

SUPPLEMENTARY INFORMATION

Experimental and Theoretical Studies on Polar Diels-Alder Reactions of 1-Nitronaphthalene developed in Ionic Liquids.

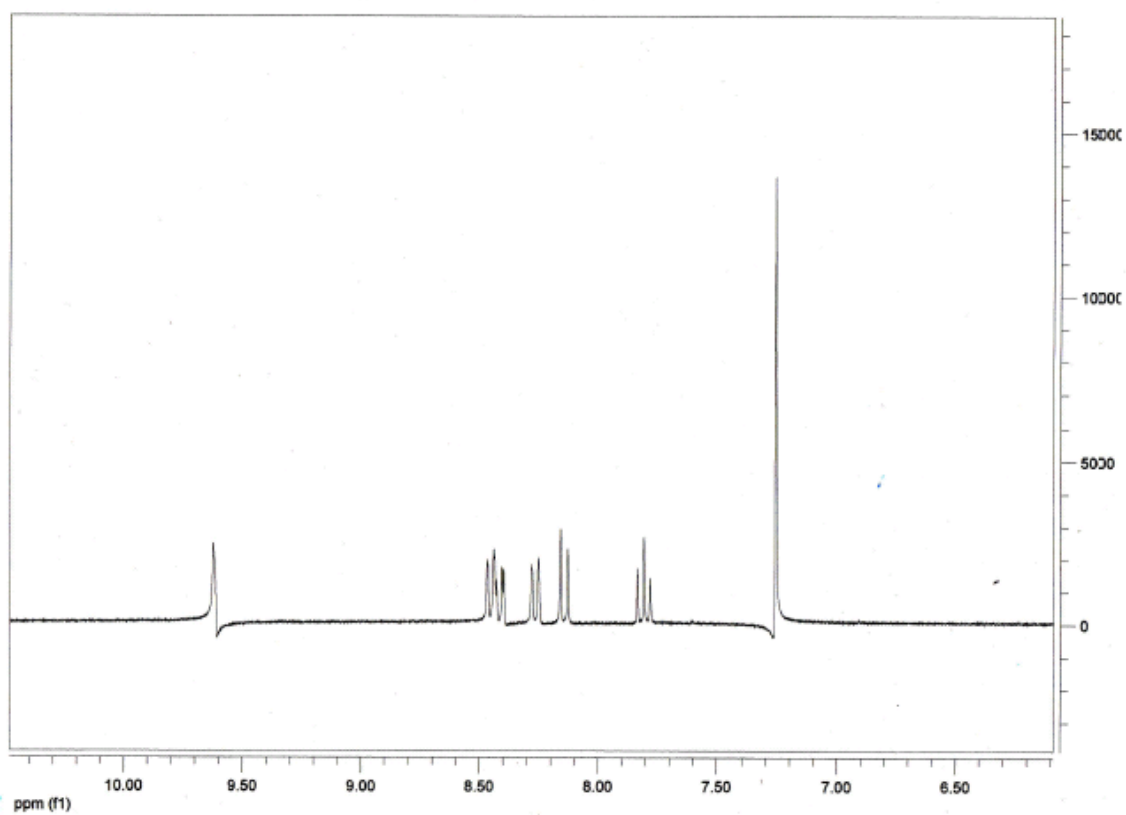
Pedro M.E. Mancini, Claudia D. Della Rosa, Carla M. Ormachea, María N. Kneeteman,
and Luis R. Domingo

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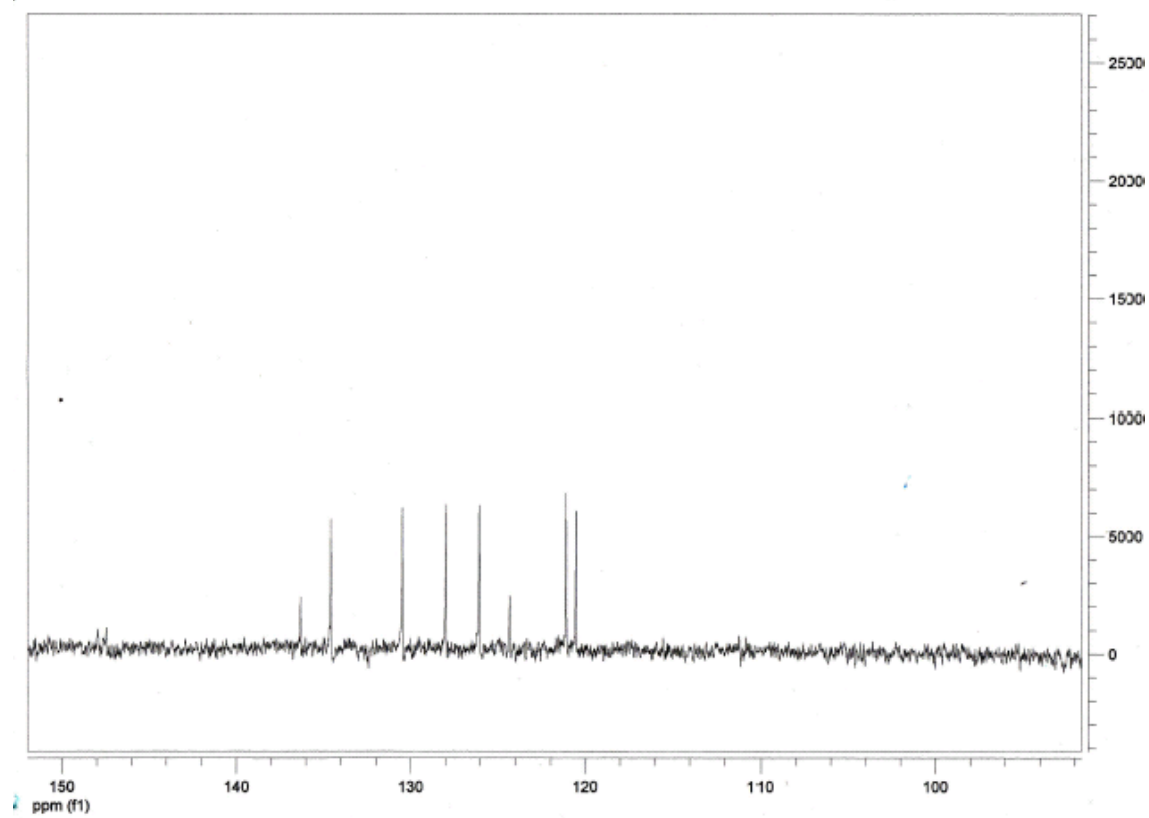
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Table S2. Total (E, in au) and relative (ΔE , in kcal/mol) energies, in gas phase and in 1-heptanol, of the stationary points involved in the reaction between complex **1-PIL** and 1-trimethylsilyloxy-1,3-butadiene **3**.
- S14** **Table S3.** MPWB1K/6-311G** Total enthalpies (H, in au), entropies (S, in eu) and free energies (G, in au) in 1-heptanol, computed at 60 °C and 1 atm, of the stationary points involved in reaction *Model II*.
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- S16** MPWB1K/6-31G* computed total energies, unique frequency imaginary, and cartesian coordinates of the stationary points involved in the reaction between 1-nitronaphthalene **1** and 1-trimethylsilyloxy-1,3-butadiene **3**, and in the reaction between complex **1-PIL** and 1-trimethylsilyloxy-1,3-butadiene **3**.

Compound 7

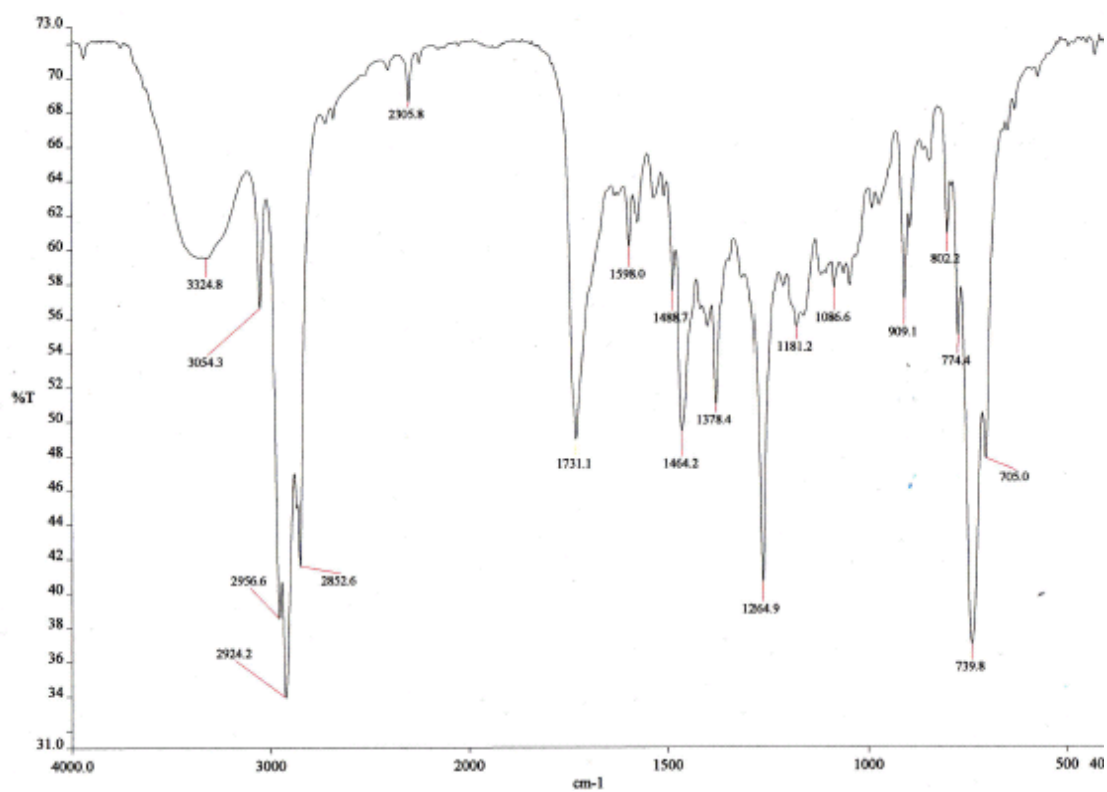
Captions ^1H NMR spectra



Captions ^{13}C NMR spectra

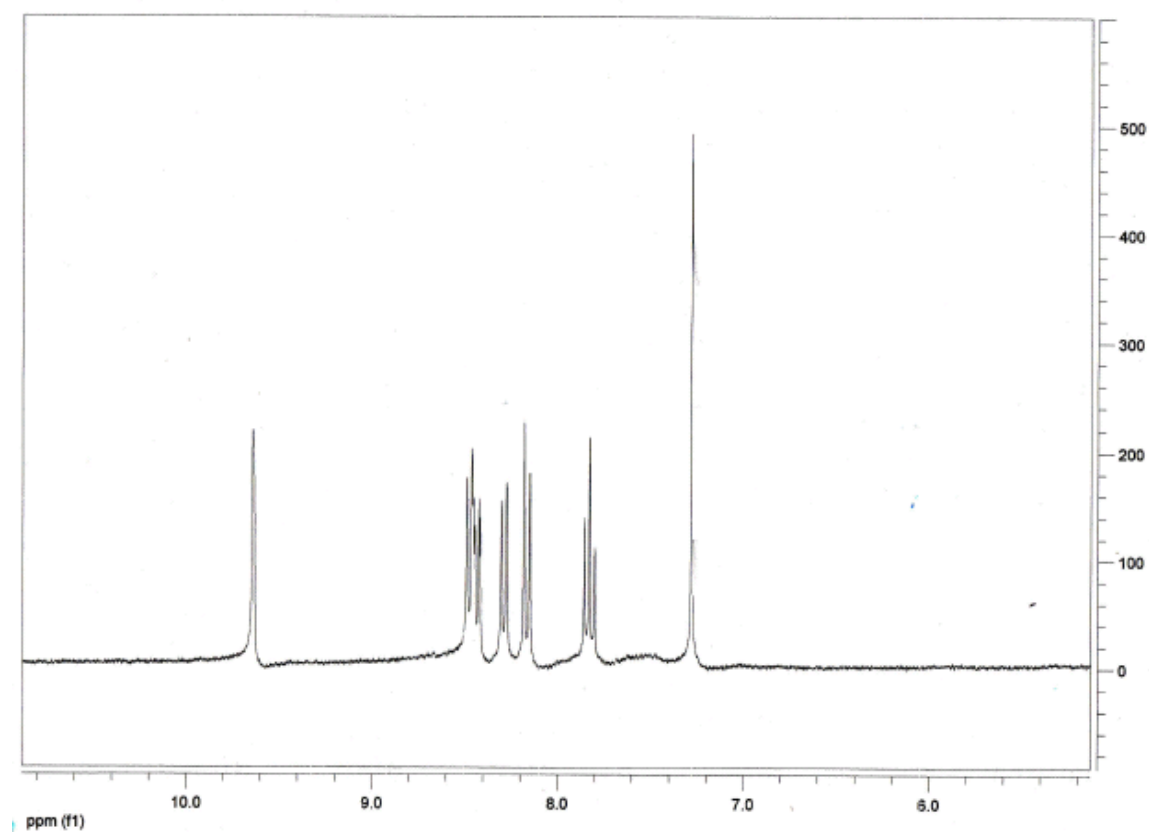


Captions **IR spectra**

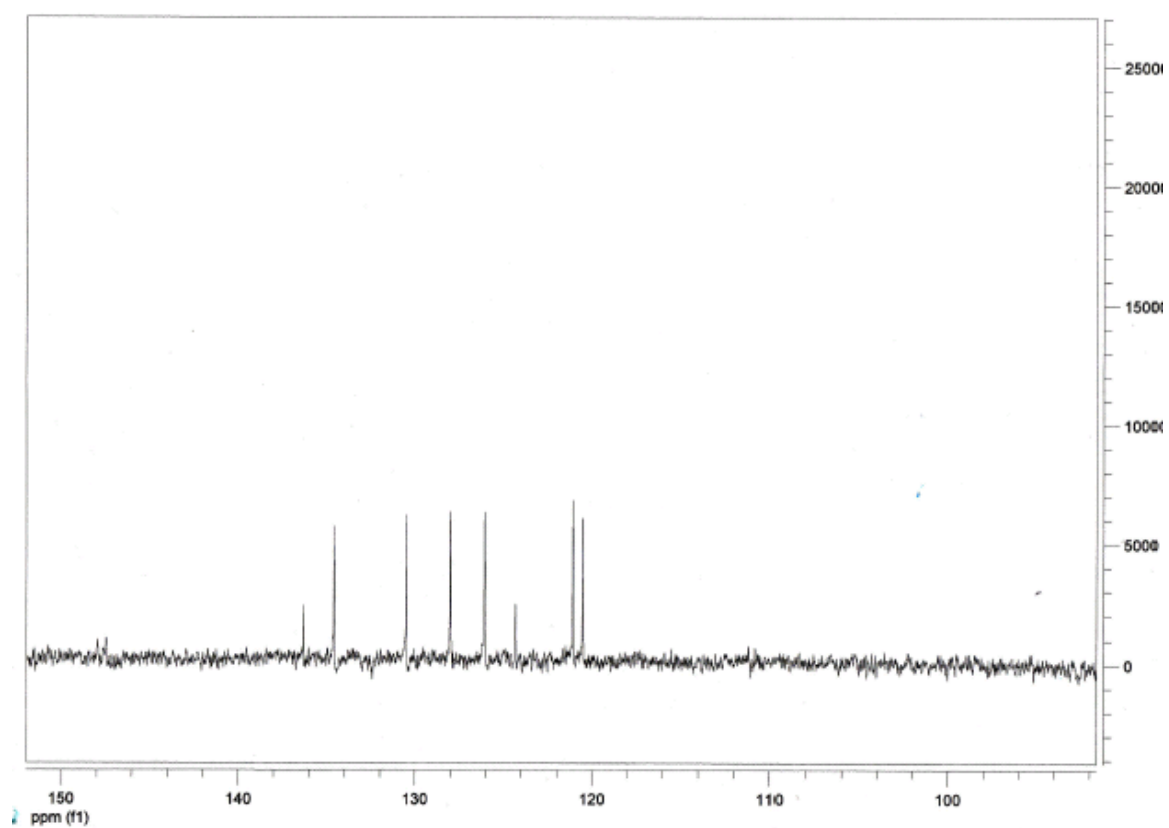


Compound 8

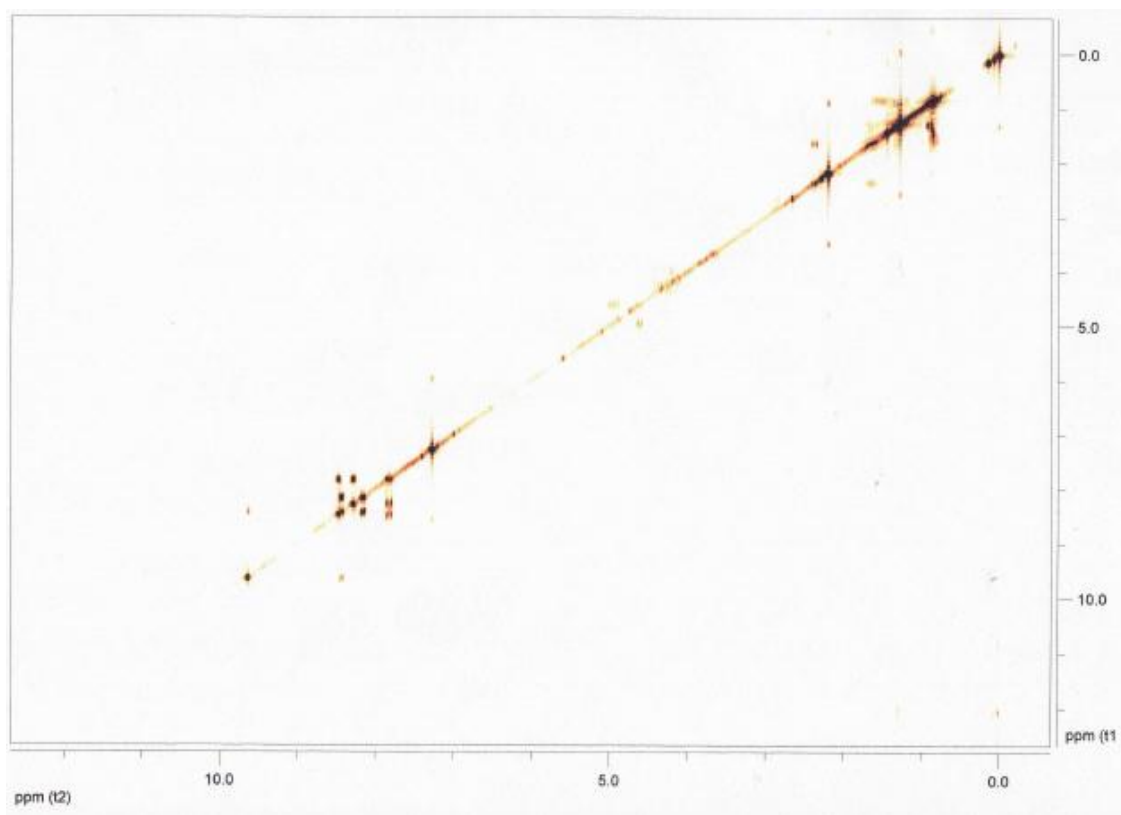
Captions: ^1H NMR spectra



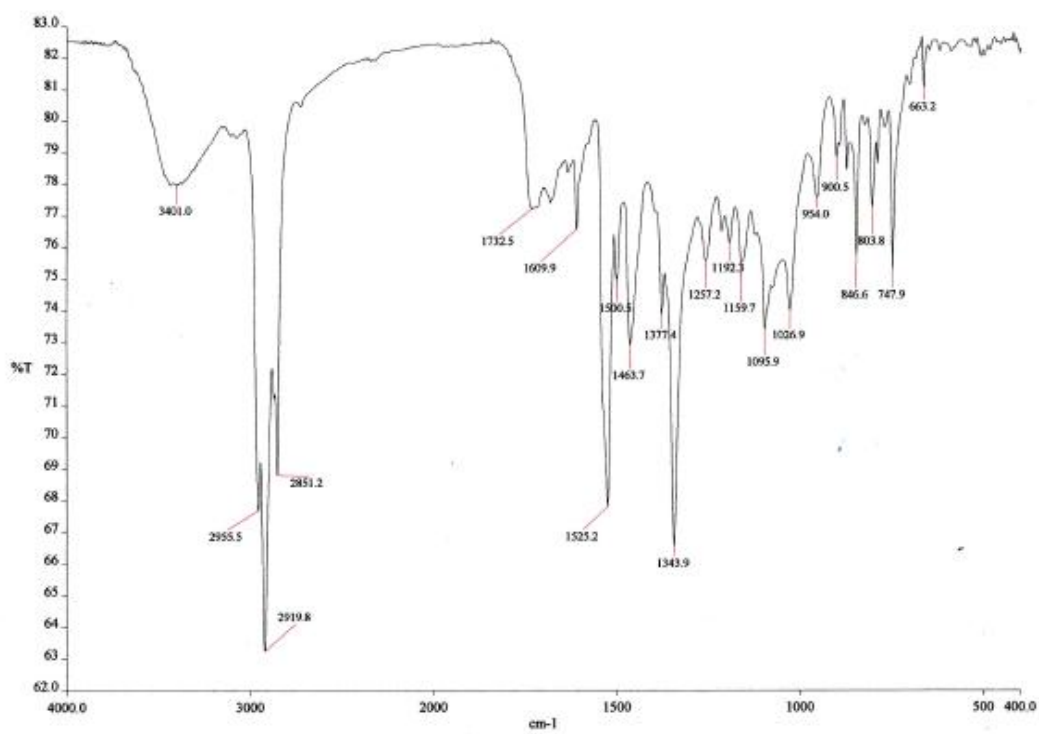
Captions: ^{13}C NMR spectra



Captions: COSY ^1H - ^1H (Connectivity ^1H - ^1H)

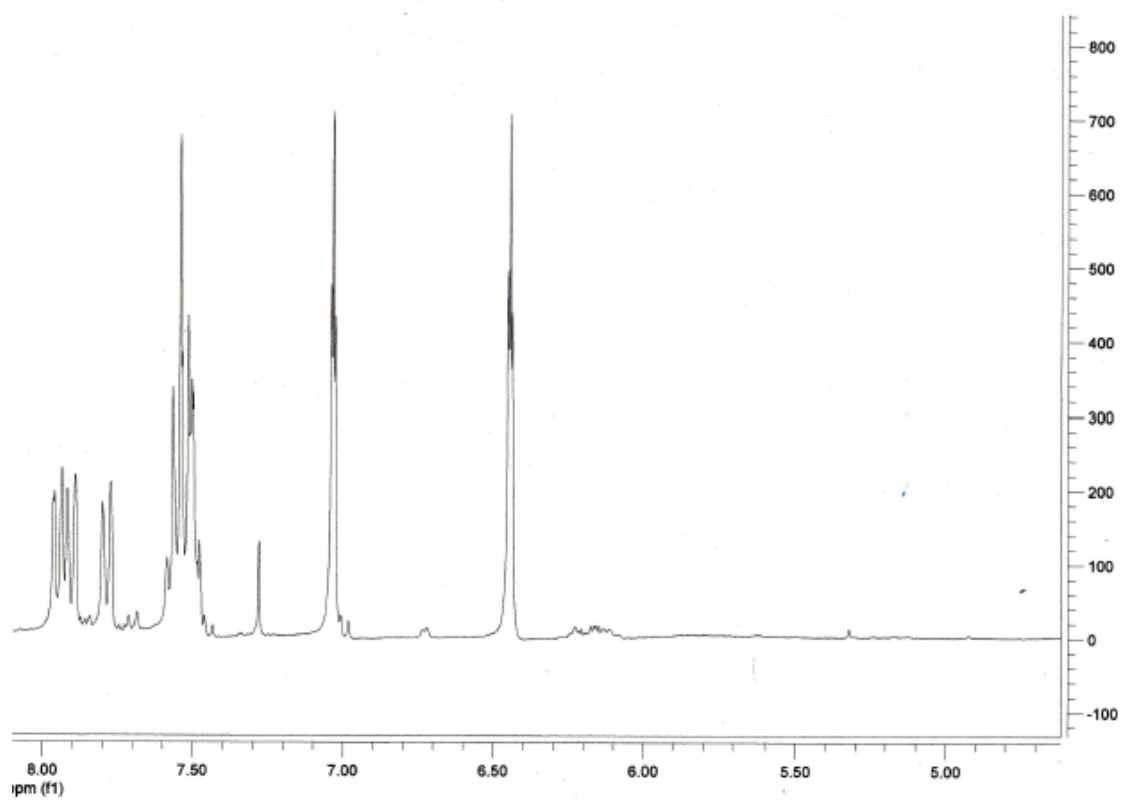


Captions: **IR spectra**

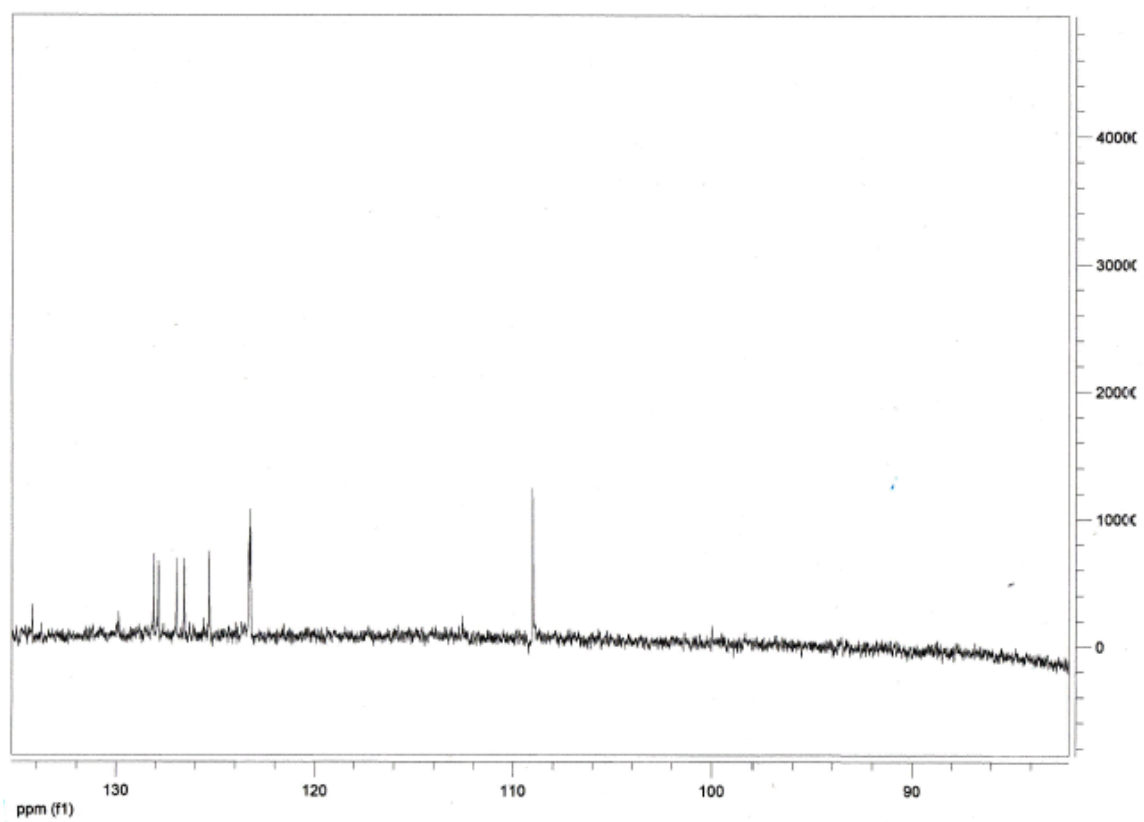


Compound 9

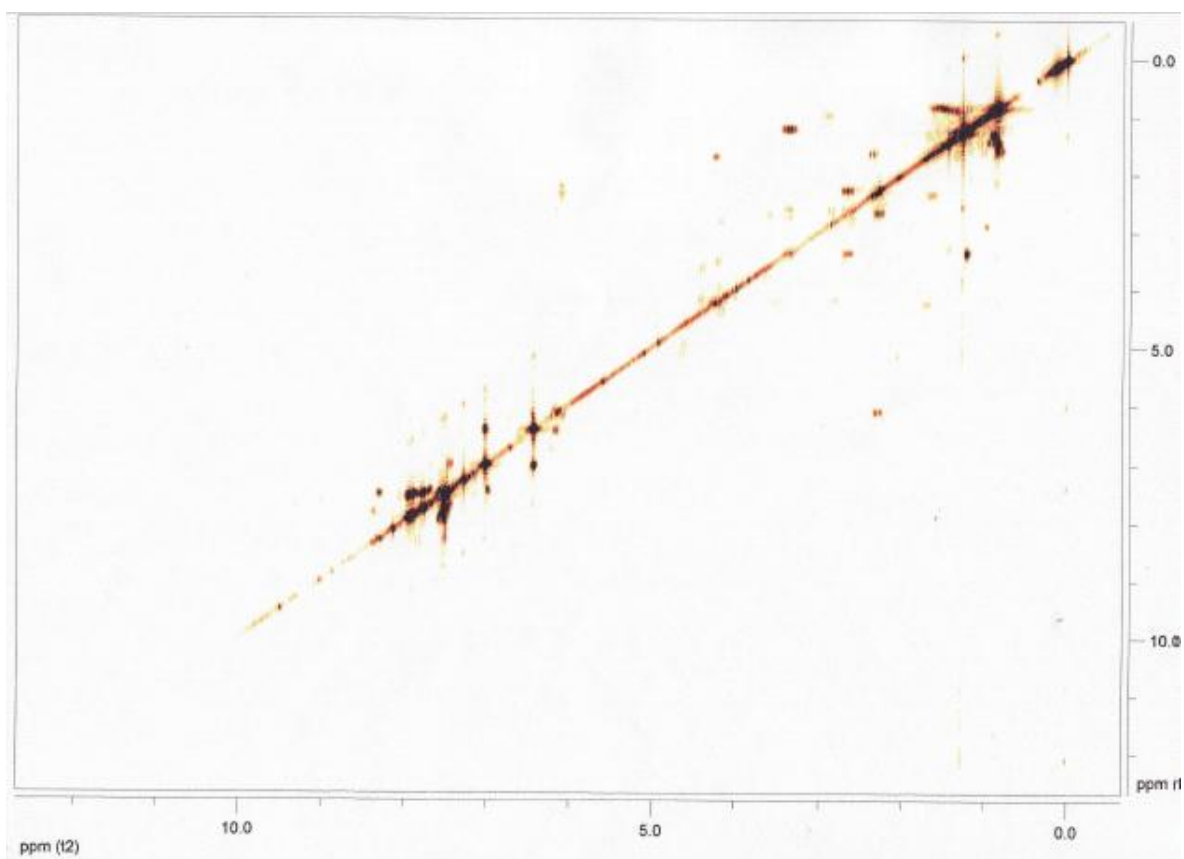
Captions: ^1H NMR



Captions: ^{13}C NMR



Captions: COSY ^1H - ^1H (Connectivity ^1H - ^1H)



Captions: **IR spectra**

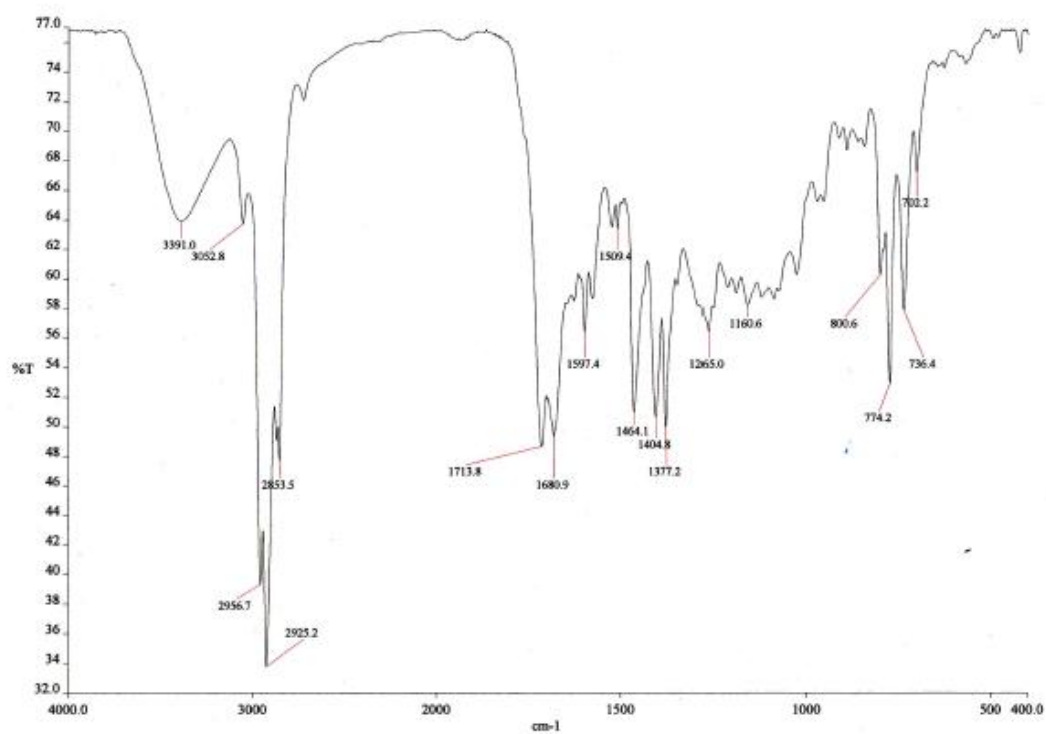


Table S1. Total (E, in au) and relative (ΔE , in kcal/mol) energies, in gas phase and in benzene, of the stationary points involved in the reaction between 1-nitronaphtalene **1** and 1-trimethylsilyloxy-1,3-butadiene **3**.

	MPWB1K/6-31G*		MPWB1K/6-311G**// MPWB1K/6-31G*		MPWB1K/ 6-311G**(benzene)// MPWB1K/6-31G*	
	E	ΔE	E	ΔE	E	ΔE
1	-590.107302		-590.240443		-590.244204	
<i>s-trans</i> 3	-639.737143		-639.850635		-639.852978	
TS1	-1229.816697	17.4	-1230.063949	17.0	-1230.068926	17.7
10	-1229.869528	-15.7	-1230.116730	-16.1	-1230.121052	-15.0
TS2	-1229.815905	17.9	-1230.065528	16.0	-1230.070252	16.9
11	-1024.284501	-24.8	-1024.474194	-28.0	-1024.476860	-27.6
5	-205.599532		-205.661551		-205.664244	

Table S2. Total (E, in au) and relative (ΔE , in kcal/mol) energies, in gas phase and in 1-heptanol, of the stationary points involved in the reaction between complex **1-PIL** and 1-trimethylsilyloxy-1,3-butadiene **3**.

	<i>Model I</i>				<i>Model II</i>	
	MPWB1K/6-31G*		MPWB1K/6-311G**// MPWB1K/6-31G*		MPWB1K/6-31G*	
	E	ΔE	E	ΔE	E	ΔE
1-PIL	-1280.437256		-1280.763019		-1280.795405	
<i>s-trans</i> 3	-639.737143		-639.850635		-639.855551	
TS1-PIL	-1920.157280	10.7	-1920.596159	11.0	-1920.627254	14.9
10-PIL	-1920.200005	-16.1	-1920.639392	-16.2	-1920.673716	-14.3
TS2-PIL	-1920.152288	13.9	-1920.593123	12.9	-1920.629917	13.2
11	-1024.284501	-19.3	-1024.474194	-22.7	-1024.479967	-25.0
5-PIL	-895.920578		-896.175689		-896.210760	

Table S3. MPWB1K/6-311G** Total enthalpies (H, in au), entropies (S, in eu) and free energies (G, in au) in 1-heptanol, computed at 60 °C and 1 atm, of the stationary points involved in reaction *Model II*.

	H	S	G
1-PIL	-1280.481067	168.9	-1280.570753
<i>s-trans</i> 3	-639.646095	113.2	-639.705128
TS1-PIL	-1920.101516	220.3	-1920.218491
10-PIL	-1920.143554	218.9	-1920.259780
TS2-PIL	-1920.106364	219.1	-1920.222692
11	-1024.126530	142.8	-1024.202342
5-PIL	-896.037057	132.7	-896.107507

Complete citation for reference 34

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09, Revision A.01*, Gaussian, Inc., Wallingford CT, **2009**.

MPWB1K/6-31G* computed total energies, unique frequency imaginary, and cartesian coordinates of the stationary points involved in the reaction between 1-nitronaphtalene **1** and 1-trimethylsilyloxy-1,3-butadiene **3**, and in the reaction between complex **1-PIL** and 1-trimethylsilyloxy-1,3-butadiene **3**.

1

E(RmPW+HF-B95) = -590.107302003 A.U.

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.36385105
C	1.18756638	0.00000000	-0.77290276
C	1.21340689	0.03248501	2.05914069
C	2.38605194	0.04521834	1.36513981
C	2.40482672	0.01781635	-0.04306537
C	3.63040154	0.00019587	-0.73953843
C	1.25113852	-0.06321646	-2.18174299
C	2.45663396	-0.09013251	-2.81838600
C	3.66056746	-0.05006628	-2.09889973
N	-1.31730460	0.01916049	-0.61749377
O	-2.23211430	-0.46112683	0.01021157
O	-1.43466158	0.53684513	-1.70435155
H	-0.94271869	-0.01639406	1.88358619
H	1.20983642	0.04993783	3.13721636
H	3.32999319	0.07076746	1.88954994
H	4.54641129	0.02076654	-0.16771724
H	0.34257778	-0.08695915	-2.75395895
H	2.48222686	-0.14195404	-3.89604121
H	4.60309649	-0.06586802	-2.62391541

s-trans **3**

E(RmPW+HF-B95) = -639.73714301 A.U.

C	-1.00691000	-0.10511700	-0.06576500
C	-2.21867400	0.44303600	-0.03801500
C	-3.42432400	-0.34954900	-0.00227600
C	-4.65828000	0.14353400	0.02613200
O	0.11960800	0.62092800	-0.11040400
H	-0.88585200	-1.18450700	-0.06278600
H	-2.30321900	1.52064700	-0.04434800
H	-4.84027800	1.20858900	0.02361900
H	-5.52378900	-0.49924800	0.05263000
Si	1.67448500	0.00226900	0.00835600
C	2.77533900	1.47973400	-0.21970900
H	3.82675800	1.20578000	-0.14894600
H	2.61254700	1.93730800	-1.19344500
H	2.57350900	2.23281300	0.53937400
C	1.88689300	-0.77493200	1.68951600
H	1.73090700	-0.04234000	2.47923700
H	1.17778400	-1.58631600	1.84823500

H	2.88797500	-1.18733500	1.80891500
C	1.92632400	-1.26621100	-1.33580700
H	2.93780900	-1.66928400	-1.30305300
H	1.23975400	-2.10613200	-1.23878300
H	1.77459000	-0.82691300	-2.32004600
H	-3.29035100	-1.42521700	0.00119600

s-cis **3**

E(RmPW+HF-B95) = -639.732787840 A.U.

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.33247341
C	1.22746088	0.00000000	2.11552343
C	2.35417300	0.62249871	1.78821911
O	-1.05816993	0.02808191	-0.81778291
H	0.93230228	-0.04413576	-0.54658913
H	-0.93644302	-0.03797019	1.87263469
H	2.42168508	1.24372157	0.90677194
H	3.24224724	0.53487472	2.39457771
Si	-2.68843827	0.23913357	-0.47756042
C	-3.47360843	0.32786566	-2.15973107
H	-4.55224428	0.45797898	-2.08551142
H	-3.07438355	1.16270907	-2.73223366
H	-3.28492008	-0.58271908	-2.72492011
C	-3.33573978	-1.22999805	0.47323700
H	-3.15515854	-2.15190892	-0.07675462
H	-2.87287969	-1.33476953	1.45206018
H	-4.41101448	-1.14033265	0.62453186
C	-2.93851179	1.82886902	0.46417994
H	-3.99934477	2.00171642	0.64219482
H	-2.43623115	1.82562968	1.42873672
H	-2.55599324	2.67589163	-0.10260793
H	1.19832192	-0.56236839	3.04112439

TS1

E(RmPW+HF-B95) = -1229.81669667 A.U.

1 imaginary frequencies -467.4844 cm-1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.36638874
C	1.18032305	0.00000000	2.10649916
C	2.46004712	0.00364808	1.55671285
O	-1.03275254	0.24864149	-0.75963839
H	0.87414621	-0.28263394	-0.56674174
H	-0.92746694	0.17623692	1.88590852
H	2.61678555	-0.49249083	0.60910988
H	3.28671911	-0.12185365	2.24165109
C	1.79519804	2.09642745	-0.08046034

C	2.79110792	1.77970763	0.88222444
C	2.02021091	1.92006399	-1.49220229
C	4.14539645	1.62644659	0.39079227
C	4.38762028	1.50541038	-0.91912074
C	3.33644279	1.58648566	-1.89129331
C	3.62687963	1.37271114	-3.24015784
C	1.04117454	2.01381078	-2.49535924
C	1.35664806	1.79124106	-3.81415419
C	2.65303176	1.47096012	-4.20081478
N	0.65627724	2.72409074	0.44540016
O	0.58581294	2.85730837	1.66517089
O	-0.23212211	3.12100235	-0.30263057
H	2.67773210	2.29779231	1.81972338
H	4.94604214	1.57431082	1.11303993
H	5.39652383	1.36203796	-1.27880822
H	4.64310690	1.12860603	-3.51492411
H	0.03170660	2.25304278	-2.22451240
H	0.57749033	1.86754319	-4.55767858
H	2.88995880	1.30328526	-5.24014840
Si	-2.59074246	0.89802309	-0.48923710
C	-2.87550055	2.00328186	-1.95126149
H	-3.92554503	2.28474466	-2.02193694
H	-2.28582480	2.91201372	-1.86226112
H	-2.60170366	1.50113036	-2.87734631
C	-3.71654867	-0.58719152	-0.53539989
H	-3.63156855	-1.11955619	-1.48074459
H	-3.48085529	-1.28779379	0.26422050
H	-4.75664718	-0.28654102	-0.41364202
C	-2.75653681	1.80201010	1.12879860
H	-2.97112317	1.13541778	1.96222864
H	-1.87480080	2.39590504	1.36099666
H	-3.59753022	2.49084015	1.04093099
H	1.08590061	0.15735188	3.17117369

10

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C	0.56479900	0.38255200	-0.84294900
C	1.18593800	1.69592300	-1.18975700
C	0.42961800	2.75639000	-1.41797800
C	-1.02836700	2.66940400	-1.12681200
O	1.43685800	-0.58379700	-0.36347500
H	0.12858100	-0.00481000	-1.76768700
H	2.25177400	1.71297300	-1.36207900
H	-1.57397700	2.14581300	-1.91557100
H	-1.47515200	3.65765100	-1.04447400
C	-0.66522700	0.49830900	0.13078100
C	-1.20144900	1.92960900	0.20486700
C	-1.71036000	-0.54082500	-0.18165700
C	-2.60235600	2.02208300	0.69660400

C	-3.45037700	1.00514400	0.63948300
C	-3.05284200	-0.28092800	0.09625400
C	-4.00640500	-1.25730200	-0.16483100
C	-1.35360900	-1.77606200	-0.70016900
C	-2.31076300	-2.73802700	-0.96140200
C	-3.64323000	-2.47760300	-0.69456700
N	-0.06895900	0.18740100	1.50403600
O	0.69281200	1.01208700	1.95154500
O	-0.33858100	-0.85723800	2.02715200
H	-0.54615000	2.44459300	0.90303000
H	-2.92086800	2.98494700	1.07008200
H	-4.47246900	1.11514800	0.97229400
H	-5.04382800	-1.04561100	0.05044200
H	-0.31190500	-1.99581200	-0.87564500
H	-2.01300900	-3.69470400	-1.36221700
H	-4.39525600	-3.22586100	-0.89390700
Si	3.07549000	-0.64809500	-0.04127100
C	3.27882200	-2.31987300	0.74487000
H	4.31102600	-2.49248600	1.04603300
H	2.65134500	-2.39921300	1.63063500
H	2.99140500	-3.11616000	0.06100200
C	4.03305300	-0.56871400	-1.64730200
H	3.97572200	0.40236200	-2.13618500
H	5.08748000	-0.77526200	-1.46482200
H	3.66990200	-1.31529500	-2.35184900
C	3.63868100	0.69750400	1.11874900
H	4.72372900	0.66279100	1.22014100
H	3.36644400	1.69368400	0.77678700
H	3.19722000	0.56547200	2.10321500
H	0.85957200	3.68738900	-1.75656100

TS2

E(RmPW+HF-B95) = -1229.81590509 A.U.

1 imaginary frequencies -1025.4338 cm-1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.49387621
C	1.09225350	0.00000000	2.23674692
C	2.44684811	-0.07895497	1.63642955
O	-1.12072748	-0.61908372	-0.54181190
Si	-2.41833271	-1.44895088	0.10871757
C	1.29513652	-0.52730806	-0.60353724
C	2.42893203	-0.71297575	0.25619127
C	1.48716576	-0.43247348	-2.03080967
C	3.73294007	-0.85725118	-0.37106567
C	3.88763974	-0.87966730	-1.69895226
C	2.77528244	-0.63580152	-2.56710259
C	2.96430120	-0.54647982	-3.94804137
C	0.43723972	-0.11395016	-2.90368313
C	0.65216443	-0.01266295	-4.25489687

C	1.92079215	-0.23894396	-4.78312493
N	0.73693779	-2.66259234	-0.47671931
H	2.14662019	-1.91094541	0.52255208
H	4.58200787	-0.99362991	0.28362031
H	4.86009269	-1.03271326	-2.14274376
H	-0.55196046	0.02650750	-2.50509059
H	-0.16989086	0.22956141	-4.91049343
H	2.08365859	-0.16910785	-5.84797864
H	3.95369789	-0.71240818	-4.34832586
H	-0.03471210	1.04991105	-0.32228312
H	2.88332729	0.92179775	1.57678452
H	3.11240128	-0.65382410	2.27985591
H	-0.97342533	0.09196255	1.95431675
O	1.49924093	-3.11485652	0.39598105
O	-0.01917833	-3.37987504	-1.06366464
C	-1.91991268	-2.73376509	1.37169104
H	-1.65690895	-3.67071919	0.88762450
H	-1.06275521	-2.42434136	1.96661291
H	-2.74725867	-2.92312795	2.05534326
C	-3.22150371	-2.22325146	-1.37562986
H	-4.07383588	-2.83724527	-1.08803087
H	-3.57292198	-1.46806273	-2.07638209
H	-2.50005289	-2.85537563	-1.88729463
C	-3.60012780	-0.22306438	0.89339030
H	-3.82364519	0.59319304	0.20815945
H	-4.54192562	-0.71835000	1.13038887
H	-3.22699179	0.21347457	1.81874794
H	1.01476848	0.07277938	3.31206950

11

E(RmPW+HF-B95) = -1024.28450085 A.U.

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.48873060
C	1.10241825	0.00000000	2.22037634
C	2.46766588	0.05557314	1.63760933
O	-0.69152668	-1.13106334	-0.49042766
Si	-0.45947322	-2.73519021	-0.10664024
C	1.36559132	0.12780605	-0.61668697
C	2.50188953	0.14769233	0.14423230
C	1.45327051	0.25167074	-2.03373737
C	3.76315026	0.26954540	-0.48060875
C	3.87336248	0.37986087	-1.82824511
C	2.72146920	0.38315406	-2.64301506
C	2.81228652	0.52546587	-4.04091005
C	0.31194635	0.26810436	-2.86404165
C	0.42971562	0.41568615	-4.21604739
C	1.69095590	0.54496279	-4.81557548
H	4.64923137	0.27671412	0.13870243

H	4.84322472	0.47585146	-2.29486685
H	-0.66364743	0.13800583	-2.42649350
H	-0.45729057	0.42734028	-4.83133836
H	1.77003682	0.65713107	-5.88624630
H	3.79149206	0.62351704	-4.48744902
H	-0.59649427	0.85083940	-0.33933537
H	3.00717982	0.90710390	2.06077432
H	3.03605498	-0.82183536	1.96079296
H	-0.97515446	-0.03821213	1.95370436
C	1.35159339	-3.15797715	0.05926616
H	1.91497640	-2.86941441	-0.82619400
H	1.79689354	-2.65608181	0.91709631
H	1.47403192	-4.23125829	0.20519728
C	-1.23070998	-3.64756241	-1.53571844
H	-1.17901142	-4.72621771	-1.39395406
H	-2.27889608	-3.37610343	-1.64794465
H	-0.72389973	-3.40508335	-2.46786345
C	-1.34711943	-3.17321709	1.47968301
H	-2.39541842	-2.88167920	1.43578109
H	-1.31042602	-4.24807321	1.65656225
H	-0.89677324	-2.68010199	2.33875219
H	1.03387127	-0.02843146	3.29951038

1-PIL

E(RmPW+HF-B95) = -1280.43725617 A.U.

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.36867502
C	1.19820315	0.00000000	-0.77025948
C	1.19987505	-0.01811155	2.07636987
C	2.37626184	-0.02664480	1.38789595
C	2.40588903	-0.01104871	-0.01914832
C	2.51976274	0.05985577	-2.78639520
C	3.70857726	0.02949592	-2.04534261
N	-1.30780390	-0.01768661	-0.60634696
H	-0.94436607	0.00349780	1.88548541
H	1.18556970	-0.03049853	3.15394622
H	3.31737068	-0.04414490	1.91759466
H	2.56369288	0.09318658	-3.86396928
H	4.66128477	0.03612385	-2.55116167
O	-2.26780883	0.29026109	0.06656899
O	-1.40933794	-0.35659710	-1.77052025
H	-7.31110715	-1.04534579	-4.77956155
C	-6.91043376	-0.03943419	-4.73943741
N	-4.22038237	0.02257134	-2.43334251
C	-4.71580469	-0.19411235	-3.63895853
C	-5.21355718	0.44449918	-1.59827156
N	-6.00543821	0.08160650	-3.60893664

H	-7.70669232	0.68449155	-4.61062548
H	-6.34824365	0.15323671	-5.64428204
C	-6.34023453	0.48048953	-2.34093218
H	-7.34375482	0.75667471	-2.08483192
H	-4.13732514	-0.53718218	-4.48150212
H	-5.03067659	0.68054184	-0.56955793
H	-3.24713954	-0.11899185	-2.17961158
B	-4.04500994	-1.11316152	-6.61096238
F	-5.01961751	-1.89855206	-5.97380783
F	-4.53679049	0.20611296	-6.63107011
F	-2.90931007	-1.11361641	-5.78093997
F	-3.76281964	-1.56628920	-7.85993564
C	1.29773456	0.04470090	-2.17704084
H	0.41311684	0.06140441	-2.78276028
C	3.64666743	-0.00212325	-0.68675082
H	4.54813003	-0.01696578	-0.09244560

TS1-PIL

E(RmPW+HF-B95) = -1920.15728045 A.U.

1 imaginary frequencies -469.3229 cm-1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.36242811
C	1.14943073	0.00000000	2.15848200
C	2.46442453	0.03227430	1.70594472
O	-1.10785417	0.14946586	-0.66126166
H	0.91066683	-0.13011587	-0.57583537
H	-0.96237191	0.09769212	1.84125485
H	2.67840724	-0.33577731	0.71223910
H	3.23457852	-0.19606569	2.42838505
C	2.00116750	2.32956712	0.32325304
C	2.91563495	1.88949296	1.31937102
C	2.33485909	2.30609302	-1.07654348
C	4.29855159	1.74861231	0.92966824
C	4.63904315	1.75408213	-0.36477520
C	3.67379279	1.97557835	-1.40016049
C	4.07949610	1.91474801	-2.73443653
C	1.46488790	2.59605297	-2.13978502
C	1.89580881	2.52886926	-3.44514556
C	3.20446505	2.17809877	-3.75687351
N	0.78406346	2.75256690	0.82098918
O	0.62340436	2.78149893	2.04535105
O	-0.15206757	3.03157887	0.05552002
H	2.72822887	2.26904357	2.30891881
H	5.03634471	1.59633486	1.70221349
H	5.66919845	1.61582746	-0.66014771
H	5.10811858	1.66195794	-2.94751999
H	0.45613672	2.89252077	-1.92839064
H	1.19925778	2.76315371	-4.23654121
H	3.52967816	2.12955266	-4.78433163

Si	-1.53956886	-0.14827051	-2.29784238
C	-3.00823680	-1.27189293	-2.14762347
H	-3.36443313	-1.57268745	-3.13193759
H	-2.77763022	-2.17341766	-1.58358635
H	-3.82634268	-0.75442838	-1.64940420
C	-1.99171249	1.44356417	-3.11759777
H	-2.71983523	2.02157485	-2.55002113
H	-1.12550148	2.07094178	-3.30848777
H	-2.44913956	1.21688954	-4.08145350
C	-0.07334995	-0.98404778	-3.09004817
H	0.79789361	-0.33156220	-3.12801527
H	0.20417276	-1.90236475	-2.57435287
H	-0.31918865	-1.25113825	-4.11727759
H	0.99026637	0.06595856	3.22544030
H	-6.29155952	1.69024817	1.92824216
C	-5.92094141	2.68096806	2.16216701
N	-2.42021739	2.81406623	1.62878038
C	-3.66435475	2.92053235	1.20676531
C	-2.41482770	2.47589828	2.94947743
N	-4.47094143	2.66183943	2.22123937
H	-6.29258935	3.00616993	3.12726253
H	-6.21758682	3.36633870	1.37926401
C	-3.70862793	2.37368214	3.32302671
H	-4.15445977	2.13627022	4.26853045
H	-3.95099252	3.19166398	0.20603495
H	-1.49854228	2.35896928	3.49215791
H	-1.57922271	2.99154609	1.06498583
B	-5.54683152	3.41812115	-1.34691566
F	-5.76659054	2.17459310	-0.73566424
F	-5.76136059	4.40473419	-0.37334408
F	-4.17507690	3.46508590	-1.68602546
F	-6.33797530	3.59837459	-2.43628228

10-PIL

E(RmPW+HF-B95) = -1920.20000475 A.U

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.49307773
C	1.14712063	0.00000000	2.15334253
C	2.41600894	0.17375350	1.38962463
O	-1.21781179	0.29579936	-0.59720176
H	0.28806242	-1.00705759	-0.31371311
H	-0.94823005	-0.10355454	1.99765344
H	2.71977690	-0.74798202	0.88817763
H	3.23697893	0.45513892	2.04468347
C	1.10497360	0.90963558	-0.64521635
C	2.20186562	1.28548007	0.35373870
C	1.60337909	0.32642739	-1.94171121
C	3.47954411	1.70061391	-0.28617651
C	3.79635428	1.38244571	-1.53346188

C	2.90430992	0.59686784	-2.36677261
C	3.34346380	0.09026295	-3.58383419
C	0.77036680	-0.43531602	-2.74674509
C	1.21964173	-0.93772262	-3.95286395
C	2.51060947	-0.67433037	-4.37360578
N	0.35625075	2.20499887	-0.96271292
O	0.00427272	2.88711639	-0.02973122
O	0.10525103	2.46425441	-2.11297145
H	1.80546726	2.12334487	0.92243841
H	4.17127191	2.25165130	0.33476992
H	4.74649073	1.67752426	-1.95448630
H	4.35239444	0.30319136	-3.90546236
H	-0.24966729	-0.61142586	-2.44407499
H	0.55439112	-1.52072200	-4.57038589
H	2.86413714	-1.05741922	-5.31843333
Si	-2.78579684	0.50313568	-0.05101376
C	-3.73646712	0.81000381	-1.61591539
H	-4.77592253	1.05833328	-1.40697123
H	-3.30083575	1.63890248	-2.17120257
H	-3.72647390	-0.06162421	-2.26713118
C	-3.39325867	-1.04230747	0.80460632
H	-2.91105587	-1.23013255	1.76188843
H	-4.46356525	-0.96204396	0.99331150
H	-3.23871054	-1.91886014	0.17743100
C	-2.90092958	1.98395527	1.07991004
H	-3.89816903	2.05302588	1.51380256
H	-2.18106765	1.95352386	1.89540557
H	-2.71898260	2.89758502	0.51783192
H	1.17265496	-0.07934519	3.22997978
H	-3.98277134	7.62161365	-3.39526430
C	-2.92857792	7.84655675	-3.28611749
N	-1.26949380	5.02522660	-1.92436636
C	-1.74651899	5.71766930	-2.94411307
C	-1.52204621	5.69414768	-0.76118676
N	-2.29239742	6.82241177	-2.47430717
H	-2.78894147	8.80162408	-2.79274484
H	-2.46287708	7.83611628	-4.26347424
C	-2.16661610	6.82750629	-1.10911389
H	-2.53976310	7.63595582	-0.51237426
H	-1.68239372	5.40510272	-3.97416348
H	-1.21548992	5.31273194	0.19181844
H	-0.80432630	4.12466564	-2.00245449
B	-2.10204689	5.80102943	-6.09759772
F	-3.31592518	5.91131906	-5.39808383
F	-1.29300072	6.87012657	-5.66388957
F	-1.48344712	4.61693139	-5.66529423
F	-2.28615259	5.82097046	-7.44328615

TS2-PIL

E(RmPW+HF-B95) = -1920.15228811 A.U.

1 imaginary frequencies -246.9239 cm-1

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.49558088
C	1.09059799	0.00000000	2.24049370
C	2.44607705	0.08435887	1.64042519
O	-1.10395907	0.62189491	-0.55547527
H	-0.02295316	-1.05458657	-0.31577792
H	-0.97470651	-0.09130601	1.95319302
H	2.88118532	-0.91328680	1.54570166
H	3.11711649	0.64432796	2.28975013
C	1.30111292	0.51460366	-0.59692566
C	2.41817788	0.76017873	0.27768868
C	1.48644301	0.53516807	-2.00957914
C	3.72648082	0.95953651	-0.33365520
C	3.88102733	1.03346458	-1.65921276
C	2.77232347	0.81101465	-2.53371328
C	2.95892886	0.82475190	-3.91734110
C	0.44038128	0.24348456	-2.90602280
C	0.65646629	0.24470094	-4.25719882
C	1.91949359	0.54807430	-4.76728118
N	0.58680905	2.81490939	-0.29315406
O	1.38655897	3.22866035	0.56295542
O	-0.24793273	3.58116974	-0.72463948
H	2.11047614	1.88398321	0.55424675
H	4.56546662	1.10061737	0.33191113
H	4.84839513	1.22729027	-2.09751016
H	3.93998555	1.04838075	-4.30855460
H	-0.54209061	0.04553457	-2.51654757
H	-0.15731698	0.02566516	-4.93024385
H	2.07928549	0.56105965	-5.83461292
Si	-2.49260229	1.32274900	0.08087637
C	-3.25452636	2.17851565	-1.37508159
H	-4.17632106	2.68410999	-1.09097743
H	-2.56982057	2.92724436	-1.76627155
H	-3.49168319	1.47713853	-2.17304325
C	-3.60844551	-0.05166602	0.69126892
H	-3.20012028	-0.58966728	1.54628514
H	-4.56959760	0.35886379	1.00038360
H	-3.80146536	-0.77865680	-0.09599630
C	-2.13277843	2.50560435	1.49049966
H	-2.78039175	2.29987590	2.34168935
H	-1.10295517	2.45110925	1.83729933
H	-2.31583862	3.52964358	1.17109487
H	1.01260712	-0.07687588	3.31510374
H	-1.34837219	9.46252370	2.17428505
C	-0.62802078	9.41302484	1.36744023
N	0.14969050	6.03524575	0.61443154
C	-0.55555900	7.13811029	0.43302504
C	1.08107069	6.25346087	1.58654133

N	-0.10431233	8.06320383	1.25961371
H	0.20214862	10.08337360	1.56058250
H	-1.11595634	9.66303105	0.43408212
C	0.92057490	7.52891972	1.99605582
H	1.44117584	8.10378650	2.73594886
H	-1.35624106	7.23950734	-0.28236918
H	1.76295013	5.48388564	1.88744008
H	0.01468656	5.15825938	0.10010539
B	-2.99413610	8.47842342	-1.18866054
F	-3.16601666	8.45243747	0.20538232
F	-1.85355617	9.26004124	-1.44323332
F	-2.69824075	7.16503210	-1.59336539
F	-4.09641745	8.96490059	-1.82002240

5-PIL

E(RmPW+HF-B95) = -895.920578372 A.U.

N	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.36446724
O	1.09277824	0.00000000	-0.41316331
H	-0.93474819	-0.00675958	1.60373887
H	6.71391216	1.78224143	3.02081475
C	6.43649647	0.74282960	3.14868130
N	3.17415040	0.24206750	1.84705641
C	4.48937899	0.26962513	1.69668448
C	2.84411976	0.55534613	3.13317750
N	5.01852898	0.58465545	2.86549307
H	6.60899040	0.42095166	4.16935793
H	6.99434398	0.14003394	2.44444517
C	4.01033394	0.77068263	3.77438067
H	4.21457420	1.03528888	4.79283262
H	5.00734022	0.06462510	0.76965500
H	1.82854997	0.59188040	3.47032314
H	2.52236785	0.05319571	1.09967231
B	6.97816542	0.18828185	-0.26824152
F	6.77346211	1.39659862	0.41804741
F	7.21290059	-0.80112334	0.70374188
F	5.75583900	-0.13650119	-0.89050475
F	7.99539808	0.27388859	-1.16131638