethylphenol>

C	1.144748214460	0.206193485727	-1.145519255510
C	1.135206614699	0.223465280373	0.248439514656
C	-0.052681192435	-0.012810972350	0.951469694358
C	-1.232394581612	-0.270194983743	0.239421436138
C	-1.230180748445	-0.290698942045	-1.152338765916
C	-0.039328276549	-0.050397042409	-1.855545739263
C	-0.064152292221	0.059524209177	2.454676034932
F	-0.136612599650	1.332247806915	2.898215648723
F	-1.113100996143	-0.595683112299	2.984743739736
F	1.053320454832	-0.468491010933	2.990419895364
O	-0.089508902816	-0.081787536252	-3.207926078167
H	2.077136938978	0.388908165208	-1.689425530447
H	2.062494926792	0.416626261573	0.792492620083
H	-2.159554458593	-0.462758741113	0.782503376754
H	-2.141869209243	-0.494190973816	-1.717480559947
H	0.786476097947	0.100048085985	-3.574146041493

The noncatalytic concerted mechanism for 4-CF₃-Ph ester aminolysis (Figure S7)

<Init_{non_C}>

C	-1.498052003705	1.481631824843	1.695996566392
C	-1.113315008809	1.731011259809	3.010969233163
C	0.237154672427	1.645271122675	3.372641399113
C	1.193766890339	1.318482610613	2.405273837602
C	0.819547027631	1.067115332632	1.083759772155

C	-0.534927361002	1.146151927063	0.736213569607
C	0.650779140586	1.853960122425	4.806925817918
F	0.647459463298	0.697044885087	5.499891260182
F	1.893366963856	2.360433275593	4.902606608736
F	-0.180503340110	2.694977777466	5.448591215570
O	-1.024901863716	0.971865484589	-0.545378283110
H	-2.543526188005	1.548341623056	1.388944106569
H	-1.863306068678	1.998610106519	3.757711390987
H	2.248402711403	1.264469462937	2.682970893254
H	1.568368269253	0.805863627908	0.340006060710
H	1.574184213300	-2.188986292055	-4.440631168079
C	-1.274231893143	0.155133987315	-2.746516204309
C	-0.482378490571	0.122302684319	-1.468858910448
N	0.772680277016	-2.376020946253	-3.837484078730
O	0.497118272855	-0.547457725490	-1.258157362876
C	0.536669327670	-3.809485191073	-3.728311233888
H	-0.867244849016	-0.594254839866	-3.440615295155
H	-2.336638661317	-0.040362055548	-2.533802490480
H	-1.215155957995	1.163827297300	-3.187082708854
H	0.991504511435	-1.970012950712	-2.925311589537
H	0.272334648093	-4.227541438050	-4.714645149271
H	1.386274972440	-4.408399957287	-3.335296375763
H	-0.323621675536	-3.994954015814	-3.063982881455

<TS_{non_C}>

C	-1.131442519221	-0.502976926238	1.418782987904
C	-0.794895049445	-0.197131648866	2.732150838266
C	0.053387856916	0.884458318920	3.018509867289
C	0.549216522145	1.655643578319	1.958227157772
C	0.209402218803	1.361803850546	0.640280080774
C	-0.643447405255	0.271445590669	0.332840883322
C	0.380363428859	1.219844183780	4.442994432786
F	0.644451978272	0.115421436548	5.175959627521
F	1.452770522948	2.029483444637	4.546076356329
F	-0.638380705852	1.849291476556	5.074840742721
O	-0.987856155708	-0.026823246873	-0.906105510487
H	-1.793090446582	-1.345008820943	1.196957263133
H	-1.186086034420	-0.810084417137	3.548559780412
H	1.213941643063	2.496243168645	2.169368315077
H	0.609755234792	1.968994094243	-0.173302268104
H	-0.897772061378	-1.433528483412	-1.801053987635
C	-0.388588986552	0.950372522752	-3.268478934774
C	0.365127788807	-0.002892007275	-2.381220477447
N	-0.196097506742	-1.522815454432	-2.584454072221
O	1.493949131289	0.082222517420	-1.995134342871
C	0.815607938430	-2.566680329859	-2.348022261822
H	-1.466512223110	0.745620344772	-3.272426357231
H	-0.224657550724	1.969883490403	-2.895555811380
H	0.018750687734	0.888832691520	-4.293398584768
H	-0.673024451133	-1.631554220098	-3.483655874160
H	1.321621997056	-2.345214277652	-1.400673229678
H	0.330769529002	-3.551710139630	-2.299174999703
H	1.562734618007	-2.553140737316	-3.152891621025

The noncatalytic stepwise mechanism for 4-CF₃-Ph ester aminolysis (Figure S8)

<Init_{non_S}>

C	-0.916472781897	1.595721014253	2.167759566435
C	-0.933189414643	1.657718518938	0.781266828319
C	-0.061170551131	0.862177998589	0.046949294621
C	0.834308331678	0.001412930750	0.678363736499
C	0.846529256705	-0.050774126827	2.064632102953
C	-0.022220490133	0.744553435820	2.810963713483
C	-0.027862384474	0.625104464644	4.305523259942
F	-0.753656174487	-0.449175317548	4.718484172290
F	1.218891984818	0.460998090034	4.807379467580
F	-0.565055601114	1.711001205252	4.905939785528
O	-0.207797035325	0.917562459834	-1.328034274433
C	0.898716020822	0.876863822592	-2.155517383493
N	0.307294004141	-2.176195420835	-2.090477769116
O	2.032278796070	0.922764227766	-1.763645029266
C	0.449916882556	0.867984160089	-3.584839605952
C	-1.050527637041	-2.289253059109	-1.533559194544
H	-1.593929303183	2.214446467755	2.746282771293
H	-1.619275296491	2.315177039885	0.257617319864
H	1.507880304809	-0.608518372879	0.091143763395
H	1.541877768485	-0.713647670018	2.570152028861
H	0.326413178247	-2.561614553806	-3.028932409257
H	0.947038027136	-2.748834910848	-1.549955037312
H	-0.392192014754	0.186789692136	-3.719323180866
H	0.119623700816	1.876113225257	-3.859234826241
H	1.286810067463	0.579867506902	-4.220387461033
H	-1.051884236660	-1.909373081495	-0.506637131120
H	-1.463017072760	-3.310722033232	-1.520521817219
H	-1.733130329653	-1.654723713900	-2.109053691210

<TS1_{non_S}>

C	-1.104267781374	0.820583019199	2.457076969629
C	-1.296820221906	0.322056800482	1.173335147167
C	-0.193952182771	-0.020060650922	0.368475961841
C	1.108362830718	0.132259174942	0.875724944188
C	1.287917565700	0.643415778046	2.163125351407
C	0.193798568930	0.993177581108	2.961071529855
C	0.387140543350	1.589257025923	4.328418583519
F	-0.480582677577	1.078460871426	5.226175563099
F	1.627909186424	1.382422547740	4.805893619204
F	0.187553049691	2.925683597418	4.328852853716
O	-0.494208797178	-0.497158000885	-0.870284432698
C	0.517248720261	-0.588044469063	-1.912501508248
N	-0.136514451528	-1.609791541637	-2.911497692931
O	1.590313562577	-1.307258433302	-1.645494225784
C	0.721730985105	0.797120230101	-2.519825795564
C	-1.541874591740	-2.029792742551	-2.832258828709
H	-1.968213240494	1.078906006495	3.073981351687
H	-2.301407343073	0.188676647828	0.766187111458

H	1.958246196499	-0.179746185182	0.270015371152
H	2.300407769254	0.758486090324	2.555263832142
H	0.117847337566	-1.333711864315	-3.863572501114
H	0.834070471527	-2.153401951908	-2.394610852898
H	-0.227264057031	1.257597666526	-2.835260692641
H	1.187385525178	1.448279682140	-1.765418648953
H	1.415040097983	0.727899226785	-3.371865338137
H	-1.746923762964	-2.414115039164	-1.826791279408
H	-1.721400085773	-2.824426652169	-3.571930857181
H	-2.221543217359	-1.186774415388	-3.032285535799

< IM_{non_S} >

C	0.834832819455	0.880000684800	-0.491600284163
C	1.081639069700	1.460130838406	-1.737295951786
C	0.198665433490	1.276029371607	-2.807046512703
C	-0.951842107717	0.497326207839	-2.616269419020
C	-1.202696374735	-0.092712989919	-1.381166535736
C	-0.313086363366	0.087447437614	-0.305486133802
C	0.504634391309	1.869306300206	-4.156563733894
F	1.243006008214	1.037071921188	-4.921866394725
F	-0.615651346054	2.139781239662	-4.853589081444
F	1.203115044936	3.016352929050	-4.056157799665
O	-0.675095460126	-0.505278794085	0.865624384950
H	1.517131996909	1.052121767289	0.339095524056
H	1.971362486605	2.079354411088	-1.870961671995
H	-1.655320276312	0.353889610128	-3.439210553253
H	-2.093462822992	-0.703424643586	-1.219323258667
H	0.252869660436	0.856127370435	2.710636528273
C	1.305735035649	-1.874112406662	1.377557483896
C	0.260930337822	-0.909634452715	1.923072476605
N	-0.524277675568	-1.554173645783	2.931028037698
O	0.917247753425	0.213150463482	2.423411174030
C	-1.536593127019	-0.762040791612	3.613264632331
H	0.818022833486	-2.787639736428	1.007037363049
H	1.871426164318	-1.420523533577	0.553642986603
H	1.999705026276	-2.137697861214	2.186576451223
H	-0.921550634943	-2.412036659980	2.555738293759
H	-2.078086266814	-1.408670333121	4.319763103776
H	-1.059417250721	0.026296377164	4.219412749214
H	-2.276695643068	-0.287135958576	2.939486041177

< TS2_{non_S} >

C	0.916597178632	1.728690263187	-0.622914492377
C	1.050956426084	1.886020295567	-1.997925380347
C	0.227602652385	1.174821464565	-2.886104612333
C	-0.750765567121	0.315418069026	-2.363132784024
C	-0.898456185773	0.161480553693	-0.988484868519
C	-0.059810508382	0.853404557165	-0.069651169992
C	0.433672159570	1.282768585714	-4.367198187146
F	1.352229442102	0.398464702494	-4.827256965245
F	-0.698125198978	1.039021656641	-5.060116250841
F	0.873531326977	2.503484833266	-4.735477653454
O	-0.177108685788	0.680673746736	1.221611680971

H	1.555604006575	2.288213382147	0.065958457425
H	1.805121840731	2.570932876416	-2.393710217541
H	-1.411017190931	-0.226192907855	-3.045004364205
H	-1.680500079020	-0.488421336802	-0.585203556116
H	0.673665933704	0.677776984848	2.640803467220
C	1.269680574046	-1.643796451323	1.393716917529
C	0.296295448979	-1.049817112658	2.365633877306
N	-0.811078419600	-1.722877507343	2.658532985581
O	0.695637824516	-0.135926248227	3.237320452224
C	-1.846770843919	-1.210826795249	3.546039539003
H	0.765571034660	-2.029077414541	0.495758799282
H	1.996029884662	-0.881637215898	1.089314188605
H	1.812525988438	-2.468159049225	1.888666456511
H	-1.070291329455	-2.466454696935	2.018225820881
H	-2.474422964053	-2.044089424758	3.890215168829
H	-1.377321202432	-0.726267961813	4.410375713516
H	-2.469053546609	-0.467627848838	3.020006977257

<The Ph ester aminolysis>

< phenyl acetate >

C	-0.007511146567	2.653707276085	-0.337916578410
C	0.024984456215	2.793895447328	1.053043397530
C	-0.044807530061	1.656598077710	1.863827781414
C	-0.145584269885	0.380995325192	1.300925408686
C	-0.173506024399	0.256245070302	-0.091919233342
C	-0.105167568281	1.384896674956	-0.913609867430
O	-0.339804295216	-0.961970876928	-0.738278303338
C	0.355622526182	-2.082349919221	-0.375885675986
C	-0.049399746343	-3.239065837782	-1.254489366185
O	1.163056768031	-2.117435326537	0.511491506595
H	0.044229298712	3.535778733436	-0.981598746772
H	0.103537500562	3.786131028550	1.504259361446
H	-0.021314027137	1.758550577409	2.952090952822
H	-0.192824105887	-0.503950806804	1.934422321211
H	-0.134906152471	1.250961679877	-1.997106018947
H	0.131637802189	-2.991899352702	-2.311889708199
H	-1.128840033653	-3.429222268655	-1.146735996042
H	0.520596538011	-4.131865502216	-0.970631225054

< phenol >

C	1.160469183035	-0.000000012598	0.945768878826
C	-0.034903394391	0.000000078901	1.669709911424
C	-1.253051181724	0.000000041391	0.978205982424
C	-1.282024495924	-0.000000061513	-0.416580559645
C	-0.078882346867	0.000000045836	-1.139632718263
C	1.144159396562	-0.000000036412	-0.452531197765
O	-0.156093869789	0.000000184362	-2.496736183000
H	2.120281760380	0.000000000752	1.469733745532
H	-0.019157222073	0.000000082039	2.762161787576
H	-2.195580086071	0.000000002906	1.532819978238
H	-2.224685959770	-0.000000215018	-0.968326841347
H	2.083977507816	-0.000000241045	-1.015186745749
H	0.735490698816	0.000000130399	-2.869406048253

The noncatalytic concerted for Ph ester aminolysis (Figure S9)

< Init_{non_C} >

C	1.555851766605	2.933844681827	0.288102734368
C	0.436932704821	3.667588174264	0.693858035695
C	-0.844080483013	3.197755108832	0.385886725131
C	-1.002235350044	2.001488526717	-0.316917059366
C	0.125490687393	1.272854522424	-0.714038792879
C	1.413790047189	1.734934016276	-0.418266575822
O	-0.135117955575	0.129888516901	-1.453995188428
H	2.560665623565	3.296142041627	0.521791427351
H	0.562486756017	4.602840582014	1.245239639231
H	-1.727160278669	3.765002324730	0.692073120720
H	-1.991800610764	1.618326751200	-0.575927259587

H	2.287028721455	1.162604247445	-0.724753131770
H	-1.242341430355	-1.197729237497	1.247713311857
C	-0.037347803717	-2.115436779697	-2.156860864184
C	0.587737484322	-1.026083027496	-1.330677204143
N	-1.273454118077	-2.201503526982	1.063824728152
O	1.557394472520	-1.138790369366	-0.628092233905
C	-0.237285307742	-2.887215340013	1.832359993491
H	-0.850309964815	-2.536056091511	-1.541287428062
H	-0.460028016933	-1.721963978414	-3.091485534046
H	0.705734040096	-2.898141225769	-2.356134630977
H	-2.202015216207	-2.511757155301	1.352291211121
H	-0.282824393038	-3.970574589507	1.631669550750
H	0.751685156494	-2.537815231759	1.497463336072
H	-0.292862711035	-2.752516347300	2.933209932978

< TS_{non_C} >

C	1.478268459170	2.828496927466	-0.318437070139
C	0.737749240808	3.625452014432	0.562843997086
C	-0.504630613247	3.161739078113	1.010877277454
C	-0.995306794101	1.923565865307	0.593455839893
C	-0.262062832829	1.111549468961	-0.306688062488
C	0.992177952889	1.594660420168	-0.753068122497
O	-0.748019791124	-0.055112251062	-0.715480863697
H	2.451822772531	3.175884508809	-0.678479662285
H	1.122480498659	4.593540127709	0.893857497548
H	-1.100413858437	3.772001888291	1.697177588838
H	-1.970057352922	1.565301295103	0.939014203789
H	1.577235414222	0.983003291341	-1.443163872602
H	-1.366622192794	-1.264654989862	0.158445630617
C	0.182607950667	-2.126042210517	-2.030600666452
C	0.394321736535	-1.697852493358	-0.603146736666
N	-0.851496449478	-2.183846275743	0.322251753827
O	1.431898822389	-1.526840318245	-0.030720686413
C	-0.491909030950	-2.417186643540	1.729832758872
H	-0.853186142669	-1.969674847174	-2.357297541114
H	0.847169539926	-1.529535787724	-2.669234961754
H	0.463738781457	-3.189098870968	-2.137280443919
H	-1.354265751539	-2.971160120014	-0.095726143993
H	0.136603271997	-3.314120777688	1.816085754999
H	0.085047715143	-1.554020542083	2.082655190705
H	-1.403151346304	-2.536048757722	2.332827340390

The noncatalytic stepwise mechanism for Ph ester aminolysis (Figure S10)

< Init_{non_S} >

C	-2.090045684845	2.907691944251	2.162958045755
C	-1.987376948081	1.547930558034	1.859903988978
C	-0.733119795007	0.993378367462	1.589354775964
C	0.421848875772	1.781587558225	1.620582873951
C	0.304334602134	3.141648242345	1.922576883078
C	-0.944692906282	3.709769524079	2.192687697926
O	-0.707185608893	-0.377706062904	1.362194947726
C	0.021342317430	-0.940043376135	0.355599632285

C	-0.150272899571	-2.435128209849	0.346263532620
O	0.703658590839	-0.300739314445	-0.405656295565
N	1.647098265000	-2.418043475571	-2.574707505236
C	1.176496522482	-2.311665684028	-3.948790090706
H	-3.070888764219	3.341073156909	2.375670063583
H	-2.867207658317	0.901450932239	1.832721650106
H	1.394364101809	1.341770887171	1.403175268329
H	1.204107889973	3.762224608781	1.946182484596
H	-1.024893735674	4.774322604948	2.426514214924
H	0.347079293200	-2.851089379417	-0.541565192533
H	0.288621412575	-2.856415121303	1.265613216752
H	-1.220736208090	-2.691539134886	0.356119955595
H	1.533500093572	-1.531619069103	-2.077420492331
H	2.643081623408	-2.638704840284	-2.552247757002
H	1.694141867959	-1.555962751063	-4.578373988364
H	1.274856095238	-3.284055860549	-4.460913437247
H	0.103698158662	-2.056897256542	-3.955453036053

< TS1_{non_S} >

C	-1.879550664933	2.643899643914	0.962596911348
C	-1.541628885628	1.585982041051	0.118012658479
C	-0.352973494155	0.866518284463	0.326730511064
C	0.497584385972	1.217209008113	1.388931172433
C	0.137249572406	2.273840230437	2.232076427620
C	-1.043798705544	2.993369261571	2.029459763848
O	-0.102383513591	-0.139570547461	-0.567166052101
C	0.834715440568	-1.198451900104	-0.263936470224
C	0.172389977138	-2.199303863167	0.680406392233
O	2.082370719316	-0.850943332228	-0.005985346690
N	1.116584759016	-1.800939076296	-1.694715488563
C	0.326823645467	-1.454452202947	-2.882838802656
H	-2.807148021361	3.196470043316	0.787530066325
H	-2.187663380444	1.296483955999	-0.714275292948
H	1.435403475829	0.678031789846	1.519059740840
H	0.804419812301	2.541864698536	3.056557860629
H	-1.309772969615	3.820046210610	2.693042989805
H	-0.806540379250	-2.538837463868	0.307659090540
H	0.841904237662	-3.058928669172	0.836741731099
H	0.021195455250	-1.714144902158	1.656055167040
H	2.139218091952	-1.256061176572	-1.305376974696
H	1.230098982467	-2.813668611112	-1.601790319879
H	0.793040133522	-1.908514816170	-3.770412270595
H	-0.709721371991	-1.815215351030	-2.792120306618
H	0.308182697653	-0.364683255570	-2.996243158334

< IM_{non_S} >

C	0.565390051684	3.004688755917	0.531305144485
C	-0.659389794656	3.529973404391	0.950879829078
C	-1.787932412371	2.701611233234	0.962349026324
C	-1.688275795864	1.367337988799	0.567903445022
C	-0.455687010449	0.840579049797	0.144814096330
C	0.678462949391	1.671049238933	0.121649476147
O	-0.478247889000	-0.466123043350	-0.263741824810

H	1.454666010080	3.641389958732	0.512079435671
H	-0.735658149860	4.574451552034	1.263172932561
H	-2.755309022661	3.095898114925	1.286267567538
H	-2.557951544936	0.706152379418	0.575230711057
H	1.633588558185	1.275463634315	-0.221559571624
H	1.317306207033	-0.759900520089	-1.878167410538
C	1.186905836461	-1.458728998447	1.253076379410
C	0.654678033019	-1.379643964137	-0.172327673258
N	0.173378406665	-2.666528845465	-0.586463743272
O	1.687474698899	-0.935233011822	-1.001105057017
C	-0.307542711766	-2.794608512511	-1.953977537149
H	2.049426829026	-2.138134244942	1.271886134238
H	1.499884021613	-0.470095267056	1.612508170172
H	0.406650074633	-1.845490327717	1.925130499598
H	-0.526469301499	-2.992100446181	0.076375244739
H	-1.109795869020	-2.080205505332	-2.225382638373
H	0.527409912571	-2.667623038110	-2.663203398495
H	-0.690295137111	-3.815474221657	-2.103236947893

< TS_{2non_S} >

C	0.437250026954	3.326981852854	0.722161815839
C	-0.835643986753	3.419476757423	1.298650724610
C	-1.753772251550	2.383884004446	1.080741003704
C	-1.411074285588	1.277610870346	0.303106675391
C	-0.122609402064	1.161026633749	-0.283763789980
C	0.794374540218	2.219966312109	-0.049333576326
O	0.203394744455	0.105219910259	-1.000470631539
H	1.164530361551	4.130325262391	0.877344771508
H	-1.110355343706	4.287346355678	1.903581399103
H	-2.755777638899	2.444647425815	1.517638285587
H	-2.134370537682	0.478211241599	0.115723089445
H	1.786450143854	2.155236732249	-0.506797600637
H	1.506102537405	-0.650741723725	-1.502957043200
C	1.235496337836	-1.382349099551	1.090788157416
C	0.861174988544	-1.783979978068	-0.302690995328
N	-0.115547857453	-2.673574533000	-0.471470728499
O	1.725310383433	-1.628161754452	-1.293847394803
C	-0.602664483498	-3.076436920987	-1.782681963026
H	1.885217020521	-2.162583651322	1.524827364710
H	1.794433104981	-0.439116672453	1.064827417212
H	0.351135643162	-1.248658658641	1.730496475302
H	-0.738829146813	-2.810091128183	0.317549217591
H	-1.276680630930	-2.306903938618	-2.195302535717
H	0.249834629622	-3.194823573063	-2.462082499810
H	-1.137378897602	-4.032511726850	-1.696037638555

< *The aminolysis of oligo-CF₂CO₂Et by n-hexylamine* >

< oligo-CF₂CO₂Et >

C	-5.467224781383	-4.042657583574	0.023676617161
C	-4.663054788618	-4.991493692628	0.643246065199
C	-3.407886126771	-5.312792794905	0.128688428499
C	-3.001094306177	-4.716411327732	-1.066999618435
C	-3.799046164600	-3.775921938231	-1.701728551358
C	-5.026948490161	-3.421004021402	-1.142934631242
C	-5.777687039654	-2.241102699325	-1.695773367986
C	-2.447582990379	-6.215017545303	0.893577598433
C	-2.196365117298	-7.527658169431	0.147904686530
C	-1.195888854350	-5.403099104516	1.181598602909
C	0.028380211039	-5.647947984062	0.570038858122
C	1.112635047451	-4.774132806427	0.717550924195
C	0.961784620526	-3.588738714711	1.443579893768
C	-0.238726901711	-3.391016886841	2.126637746354
C	-1.298450710121	-4.277548293068	2.013738043302
C	2.040753029423	-2.522473896543	1.592229429682
C	1.488858322159	-1.098836058961	1.677696149207
C	3.176904471915	-2.485971207841	0.577046700777
C	4.489854909040	-2.649110692614	1.019282941637
C	5.563887569948	-2.486072311218	0.154653599657
C	5.333791593916	-2.150175769124	-1.177833337233
C	4.026261613266	-1.994563539121	-1.636235625316
C	2.959167421921	-2.167400883869	-0.765636674370
C	6.519067144613	-1.887966571668	-2.066507732941
C	2.092464209033	-0.217506700788	2.577333958871
C	1.757384760413	1.132622208315	2.618521617885
C	0.775676800403	1.635896291250	1.753745498811
C	0.140390447939	0.753707706430	0.888907819492
C	0.494819526816	-0.595771580848	0.824667104415
C	0.571578794337	3.136081503796	1.664271196616
C	1.730731859791	3.765166306581	0.905171613915
C	-0.787722101829	3.514912889769	1.093641611323
C	2.399738679923	3.066352047799	-0.097385759552
C	3.438244534683	3.650740633500	-0.816456229848
C	3.847695301022	4.959277824668	-0.532247568752
C	3.175039218302	5.658740257896	0.468519117954
C	2.120835221936	5.079596404141	1.178832491915
C	4.980874494611	5.577883144460	-1.297409914806
C	-1.942615549031	3.155348600425	1.795089819290
C	-3.203089291771	3.489514524658	1.320827546342
C	-3.328419409805	4.206225010784	0.130232478264
C	-2.186722813560	4.561303549477	-0.583967156626
C	-0.928688557811	4.217382640973	-0.102496937808
C	-4.685277034119	4.585448392654	-0.403282239755
O	2.346593642620	-5.022825473455	0.182141667994
C	2.488686765965	-6.117952695481	-0.710744313431
O	-2.501601394566	-4.110018547123	2.649275445986
C	-2.744583003838	-2.861821297411	3.281694692034

O	-0.062002603424	-1.454428434044	-0.080351113851
C	-1.300251593512	-1.075483630771	-0.680678205492
O	2.351962625801	2.046388873140	3.443656318560
C	3.444730956962	1.606688430531	4.239053180337
O	4.123581021659	3.011827591930	-1.819080512381
C	3.680629310623	1.703229942731	-2.177384575571
O	1.405975333574	5.724978746937	2.153045393109
C	1.747540472862	7.073479079729	2.441396094875
F	-5.598273824976	-2.124640661418	-3.044027839889
F	-7.121066158801	-2.350297258287	-1.467143781676
C	-5.218558104176	-0.957294588456	-1.030811525803
O	-5.846503874007	-0.706833236373	0.112281763787
C	-5.304885957790	0.391876796459	0.911444352970
O	-4.263585153798	-0.363728928824	-1.473422309399
F	7.367540929831	-2.958301516644	-2.068583347678
C	7.314567112785	-0.658976152584	-1.557193079983
F	6.132061536702	-1.675175142607	-3.363888223821
O	6.674203615953	0.463885447466	-1.889771204769
C	7.212118633233	1.703494971664	-1.332464262131
F	-5.637135461841	4.464568539847	0.566151720463
F	-4.686913263403	5.895141558968	-0.815319182891
C	-5.114200205438	3.681380909193	-1.586779782338
O	-4.536108405986	4.089820043712	-2.714551252222
C	-4.727956374350	3.233552600227	-3.886189043499
O	-5.833794152438	2.722809807161	-1.449711871827
O	8.319767300449	-0.748076741166	-0.898932097564
C	-6.083240995461	0.418134820450	2.203514774139
C	6.757148625794	1.886968320790	0.099507999803
C	-3.703496235834	2.120779242158	-3.893194862893
H	-6.421536956837	-3.761554105762	0.457561411019
H	-4.989775623214	-5.450550033643	1.572641106382
H	-2.020057500107	-4.950263014719	-1.473598688358
H	-3.463293425814	-3.290234327998	-2.612613523626
H	-2.924187853733	-6.453375544581	1.853084358429
H	-3.139926012104	-8.066496007125	0.021327344900
H	-1.782578983506	-7.354551213583	-0.850990740420
H	-1.504141349696	-8.168988118819	0.703761356574
H	0.137465816855	-6.533283801207	-0.043749241429
H	-0.341554290788	-2.484839120341	2.713917849414
H	2.520626676557	-2.713293919759	2.563572233100
H	4.676794726780	-2.908080550240	2.058566142306
H	6.582323270114	-2.609288893765	0.513543831444
H	3.845925904672	-1.733176575471	-2.673854541297
H	1.942742101914	-2.047182130979	-1.126189191267
H	2.864019237456	-0.611458162411	3.230573633236
H	-0.610192892023	1.149966326613	0.213780660779
H	0.603785111776	3.539458406337	2.684072875092
H	2.093406041425	2.047151444539	-0.300447425213
H	3.492010593088	6.673823688474	0.682335680009
H	5.905955641532	5.004912408482	-1.163359589367
H	4.773331169281	5.585096989007	-2.373023307548
H	5.160491149601	6.604631284487	-0.968764085899
H	-1.845838798819	2.606020400691	2.728954740607

H	-4.089572825990	3.219375965587	1.884667737851
H	-2.282411700381	5.119907784370	-1.509707504113
H	-0.042469249536	4.507664262556	-0.658494860749
H	3.521458166421	-6.079653984165	-1.062565241015
H	1.808832803529	-6.027035059731	-1.569413226612
H	2.313177260074	-7.078485821298	-0.206313695408
H	-3.780455245451	-2.896990726227	3.625610681760
H	-2.082486081953	-2.707348142851	4.144858051807
H	-2.620321909771	-2.026811865767	2.576784995171
H	-2.029654464073	-0.765903333219	0.077777300599
H	-1.671190020342	-1.965195530981	-1.190236813938
H	-1.176673739841	-0.263460782659	-1.408697484922
H	3.801320502658	2.490567386537	4.770681505883
H	4.254769352171	1.204134124289	3.615242172805
H	3.133144764631	0.846614856793	4.968966051262
H	2.635350903717	1.720408545175	-2.515594591331
H	3.781236141786	0.997073939513	-1.342040227233
H	4.328909076495	1.377386181632	-2.991971321782
H	2.777748279376	7.157367543730	2.814629427618
H	1.054517656523	7.397255187121	3.219905535911
H	1.626173160349	7.715611103953	1.558184297124
H	-5.418393796495	1.314698232666	0.336135050177
H	-4.235816762404	0.204397468387	1.068892247761
H	6.804572963105	2.479865495353	-1.983579190678
H	8.302912127206	1.675266372951	-1.414253402785
H	-5.750800717566	2.846930018743	-3.870147311097
H	-4.604146298203	3.916376457460	-4.730148179225
H	-5.707756138435	1.226849035339	2.838468324242
H	-5.978650935509	-0.525370932516	2.747754046012
H	-7.144703540671	0.598798421059	2.013541806110
H	7.119707473308	2.850870248424	0.472554511133
H	7.158005571061	1.098033605264	0.741697609001
H	5.665085802894	1.890707775855	0.162850876269
H	-3.838994653635	1.456682032831	-3.036023221613
H	-2.688567798713	2.529943194171	-3.879567568358
H	-3.823391976999	1.524655541356	-4.803999111742

< *n*-hexylamine >

C	-3.845555261108	-0.348777174165	0.000602768072
C	-2.573834588250	0.496772892929	0.000848295786
C	-1.301724485996	-0.350069178728	-0.000840410718
C	-0.020428171510	0.482144228737	-0.000606808198
C	1.250394785877	-0.366850679656	-0.001141206188
C	2.530886026548	0.473201208310	0.000015449612
N	3.791754952762	-0.278176975248	0.000923568620
H	-3.886015105275	-0.996508257277	0.883724954366
H	-3.887402101406	-0.993989175773	-0.884295275026
H	-4.744997182489	0.275280041654	0.002200202246
H	-2.568923509577	1.158085740501	-0.876612126559
H	-2.567900806610	1.155985000739	0.879882043611
H	-1.305946039372	-1.012696047437	0.877135045338
H	-1.306940461528	-1.010785703112	-0.880245359524
H	-0.017001774606	1.144163432947	-0.879028285422

H	-0.016764117551	1.143230037208	0.878525352600
H	1.252181807506	-1.025892678567	-0.882308303971
H	1.251751204560	-1.027513581166	0.878817757782
H	2.531372040944	1.135567972635	-0.877172536964
H	2.529901485620	1.135240276264	0.877457124217
H	3.822560283324	-0.890011155915	0.810571202985
H	3.824031744536	-0.889615628680	-0.808965646665

< oligo-CF₂CONH-hexyl >

C	-2.562090826098	5.837511191209	-5.381388173239
C	-2.126283141308	6.920073164468	-4.627658522498
C	-2.413544989630	7.008034113578	-3.266155894439
C	-3.220903393982	6.025994449040	-2.688042453315
C	-3.673468933718	4.946184460909	-3.432504428925
C	-3.321557187136	4.837316015185	-4.777789039582
C	-3.596379574513	3.555123353115	-5.513858866143
C	-1.781999493674	8.085938165458	-2.394455683188
C	-2.833077920478	9.053583472654	-1.846420707675
C	-0.954452008762	7.382113710207	-1.331078888717
C	-1.292779805923	7.374740746076	0.017391081601
C	-0.612634065250	6.573640682018	0.942990332287
C	0.393397446491	5.704491130808	0.509203990500
C	0.786167781586	5.777775171036	-0.827623041509
C	0.141803758383	6.604353745783	-1.734910135238
C	1.136369383739	4.720700639053	1.404374497296
C	1.495618527826	3.405119028356	0.709451974145
C	0.526637799286	4.327685709208	2.743952532438
C	1.254994515452	4.551316506420	3.912157030257
C	0.834527890968	4.038853245073	5.131830510240
C	-0.338186232559	3.288916234174	5.198693590806
C	-1.098150499325	3.093873605462	4.044449647993
C	-0.668980307695	3.611139608938	2.829976942265
C	-0.688748029839	2.618213357438	6.500008519649
C	2.733379505667	2.829929784796	1.002776950411
C	3.081234283610	1.558401772741	0.552402843366
C	2.184856854093	0.831626262470	-0.241794182666
C	0.970926096970	1.421055625156	-0.576790584538
C	0.604706484569	2.679726369464	-0.096458268131
C	2.480873467466	-0.616140640837	-0.580420212694
C	2.118012040154	-1.518898179878	0.589623444546
C	1.816510974845	-1.053289822652	-1.880961961100
C	1.101471204801	-1.179163587268	1.479399617294
C	0.710292589384	-2.046000479407	2.495796160901
C	1.339364807939	-3.285876439390	2.653916712448
C	2.367782527285	-3.618082264499	1.773294036304
C	2.757362145527	-2.753703525761	0.747495347220
C	0.892873900621	-4.231116041537	3.730902144335
C	2.179148959344	-0.418521660540	-3.072568755933
C	1.603695056657	-0.779918843414	-4.282492236919
C	0.652570349744	-1.800148037915	-4.321786786913
C	0.277597183726	-2.436174176166	-3.140673120207
C	0.856263665164	-2.062986290176	-1.933000903946
C	0.024164196667	-2.225797417857	-5.623935141814

O	-0.881503180999	6.594559231441	2.283705407770
C	-1.993723214493	7.350119218665	2.739664575410
O	0.487345088863	6.696485155930	-3.058400439331
C	1.356234933942	5.702845445260	-3.582891865293
O	-0.621235650347	3.228244162503	-0.344495308334
C	-1.375955137942	2.697099178641	-1.432796043879
O	4.260696014587	0.935377991376	0.854861965314
C	5.187273288322	1.644195016274	1.668544325984
O	-0.294593663439	-1.763917005877	3.391091443911
C	-1.037804663166	-0.569335248627	3.169194218561
O	3.738695809941	-3.038688921038	-0.163126469993
C	4.399467512077	-4.293152434381	-0.054358198403
F	-4.743006207617	2.962519113315	-5.070364488612
F	-3.734917404144	3.767507933091	-6.857406092861
C	-2.420890520203	2.581469339637	-5.241113975033
O	-1.421049566868	2.808867798324	-6.085101564971
C	-0.185863203564	2.070108564968	-5.828623521948
O	-2.413256293943	1.819423410262	-4.303366230821
F	-0.830609480280	3.528340200144	7.504998888536
C	0.432441266544	1.617226523892	6.894643669809
F	-1.898291051771	1.952606231491	6.388356058791
F	0.687334859187	-1.676672282524	-6.682052942193
F	0.098733992174	-3.590795189616	-5.761968574242
C	-1.459805301045	-1.789908573474	-5.736926502987
O	-2.243986389853	-2.633789525847	-5.068430201418
C	-3.658442959059	-2.267490919016	-4.976658350025
O	-1.805814889289	-0.795364720156	-6.325123248954
O	1.412481488874	2.004092828926	7.509718878864
C	0.850777900764	2.602955577731	-6.786283869002
C	-3.881758894512	-1.332974651607	-3.808689515326
H	-2.288963265460	5.750273421304	-6.428198816393
H	-1.502273946897	7.680637432713	-5.089662884837
H	-3.448345089316	6.077255943921	-1.625800989899
H	-4.272593626694	4.168319656145	-2.969394306302
H	-1.095237874730	8.655240269287	-3.033957490314
H	-3.351148684494	9.542743085637	-2.676431505721
H	-3.590396982151	8.536356053645	-1.248114237193
H	-2.369726753302	9.827301220239	-1.224985611909
H	-2.112650747801	7.997185285559	0.353120801300
H	1.586908794047	5.122563369155	-1.154345736886
H	2.096802138297	5.199502583938	1.646204920178
H	2.179539736926	5.121823222940	3.865588195606
H	1.426921933169	4.189826676488	6.029259154929
H	-2.023462596412	2.528763843458	4.095299825100
H	-1.257708398948	3.447457347379	1.932860273751
H	3.412969160757	3.392273528944	1.634265174895
H	0.278638915455	0.851806450723	-1.187831478106
H	3.562746354325	-0.710081040888	-0.735386344097
H	0.620683728083	-0.215637132153	1.360421637149
H	2.854111479947	-4.579655594082	1.896958147915
H	0.906668794493	-3.751858454277	4.715593254986
H	-0.139818670023	-4.556977990074	3.560981607500
H	1.534308185295	-5.115394040015	3.766465147530

H	2.926130898799	0.371750281930	-3.045891009834
H	1.909036635467	-0.289397467583	-5.200527081349
H	-0.458502080941	-3.233390963467	-3.168177067231
H	0.563604088070	-2.571938726924	-1.019690103977
H	-2.048257594189	7.174053253439	3.815721912863
H	-2.928808376488	7.014816700791	2.269327924410
H	-1.857439660990	8.424892392537	2.554611455547
H	1.397195327328	5.878974525060	-4.659982749050
H	2.369450165545	5.784444792690	-3.165944473698
H	0.965721390908	4.692700911338	-3.390502337637
H	-0.765253485440	2.620811347345	-2.340288318154
H	-2.187613450113	3.403655580929	-1.607768336091
H	-1.793144618582	1.708138787499	-1.201643588997
H	6.045093932769	0.981131558791	1.788998777783
H	4.760725692567	1.869117657461	2.655483387466
H	5.510051257077	2.576962029561	1.185667122929
H	-1.499164022894	-0.564958206669	2.171999093913
H	-0.413922563052	0.329242826553	3.279273888116
H	-1.828613113964	-0.561414981220	3.924080812859
H	4.914849378899	-4.392839416969	0.910755141333
H	5.135851038120	-4.312504414103	-0.859605481246
H	3.696951145121	-5.127630360928	-0.184304248080
H	-0.392374448541	1.008179693003	-5.985967515303
H	0.093192131745	2.223123466901	-4.779096931039
H	-3.961731723326	-1.815303081940	-5.925040712073
H	-4.167003181249	-3.225548129423	-4.844747984956
H	1.798569053940	2.079851233434	-6.624082878421
H	1.016643256405	3.673838098667	-6.634075195383
H	0.543125830352	2.438927102713	-7.822602288533
H	-3.347834872351	-0.390387514536	-3.952316855545
H	-3.552669602321	-1.796838240021	-2.873624640512
H	-4.950288015455	-1.108087918657	-3.724783366973
N	0.256397333362	0.368279650076	6.413428181383
H	-0.576970251935	0.174833142427	5.881314136222
C	1.346791395814	-0.604622626368	6.385729132379
C	2.346079006026	-0.322682140472	5.263134741019
H	0.899011403921	-1.596422855751	6.253336584193
H	1.849762535979	-0.583571335713	7.359085519676
C	3.390870741255	-1.426661944109	5.127138171694
H	1.802209850745	-0.227506207171	4.313999031413
H	2.830883345314	0.643635292785	5.453612175137
H	3.965942712304	-1.517112755759	6.060300549234
H	2.880313243594	-2.389554455244	4.980220318964
C	4.339075663257	-1.192220267991	3.953390187869
C	5.298071304736	-2.355042479961	3.708917989443
H	4.917806221658	-0.273562217161	4.130466958391
H	3.748815617313	-1.018922803264	3.041803868590
C	6.220407954735	-2.108593543542	2.516681995091
H	5.896239630971	-2.538411670133	4.612431344392
H	4.707563896918	-3.265992060438	3.537483350841
H	6.870067626818	-2.968676555080	2.320891325078
H	5.637846781130	-1.905300747854	1.609746917605
H	6.868843847491	-1.243569300170	2.698565972771

<Ethanol>

C	1.250450142695	-0.286873873864	-0.003659216471
C	0.006031972615	0.573386298063	0.049639037191
O	-1.128329448135	-0.295928560868	-0.044672943720
H	1.287030248082	-0.848100658714	-0.942239915663
H	1.256044259977	-1.001984976461	0.824470079657
H	2.148436596289	0.335223912353	0.066250157195
H	-0.019446858181	1.143533801180	0.992591944560
H	0.010612153683	1.297096035012	-0.781694109935
H	-1.925133138525	0.243072514798	-0.011308490914

The noncatalytic concerted mechanism for the aminolysis of oligo-CF₂CO₂Et by n-hexylamine (Figure 6)

< Init_{non_C} >

C	-4.450091706969	4.681209156677	-4.521595469222
C	-3.212704741839	4.990994637183	-5.074037896506
C	-2.112896267321	5.265166817295	-4.262829564234
C	-2.296204730588	5.306857570519	-2.878246563222
C	-3.529588379648	5.018631189940	-2.315245798849
C	-4.604188832558	4.678034763128	-3.138619717973
C	-5.845346051215	4.120553496049	-2.504275625335
C	-0.710798215373	5.386746417936	-4.848201670521
C	-0.107661955017	6.772319133369	-4.611337797896
C	0.096209665031	4.234812496505	-4.270623834617
C	1.082188738018	4.407910213436	-3.305680437381
C	1.656281714266	3.322798498044	-2.632498708119
C	1.204302608443	2.025831678500	-2.891532215705
C	0.277729634931	1.849142034246	-3.920219432153
C	-0.264374334110	2.922209953136	-4.610911246496
C	1.628097273501	0.759263161202	-2.154344842413
C	0.437184895983	-0.111410479749	-1.747294711280
C	2.547441471551	0.850908523083	-0.943887620951
C	3.833153853216	0.317904117556	-1.022249661276
C	4.640119234883	0.217379560339	0.105511767288
C	4.165190451825	0.662020120398	1.335849108245
C	2.891731398124	1.225571712708	1.422253646217
C	2.094409542861	1.318614825848	0.292558275971
C	4.980682755611	0.398710672662	2.575829681760
C	0.578222167367	-1.495424110452	-1.847116442956
C	-0.388061380269	-2.368618093963	-1.354969028885
C	-1.560368796172	-1.861635697287	-0.777641816113
C	-1.725895228938	-0.481296623076	-0.718323280387
C	-0.734416174871	0.395813487685	-1.166444882639
C	-2.511907239848	-2.824663286713	-0.094116458519
C	-1.998861480918	-3.188687847752	1.293861061116
C	-3.951722116844	-2.340637170440	-0.049365910452
C	-1.116443900966	-2.371935645293	1.996981626160
C	-0.683466831254	-2.714214330462	3.276237798546
C	-1.115344027455	-3.901204954427	3.878785785580
C	-1.999551838352	-4.716355723151	3.173740217183
C	-2.447563559804	-4.368228824508	1.898704593772

C	-0.630263638507	-4.270652781404	5.250244798007
C	-4.840598220866	-2.730792244237	-1.052447784311
C	-6.172808111259	-2.339565980334	-1.022795666607
C	-6.634702040564	-1.542522379758	0.023296639751
C	-5.753529622757	-1.122368917461	1.018093611713
C	-4.425966157186	-1.531289227322	0.984815533434
C	-8.074370711537	-1.105459807027	0.066715278110
O	2.644622642053	3.468031788561	-1.698410477033
C	3.064612987433	4.779406985639	-1.356165321662
O	-1.190399143231	2.793868230117	-5.612721290392
C	-1.812352307326	1.526677526714	-5.776629829612
O	-0.826480827589	1.753307659259	-1.033456025562
C	-1.928774449463	2.278361992042	-0.299795601085
O	-0.261148977530	-3.730638099992	-1.363661353719
C	0.982832059944	-4.275700735402	-1.783888408613
O	0.180362206664	-1.949273283510	4.019467683392
C	0.541515711622	-0.674565096983	3.493373322455
O	-3.325237103693	-5.117400357225	1.160953045799
C	-3.847286333909	-6.299021700617	1.752193219821
F	-6.212179240572	4.848058412140	-1.406537372454
F	-6.907342584361	4.125647979437	-3.367916355285
C	-5.562501849512	2.667236730621	-2.035816394029
O	-5.479792419257	1.863964675161	-3.086564160381
C	-5.077735059206	0.482639919929	-2.821138637860
O	-5.365715027494	2.374024394791	-0.878849450655
F	6.287809263894	0.741289731563	2.373318561850
C	4.918766186075	-1.115248342589	2.893879995044
F	4.516714132063	1.145510291566	3.624413756667
F	-8.866806731463	-1.994316277846	-0.611738824276
F	-8.522248907138	-1.072434841760	1.358362398144
C	-8.279631939728	0.273367802163	-0.613604828458
O	-8.470798018535	1.236055251135	0.279959774038
C	-8.681983940339	2.588595682676	-0.236436239850
O	-8.222933387325	0.392872879798	-1.814718742960
O	5.707862145286	-1.910360280531	2.443653081625
C	-5.462283101695	-0.332252346969	-4.028784567232
C	-8.237862100163	3.553984797704	0.832895167704
H	-5.284151769818	4.408043890126	-5.159282933547
H	-3.082086403725	4.957029094838	-6.152266552631
H	-1.444989353388	5.506338346912	-2.232049661685
H	-3.658138120877	5.017618664857	-1.236603475153
H	-0.797697756441	5.232724829485	-5.930894917189
H	-0.721821848664	7.530988174258	-5.105303402546
H	-0.068895150148	7.027352083751	-3.547276868513
H	0.907638888918	6.831200441690	-5.017551746611
H	1.391639080869	5.414680128744	-3.054344447553
H	-0.052948464196	0.837159624719	-4.131056271748
H	2.183120745582	0.165667198210	-2.895289848210
H	4.205291244169	-0.044212322218	-1.977700326067
H	5.627346179010	-0.230003557549	0.038850282811
H	2.524068035563	1.577474718454	2.380470650329
H	1.102443126224	1.752676503425	0.365347649684
H	1.496644723533	-1.879072879193	-2.279410266535

H	-2.630717121045	-0.095134929328	-0.262129738838
H	-2.514768197766	-3.751753836532	-0.677394434197
H	-0.767752065924	-1.463601918711	1.519289333958
H	-2.335776510313	-5.633186280029	3.645859749565
H	0.460501090422	-4.378468280545	5.267653469004
H	-0.876738877539	-3.490854886404	5.979077187680
H	-1.075786656089	-5.212096306871	5.581445323547
H	-4.485766794943	-3.373771916290	-1.854604398931
H	-6.859483950965	-2.662117789907	-1.798566513264
H	-6.113102594806	-0.496196926994	1.828665742972
H	-3.752838814516	-1.243967193352	1.788386649679
H	3.835019176929	4.651918764973	-0.593105649587
H	2.238350231103	5.374037222936	-0.940867338333
H	3.493160535511	5.306604463486	-2.220188778091
H	-2.594156353819	1.670645755816	-6.525347281277
H	-1.102992922771	0.768865374692	-6.136732556027
H	-2.265419992799	1.182863771403	-4.835896648175
H	-2.887494537328	2.073388215449	-0.790132890290
H	-1.768738814976	3.357414343407	-0.266120193064
H	-1.954428847012	1.877050086462	0.723530090897
H	0.896470255893	-5.355037103421	-1.647321509374
H	1.811165416505	-3.894556311486	-1.170921049817
H	1.182032836485	-4.060431847690	-2.842912029134
H	-0.346974151264	-0.043987389009	3.345967998984
H	1.086725683632	-0.762033854191	2.544701262387
H	1.202066959093	-0.220212279947	4.233730893683
H	-3.052739517438	-7.026899593813	1.968153014984
H	-4.534017799973	-6.722477499561	1.017072874338
H	-4.398464901144	-6.075408104262	2.675850013835
H	-5.581448289573	0.138418017543	-1.916285794176
H	-3.994635972563	0.484081554662	-2.642152012567
H	-8.120318678930	2.703633165136	-1.165934747684
H	-9.750257537497	2.676873711149	-0.464850999011
H	-5.122574223285	-1.362589726920	-3.886296756032
H	-4.998872910461	0.063326135688	-4.937871252324
H	-6.548628699486	-0.336980659512	-4.152901790876
H	-7.165997225530	3.446904691929	1.018034899218
H	-8.787328331544	3.388367304905	1.764103357089
H	-8.424297470109	4.577048092537	0.492662700212
N	6.277380441252	-0.704513812092	5.235185867024
H	6.666695165605	0.208770751280	5.445970657319
C	7.337424241463	-1.722282743962	5.216602838775
C	8.472007510303	-1.296100046755	4.293843003210
H	6.901452783754	-2.655450653702	4.831795459738
H	7.747033189224	-1.944914047073	6.219118248446
C	9.537940265893	-2.378246912514	4.139229846300
H	8.048319399305	-1.045880288569	3.314457015872
H	8.935490056800	-0.378284645649	4.687977985241
H	9.939460528441	-2.652213510635	5.126378356417
H	9.070162023073	-3.286447114859	3.732312153353
C	10.687789996685	-1.954327610314	3.227081378452
C	11.747603744396	-3.040248427863	3.047247693558
H	11.161512135386	-1.048499817020	3.633360400200

H	10.283873685815	-1.672815659674	2.243897781430
C	12.893319795010	-2.603444783592	2.136564676751
H	12.145793019612	-3.324163055155	4.031368622982
H	11.273153329952	-3.942664546407	2.637549631338
H	13.639952669013	-3.395608136931	2.019246534870
H	12.522695692724	-2.341519172125	1.139048343553
H	13.401803821809	-1.721330319599	2.542068272177
C	2.912590779727	-3.409564160484	2.385396800017
C	3.467710179318	-2.822126144515	3.667098475662
O	3.766555180155	-1.404223397409	3.512279456681
H	2.014219274218	-2.873616319343	2.065732964801
H	2.633845551658	-4.454933013159	2.557563104515
H	3.658876513056	-3.374956481413	1.587488167944
H	2.725615499792	-2.847789135551	4.468641216887
H	4.380677481605	-3.337281707450	3.983191709530
H	5.591240791266	-0.902264653064	5.955403462912

< TS_{non_C} >

C	-4.468855519636	4.759668560651	-4.382525732163
C	-3.249880443116	5.009635206470	-5.002350395295
C	-2.094458375434	5.224756614403	-4.253235418893
C	-2.197924572994	5.268376064790	-2.860358662609
C	-3.411029896233	5.039743870023	-2.230377599532
C	-4.545749378406	4.758074514435	-2.993337917817
C	-5.776025749117	4.265187670581	-2.288324352109
C	-0.723083559018	5.276590442450	-4.916027337902
C	-0.034750084531	6.626792869557	-4.708692983954
C	0.052664837121	4.080155858533	-4.388143450783
C	1.097967268814	4.196138551731	-3.478442184796
C	1.649275039187	3.078897428963	-2.840153697348
C	1.118248258266	1.807716246433	-3.079647166957
C	0.126858048070	1.686382960658	-4.053878379731
C	-0.396806043644	2.790652654238	-4.708938867132
C	1.515681277406	0.516759440320	-2.368137951505
C	0.305089939272	-0.289585833207	-1.895758153417
C	2.507447761366	0.575909022959	-1.213805233096
C	3.805760522965	0.100110599995	-1.390000815952
C	4.694174086606	0.013283002486	-0.323258779170
C	4.280475798897	0.396208145042	0.950269795294
C	2.994157734683	0.902170134515	1.132578427099
C	2.120422473514	0.989550954107	0.062255108237
C	5.197125050399	0.217849111111	2.121164881625
C	0.349345614645	-1.677066355283	-2.030726354087
C	-0.622551828661	-2.501000841612	-1.468058651592
C	-1.694691120125	-1.936680326549	-0.763151046695
C	-1.773849684279	-0.549985380200	-0.678928094558
C	-0.785956008007	0.275935144782	-1.219227578632
C	-2.637949560009	-2.848740545218	-0.002923734085
C	-2.040576458886	-3.255522007418	1.338837694711
C	-4.035935915646	-2.276374487442	0.164683387025
C	-1.044163837679	-2.514189111925	1.970658476761
C	-0.547614796548	-2.893186379564	3.217214648435
C	-1.034986682219	-4.039590862039	3.856614831348

C	-2.030910124879	-4.779438195833	3.221928787021
C	-2.539069352717	-4.394793566339	1.980995862437
C	-0.482881437007	-4.447335965356	5.191200384746
C	-5.031536621393	-2.603198977899	-0.757424395417
C	-6.326636691606	-2.122771876078	-0.615774613987
C	-6.643190318105	-1.298205295387	0.462909897327
C	-5.655296659956	-0.944732328354	1.379931538973
C	-4.366275173594	-1.443561655295	1.235328456592
C	-8.042097017574	-0.767056793732	0.620519055933
O	2.690191553688	3.168803460575	-1.958205723998
C	3.183208900474	4.455425671504	-1.620716392365
O	-1.385067776206	2.715260515114	-5.655587706883
C	-2.114277076665	1.498648549239	-5.748882466636
O	-0.801296872239	1.637640613554	-1.087525135224
C	-1.810377746836	2.216527310043	-0.265837171557
O	-0.589916737699	-3.867369348500	-1.525215775243
C	0.444265180628	-4.473019800252	-2.289110704556
O	0.427178775956	-2.209847993145	3.894717484155
C	0.866646493618	-0.969815617148	3.346409727086
O	-3.528327626866	-5.069344040752	1.313017410842
C	-4.116558722607	-6.188541538754	1.959752101863
F	-6.070188483657	5.038813741863	-1.200326804096
F	-6.874292443944	4.282575459160	-3.105948710029
C	-5.525791219231	2.816866335319	-1.786202359854
O	-5.513002913731	1.982936576942	-2.816363934378
C	-5.151167266805	0.593745944303	-2.533429790807
O	-5.296402311424	2.549983586876	-0.629122736469
F	6.329308842954	1.004790442306	1.987106260108
C	5.714994916966	-1.223087272497	2.319332133668
F	4.590983007783	0.652989095190	3.285162736203
F	-8.951019611543	-1.650200426303	0.092428756740
F	-8.350463606578	-0.618913516108	1.943401607255
C	-8.246829245661	0.569429652020	-0.139810286562
O	-8.386343905860	1.593806044411	0.691738037882
C	-8.597854199845	2.910319851556	0.090731475666
O	-8.241837442172	0.605914269379	-1.347938301274
O	6.434614023499	-1.760354858023	1.500492323909
C	-5.662492800171	-0.241125816256	-3.679300330902
C	-8.120013335996	3.939323691645	1.083470792643
H	-5.349432339734	4.531044051996	-4.973386207033
H	-3.180486917975	4.973350705912	-6.086176112242
H	-1.303352262812	5.420914405559	-2.261695841001
H	-3.478985885345	5.038579566347	-1.146081656556
H	-0.877580049901	5.134422011858	-5.992851518770
H	-0.634826113969	7.420282726307	-5.163782264640
H	0.078402196643	6.872005931797	-3.647674606149
H	0.957405933735	6.634561392442	-5.172281595709
H	1.474475820156	5.183589736102	-3.242431082751
H	-0.268339407815	0.694494196733	-4.248858666411
H	1.999480827031	-0.103215605101	-3.137020945543
H	4.129149744505	-0.219620931471	-2.377813178751
H	5.693800842473	-0.380907797994	-0.470581513924
H	2.668474518220	1.209739972248	2.119750559756

H	1.121511396691	1.382330400527	0.216814003889
H	1.203472449314	-2.106973786582	-2.543784611834
H	-2.610730469366	-0.119353564640	-0.140637641649
H	-2.746751547783	-3.767430360882	-0.589357336620
H	-0.650541057505	-1.640734829431	1.463251021125
H	-2.405716081379	-5.665971518096	3.722071156034
H	0.596253832745	-4.627911677254	5.131026028724
H	-0.623266183587	-3.654016512863	5.933717809241
H	-0.970020379276	-5.356162439496	5.553946301540
H	-4.791473435574	-3.267032711306	-1.584806371316
H	-7.096859792954	-2.395303627298	-1.330012832947
H	-5.900889515985	-0.301424964539	2.218886918590
H	-3.610180674913	-1.208862243199	1.980215324284
H	3.981239809351	4.283367848486	-0.895659948638
H	2.403684393886	5.079792498110	-1.161007290096
H	3.595332569137	4.975472416280	-2.497112221769
H	-2.938572123312	1.694115851363	-6.438137853230
H	-1.496350538469	0.683018131440	-6.149037934707
H	-2.517533904268	1.203316946279	-4.769892678014
H	-2.816261001172	2.055972475301	-0.671483760036
H	-1.597369169281	3.286918293164	-0.253253205916
H	-1.768341346487	1.820098264742	0.758865107130
H	0.272285771579	-5.548792208159	-2.223036362246
H	1.436390602934	-4.239804688664	-1.881405058097
H	0.399561923263	-4.159052413060	-3.341508920505
H	0.028318143284	-0.264045509643	3.249006060230
H	1.357876258547	-1.101342261835	2.376148771537
H	1.601190544565	-0.576682253546	4.051669148081
H	-3.383502624862	-6.990473151802	2.125692180644
H	-4.896897639866	-6.547403056907	1.286063109058
H	-4.568761344854	-5.903788968503	2.919625999937
H	-5.594849769191	0.301237510824	-1.579944239059
H	-4.058121254651	0.552466054316	-2.441249633932
H	-8.056942138282	2.956916834466	-0.857044468874
H	-9.670070450476	2.995174988170	-0.120103347414
H	-5.347464900198	-1.278518220462	-3.532238459583
H	-5.261764034159	0.110920819375	-4.634934068743
H	-6.754789804172	-0.209332146808	-3.714020848397
H	-7.046566927424	3.828287687089	1.256759721527
H	-8.653587865723	3.845235633849	2.033732513876
H	-8.298213113765	4.939857875123	0.678163739865
N	5.874017232411	-1.601509708271	3.822589674172
H	5.748116640788	-0.790286789070	4.424826918154
C	7.107093285539	-2.349794676336	4.139371753350
C	8.339312572784	-1.454277687065	4.154107442581
H	7.211418891977	-3.133993903095	3.382446909837
H	6.960107871683	-2.831612779184	5.114501416256
C	9.608217822644	-2.235783682420	4.490843703706
H	8.442741111308	-0.977260343419	3.171681578606
H	8.198006982925	-0.648154397552	4.889708123206
H	9.491788858464	-2.724634628245	5.469491653164
H	9.742090778214	-3.042672067165	3.756245752059
C	10.857499192437	-1.356944322079	4.510101518510

C	12.129838023257	-2.129832879363	4.855016913127
H	10.719725009347	-0.541717449742	5.235468620862
H	10.977950991650	-0.875694603724	3.528996948731
C	13.372436452294	-1.242444564979	4.869131561786
H	12.006816399182	-2.609679417261	5.835810795903
H	12.265200760824	-2.944507725587	4.130332977051
H	14.271751714113	-1.814459883282	5.118464034489
H	13.532802491778	-0.776139136568	3.890568114844
H	13.272186524781	-0.437984527174	5.606474990998
C	2.635879327023	-3.111730557228	0.841132353529
C	3.927974291939	-3.185942483671	1.639560714995
O	4.054249019620	-2.099025817630	2.540837271800
H	1.757148215755	-3.218998771401	1.484537377904
H	2.610944807821	-3.925874187982	0.106918816314
H	2.565086053798	-2.160191041497	0.301969325771
H	3.968853200482	-4.135042728513	2.198230822824
H	4.795707137927	-3.179111215124	0.956366707958
H	4.854291675642	-2.173734669807	3.615445814015

The noncatalytic stepwise mechanism for the aminolysis of oligo-CF₂CO₂Et by n-hexylamine (Figure 7)

< Init _{non} S >			
C	-4.575049707778	5.837743613903	-3.955709142897
C	-3.434395986934	5.914161630209	-4.745531523530
C	-2.163721289027	5.924507497827	-4.171349183832
C	-2.059310385350	5.932022414215	-2.778676666853
C	-3.190700414504	5.866659930307	-1.978378283955
C	-4.452589901880	5.796412130794	-2.568283427437
C	-5.653678480612	5.489060817777	-1.717052067435
C	-0.908577689150	5.827301268315	-5.029804027967
C	-0.061823895357	7.098300520401	-4.934493907149
C	-0.182982372867	4.553446972740	-4.629436667171
C	1.023261777816	4.549716592861	-3.937502918665
C	1.574774116271	3.369330961752	-3.424750655300
C	0.881772317021	2.161027375361	-3.551214205974
C	-0.280674353893	2.155076315398	-4.322526019233
C	-0.807906638770	3.318834661586	-4.860783314301
C	1.331148367020	0.835126946605	-2.946984972894
C	0.174056148804	-0.047303105893	-2.474436880571
C	2.344374679105	0.853062461305	-1.809068201543
C	3.569500967311	0.207405945451	-1.974351748696
C	4.454950734044	0.064101298841	-0.914049428097
C	4.119660616495	0.569633842261	0.340150932711
C	2.906139438043	1.234868968770	0.513582910973
C	2.030733667373	1.378286482192	-0.553540723495
C	5.045634257705	0.308858945027	1.501518074684
C	0.279909885442	-1.425010288275	-2.677630422699
C	-0.646086485031	-2.318717872764	-2.147676096018
C	-1.734205617483	-1.839827555103	-1.405737915966
C	-1.865024435145	-0.467640046426	-1.234491510940
C	-0.920234248232	0.429589898746	-1.737170455888
C	-2.624869469165	-2.828599678065	-0.677188825735

C	-1.889139755964	-3.390687179582	0.529949362367
C	-3.984587750453	-2.242753771062	-0.325678493366
C	-0.944999132895	-2.630291980728	1.217122783365
C	-0.290239562753	-3.132406069382	2.338385572887
C	-0.556786908243	-4.430561228752	2.791364822136
C	-1.506121527068	-5.187428891183	2.106871354268
C	-2.176949272294	-4.678203257031	0.992384950133
C	0.171259145623	-4.976331006081	3.984785636818
C	-4.852697380243	-1.873837362801	-1.357685446581
C	-6.100039554820	-1.330211717944	-1.086002686203
C	-6.507794974239	-1.154959778907	0.236942318214
C	-5.650866561800	-1.514816501538	1.274573648869
C	-4.401154494039	-2.054059585565	0.991449971384
C	-7.857998139128	-0.569104050813	0.558259342831
O	2.786146796643	3.329054592796	-2.791422906741
C	3.446605123643	4.554634452432	-2.514653790327
O	-1.962106916772	3.359281045742	-5.600627291129
C	-2.794577319450	2.208441100542	-5.582923133601
O	-0.992362235118	1.772782463820	-1.500411496695
C	-2.245502732410	2.305267541463	-1.073397996942
O	-0.561441527171	-3.677616555620	-2.275101576570
C	0.617156723076	-4.213006199538	-2.862555028227
O	0.642663265570	-2.428637239047	3.055944471640
C	0.891313398846	-1.081192749505	2.656168513186
O	-3.136456623733	-5.364182139775	0.294793264668
C	-3.470656920164	-6.670857922551	0.740170929374
F	-5.515217914412	6.001374984264	-0.459150932002
F	-6.795540322754	6.016430302907	-2.252913786521
C	-5.775740023407	3.949033582702	-1.591392621890
O	-6.489337407262	3.449259038784	-2.593825988563
C	-6.539119369382	1.990367716740	-2.675905165133
O	-5.185452087744	3.321281844039	-0.744406940225
F	6.302077656818	0.781481472089	1.221213314627
C	5.150406384383	-1.216666984289	1.742226142192
F	4.608396454850	0.958924687995	2.621508187648
F	-8.655723424693	-0.558863009981	-0.548428940274
F	-8.493137221386	-1.329482872669	1.510371842154
C	-7.760203062440	0.891672284334	1.068886786214
O	-7.404499858830	0.907858055232	2.352440035214
C	-7.128925975332	2.222786940263	2.932436648750
O	-7.948473324655	1.848488198273	0.359331445264
O	5.972493841102	-1.909063436278	1.191856836829
C	-7.288369517215	1.647621641983	-3.939603639418
C	-5.694868863282	2.621017920301	2.663673503095
H	-5.557967085934	5.781778797452	-4.412936673018
H	-3.528169206267	5.910134678492	-5.828328158934
H	-1.075518001173	5.930042900546	-2.315100179090
H	-3.100574097009	5.837983323327	-0.897026446864
H	-1.238363542967	5.715263336509	-6.070541635070
H	-0.642721543199	7.955769545195	-5.286699819443
H	0.240715223505	7.310039478962	-3.903738291233
H	0.840124402259	7.015302187361	-5.550086797201
H	1.536829880575	5.489850571839	-3.780200637042

H	-0.800843448143	1.210583518176	-4.442229913769
H	1.814037287847	0.279908424424	-3.764987271329
H	3.834631690547	-0.197034501591	-2.948359317069
H	5.398033281308	-0.457437180183	-1.050198268877
H	2.644400697058	1.631762523409	1.488906112400
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O	0.695481137667	0.682513932375	-1.006437407687
C	0.142499033259	1.185760789811	0.202150468241
O	-0.711677572080	-4.399021788781	-2.653104659024
C	-0.262824921925	-4.875707703394	-3.914086900286
O	-1.018481994859	-1.937304408679	4.555837564755
C	-1.983998997070	-0.920229151786	4.331348403162
O	0.231776962386	-5.414516086728	0.455158085178
C	1.259440484922	-6.376394878689	0.643449778176
F	-2.937365712226	7.250164257954	0.337369978294
F	-4.519492200981	8.030705242865	-0.983865088277
C	-4.711336195043	5.791023949152	-0.187193867558
O	-5.805443770392	5.737684415243	-0.942792073593
C	-6.685869278822	4.596185714183	-0.703538876294
O	-4.420460365913	5.033233509131	0.707050568551
F	7.444817084787	-0.261325781651	-0.377186051080
C	5.864046905673	-0.698711505920	1.361312612855
F	6.457508309827	1.460924674537	0.585849536360
F	-7.657743623661	-1.101240392397	-1.112145252087
F	-7.744253082805	-1.560280851205	1.039681705783
C	-6.588912014285	0.414507588027	0.345984368700
O	-6.139751838784	0.530310985925	1.593986317748
C	-5.468522639412	1.787129170254	1.928116035209
O	-6.633221656957	1.284213724471	-0.490580613506
O	5.948223942366	-2.026686459178	0.926532414159
C	-7.727568054735	4.590912071281	-1.793584362565
C	-4.044523006017	1.767096714142	1.415694376976
H	-4.592520138254	6.931225612658	-3.259633844762
H	-3.440882100569	5.946597288508	-5.214888918204
H	-0.121838095783	4.867779940109	-2.729383981310
H	-1.272008482134	5.848845754628	-0.767019418131
H	-1.850676819242	4.398144312936	-5.992460272348

H	-0.777868103692	6.595500322517	-6.301574586231
H	0.645986473384	6.076168087453	-5.395311643022
H	0.256219413340	5.314201008076	-6.957762844829
H	1.614168390771	3.987549324357	-5.686867977268
H	-0.896652381715	0.504138463436	-3.272277394008
H	2.004196529408	-0.747070689813	-4.379678786842
H	3.756040815796	-1.883482285351	-3.206319408305
H	5.700464551630	-1.761089401771	-1.683365728152
H	4.539165452120	2.204447141130	-0.545542563296
H	2.629715687725	2.098146572279	-2.111464026344
H	0.852521448595	-2.643655838540	-4.013817876063
H	-0.749618814578	-1.105954979240	0.377870525997
H	-1.719653194571	-4.550560893357	-0.547467036842
H	-2.176397154587	-2.016171644671	2.100824951503
H	1.327615474718	-5.385133332748	2.942332566685
H	1.466704771114	-2.854822144606	5.284450276544
H	0.220742153474	-3.917914561398	5.918745136150
H	1.653687078266	-4.615156586214	5.131799493761
H	-2.801473020525	-1.744688181710	-1.888133707105
H	-5.062150928036	-0.756361649434	-1.828855344666
H	-5.990719320849	-3.090438140409	1.648793920669
H	-3.746543995731	-4.118418378178	1.553048136314
H	4.814600969853	2.378434878044	-5.693179986947
H	3.826271410728	3.699729958069	-5.010405774470
H	3.445928419038	3.037452070481	-6.633787361041
H	-4.074833713381	2.144275988175	-3.170291054096
H	-3.109141348279	0.713239747456	-3.628981644353
H	-2.600517336362	1.731893605769	-2.244316751949
H	-0.957272827679	1.182269601059	0.171275202714
H	0.498933503608	2.214310883314	0.285359520426
H	0.484509709777	0.613014743996	1.075359374379
H	-0.690144006016	-5.873909498634	-4.024717161463
H	0.833359970173	-4.943682399193	-3.950969844838
H	-0.616537170542	-4.237898347997	-4.736009198341
H	-2.972738081256	-1.342354621287	4.101585240899
H	-1.677988146466	-0.250955039128	3.513538083327
H	-2.041836269353	-0.349690104621	5.260111873678
H	2.219439440495	-5.896643903898	0.879475875939
H	1.346209838668	-6.908720571350	-0.305488811314
H	1.003227467697	-7.090866365431	1.438023258455
H	-7.128344992952	4.711769155085	0.292545287381
H	-6.081762850116	3.684944680434	-0.711522804204
H	-6.036288624315	2.622671426139	1.511191080165
H	-5.511266349068	1.825015526108	3.018741636449
H	-8.384819932828	3.727997404787	-1.651097144508
H	-7.257427925986	4.502810515963	-2.777316764753
H	-8.331648480691	5.502481339345	-1.772086478997
H	-4.025150125631	1.732185720510	0.322156329946
H	-3.506490828113	0.897564211675	1.808432630348
H	-3.535600231721	2.683092678514	1.729225329603
N	6.811361426180	-0.412066735922	2.401007351465
H	5.615177741227	-2.586450778052	1.640054967295
C	6.966404824298	-1.379302528282	3.487618675390

C	5.744314582068	-1.658248838328	4.372903173565
H	7.781725196515	-1.001851211334	4.119603901347
H	7.343565216736	-2.318742852476	3.059664277865
C	6.076612189447	-2.583650194360	5.541905369994
H	5.341851817562	-0.706710316074	4.745910850946
H	4.933941872671	-2.100382431673	3.779166851250
H	6.544085984248	-3.504792473909	5.162252148484
H	6.827226124194	-2.105863055691	6.188499753872
C	4.845430891794	-2.948511183323	6.369635261436
C	5.150732800116	-3.863168433025	7.554495566323
H	4.105340136476	-3.437302834523	5.718367906210
H	4.365445421829	-2.028392289179	6.734180515752
C	3.899556163311	-4.226165706541	8.351486679192
H	5.636380169296	-4.778753967621	7.189411574067
H	5.880001040203	-3.371920108065	8.213165614178
H	4.133918402444	-4.884226416662	9.194303155253
H	3.415405860398	-3.328206305703	8.751777210885
H	3.166834832764	-4.740485016265	7.718491669772
C	2.419933030529	-1.441163662433	2.182057251074
C	3.379836990423	-0.880685500978	1.150988996308
O	4.553005954668	-0.368620388247	1.831140023186
H	2.841471384606	-2.311868256775	2.695530992491
H	1.495257418796	-1.766931841069	1.690981793122
H	2.169308925492	-0.690642494133	2.939730654518
H	3.661913863012	-1.651602897587	0.428006499357
H	2.914547289162	-0.061855376060	0.588986309122
H	6.644564972744	0.522846426226	2.752939415766

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C	-1.676024641440	5.227211112764	-4.714773996596
C	-1.782017265606	5.538532399898	-3.356430065029
C	-3.002395509494	5.473384632902	-2.703183267978
C	-4.145094834157	5.092098483583	-3.407821955563
C	-5.401364195204	4.793100649139	-2.641436182151
C	-0.304077691350	5.118446691717	-5.368372296494
C	0.471257016427	6.436642383175	-5.319404369497
C	0.392738935598	3.946000359345	-4.696760112936
C	1.347542056674	4.114437711412	-3.699564955739
C	1.822625357044	3.040687622231	-2.939834227194
C	1.341258739603	1.750155409920	-3.181973447095
C	0.433815730776	1.573706344159	-4.227111674870
C	-0.043699772801	2.642320649752	-4.974138366032
C	1.670556636211	0.493912220246	-2.376530101928
C	0.435432466984	-0.143780458714	-1.748824096416
C	2.809626215291	0.559162866265	-1.370260272166
C	4.110269411566	0.287679910520	-1.794390644225
C	5.167430174042	0.256754360682	-0.896209178039
C	4.932109668458	0.484609532545	0.459968286478
C	3.641129375570	0.790598640501	0.889006107302
C	2.591601778280	0.817600612378	-0.018411649152
C	6.075867396593	0.459036536645	1.427546209899

C	0.365394537110	-1.537304760292	-1.723716704562
C	-0.681162074826	-2.205078143843	-1.096628777541
C	-1.722379743770	-1.476334967619	-0.501487361860
C	-1.674107126831	-0.087070489529	-0.555279040238
C	-0.594245669600	0.584036899361	-1.140069321348
C	-2.753157764796	-2.236170205536	0.311914045592
C	-2.169937323388	-2.646511282750	1.659139619420
C	-4.077740897599	-1.513319860558	0.484321806302
C	-1.087999357720	-1.981760647270	2.230479941391
C	-0.584856344385	-2.361158810229	3.472545081692
C	-1.154362446151	-3.430195373478	4.173874353534
C	-2.238268699752	-4.092903939160	3.600270754262
C	-2.750521873298	-3.708764450217	2.360330089483
C	-0.597953298631	-3.839511485677	5.506208122039
C	-5.157383716364	-1.843137549947	-0.335692004418
C	-6.395169260060	-1.234333611755	-0.173115499910
C	-6.566895564212	-0.274898851439	0.822559616230
C	-5.493036937649	0.080642708712	1.637251586304
C	-4.264264190428	-0.546840371375	1.475095834249
C	-7.897750882578	0.404337850112	0.997791012461
O	2.720867583238	3.196104169398	-1.922518757091
C	3.216293949608	4.496345638468	-1.647666974785
O	-0.963001300579	2.516053690667	-5.983757754170
C	-1.599351369374	1.255101073701	-6.139648934149
O	-0.447860526083	1.941330529708	-1.103149758606
C	-1.541191914301	2.720255168171	-0.630395795588
O	-0.765023753033	-3.565667419239	-0.992275207833
C	0.337586911994	-4.333075945912	-1.459546031126
O	0.477178113154	-1.744572061225	4.085219797061
C	0.988365234422	-0.569797542240	3.468343774945
O	-3.816772353198	-4.313746841541	1.747792405800
C	-4.471889529526	-5.363285213458	2.445431336780
F	-5.602204266093	5.706006524965	-1.643258180456
F	-6.507085314844	4.820859308208	-3.446313366202
C	-5.261129569412	3.393108961462	-1.986236784731
O	-5.420066216305	2.452163476502	-2.905389403009
C	-5.168349201027	1.073848598561	-2.486460443364
O	-4.954752457000	3.237935849925	-0.826565676820
F	6.993575919927	1.442483265306	1.065973042175
C	6.899282157472	-0.838393207814	1.533104324202
F	5.657161084643	0.796315275091	2.696962362315
F	-8.912378617076	-0.405983348648	0.556949379547
F	-8.133534336504	0.657611876479	2.320540501367
C	-7.991222045876	1.712440438594	0.168730386354
O	-7.923081453425	2.787337062460	0.944198342621
C	-8.012413749360	4.092571624373	0.289906836848
O	-8.080537111168	1.683018098008	-1.036009254657
O	7.144702926447	-1.539217530636	0.444786083677
C	-5.858025760992	0.176143581342	-3.481778831554
C	-7.227328738126	5.072397713167	1.124735419759
H	-4.952995640960	4.517954709334	-5.314297185344
H	-2.768323122929	4.666229892843	-6.474890449410
H	-0.887024652952	5.781708760680	-2.789691405207

H	-3.071408427060	5.683040181663	-1.639716787059
H	-0.463521956961	4.858391034693	-6.421296006713
H	-0.067998683840	7.202244107145	-5.885032365376
H	0.589527675727	6.812651690729	-4.298445429037
H	1.467560860528	6.317039695577	-5.757621105761
H	1.703536016073	5.114822988323	-3.487350718778
H	0.067127408524	0.568192901909	-4.408258659811
H	2.008212285228	-0.231660756463	-3.131055050050
H	4.299686208773	0.098088008683	-2.848464642969
H	6.171851800468	0.043254481869	-1.243587125436
H	3.453531681571	1.002719549951	1.935611908107
H	1.589112754808	1.051976626179	0.326334221339
H	1.178007264875	-2.093846497318	-2.179497566677
H	-2.475141755880	0.474150353226	-0.086757845295
H	-2.974014404157	-3.164413363080	-0.226458555423
H	-0.635806883824	-1.167988695048	1.675422064719
H	-2.677452402845	-4.920421273083	4.146946003896
H	0.456120540197	-4.126290233930	5.421340413720
H	-0.637379139195	-3.009805853883	6.220623696197
H	-1.157066899862	-4.682856424295	5.919462239450
H	-5.031194388180	-2.610040478440	-1.096298485443
H	-7.231375735590	-1.508588588809	-0.807930166263
H	-5.626625190065	0.828593841564	2.412592393588
H	-3.443752569064	-0.306532669435	2.146244020422
H	3.919394535780	4.373832886283	-0.821321319756
H	2.412208921265	5.180904627242	-1.341089384808
H	3.744594916067	4.920462958646	-2.513195839724
H	-2.352644486695	1.393085132655	-6.917935568477
H	-0.889640482161	0.479414031485	-6.458861517401
H	-2.088879662305	0.938531702547	-5.207853605895
H	-2.449404719271	2.540089878296	-1.217796729604
H	-1.235369327828	3.760369054961	-0.754406045272
H	-1.754211840410	2.524874381797	0.429604859890
H	0.102092036764	-5.370544554652	-1.216069790623
H	1.267897526086	-4.040878929000	-0.954619011669
H	0.463862540860	-4.236096559076	-2.547025844063
H	0.213940503373	0.207162199145	3.390679517596
H	1.393600915927	-0.777359746439	2.468592039743
H	1.794504352273	-0.218276333590	4.115753298285
H	-3.798557784146	-6.214418601152	2.618601252463
H	-5.295803977961	-5.680346369650	1.803401329552
H	-4.875017692317	-5.015437510176	3.406393125116
H	-5.551980102524	0.939164971120	-1.473910920022
H	-4.080535487598	0.928086599328	-2.473814316195
H	-7.626744211566	4.006930522453	-0.728056111017
H	-9.077765861304	4.344779314446	0.238772253039
H	-5.632756940337	-0.866747024834	-3.239836386717
H	-5.512833504794	0.377569971820	-4.500454382147
H	-6.941032442965	0.319662830569	-3.434837703847
H	-6.169684929711	4.796988018864	1.134509079080
H	-7.605485351962	5.106137841256	2.150618418808
H	-7.316179692209	6.070380808340	0.685012529245
N	7.760842883129	-0.867604395215	2.549400280496

H	6.236370639428	-2.113753964383	0.542043387496
C	8.608085046433	-2.024717834569	2.837632804828
C	7.966035848307	-2.960712669676	3.861215423715
H	9.576385302029	-1.655362069573	3.200160717222
H	8.780344943304	-2.545378483773	1.892000556783
C	8.846861861685	-4.174346027096	4.150646652951
H	7.780727981125	-2.409537097109	4.795021089222
H	6.989168178962	-3.272503373492	3.472041234050
H	9.016508596565	-4.731170682992	3.217821755228
H	9.837427184004	-3.841809335039	4.495667030649
C	8.237548888083	-5.109914322698	5.193438599350
C	9.106664744267	-6.332047842939	5.486960812710
H	7.246963303232	-5.440483737900	4.849550412755
H	8.066963019080	-4.553105830752	6.126474067628
C	8.491195313047	-7.255074208955	6.536425126339
H	9.272027754235	-6.890349876319	4.555274505262
H	10.097958733185	-5.998725816225	5.824036818997
H	9.129307231854	-8.122748322478	6.731906538699
H	8.343721972361	-6.727319851714	7.485459207686
H	7.513482882216	-7.625720519926	6.208516756591
C	3.182141709529	-2.742592506419	0.981341132562
C	4.095779883266	-2.302628344501	2.121544539010
O	5.430295914893	-2.204137204894	1.701951586705
H	3.208434621885	-2.011006143514	0.166250923977
H	2.143934059727	-2.847464569978	1.324207449436
H	3.514523172194	-3.711728704306	0.592070946930
H	3.745834764154	-1.333085734063	2.514968872573
H	4.011373743675	-3.022756504709	2.956486403062
H	7.552843263865	-0.247798226304	3.320275330107

The self-catalytic concerted mechanism for the aminolysis of oligo-CF₂CO₂Et by n-hexylamine (Figure 8)

< Init _{cat_C} >			
C	-6.051718055669	5.499886961937	-4.037680510991
C	-5.053681013420	5.770963225293	-4.965825638736
C	-3.741553866817	6.008569298046	-4.558560060201
C	-3.462298073777	6.045429024609	-3.190563430060
C	-4.451334098663	5.785745685932	-2.253283738082
C	-5.746066545136	5.488730858647	-2.678398059837
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H	-3.573580633536	1.742833302553	-5.031355236972
H	-3.137469565272	2.381219668506	-1.061547822851
H	-2.116557966210	3.805526980802	-0.743014131093
H	-1.878693343344	2.306129461022	0.203986154080
H	1.045901020308	-4.438012138743	-3.474991920674
H	1.936620330899	-2.903359133256	-3.272106688278
H	0.688384897591	-3.056921496880	-4.551469310683
H	0.249951424576	0.738022864153	2.353493992890
H	1.664031451437	0.393973267767	1.296605237529
H	1.911694567232	0.945581849617	2.972299315546
H	-0.989720032684	-6.651159751279	1.159836121160
H	-2.682247932638	-6.718313809541	0.590473553641
H	-2.323371843697	-6.103493126569	2.228084986565
H	-5.919012674478	0.146771927618	-1.320447191799
H	-4.543574643861	0.735195556495	-2.274225215627
H	-8.545935676539	1.591927614960	-0.922700263468
H	-10.094460084136	1.096584831919	-0.224219327975
H	-5.631789977681	-1.192569942902	-3.424291309610
H	-5.835796118669	0.280460927042	-4.397778260190
H	-7.189744128628	-0.347201243137	-3.418159162627
H	-8.003047311970	2.856051430740	1.202106316952
H	-9.579758722759	2.377059413419	1.876655826413
H	-9.498835848821	3.452458724285	0.463794062309
N	6.987020670996	-0.106354485972	1.209684524276
H	7.588732842549	0.690494266981	1.015098591013
C	7.808774609631	-1.331666946951	1.142491411124
C	7.235820680162	-2.443382028173	2.016256314237
H	8.821923773361	-1.083761019505	1.486126482773
H	7.875253089006	-1.674489905738	0.100042422473
C	7.941328810268	-3.781023345458	1.811901206952
H	7.309129441175	-2.152465946647	3.075755447247
H	6.167662557813	-2.560170380170	1.789921508814
H	7.847296054563	-4.077167209672	0.757769335342
H	9.018310168718	-3.664825843890	2.004857970996
C	7.381506191342	-4.887365580246	2.704408084473
C	8.065535513941	-6.238162225838	2.499225541748
H	6.303128228316	-4.994860796996	2.513500386848
H	7.477184604830	-4.589827327347	3.759710180018
C	7.496056443588	-7.331924704661	3.400273164545
H	7.965053582013	-6.536343346445	1.446749944703
H	9.142991767929	-6.129611478741	2.684987429824
H	7.998988890164	-8.290553475236	3.237381685598
H	7.611613781754	-7.069325301092	4.458136114356
H	6.426634218350	-7.478926403248	3.210720624267
C	2.955410616107	-1.510216466865	-0.694355256988
C	3.924507261606	-1.704985541684	0.461713870345
O	4.498032600601	-0.488177746851	0.933056744448
H	2.176907992817	-0.780076897636	-0.455960179213

H	2.456753014926	-2.461486477505	-0.919313493286
H	3.490549240615	-1.159576755737	-1.580736209112
H	3.402200869256	-2.161687493747	1.317245779414
H	4.721631195869	-2.390222011375	0.138726918516
H	6.151618190248	0.097062300108	2.723864672669
N	5.221562216778	0.155920214134	3.270120253338
H	5.032186378826	1.132606998928	3.481967678510
C	5.101903843452	-0.713613392972	4.464490888239
C	3.801512297511	-0.456961465583	5.211348399283
H	5.967938472348	-0.547894610450	5.118361928898
H	5.145118236385	-1.751809124520	4.115904057506
C	3.609814880994	-1.401658742867	6.396397316422
H	3.783253775136	0.584656359877	5.566825991972
H	2.960742112869	-0.581501866684	4.517872148368
H	3.578499158729	-2.437077022854	6.028130020904
H	4.473180653802	-1.339385633249	7.074652360097
C	2.328475649531	-1.104961549045	7.174061996928
C	2.036043065209	-2.133015832285	8.265721045405
H	1.480335988945	-1.067164226292	6.474795194253
H	2.397219327011	-0.103644405675	7.623454086449
C	0.759981321143	-1.818453354768	9.042947113486
H	1.953299184091	-3.128332961291	7.807173586077
H	2.889324445770	-2.182954995237	8.956097777213
H	0.563194064115	-2.570730450102	9.813184021429
H	0.830821762441	-0.843467182555	9.538040155882
H	-0.108102624223	-1.788800063741	8.374811408675
H	4.629960782645	-0.161594155883	2.399395265127

The self-catalytic stepwise mechanism for the aminolysis of oligo-CF₂CO₂Et by n-hexylamine (Figure 9)

< Init _{cat_S} >			
C	-5.397554066193	6.186218972999	-4.682317263351
C	-4.256955128981	6.054292093966	-5.464976247781
C	-2.997563998324	5.926591052710	-4.881095644979
C	-2.892567487529	6.008391902795	-3.490790233048
C	-4.022075799093	6.152438821405	-2.698366537516
C	-5.281552451360	6.219465169358	-3.294418192499
C	-6.511310076202	6.139901376419	-2.433002215279
C	-1.767071288802	5.605785963607	-5.719742216100
C	-0.783635877136	6.778189152677	-5.739146929652
C	-1.187023200970	4.302970596108	-5.195103383148
C	0.030085061446	4.222887636210	-4.527497949928
C	0.443679589773	3.044870632083	-3.894237777311
C	-0.404624893513	1.933142489704	-3.858467313530
C	-1.581126894281	1.988287156925	-4.605625967255
C	-1.967060151702	3.139216220828	-5.275340155823
C	-0.086911400394	0.645887012140	-3.108808611938
C	-1.321251845359	-0.101319521363	-2.601675350549
C	0.881361660275	0.718493094838	-1.933256146707
C	2.020483086441	-0.086739278116	-1.940903319174
C	2.862025449287	-0.151004076732	-0.838741478729
C	2.567860844950	0.593586027018	0.301782527204

C	1.437547088577	1.409615753988	0.318824598882
C	0.606902424523	1.474710673968	-0.791850680113
C	3.460098338428	0.454354735734	1.510376929051
C	-1.328354234896	-1.493903283993	-2.707169657119
C	-2.329246394049	-2.270342588505	-2.130186949429
C	-3.377364544760	-1.653717242336	-1.434677349546
C	-3.399833825378	-0.266038666215	-1.366474009304
C	-2.384056936157	0.514706521816	-1.921820789518
C	-4.336239904912	-2.509508334719	-0.629713836530
C	-3.644872829960	-2.992727329711	0.637493475142
C	-5.659186936562	-1.809341674436	-0.351566071067
C	-2.671927643315	-2.217402304710	1.264838895215
C	-2.070256605554	-2.631366235007	2.449647941429
C	-2.418899641011	-3.857730257781	3.029322553079
C	-3.392879921023	-4.632180209398	2.401236457795
C	-4.011812038850	-4.208166705673	1.222456213273
C	-1.752988198810	-4.306685960840	4.296947772249
C	-6.469101618181	-1.431278978084	-1.427155264297
C	-7.683364244157	-0.791690585565	-1.221589858558
C	-8.118080284451	-0.530657110421	0.078403284802
C	-7.319139917867	-0.897878020401	1.158535691170
C	-6.101214460755	-1.531469866802	0.941354539649
C	-9.429535478336	0.165706135966	0.330675379351
O	1.667490498677	2.909514003381	-3.299009458573
C	2.463101071086	4.071430196847	-3.115250144881
O	-3.123691966347	3.242491053895	-6.004474244133
C	-4.093245251111	2.216146880565	-5.849733780304
O	-2.357852845109	1.874727744921	-1.797394588438
C	-3.561774336731	2.532189408653	-1.404852259891
O	-2.354491184691	-3.637276729515	-2.160723638821
C	-1.240810535755	-4.306301377498	-2.736907114975
O	-1.120034386001	-1.901936868121	3.116785135888
C	-0.770098103004	-0.631150638305	2.567794121750
O	-4.996106580756	-4.910067833481	0.577038810354
C	-5.423304651680	-6.134725046966	1.156082953482
F	-6.316995163147	6.756163533753	-1.230556870279
F	-7.583452583185	6.738443164487	-3.034164117254
C	-6.811651823118	4.644940923620	-2.155208125130
O	-7.560942339914	4.125880107981	-3.121242475088
C	-7.775530753495	2.680138147284	-3.052943391909
O	-6.316243763005	4.047886340775	-1.228685562908
F	4.743828045855	0.810572709063	1.191940379063
C	3.483437447207	-1.018624563819	1.986057425226
F	3.045629018352	1.282047463637	2.514527299322
F	-10.216158733766	0.138259866632	-0.782680719052
F	-10.120518085926	-0.467613105203	1.334650764655
C	-9.227187450594	1.652411941855	0.718751829478
O	-8.879606237038	1.751903604409	2.000278887192
C	-8.492187388186	3.085175184097	2.463164574156
O	-9.329965889075	2.556710593906	-0.073264272259
O	4.310511896030	-1.812983469798	1.598803296239
C	-8.636691168838	2.307434748587	-4.233768292513
C	-7.037043362418	3.346036466182	2.143461423439

H	-6.378761015393	6.234796714651	-5.143720780772
H	-4.350843473244	5.990987240912	-6.546032125086
H	-1.918207627230	5.899989136643	-3.020052724560
H	-3.937012037305	6.183106680578	-1.616539285735
H	-2.113170738175	5.433414190353	-6.747113384537
H	-1.271358046991	7.660943827206	-6.162969567638
H	-0.448088458410	7.042782175894	-4.730913626146
H	0.096277900409	6.544714358009	-6.348099111490
H	0.665144720572	5.099167514741	-4.488698597125
H	-2.222484751251	1.113565086811	-4.604171339622
H	0.386015682116	-0.024803788723	-3.841467851224
H	2.255090956714	-0.673123668575	-2.826044565814
H	3.743212942359	-0.786361744787	-0.855761073343
H	1.206434575982	1.990622983750	1.205508062014
H	-0.269531004507	2.114105746692	-0.774644789069
H	-0.501385466936	-1.964758400075	-3.228210753733
H	-4.205534187612	0.204326053524	-0.813767722253
H	-4.572216660978	-3.400858054742	-1.224259606134
H	-2.389170044031	-1.279441559115	0.802230059187
H	-3.663339843484	-5.578922027296	2.856256097903
H	-0.668208351562	-4.390238110665	4.162737166114
H	-1.910591605632	-3.581693105751	5.103151415354
H	-2.137776362371	-5.277406907792	4.619911426520
H	-6.135886112882	-1.641516120654	-2.441005726115
H	-8.306394565243	-0.516052729048	-2.065937170789
H	-7.655958890495	-0.697129609370	2.170637439611
H	-5.488101301755	-1.820852055089	1.789295673873
H	3.337175420224	3.743956390989	-2.548917884065
H	1.925497872488	4.839270285896	-2.541526956698
H	2.790907812369	4.495245782603	-4.074884596308
H	-4.975309333318	2.551464385095	-6.399683708493
H	-3.747565203986	1.261334985254	-6.269426064995
H	-4.353816114258	2.072681823986	-4.790971145589
H	-4.414840744141	2.192459542235	-2.004636945767
H	-3.398312771386	3.594687340248	-1.588288814369
H	-3.789468837101	2.375026174680	-0.342321050006
H	-1.436287236129	-5.372699167385	-2.611732061668
H	-0.307257616674	-4.043281740165	-2.220623548044
H	-1.142958153445	-4.079646762286	-3.807773306172
H	-1.646185069166	0.029620854475	2.512448746088
H	-0.323470140196	-0.730688376178	1.569370503283
H	-0.025744508427	-0.205868227591	3.241883260616
H	-4.605572809776	-6.867758183095	1.198279964891
H	-6.213515570199	-6.513487550396	0.505358911340
H	-5.827891549631	-5.981490097008	2.166051565252
H	-8.256622454908	2.451028169674	-2.098666248932
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H	-9.151754883146	3.821297119705	1.994978065121
H	-8.680759577411	3.051561869494	3.538861447572
H	-8.818037847455	1.228014046215	-4.224092645934
H	-8.150745145854	2.568763218642	-5.178689119050
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H	-6.745639912107	4.320123231535	2.550209541159
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H	4.982200861749	-1.459729989931	4.581531646518
C	6.276134060441	-0.058970881604	3.867266539877
C	7.366634371918	-0.195218665466	4.933085320422
H	6.218457598634	0.983258216532	3.525789402610
H	6.552406847808	-0.647464547381	2.980295234023
C	8.766072147551	0.068881225549	4.378702237792
H	7.159007311878	0.495499109565	5.763896673047
H	7.324929031632	-1.208841096860	5.358057453524
H	8.944847120372	-0.599058308603	3.521971664716
H	8.816861617723	1.092050605247	3.978562313507
C	9.875528375490	-0.133571476350	5.408400648639
C	11.275984451166	0.083516473541	4.836509688810
H	9.806302188365	-1.152004321393	5.819007695714
H	9.718053274241	0.548936187152	6.256478606019
C	12.377423430302	-0.116887978823	5.875130787068
H	11.431256565387	-0.606447833674	3.995189868122
H	11.342226202508	1.096882110475	4.417016083448
H	13.371478990042	0.041958014143	5.444706579241
H	12.259224962728	0.581408180209	6.711491283801
H	12.348770409291	-1.132531521203	6.285934311177
C	1.693921585169	-3.541772952603	1.972658883473
C	2.202185545112	-2.671754798130	3.103414435100
O	2.376386415980	-1.290600160043	2.674283933347
H	0.748053317798	-3.154798400617	1.582171880159
H	1.513084037818	-4.554423075114	2.350052258935
H	2.424814146988	-3.600755379644	1.162297556445
H	1.466922413950	-2.602275270600	3.908863466539
H	3.156227696309	-3.027183273694	3.506661511761
H	4.614003738913	0.061976031196	5.066747278233
N	5.818279728585	-3.671376711698	3.693967842591
H	5.477387307785	-3.233419370115	2.840036089950
C	7.286495485646	-3.722204087143	3.670277624795
C	7.914450225843	-4.422466340620	2.463488718401
H	7.630374078909	-4.204938709636	4.596417569691
H	7.661071799807	-2.691096074592	3.708788671163
C	9.441683480836	-4.366244680646	2.492066615289
H	7.581430630280	-5.470583545400	2.430372558657
H	7.543953610573	-3.946703775012	1.543656962276
H	9.761828228997	-3.314358320101	2.538017739853
H	9.807324009355	-4.836215107907	3.417111911217
C	10.099242618219	-5.040171140357	1.289263900081
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H	11.938201786098	-3.919217184527	1.367983702458
H	11.989354454049	-5.440278733749	2.245703645646
H	13.365823149598	-5.585462635099	0.156200699383
H	11.999282041551	-6.706222489553	0.062252017383
H	11.948279795535	-5.175057152498	-0.820726537852

H	5.450593481090	-4.618267113917	3.688768533475
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C	-3.693959886475	5.772786153935	-3.224153895030
C	-4.817813042457	5.460589730990	-2.475023870815
C	-6.002363831651	5.099453755207	-3.119579890797
C	-7.109874672039	4.502500421868	-2.300272268572
C	-2.438664991048	5.858078899623	-5.419741380693
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H	-6.120144327077	0.910839834263	-2.993565156488
H	-9.143850062883	2.229274442503	1.769758716310
H	-8.584707892648	1.638124125544	3.362043651118
H	-7.530897631713	-0.621563476188	-4.414595018682
H	-7.109180709344	0.848039105595	-5.317513034994
H	-8.732621343952	0.664775885886	-4.614759885447
H	-6.767569769371	2.401874887912	0.990950608752
H	-6.203705006266	1.793480763415	2.570892126812
H	-7.005890633583	3.373557531519	2.451347962231
N	6.150827607665	0.729313204464	3.217579020809
H	5.533904373307	-2.084603708114	3.182016349868
C	7.479780088097	1.176749320554	2.795169862801

C	8.565610898463	0.486201610066	3.618876970093
H	7.596983288872	2.269445737963	2.871411251085
H	7.605455617026	0.921429916738	1.738198452323
C	9.969897440006	0.938250224007	3.223018313693
H	8.400959577295	0.685778899466	4.687741459865
H	8.467445532680	-0.599952201803	3.487018920820
H	10.121436051846	0.752997734377	2.149325614687
H	10.058070793266	2.026008298500	3.359698087951
C	11.072394944418	0.238621488109	4.015945624904
C	12.479145687516	0.682338487229	3.616198609363
H	10.983826111127	-0.849484380984	3.880484856379
H	10.924603835517	0.424836448164	5.089929286397
C	13.572216967453	-0.028176705168	4.411707492929
H	12.623897919248	0.498142499925	2.542731402493
H	12.568270148931	1.768683081639	3.754449906734
H	14.570847334301	0.303989973126	4.110117005290
H	13.465335003572	0.165305463965	5.485159833842
H	13.522010834813	-1.113166004017	4.265069729708
C	2.446938652891	-1.101776459253	1.445323118877
C	2.734672722467	-0.225230112341	2.653547347779
O	4.115461449342	-0.134720876691	3.041823009544
H	2.974169466098	-0.753695861038	0.553945925043
H	1.370442570602	-1.084275730551	1.235864245736
H	2.725929644628	-2.140493457295	1.647024427526
H	2.318390355862	0.776038808712	2.513113078699
H	2.251378199264	-0.653782359032	3.538028326643
H	5.805508343278	1.212054626499	4.037207625056
N	6.086457799424	-2.557762987721	2.468202816326
H	5.945246536401	-0.992775479380	1.513295385298
C	5.266597436653	-3.561882263259	1.771264916813
C	4.355269190361	-4.397352773462	2.670737930968
H	5.938003492264	-4.219134195629	1.203100635464
H	4.651989408769	-3.036028195848	1.027270213496
C	3.420618921213	-5.306742235886	1.874772362229
H	4.966631053454	-4.998394345159	3.359665735322
H	3.756683702633	-3.718041555272	3.296745718647
H	2.767219788878	-4.688666888468	1.240493433395
H	4.013154509968	-5.932744191353	1.190862222865
C	2.557363381552	-6.204941351269	2.758337174659
C	1.609916954454	-7.101165113626	1.963700973575
H	1.970646029914	-5.580244421777	3.447844284652
H	3.208524758654	-6.831059942056	3.385810650375
C	0.822458577427	-8.058425059034	2.855677039476
H	0.920205828393	-6.467698246400	1.387420974258
H	2.186630684776	-7.679302175357	1.228266806623
H	0.151452879775	-8.699584649086	2.274128078574
H	1.498191848002	-8.711918780011	3.418771717786
H	0.215394725034	-7.510892144169	3.586909823771
H	6.869440414484	-2.992408473428	2.943178437805

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C	-6.155517468820	4.705717992966	-4.664240136657
C	-5.003311440541	5.104091843339	-5.330756674697

C	-3.819565737757	5.343613455685	-4.634430642592
C	-3.833259351935	5.261477863845	-3.240485987547
C	-4.978838621480	4.873449076433	-2.562396568726
C	-6.137025404067	4.570763181454	-3.277267597543
C	-7.287865208084	3.918044955369	-2.567351067320
C	-2.505715159046	5.592381852406	-5.363589634099
C	-2.083174798140	7.059324531944	-5.253063968515
C	-1.484924829087	4.600624174694	-4.829191771097
C	-0.334209754396	4.976439549844	-4.143236785343
C	0.481601364724	4.035156495284	-3.502191774450
C	0.120671187062	2.682587228004	-3.497144946836
C	-0.987170793101	2.304993399519	-4.254895627614
C	-1.773945077318	3.232615282041	-4.917182712484
C	0.866888012897	1.567120242713	-2.774175704834
C	-0.063459429759	0.543552080060	-2.116435217698
C	1.942978785480	1.905036648231	-1.753980872294
C	3.253754163520	1.498056010945	-1.994116647472
C	4.228102669545	1.581596944399	-1.007330476512
C	3.898690555902	2.076888938597	0.252966483750
C	2.610705300288	2.572511220813	0.470935525982
C	1.640732481885	2.475673764484	-0.516209121095
C	4.922552765850	2.017932270940	1.349991257382
C	0.340677041383	-0.792112962825	-2.125987146868
C	-0.386110576851	-1.785795781982	-1.477344255197
C	-1.600466885612	-1.468786318457	-0.856364966847
C	-2.014065982789	-0.140699662160	-0.851262741930
C	-1.238903454057	0.871593075188	-1.423128355729
C	-2.365998179692	-2.553627113750	-0.122027488775
C	-1.759532002314	-2.816507540159	1.245773236963
C	-3.858332132709	-2.263000980207	-0.055050470288
C	-1.178817929553	-1.792477276934	1.988722506589
C	-0.676651751659	-2.021655991139	3.266587404405
C	-0.718362060353	-3.304522096867	3.824986823954
C	-1.304556014858	-4.328161811464	3.081451778069
C	-1.837599290743	-4.093035025527	1.812662997999
C	-0.161162670754	-3.548752619226	5.197166986307
C	-4.625116813036	-2.395140019801	-1.215297674190
C	-5.989017441799	-2.140717782200	-1.205325332481
C	-6.613667345689	-1.741432616541	-0.023529353563
C	-5.858192230899	-1.594875911387	1.137145826685
C	-4.494044391742	-1.861113146910	1.119426509454
C	-8.093155110564	-1.469080288282	0.006974249979
O	1.636045049405	4.374381609201	-2.855844151850
C	1.979431596476	5.747398419630	-2.754443783123
O	-2.879847138998	2.887049359823	-5.655281315380
C	-3.618696880163	1.751196033392	-5.214864320019
O	-1.563456042104	2.196399950250	-1.324695708883
C	-2.774426996281	2.537876742249	-0.658856934100
O	0.008000588813	-3.094998909660	-1.395143665420
C	1.308501890387	-3.419859462204	-1.867454443549
O	-0.122078561340	-1.043925220715	4.053837937341
C	-0.336771739518	0.307057907111	3.656572141587
O	-2.460939711087	-5.049651244633	1.055529607127

C	-2.710876696385	-6.311520466057	1.659520488037
F	-7.400824836358	4.377495030877	-1.281173508241
F	-8.474645330817	4.166162569394	-3.194132244559
C	-7.018913834589	2.392256777781	-2.499269858481
O	-7.476413856483	1.790178830062	-3.588963899722
C	-7.187502816760	0.363007005217	-3.704362094862
O	-6.379700695967	1.886044554800	-1.605964305762
F	6.037783699665	2.747627567388	0.949854582728
C	5.501863348035	0.603047625538	1.725143966199
F	4.459510839774	2.653291935971	2.483767564184
F	-8.715410525764	-2.094791464361	-1.032070719195
F	-8.642514974597	-1.967622610681	1.168761046707
C	-8.477418943807	0.035400907246	-0.066358829453
O	-8.009950905982	0.662055127844	1.008503784920
C	-8.248726308210	2.099453606937	1.117486293757
O	-9.101849464080	0.514106172069	-0.980154905807
O	5.806092154588	-0.124487993936	0.726203484060
C	-7.625822002456	-0.067060914295	-5.082307348541
C	-6.999813642834	2.729498702742	1.684103102274
H	-7.057283501109	4.465545077180	-5.218599492917
H	-5.004202068449	5.164386930837	-6.416288545293
H	-2.913973070465	5.441686807549	-2.688227743704
H	-4.973919199776	4.769927221006	-1.482133729176
H	-2.679852238636	5.365256861692	-6.423862256346
H	-2.859777692017	7.700715225007	-5.680126924574
H	-1.946055221204	7.359134401528	-4.208506816169
H	-1.149429807572	7.244210830048	-5.794652044745
H	-0.081126706907	6.027364941891	-4.082534751261
H	-1.254786270266	1.252831650147	-4.277592200743
H	1.386416135655	1.010035521844	-3.567947418002
H	3.515270745887	1.082162923878	-2.964768861842
H	5.232994419323	1.222766107111	-1.192693252816
H	2.358854540280	3.012115568206	1.430669676600
H	0.633058162153	2.834021619323	-0.326018173523
H	1.271201442947	-1.032735803210	-2.630035403669
H	-2.954202906582	0.096959758632	-0.365377268679
H	-2.254345547154	-3.476991316491	-0.701297996791
H	-1.128599138342	-0.805515530277	1.542856709848
H	-1.354351723426	-5.317174540333	3.524045573910
H	0.899744827499	-3.277856196774	5.249637874555
H	-0.673329550369	-2.932578320309	5.944532365865
H	-0.266544739455	-4.599559459090	5.480795376601
H	-4.142645363169	-2.712959066783	-2.136946950368
H	-6.575242634559	-2.278856520634	-2.107641375344
H	-6.341741384769	-1.290327236525	2.059305079465
H	-3.916650121612	-1.768800344047	2.034535642869
H	2.908308595145	5.775866196516	-2.181473781355
H	1.206852723658	6.319269610977	-2.221011860931
H	2.147851013090	6.197325255511	-3.743145162648
H	-4.586948924604	1.806233235196	-5.719634619273
H	-3.125507572295	0.808379574521	-5.487551563807
H	-3.769919783075	1.781712683833	-4.126152928465
H	-3.655112192867	2.132255257774	-1.174969439082

H	-2.817625902459	3.628160826241	-0.675952255622
H	-2.771918185599	2.191485187177	0.384515071045
H	1.456798332457	-4.475512171616	-1.630809239452
H	2.075996241788	-2.816668598038	-1.361957851761
H	1.393088810310	-3.279559913793	-2.954135810002
H	-1.410991079069	0.523792454096	3.572997815492
H	0.154034195359	0.541061588390	2.702755033128
H	0.105039762839	0.923956286828	4.441450105723
H	-1.778109502260	-6.841150248031	1.896786619511
H	-3.273947224226	-6.888567610842	0.923665733019
H	-3.310081268774	-6.203205093859	2.573972194163
H	-7.745262949517	-0.150030722021	-2.915767846616
H	-6.114648853029	0.215221551472	-3.534100268346
H	-8.494630180620	2.492305816575	0.129726716150
H	-9.113999498362	2.222172534922	1.778607029748
H	-7.430479856646	-1.136841616276	-5.206725239887
H	-7.080701742498	0.476163651182	-5.860006357481
H	-8.696868751795	0.104475658458	-5.219417184705
H	-6.163949891945	2.586198382783	0.994035229588
H	-6.745475520889	2.300267193163	2.657925079365
H	-7.164750366778	3.804433973225	1.809385104522
N	6.473463728224	0.653939633743	2.795117009175
H	4.916615174575	-1.449500716579	2.634295761096
C	7.868535028625	0.910822311618	2.424670540940
C	8.822568733722	0.220621247947	3.397737460140
H	8.098481467412	1.988400999895	2.386526487322
H	8.016954397139	0.517290960812	1.412865544590
C	10.292233672513	0.471662167782	3.067047482295
H	8.612942093363	0.562465188674	4.421933559478
H	8.619085513026	-0.860233689714	3.388288615617
H	10.498028916756	0.131894302167	2.041328236677
H	10.490427752339	1.553175771628	3.075307570219
C	11.248310873020	-0.225250191698	4.033929553612
C	12.722417543703	0.007755482148	3.705824912197
H	11.044143108578	-1.306436174286	4.032706399363
H	11.045766360231	0.120881101159	5.058248796704
C	13.662591540678	-0.693585264981	4.684135324095
H	12.924616697358	-0.341050705614	2.683720984086
H	12.926530413948	1.087285348693	3.706299043141
H	14.713032292272	-0.514469869983	4.433151772831
H	13.498158428195	-0.339343578760	5.708166231298
H	13.497292906295	-1.777091969770	4.679024833917
C	2.474737119338	-0.812941055510	1.131193802489
C	2.889668095993	-0.081875634388	2.407664741504
O	4.278058724930	-0.121434188803	2.716284664307
H	3.129547018516	-0.544567005318	0.297872796997
H	1.449273198848	-0.543626358111	0.851658334916
H	2.491961171060	-1.900458090586	1.269931776063
H	2.558344030546	0.961648859934	2.362841555265
H	2.375986063754	-0.533969861431	3.270581995983
H	6.151809066095	1.245292395334	3.552299486327
N	5.618033420424	-2.237280501448	2.261645980708
H	6.063466115335	-1.612325551292	1.529849759693

C	4.920074725478	-3.397717162187	1.661111181567
C	3.962584739129	-4.059432015475	2.643410112908
H	5.659945508545	-4.119018987651	1.292190967346
H	4.374811669310	-3.014308367821	0.791447764927
C	3.090449093877	-5.113562502522	1.961859782620
H	4.534058000553	-4.521178867292	3.461762249615
H	3.320819207560	-3.292765720613	3.100351755148
H	2.429649226232	-4.617947950416	1.235145979643
H	3.727427118291	-5.803103824863	1.387837005481
C	2.245600731226	-5.916138888453	2.948741952939
C	1.356272186362	-6.952923868069	2.264963372684
H	1.615644963043	-5.229434454284	3.531667309358
H	2.908926566905	-6.421422111089	3.666276617303
C	0.622266779896	-7.845595728309	3.262839191156
H	0.635194146313	-6.432390463934	1.618720255920
H	1.969727758933	-7.578728094041	1.601742555731
H	-0.026532046650	-8.569463865201	2.758539253376
H	1.332246841257	-8.409104606207	3.878569443661
H	0.000036165783	-7.253005174519	3.944004467262
H	6.284947884009	-2.492236048449	2.984788524348

The noncatalytic concerted mechanism for the aminolysis of oligo-CF₂CO₂Et by n-hexylamine with and without considering the polymer effect (Figure 10)

<With polymer effect>

< Init_{non_C} >

C	6.790464961784	-2.907981966945	1.851729086458
C	7.510722892774	-1.605228183062	2.118775698710
O	6.931704198296	-0.483184908843	1.368436637771
H	6.830165358114	-3.176478698470	0.792478388489
H	5.747862644927	-2.867463286509	2.177745607823
H	7.286412414534	-3.701619276840	2.421344096111
H	7.393345481154	-1.293715505470	3.158601766565
H	8.569318857413	-1.669720885662	1.849806162025
H	4.666932207541	-0.654473554301	3.032661325176
C	-4.388765617156	4.557330121798	-3.070743207261
C	-3.542793456711	4.734639660527	-4.159198160173
C	-2.223545793877	5.155509774861	-3.984818169112
C	-1.789036594687	5.460512781055	-2.692053324401
C	-2.629768004297	5.305987471353	-1.599436130319
C	-3.928868160455	4.832332851604	-1.785191997731
C	-4.768135493463	4.485217854282	-0.588063701744
C	-1.246167496379	5.173527459020	-5.155328506972
C	-0.555065873306	6.527750704510	-5.323728406441
C	-0.299587818856	4.002487636854	-4.941715570208
C	0.978724033209	4.155637379403	-4.416161715934
C	1.756171349678	3.059549654643	-4.025326609455
C	1.227978533329	1.767886867688	-4.113425052984
C	-0.010755754822	1.610474832014	-4.737770512778
C	-0.767047932518	2.696919879531	-5.154135463408
C	1.845809040897	0.493296238831	-3.530908047207
C	0.808669751565	-0.297030762094	-2.733886949253

C	3.126491111140	0.613042167151	-2.711275035274
C	4.333336567130	0.166754642262	-3.250902835420
C	5.522787846046	0.262287265341	-2.536416719089
C	5.517842808714	0.812709319426	-1.256926715381
C	4.311403806599	1.219671908890	-0.686919134125
C	3.130621162775	1.114674297350	-1.406549620925
C	6.815407243816	0.979976762536	-0.511702562846
C	0.724649575228	-1.679267039131	-2.914525454327
C	-0.103282926283	-2.471439966137	-2.122486183035
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C	-0.851695671666	-0.503999076890	-0.981907336558
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H	4.382927206520	-6.379119325240	8.511937299142
H	3.532641325682	-4.827129146775	8.508302585234
N	6.327265763023	-0.144679061617	3.087936228986

<Without polymer effect>

Init_{non_C} and TS_{non_C} structures are the same as in Figure 6.