Supporting Information

for

Protonation pattern as controlling factor of thermal reactions of aryl o-divinylbenzenes in acidic media: an integrated experimental-theoretical study

Vilma Lovrinčević,[a] Monika Znika,[a,1] Jerome Le-Cunff,[b] Ines Despotović,*[c] and Dragana Vuk,*[a]

Address:

[a] Department of Organic Chemistry, University of Zagreb Faculty of Chemical Engineering and Technology, Marulićev trg 19, 10000 Zagreb, Croatia

[b] Xellia Ltd., Slavonska Avenija bb, 10000 Zagreb, Croatia

[c] Division of Physical Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia

Email:

Dragana Vuk* - dvuk@fkit.unizg.hr

Ines Despotović* - Ines.Despotovic@irb.hr

* Corresponding author

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[1] Present name and adress: Department of Reaction Engineering and Catalysis, University of Zagreb Faculty of Chemical Engineering and Technology, Marulićev trg 19, 10000 Zagreb, Croatia

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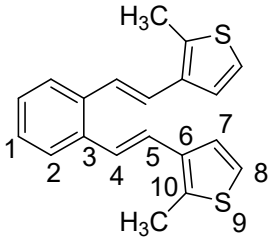
Table S1: Relative Gibbs free energies in kcal mol^{-1} and relative populations* in % (in round parentehese) of the *trans,trans*-, *cis,trans*- and *cis,cis*-isomers of derivatives **9**–**14**

Molecule	*trans,trans*-isomer	*cis,trans*-isomer	*cis,cis*-isomer
9	0.0 (98.07)	2.33 (1.93)	5.53 (0.009)
10	0.0 (99.37)	3.01 (0.62)	5.46 (0.009)
11	0.0 (97.55)	2.19 (2.43)	5.28 (0.013)
12	0.0 (95.18)	1.77 (4.79)	5.07 (0.018)
13	0.0 (95.71)	1.84 (4.26)	5.03 (0.020)
14	0.0 (99.16)	2.83 (0.83)	5.76 (0.006)

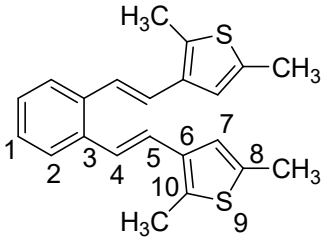
*The relative populations of the isomers are computed through the probabilities defined in equation: $P(T) = e^{-\beta\Delta G}/\sum e^{-\beta\Delta G}$, where $\beta=1/k_BT$, and k_B is the Boltzmann constant, T is the temperature in Kelvin, and ΔG is the relative Gibbs free energy of the corresponding isomer.

Table S2: Gibbs free energies, G^*, of all possible protonated forms (in a.u.) and relative Gibbs free energies, $G^*_{relat.}$, to the most stable protonated form (in kcal mol^{-1}) of compounds **9** –**14**



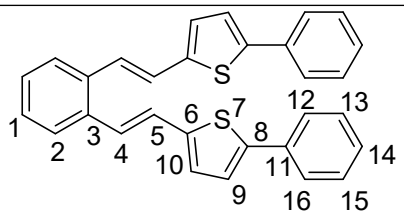
9

Protonation position	G^*	$G^*_{relat.}$
1	-1569.3729735	9.74
2	-1569.3702571	11.45
3	-1569.3614632	16.97
4	***-1569.3885014***	***0.00***
5	-1569.3761046	7.78
6	-1569.3649958	14.75
7	-1569.3774620	6.93
8	-1569.3845741	2.46
9	-1569.3536380	21.88
10	-1569.3872132	0.8

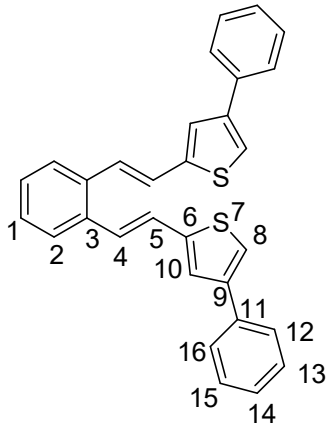


10

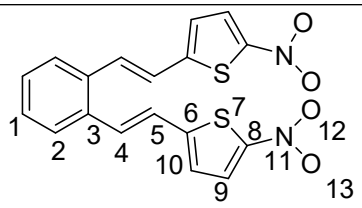
Protonation position	G^*	$G^*_{relat.}$
1	-1647.9434528	14.28
2	-1647.9414352	15.50
3	-1647.9312590	21.89
4	***-1647.9661434***	***0.00***
5	- 1647.9503955	9.88
6	-1647.9400245	16.39
7	-1647.9546417	7.22
8	-1647.9555048	6.67
9	-1647.9271327	24.48
10	-1647.9595540	4.13



11		
Protonation position	G^*	$G^*_{relat.}$
1	-1952.7363535	10.23
2	-1952.7347909	11.21
3	-1952.7264113	16.47
4	***-1952.7526624***	***0.00***
5	- 1952.7373396	9.61
6	-1952.7395994	8.19
7	-1952.7142058	24.13
8	-1952.7524224	0.15
9	-1952.7428791	6.14
10	-1952.7444034	5.18
11	-1952.7065234	28.95
12	-1952.7317920	13.09
13	-1952.7186074	21.37
14	-1952.7360856	10.40
15	-1952.7180074	21.75
16	-1952.7324687	12.67

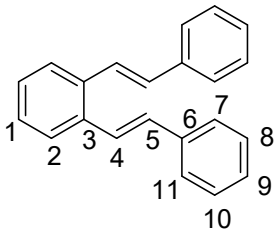


12		
Protonation position	G^*	$G^*_{relat.}$
1	-1952.7336690	16.67
2	-1952.7302299	18.83
3	-1952.7218183	24.11
4	***-1952.7602328***	***0.00***
5	- 1952.7357574	15.36
6	-1952.7261103	21.41
7	-1952.7119871	30.27
8	-1952.7441628	10.08
9	-1952.7201433	25.16
10	-1952.7442543	10.03
11	-1952.7082241	32.63
12	-1952.7290347	19.58
13	-1952.7190843	25.82
14	-1952.7321956	17.59
15	-1952.7191776	25.76
16	-1952.7282530	20.07



13

Protonation position	G^*	$G^*_{relat.}$
1	-1899.7997122	10.59
2	-1899.7979411	11.70
3	-1899.7876526	18.16
4	*-1899.7988360*	*11.13*
5	- 1899.8049971	7.27
6	-1899.7748353	26.20
7	-1899.7702541	29.07
8	-1899.8086124	5.00
9	-1899.7727413	27.51
10	-1899.8051115	7.20
11	-1899.8100039	4.11
12	-1899.8159616	0.39
13	**-1899.8165872**	**0.00**



14

Protonation position	G^*	$G^*_{relat.}$
1	-849.1886666	4.09
2	-849.1843345	6.81
3	-849.1775033	11.09
4	*-849.1908299*	*2.73*
5	**- 849.1951834**	**0.00**
6	-849.1610391	21.43
7	-849.1855096	6.07
8	-849.1745977	12.91
9	-849.1877922	10.83
10	-849.1745155	12.97
11	-849.1844830	6.71

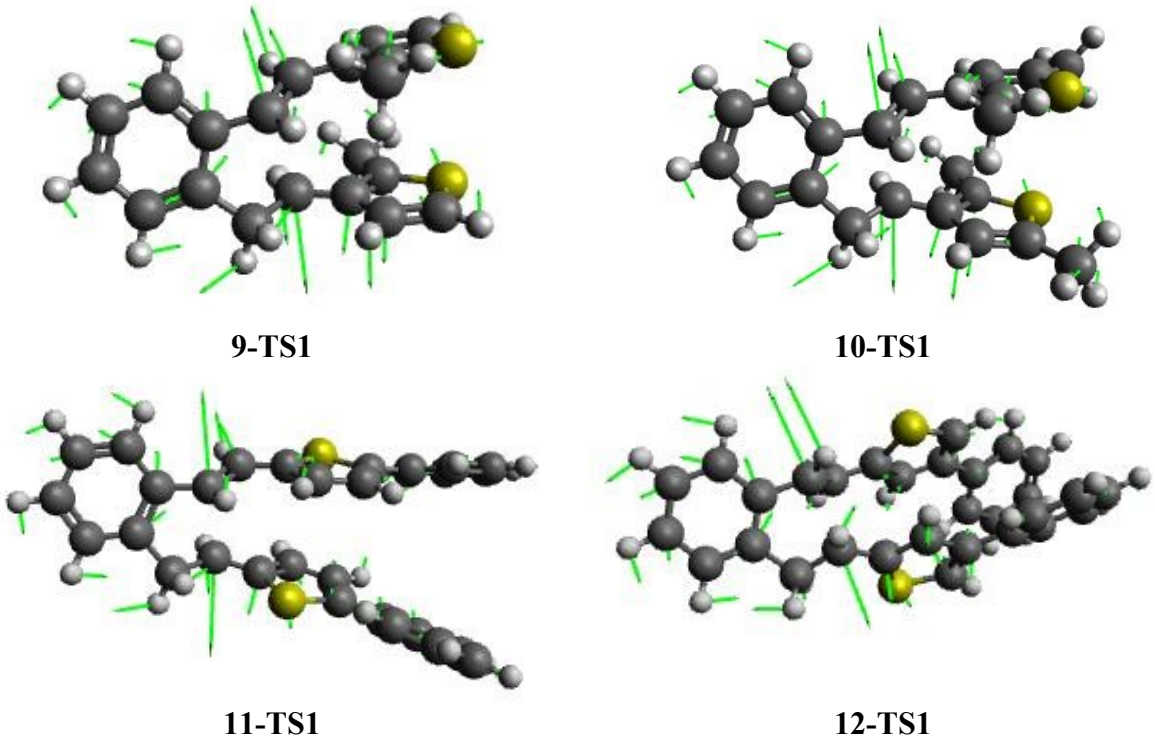


Figure S1: Pictorial presentation of imaginary normal modes for **9-TS1**, **10-TS1**, **11-TS1** and **12-TS1** transition states.

Cartesian coordinates and selected energy values for the calculated structures

Cartesian coordinates and selected energy values for the calculated structures along the pathway of formation of products **15** and **9-indene**

9
*E*elec.= -1569.2560081 a.u.
*G*corr. = 0.267236 a.u.
*E*elec. + *G*corr. = -1568.9887721 a.u.

C	-4.712617	2.821284	0.670034
C	-5.639065	2.504456	-0.386545
C	-6.918150	2.928490	-0.101381
S	-6.986391	3.703886	1.444547
C	-5.296063	3.462348	1.715109
C	-5.308072	1.812774	-1.630859
C	-4.088081	1.365506	-1.973867
C	-3.780880	0.703380	-3.254390
C	-2.737428	-0.249020	-3.345763
C	-2.466609	-0.839959	-4.589182
C	-3.187822	-0.498533	-5.726127
C	-4.210404	0.445879	-5.637760
C	-4.495628	1.038526	-4.414328
C	-1.972887	-0.647626	-2.150308
C	-0.694499	-1.061250	-2.177154
C	0.080596	-1.497043	-1.017148
C	1.392901	-1.901954	-1.122425
S	2.032122	-2.348355	0.422862
C	0.538655	-1.993361	1.218027
C	-0.400106	-1.557019	0.339455
C	2.249313	-1.966984	-2.351315
C	-8.155358	2.774087	-0.934036
H	-1.696477	-1.603099	-4.653006
H	-2.959959	-0.973098	-6.675535
H	-4.776729	0.725421	-6.520732
H	-5.266747	1.801097	-4.355850
H	-3.656502	2.578200	0.643122
H	-4.835904	3.815045	2.628421
H	-1.405933	-1.284942	0.638584
H	0.444528	-2.135144	2.286351
H	-3.260159	1.492042	-1.279432
H	-2.496622	-0.598886	-1.197926
H	-6.140155	1.646692	-2.313677
H	-0.164255	-1.069096	-3.128450
H	1.723088	-2.474671	-3.164682
H	2.517206	-0.963926	-2.699265
H	3.176369	-2.512606	-2.162142
H	-7.969995	3.085355	-1.966013
H	-8.490990	1.731992	-0.952821
H	-8.975578	3.381269	-0.544822

9-IM1
*E*elec.= -1569.673328 a.u.
*G*corr. = 0.284774 a.u.
*E*elec. + *G*corr. = -1569.388554 a.u.

C	-3.402219	-2.648700	-0.108616
C	-3.508672	-1.222755	0.134977
C	-2.922462	-0.455355	-0.907807
S	-2.308644	-1.467234	-2.115054
C	-2.788760	-2.923353	-1.276089
C	-4.035262	-0.602442	1.254513
C	-4.755400	-1.249460	2.386686
C	-4.434964	-0.544698	3.690271
C	-3.089439	-0.211236	3.930643
C	-2.746211	0.495240	5.083031
C	-3.732651	0.855066	6.001222
C	-5.061453	0.510987	5.769150
C	-5.413178	-0.182225	4.610079
C	-2.107084	-0.639616	2.911748
C	-1.296171	0.185654	2.215119
C	-0.438069	-0.268924	1.136110
C	-0.200734	-1.648607	0.790887
C	0.585731	-1.793689	-0.304358
S	1.056155	-0.259634	-0.951414
C	0.195261	0.603043	0.266148
C	0.229131	2.099015	0.301547
C	-2.886403	1.029539	-1.029954
H	-6.453259	-0.427043	4.413221
H	-5.829559	0.791724	6.482908
H	-3.460307	1.402680	6.897956
H	-1.705763	0.749113	5.263719
H	-0.595914	-2.491867	1.345167
H	0.920273	-2.707400	-0.777501
H	-3.773896	-3.405290	0.571694
H	-2.568373	-3.886368	-1.717257
H	-2.069795	-1.711389	2.713591
H	-4.539951	-2.321686	2.436510
H	-1.338319	1.256629	2.407904
H	-3.866620	1.393935	-1.356682
H	-2.658838	1.487096	-0.062779
H	-2.137290	1.353064	-1.755554
H	-0.733822	2.506244	0.619635
H	0.990425	2.450403	1.006029
H	0.464181	2.515463	-0.680641
H	-4.052867	0.486243	1.263715
H	-5.828101	-1.140707	2.165977

9-TS1
*E*elec.= -1569.6696096 a.u.
*G*corr. = 0.286774 a.u.
*E*elec. + *G*corr. = -1569.3822356 a.u.

C	0.689137	2.502850	-0.888300
C	0.292310	1.724472	0.265628
C	1.394740	1.350291	1.060544
S	2.839083	1.964617	0.412406
C	2.023688	2.703277	-0.940346
C	-1.000168	1.290816	0.585649
C	-2.279283	1.840507	0.037129
C	-3.312905	0.738584	-0.026704
C	-2.827575	-0.519560	-0.417800
C	-3.683105	-1.618416	-0.457742
C	-5.027425	-1.456414	-0.119185
C	-5.510019	-0.205319	0.256554
C	-4.651551	0.894660	0.310183
C	-1.392226	-0.554149	-0.779546
C	-0.460186	-1.378556	-0.225138
C	0.942946	-1.379999	-0.562267
C	1.932877	-1.884765	0.359263
C	3.205128	-1.723826	-0.078448
S	3.231956	-0.996510	-1.647395
C	1.520735	-0.874987	-1.724395
C	0.887531	-0.376092	-2.987933
C	1.375004	0.611561	2.356653
H	-5.022041	1.865197	0.627793
H	-6.555985	-0.085050	0.520852
H	-5.697411	-2.309820	-0.151696
H	-3.301763	-2.588205	-0.763785
H	1.673829	-2.325746	1.315542
H	4.130487	-1.989472	0.414797
H	-0.003749	2.872699	-1.635143
H	2.599900	3.239300	-1.682765
H	-1.108794	0.081149	-1.616091
H	-2.125537	2.310988	-0.939854
H	-0.759801	-2.014857	0.607854
H	1.045491	1.282550	3.157268
H	0.676702	-0.228858	2.310697
H	2.364119	0.227348	2.611754
H	0.002807	-0.972690	-3.227998
H	0.581461	0.670773	-2.900252
H	1.584990	-0.448821	-3.825551
H	-1.115804	0.723141	1.507334
H	-2.602682	2.626027	0.734655

9-IM2
*E*elec.= -1569.6887991 a.u.
*G*corr. = 0.286142 a.u.
*E*elec. + *G*corr. = -1569.4026571 a.u.

C	0.592123	1.947447	-1.754319
C	0.385254	1.690762	-0.352945
C	1.529408	1.864922	0.385448
S	2.847987	2.363899	-0.625951
C	1.865580	2.319630	-2.045503
C	-0.910482	1.187870	0.203178
C	-1.147556	-0.359693	-0.133825
C	-2.649742	-0.480044	-0.024348
C	-3.248990	0.777804	-0.129580
C	-2.206335	1.850812	-0.315291
C	-4.632594	0.897625	-0.070588
C	-5.404093	-0.253897	0.101670
C	-4.800882	-1.507495	0.207261
C	-3.411675	-1.630902	0.141636
C	-0.371365	-1.130269	0.841323
C	0.944937	-1.502396	0.697422
C	1.798579	-1.296823	-0.462398
C	3.065718	-1.688896	-0.241095
S	3.268977	-2.335281	1.376271
C	1.657576	-2.086162	1.790784
C	1.135636	-2.416240	3.143383
C	1.769560	1.656011	1.850013
H	-5.106661	1.872135	-0.145847
H	-6.485166	-0.171803	0.159369
H	-5.414561	-2.392212	0.344859
H	-2.937481	-2.605654	0.220948
H	1.455506	-0.872169	-1.398691
H	3.916061	-1.659354	-0.909320
H	-0.184145	1.853113	-2.505761
H	2.287204	2.581845	-3.006682
H	-0.799110	-0.533402	-1.158869
H	-2.114803	2.110591	-1.376392
H	-0.859589	-1.337531	1.794462
H	2.030176	2.594217	2.349790
H	0.880781	1.249766	2.337875
H	2.595003	0.954593	2.013014
H	0.911087	-1.488293	3.680974
H	0.210918	-2.993551	3.060271
H	1.861937	-2.986486	3.722975
H	-0.912685	1.279838	1.293264
H	-2.424779	2.769470	0.235298

9-indane
*E*elec.= -1569.2769372 a.u.
*G*corr. = 0.272159 a.u.
*E*elec. + *G*corr. = -1569.0047782 a.u.

C	-0.237905	1.740122	-1.487469
C	0.095043	1.684358	-0.092708
C	1.002220	2.646071	0.269018
S	1.451806	3.618202	-1.094210
C	0.416673	2.732565	-2.151458
C	-0.499230	0.711815	0.906105
C	-0.952150	-0.584607	0.241992
C	-2.406882	-0.469670	0.028460
C	-2.906395	0.621800	0.751455
C	-1.802592	1.286347	1.536780
C	-4.260474	0.935004	0.711785
C	-5.114379	0.148676	-0.062919
C	-4.617036	-0.939370	-0.786086
C	-3.261180	-1.256041	-0.747780
C	-0.220602	-1.671696	-0.062364
C	1.209909	-1.894819	0.145579
C	2.225089	-0.896665	0.371511
C	3.466671	-1.425010	0.537417
S	3.440701	-3.146121	0.420692
C	1.736519	-3.170134	0.136208
C	1.010212	-4.467787	-0.056723
C	1.587813	2.887992	1.628025
H	-4.648952	1.780044	1.273763
H	-6.172833	0.386146	-0.108799
H	-5.292757	-1.537918	-1.389271
H	-2.876233	-2.092892	-1.324462
H	2.037607	0.170411	0.372788
H	4.398982	-0.903358	0.706995
H	-0.931429	1.059032	-1.969166
H	0.356121	2.992948	-3.199745
H	-1.839642	2.377971	1.486865
H	-0.757847	-2.519899	-0.486167
H	0.816469	3.197419	2.340991
H	2.050807	1.973032	2.015131
H	2.353819	3.666289	1.603646
H	0.274412	-4.626409	0.737777
H	0.477062	-4.477873	-1.012886
H	1.698516	-5.315630	-0.050275
H	0.245206	0.511188	1.683430
H	-1.872051	1.000906	2.593095

9-IM3
*E*elec.= -1569.6899081 a.u.
*G*corr. = 0.281132 a.u.
*E*elec. + *G*corr. = -1569.4087761 a.u.

C	-1.719825	2.067610	-1.185942
C	-0.663099	1.659317	-0.415246
C	-1.055394	1.231878	0.899137
C	-2.393798	1.332533	1.107970
S	-3.201941	1.943832	-0.289864
C	0.775527	1.599122	-0.871538
C	1.254128	0.190754	-1.049353
C	2.505651	0.012298	-0.443173
C	2.886784	1.235138	0.182065
C	1.816731	2.267245	0.044893
C	3.352876	-1.130337	-0.393615
C	4.554211	-1.012707	0.262607
C	4.929816	0.212796	0.857497
C	4.112827	1.337167	0.824916
C	0.420213	-0.786794	-1.785531
C	1.153028	-1.888075	-2.502998
C	2.035506	-1.654931	-3.525170
S	2.726196	-3.142401	-4.082092
C	1.822871	-4.072196	-2.943536
C	1.028664	-3.277311	-2.175413
C	2.462152	-0.338627	-4.097727
C	-1.747295	2.540097	-2.607379
H	4.421287	2.263433	1.297403
H	5.889984	0.272016	1.361816
H	5.226900	-1.860555	0.324880
H	3.056007	-2.066147	-0.853279
H	0.370745	-3.651459	-1.398757
H	1.918401	-5.149541	-2.923037
H	-0.353051	0.871059	1.644012
H	-2.956047	1.088952	1.999512
H	1.391964	2.497865	1.028160
H	-0.249256	-1.215065	-1.020613
H	-2.398940	3.410513	-2.721589
H	-0.747547	2.826252	-2.942359
H	-2.116395	1.757113	-3.277456
H	1.673706	0.408574	-3.961798
H	3.368641	0.031986	-3.606324
H	2.669250	-0.413329	-5.168218
H	0.846239	2.030910	-1.882346
H	2.203195	3.203090	-0.367811
H	-0.242424	-0.227003	-2.458056

15

*E*elec.= -1569.2838573 a.u.
*G*corr. = 0.272059 a.u.
*E*elec. + *G*corr. = -1569.0117983 a.u.

C	1.861254	3.271621	2.230514
C	1.245297	1.979719	2.138056
C	1.271498	1.300481	3.327552
S	2.058799	2.237735	4.558478
C	2.346511	3.547281	3.472131
C	0.636076	1.408997	0.875262
C	1.384453	0.203473	0.374974
C	0.927043	-1.067210	0.257719
C	2.041735	-2.002434	-0.161331
C	3.220103	-1.079904	-0.304965
C	2.813856	0.227385	0.016012
C	4.528970	-1.344630	-0.680576
C	5.438667	-0.284783	-0.738384
C	5.036512	1.015072	-0.424344
C	3.721047	1.284888	-0.043587
C	-0.429203	-1.568966	0.518990
C	-1.586620	-1.044192	-0.006692
S	-2.971968	-1.935165	0.545268
C	-1.995952	-3.018062	1.472459
C	-0.677344	-2.713385	1.359602
C	-1.757667	0.086659	-0.973475
C	0.731244	-0.066055	3.620537
H	4.844048	-2.355137	-0.926636
H	6.467026	-0.473933	-1.030951
H	5.756850	1.825949	-0.476855
H	3.414668	2.298137	0.199909
H	1.927734	3.960808	1.394803
H	2.849363	4.441157	3.816184
H	0.110821	-3.261577	1.864530
H	-2.457102	-3.809237	2.048413
H	1.802308	-2.524485	-1.096014
H	0.617692	2.188031	0.103438
H	-2.172116	0.977468	-0.489937
H	-0.788485	0.353620	-1.402309
H	-2.429741	-0.191725	-1.790372
H	-0.173458	-0.246606	3.030773
H	1.455975	-0.846822	3.362308
H	0.476634	-0.179264	4.677330
H	2.216055	-2.779853	0.594418
H	-0.403442	1.125098	1.070187

Cartesian coordinates and selected energy values for the calculated structures along the pathway of formation of products **16** and **10-indene**

10

*E*elec.= -1647.8776369 a.u.

*G*corr. = 0.318053 a.u.

*E*elec. + *G*corr. = -1647.5595839 a.u.

C	-5.202877	-2.868319	-1.522409
C	-6.250802	-2.117528	-0.876642
C	-7.429859	-2.157458	-1.583235
S	-7.252699	-3.101173	-3.027950
C	-5.580482	-3.454449	-2.688719
C	-6.113343	-1.381802	0.377978
C	-4.981646	-1.276742	1.095616
C	-4.873772	-0.557534	2.376947
C	-3.648396	0.030028	2.775407
C	-3.582456	0.684708	4.014777
C	-4.684924	0.754437	4.857095
C	-5.890294	0.170507	4.467215
C	-5.975520	-0.479421	3.242420
C	-2.473102	-0.005920	1.887658
C	-1.198977	-0.001622	2.315870
C	-0.019738	-0.002913	1.453515
C	-0.040519	0.021216	0.012046
C	1.192205	0.002384	-0.559312
S	2.426470	-0.041060	0.669874
C	1.260580	-0.034623	1.954337
C	1.704748	-0.086535	3.385358
C	1.548270	0.021268	-2.012597
C	-8.736238	-1.495569	-1.262178
C	-4.765680	-4.301672	-3.614725
H	-6.903918	-0.965880	2.958012
H	-6.757257	0.213649	5.118978
H	-4.607297	1.269719	5.809323
H	-2.656301	1.172753	4.303740
H	-0.948826	0.053688	-0.580455
H	-4.197683	-2.969333	-1.126790
H	-2.672937	-0.035672	0.818916
H	-4.073805	-1.747876	0.725636
H	-1.003396	-0.013917	3.387054
H	-7.009637	-0.873782	0.730697
H	-8.992287	-1.633648	-0.208108
H	-8.693320	-0.419339	-1.459774
H	-9.549663	-1.912277	-1.860225
H	1.143609	0.629670	3.991877
H	1.549237	-1.083110	3.811751
H	2.765660	0.155086	3.480493
H	0.634210	0.053586	-2.609790
H	2.154976	0.895787	-2.266471

H	2.113872	-0.870458	-2.299572
H	-3.753351	-4.403510	-3.217222
H	-5.193370	-5.302837	-3.724622
H	-4.699074	-3.857208	-4.612448

10-IM1

*E*elec.= -1648.2987619 a.u.
*G*corr. = 0.336311 a.u.
*E*elec. + *G*corr. = -1647.9624509 a.u.

C	1.949671	-3.308889	3.027734
C	0.743573	-3.193155	2.363143
C	0.903690	-3.264826	0.929731
C	2.188441	-3.425844	0.524985
S	3.252847	-3.496248	1.905746
C	-0.520732	-2.945378	3.036165
C	-1.635126	-2.548427	2.387893
C	-2.899782	-2.148536	3.040506
C	-3.363789	-0.843687	2.787680
C	-4.551285	-0.407803	3.366577
C	-5.281951	-1.259624	4.196210
C	-4.816686	-2.544946	4.459904
C	-3.626902	-2.989346	3.883449
C	-2.506361	0.055823	1.917379
C	-1.072886	-0.036635	2.310800
C	0.024441	-0.004261	1.473405
C	0.029924	-0.005358	0.022389
C	1.270475	-0.009013	-0.507413
S	2.486671	-0.030380	0.773077
C	1.340333	-0.034382	2.013700
C	1.737407	0.005680	3.449168
C	1.697635	0.005669	-1.937644
C	2.723988	-3.529564	-0.867688
C	2.234659	-3.288408	4.496104
H	-4.899044	0.604512	3.180289
H	-6.207455	-0.912416	4.644389
H	-5.379011	-3.204735	5.113034
H	-3.263718	-3.994913	4.074438
H	0.082571	-3.203643	0.223696
H	-0.869194	-0.002249	-0.583133
H	-1.618755	-2.469588	1.300863
H	-2.641704	-0.158004	0.852374
H	-0.540751	-3.006170	4.122586
H	1.619307	1.025534	3.831849
H	1.100496	-0.657048	4.041788
H	2.778555	-0.294522	3.581267
H	1.337446	-3.042030	5.065817
H	2.595902	-4.263819	4.837178
H	3.002628	-2.547373	4.738600

H	-0.886330	-0.017334	3.383393
H	-2.800943	1.103339	2.079557
H	0.813292	-0.030585	-2.576746
H	2.259053	0.915492	-2.170386
H	2.334475	-0.852232	-2.171517
H	3.487194	-2.768931	-1.061522
H	3.178023	-4.508293	-1.051715
H	1.907918	-3.389985	-1.580797

10-TS1

*E*elec.= -1648.2933595 a.u.
*G*corr. = 0.338578 a.u.
*E*elec. + *G*corr. = -1647.9547815 a.u.

C	0.765181	-3.343058	0.886031
C	0.580081	-3.111612	2.246434
C	1.825729	-3.150352	2.977562
C	2.919619	-3.353199	2.202560
S	2.434055	-3.563832	0.540325
C	-0.660949	-2.800645	2.904088
C	-1.757801	-2.274159	2.283811
C	-3.035164	-1.935422	2.951802
C	-3.473957	-0.616727	2.752177
C	-4.672636	-0.189303	3.308920
C	-5.436237	-1.078973	4.068013
C	-4.995602	-2.383601	4.277497
C	-3.792061	-2.817605	3.719389
C	-2.529474	0.253770	1.954461
C	-1.118555	-0.089523	2.328703
C	0.003169	-0.006967	1.489852
C	0.007971	0.007622	0.043610
C	1.251132	0.008832	-0.490002
S	2.464190	0.010645	0.782962
C	1.302905	-0.024695	2.026224
C	1.700067	0.022578	3.464094
C	1.664268	-0.017892	-1.924923
C	4.360985	-3.387855	2.598255
C	-0.232082	-3.522304	-0.218425
H	-5.002759	0.835748	3.166473
H	-6.371587	-0.746100	4.506721
H	-5.588955	-3.067189	4.876369
H	-3.448018	-3.836743	3.868763
H	1.881338	-2.995500	4.050316
H	-0.891510	-0.002543	-0.562447
H	-1.766596	-2.202362	1.198171
H	-2.693212	0.148026	0.876506
H	-0.671233	-2.884058	3.991006
H	1.596527	1.044760	3.843565
H	1.055489	-0.628029	4.062326

H	2.735542	-0.295002	3.601001
H	-1.120011	-4.041219	0.153173
H	-0.546585	-2.561635	-0.637797
H	0.194646	-4.115301	-1.030586
H	-0.929277	-0.073502	3.400206
H	-2.674369	1.312491	2.208842
H	4.837865	-4.327641	2.305085
H	4.918780	-2.569135	2.132854
H	4.439501	-3.284227	3.682705
H	0.773767	0.002155	-2.556435
H	2.289949	0.842855	-2.177958
H	2.231636	-0.925552	-2.153466

10-IM2

*E*elec.= -1648.3135482 a.u.
*G*corr. = 0.337705 a.u.
*E*elec. + *G*corr. = -1647.9758432 a.u.

C	0.784461	-3.686551	3.984917
C	0.036353	-3.050666	2.945118
C	0.698999	-3.154900	1.655111
C	1.875925	-3.806093	1.708784
S	2.204145	-4.340830	3.366826
C	-1.119887	-2.368196	3.233952
C	-1.872071	-1.552469	2.273486
C	-1.249373	-0.080737	2.286821
C	-2.437771	0.793852	1.828286
C	-3.641117	0.050249	2.351111
C	-3.319301	-1.284677	2.613056
C	-4.934091	0.511377	2.569188
C	-5.895129	-0.376782	3.058211
C	-5.568305	-1.707628	3.320417
C	-4.271723	-2.174722	3.095123
C	0.011457	0.000295	1.483903
C	0.030057	-0.051585	0.044184
C	1.279866	-0.077166	-0.492536
S	2.476650	-0.037701	0.770830
C	1.270684	0.003397	2.023617
C	1.702856	-0.008071	3.458084
C	1.677965	-0.118499	-1.934405
C	2.860147	-4.093835	0.625511
C	0.435480	-3.772916	5.427572
H	-5.192214	1.547912	2.372033
H	-6.906358	-0.026407	3.240631
H	-6.325763	-2.383938	3.703922
H	-4.013457	-3.211328	3.294601
H	0.302639	-2.730249	0.738920
H	-0.864399	-0.075684	-0.570611
H	-1.768437	-1.944635	1.254466

H	-2.476960	0.856939	0.734382
H	-1.462765	-2.351981	4.269253
H	2.215181	0.920655	3.729270
H	0.843905	-0.125979	4.122115
H	2.394575	-0.834700	3.652067
H	0.421975	-2.766015	5.858147
H	-0.562307	-4.204852	5.544928
H	1.154055	-4.379539	5.978836
H	-1.048064	0.168083	3.333022
H	-2.352296	1.811572	2.217491
H	3.830780	-3.639312	0.844112
H	3.009104	-5.170050	0.498380
H	2.485009	-3.678358	-0.312325
H	0.782612	-0.164718	-2.558297
H	2.248201	0.771170	-2.218621
H	2.296694	-0.993857	-2.154772

10-indane
*E*elec.= -1647.8981723 a.u.
*G*corr. = 0.323283 a.u.
*E*elec. + *G*corr. = -1647.5748893 a.u.

C	-2.782352	-4.248571	2.203219
C	-2.126972	-3.044522	2.067192
C	-0.753100	-3.128861	2.498434
C	-0.388930	-4.356596	2.957421
S	-1.733979	-5.456052	2.870098
C	-2.813880	-1.870981	1.531085
C	-2.459135	-0.575587	1.614893
C	-1.253342	0.040917	2.319909
C	-1.689264	1.511451	2.593913
C	-2.794508	1.754085	1.595669
C	-3.247502	0.540540	1.060026
C	-3.383075	2.956106	1.218649
C	-4.430352	2.936961	0.296308
C	-4.882722	1.727385	-0.239357
C	-4.295053	0.521636	0.136205
C	-0.004586	-0.001439	1.462767
C	0.005527	0.055628	0.027371
C	1.254339	0.044026	-0.517872
S	2.455113	-0.040396	0.736692
C	1.254775	-0.055657	1.994762
C	1.644901	-0.117220	3.441489
C	1.641345	0.086619	-1.963217
C	0.947731	-4.799073	3.464850
C	-4.209387	-4.571239	1.874994
H	-3.032725	3.897046	1.633997
H	-4.894438	3.868620	-0.012446
H	-5.693054	1.729195	-0.961858

H	-4.638755	-0.414319	-0.295790
H	-0.044457	-2.311875	2.431125
H	-0.893592	0.095586	-0.579976
H	-0.857760	2.214020	2.491057
H	-3.755165	-2.087765	1.026622
H	1.397913	0.816053	3.958589
H	1.113671	-0.928936	3.951772
H	2.716330	-0.292721	3.561831
H	-4.897575	-3.991846	2.498490
H	-4.431011	-4.338972	0.828454
H	-4.424191	-5.630248	2.033452
H	-1.047351	-0.478367	3.261090
H	-2.079988	1.609177	3.613528
H	0.740048	0.131915	-2.578876
H	2.255163	0.963645	-2.190688
H	2.210450	-0.801445	-2.254816
H	0.892992	-5.134268	4.505150
H	1.352095	-5.624108	2.870569
H	1.649830	-3.963296	3.411423

10-IM3
*E*elec.= -1648.3116382 a.u.
*G*corr. = 0.333197 a.u.
*E*elec. + *G*corr. = -1647.9784412 a.u.

C	-1.423551	5.027167	3.120045
C	-2.015333	3.812306	2.639181
C	-3.381442	3.822172	2.693962
S	-3.948626	5.326720	3.348160
C	-2.334621	5.947775	3.542971
C	-1.224449	2.626145	2.155280
C	-1.408844	1.366429	2.911470
C	-1.271299	0.045237	2.219877
C	-1.386934	-1.009504	3.336719
C	-1.723250	-0.209896	4.552111
C	-1.698725	1.186797	4.272025
C	-2.017515	-0.658008	5.833189
C	-2.259610	0.291641	6.818961
C	-2.217440	1.680293	6.558957
C	-1.944721	2.144693	5.294927
C	-0.026394	-0.013384	1.366011
C	-0.010242	-0.038041	-0.000688
S	1.631148	-0.058751	-0.579688
C	2.292285	-0.020000	1.030649
C	1.288916	0.002221	1.948174
C	-1.142975	-0.024522	-0.979744
C	3.770495	-0.020656	1.260728
C	-4.331561	2.722308	2.336218
C	-2.092701	7.320444	4.087160

H	-2.048120	-1.717699	6.061684
H	-2.486150	-0.040970	7.827651
H	-2.408479	2.376678	7.367438
H	-1.911708	3.207171	5.082507
H	-0.352484	5.200788	3.145865
H	1.468790	0.026404	3.019329
H	-0.438511	-1.537152	3.484975
H	-0.144251	2.837970	2.226819
H	-0.999356	-0.776183	-1.760789
H	-2.090594	-0.238720	-0.480655
H	-1.231890	0.950889	-1.468492
H	-3.865598	2.037603	1.620364
H	-4.620983	2.143200	3.220428
H	-5.244315	3.112101	1.878399
H	-2.154905	-0.009436	1.565061
H	-2.148030	-1.765563	3.125103
H	-1.402244	2.414841	1.093022
H	4.247821	0.850260	0.801659
H	3.970583	0.004310	2.334167
H	4.240398	-0.916499	0.843873
H	-2.514619	7.435599	5.089944
H	-1.017387	7.503371	4.143875
H	-2.538268	8.088857	3.448176

16

*E*elec.= -1647.9050243 a.u.
*G*corr. = 0.324549 a.u.
*E*elec. + *G*corr. = -1647.5804753 a.u.

C	-0.405043	-0.358269	6.552244
C	-1.341368	-0.331998	5.454871
C	-2.159003	0.770436	5.491139
S	-1.764577	1.780616	6.851963
C	-0.497342	0.712043	7.385666
C	-1.398771	-1.397638	4.445107
C	-1.383650	-1.267891	3.095822
C	-1.445270	-2.609586	2.489729
C	-1.477613	-3.568341	3.518061
C	-1.438318	-2.858349	4.843015
C	-1.480801	-3.004138	1.152470
C	-1.546405	-4.367352	0.860359
C	-1.574803	-5.318085	1.883035
C	-1.540918	-4.922508	3.223671
C	-1.227256	-0.003784	2.295319
C	0.021032	-0.016624	1.438514
C	0.016566	0.022073	0.003474
C	1.257173	-0.014451	-0.558739
S	2.471509	-0.093830	0.684137
C	1.285125	-0.074741	1.956980

C	1.693425	-0.128731	3.397561
C	1.627318	0.012050	-2.008753
C	-3.300040	1.134465	4.592406
C	0.321171	1.025992	8.598400
H	-1.565488	-5.663978	4.017624
H	-1.625224	-6.373684	1.634272
H	-1.575938	-4.693261	-0.175013
H	-1.458972	-2.269694	0.352547
H	-0.893080	0.079148	-0.587549
H	0.325488	-1.149287	6.691755
H	-2.313192	-3.084625	5.464910
H	-2.101154	0.144002	1.649256
H	-3.052720	1.978424	3.939745
H	-3.556654	0.281266	3.959571
H	-4.185642	1.411549	5.171778
H	0.986040	0.439588	4.010008
H	1.705225	-1.158110	3.774648
H	2.689446	0.295464	3.548203
H	-0.555054	-3.136017	5.433318
H	-1.189142	0.847083	2.983688
H	-0.302023	1.108446	9.494092
H	1.050592	0.229213	8.760598
H	0.864096	1.969088	8.483495
H	0.719577	0.067426	-2.614189
H	2.252488	0.877221	-2.250253
H	2.178334	-0.887148	-2.301009

Cartesian coordinates and selected energy values for the calculated structures along the pathway of formation of products **17** and **11-indene**

11
*E*elec.= -1952.7191998 a.u.
*G*corr. = 0.365077 a.u.
*E*elec. + *G*corr. = -1952.3541228 a.u.

C	-5.044068	-5.022778	0.903748
C	-4.177538	-4.236279	1.660236
C	-3.957076	-2.906252	1.316379
C	-4.595558	-2.342475	0.203181
C	-5.459193	-3.144851	-0.557638
C	-5.684075	-4.470588	-0.205265
C	-4.384620	-0.937794	-0.174561
S	-2.926143	-0.092072	0.264901
C	-3.464540	1.371969	-0.509905
C	-4.703011	1.189294	-1.074177
C	-5.224392	-0.118010	-0.884702
C	-2.680971	2.592828	-0.536407
C	-1.460706	2.757894	0.002957
C	-0.707701	4.022204	-0.015212
C	0.707670	4.022205	0.015206
C	1.385645	5.250420	0.021609
C	0.697427	6.456491	0.012072
C	-0.697456	6.456490	-0.012082
C	-1.385674	5.250420	-0.021617
C	1.460680	2.757895	-0.002961
C	2.680939	2.592834	0.536418
C	3.464519	1.371982	0.509917
S	2.926137	-0.092063	-0.264893
C	4.384625	-0.937770	0.174567
C	5.224389	-0.117977	0.884706
C	4.702993	1.189320	1.074186
C	4.595577	-2.342447	-0.203182
C	3.957103	-2.906227	-1.316382
C	4.177577	-4.236253	-1.660239
C	5.044113	-5.022744	-0.903752
C	5.684115	-4.470550	0.205263
C	5.459220	-3.144816	0.557638
H	2.471390	5.253841	0.002801
H	1.246581	7.392756	0.014368
H	-1.246610	7.392756	-0.014378
H	-2.471419	5.253843	-0.002808
H	-5.221225	1.982564	-1.601674
H	-6.196531	-0.438899	-1.241042
H	5.221200	1.982596	1.601682
H	6.196534	-0.438855	1.241044
H	-0.981342	1.913231	0.496028
H	0.981326	1.913234	-0.496044

H	-3.160430	3.416459	-1.063693
H	3.160386	3.416466	1.063713
H	3.298057	-2.297702	-1.930270
H	5.940946	-2.728621	1.437226
H	3.677424	-4.656058	-2.527464
H	6.353534	-5.078331	0.806120
H	5.218093	-6.059482	-1.174059
H	-3.298032	-2.297723	1.930264
H	-5.940922	-2.728662	-1.437228
H	-3.677377	-4.656080	2.527458
H	-6.353490	-5.078374	-0.806122
H	-5.218040	-6.059517	1.174054

11-IM1
*E*elec.= -1953.14152 a.u.
*G*corr. = 0.383712 a.u.
*E*elec. + *G*corr. = -1952.757808 a.u.

C	5.018346	2.248109	-0.480009
C	3.946076	2.778122	-1.198611
C	2.646328	2.557797	-0.768706
C	2.399281	1.803441	0.392201
C	3.489192	1.268862	1.105728
C	4.786557	1.494080	0.670416
C	1.042813	1.545643	0.847669
S	-0.329442	2.114109	-0.026369
C	-1.430650	1.371338	1.128231
C	-0.688927	0.730694	2.160788
C	0.673385	0.828580	2.002958
C	-2.785469	1.299627	1.006884
C	-3.653268	1.846388	-0.076642
C	-4.776808	0.876827	-0.403668
C	-4.465767	-0.483738	-0.598858
C	-5.492768	-1.403204	-0.817271
C	-6.819383	-0.978265	-0.863149
C	-7.124576	0.368628	-0.689294
C	-6.104598	1.290740	-0.451651
C	-3.044625	-0.877007	-0.544576
C	-2.516473	-1.784215	0.298216
C	-1.093577	-2.015075	0.426255
S	0.041316	-1.464870	-0.769944
C	1.404584	-1.949619	0.194574
C	0.979358	-2.537481	1.366051
C	-0.429202	-2.578291	1.495475
C	2.776838	-1.749204	-0.290717
C	3.038515	-0.985345	-1.439194
C	4.339781	-0.810067	-1.894884
C	5.408079	-1.382607	-1.206395
C	5.161432	-2.134359	-0.058607

C	3.860083	-2.320220	0.394790
H	-5.244284	-2.449743	-0.967624
H	-7.611336	-1.699931	-1.036726
H	-8.156360	0.703633	-0.724916
H	-6.343249	2.337741	-0.285602
H	-1.187181	0.218839	2.977128
H	1.390622	0.395939	2.686870
H	-0.951050	-2.985417	2.354743
H	1.658085	-2.913856	2.122159
H	-2.377406	-0.318942	-1.204364
H	-3.299156	0.803013	1.830024
H	-3.153109	-2.307578	1.010190
H	2.223754	-0.510664	-1.980553
H	3.684460	-2.923168	1.280000
H	4.520412	-0.215372	-2.785151
H	5.985582	-2.587545	0.483530
H	6.424567	-1.242704	-1.560664
H	1.824546	2.981506	-1.340145
H	3.325586	0.672139	1.996286
H	4.125457	3.362080	-2.095003
H	5.619181	1.071990	1.223401
H	6.035100	2.418790	-0.820221
H	-3.063792	2.096570	-0.967520
H	-4.087759	2.783791	0.297048

11-TS1
*E*elec.= -1953.1311184 a.u.
*G*corr. = 0.382262 a.u.
*E*elec. + *G*corr. = -1952.7488564 a.u.

C	4.393366	4.046172	-0.721438
C	3.212294	4.071268	-1.464827
C	2.093434	3.372270	-1.022826
C	2.141784	2.641622	0.174836
C	3.333983	2.620537	0.916966
C	4.450199	3.318918	0.468618
C	0.977020	1.890769	0.653915
S	-0.621670	2.314256	0.162965
C	-1.312621	1.003212	1.093056
C	-0.298967	0.290834	1.747582
C	0.980767	0.796065	1.513141
C	-2.664818	0.644464	1.112574
C	-3.831629	1.505576	0.718217
C	-4.947143	0.606191	0.236481
C	-4.521108	-0.527749	-0.475112
C	-5.449202	-1.464343	-0.927551
C	-6.808594	-1.258753	-0.677007
C	-7.231853	-0.126864	0.018917
C	-6.300345	0.807217	0.483161

C	-3.059096	-0.594575	-0.701754
C	-2.248429	-1.660500	-0.403428
C	-0.850484	-1.626618	-0.675813
S	0.257878	-2.711514	0.125101
C	1.630761	-1.917469	-0.551737
C	1.243721	-0.885841	-1.394887
C	-0.147544	-0.722717	-1.466211
C	3.000946	-2.330779	-0.220461
C	3.279760	-3.055057	0.948777
C	4.586267	-3.423608	1.256518
C	5.634001	-3.068961	0.406052
C	5.365927	-2.347226	-0.758212
C	4.060662	-1.982000	-1.073242
H	-5.115527	-2.337938	-1.480800
H	-7.536118	-1.983879	-1.029068
H	-8.289285	0.026121	0.213030
H	-6.627332	1.676930	1.046947
H	-0.521870	-0.562819	2.379404
H	1.888916	0.367895	1.921439
H	-0.630562	0.025082	-2.085366
H	1.951618	-0.257567	-1.923693
H	-2.653358	0.200422	-1.328617
H	-2.900141	-0.153164	1.816950
H	-2.653825	-2.493678	0.169973
H	2.477915	-3.317876	1.634274
H	3.861043	-1.439057	-1.992049
H	4.786450	-3.980407	2.166807
H	6.175501	-2.073242	-1.427808
H	6.653366	-3.353224	0.648806
H	1.188222	3.380624	-1.624719
H	3.381073	2.074224	1.853863
H	3.163823	4.629467	-2.394534
H	5.364284	3.301090	1.053775
H	5.265830	4.592042	-1.067546
H	-3.546848	2.232772	-0.053384
H	-4.140872	2.070088	1.607579

11-IM2
*E*elec.= -1953.1552608 a.u.
*G*corr. = 0.385264 a.u.
*E*elec. + *G*corr. = -1952.7699968 a.u.

C	-3.665087	1.796109	0.541638
C	-4.781002	0.994470	-0.079049
C	-4.323867	-0.270124	-0.459928
C	-2.854434	-0.413598	-0.137050
C	-2.652954	0.711275	0.968034
C	-5.169567	-1.190905	-1.065970
C	-6.500318	-0.828997	-1.284717

C	-6.960938	0.433145	-0.908804
C	-6.103696	1.355746	-0.305068
C	-2.434258	-1.723813	0.399702
C	-1.179245	-2.235048	0.324272
S	0.155175	-1.444931	-0.514401
C	1.257894	-2.618059	0.046665
C	0.631590	-3.634312	0.811417
C	-0.711505	-3.421445	0.970745
C	-1.228223	1.120485	1.131426
S	-0.406899	2.090525	-0.053494
C	1.119764	1.929047	0.770053
C	0.975321	1.168240	1.901399
C	-0.357675	0.709036	2.103202
C	2.340224	2.560337	0.242011
C	2.280097	3.628295	-0.663397
C	3.445303	4.204627	-1.159367
C	4.691394	3.731985	-0.753321
C	4.762786	2.673311	0.151251
C	3.600059	2.087726	0.641494
C	2.678263	-2.505334	-0.237459
C	3.250215	-1.255238	-0.533103
C	4.608440	-1.156574	-0.794116
C	5.407248	-2.301079	-0.769913
C	4.847331	-3.544771	-0.476812
C	3.490840	-3.651851	-0.203444
H	-4.805732	-2.171657	-1.360792
H	-7.181866	-1.535791	-1.747510
H	-7.999211	0.698671	-1.083049
H	-6.467874	2.334888	-0.007627
H	-0.665840	0.084096	2.934817
H	1.792460	0.957505	2.581696
H	-1.381202	-4.050110	1.547590
H	1.182417	-4.454643	1.253524
H	-2.246062	-0.136204	-1.009933
H	-2.988299	0.286425	1.920897
H	-3.164218	-2.293951	0.975816
H	2.639366	-0.355057	-0.520209
H	3.054460	-4.622308	0.008923
H	5.045479	-0.185886	-1.005688
H	5.469820	-4.432889	-0.462909
H	6.469989	-2.222307	-0.975924
H	1.317620	4.023203	-0.978136
H	3.669437	1.248186	1.327243
H	3.376724	5.029964	-1.861082
H	5.728113	2.294527	0.473225
H	5.599884	4.182691	-1.139829
H	-3.222409	2.467818	-0.206375
H	-3.979443	2.407252	1.390917

11-indane

*E*elec.= -1952.7388605 a.u.
*G*corr. = 0.371241 a.u.
*E*elec. + *G*corr. = -1952.3676195 a.u.

C	-1.770300	-2.590080	2.012868
C	-2.141979	-3.364818	0.773198
C	-1.276953	-3.050132	-0.283301
C	-0.300949	-2.039264	0.159146
C	-0.803002	-1.486286	1.489172
C	-1.416203	-3.671560	-1.526525
C	-2.428361	-4.612636	-1.694871
C	-3.289664	-4.928405	-0.639538
C	-3.151156	-4.305770	0.601512
C	0.838199	-1.742840	-0.494886
C	1.866550	-0.794105	-0.101651
S	3.433064	-0.932919	-0.857776
C	4.078066	0.399342	0.050299
C	3.115971	0.919990	0.879189
C	1.866478	0.250606	0.794926
C	-1.522461	-0.169620	1.334477
S	-2.582216	0.135960	-0.007569
C	-3.034378	1.699482	0.616251
C	-2.383357	1.950069	1.794574
C	-1.526650	0.885905	2.202432
C	-3.980235	2.567666	-0.102194
C	-4.948388	2.038939	-0.967039
C	-5.842910	2.876438	-1.626288
C	-5.792607	4.254448	-1.426946
C	-4.832855	4.790134	-0.568751
C	-3.930026	3.957262	0.082604
C	5.470728	0.838774	-0.118073
C	6.457544	-0.036701	-0.592357
C	7.772107	0.391703	-0.744881
C	8.126745	1.699062	-0.418221
C	7.152995	2.576974	0.057110
C	5.835942	2.155369	0.201179
H	-0.759424	-3.416351	-2.353610
H	-2.555888	-5.099278	-2.656885
H	-4.076706	-5.660944	-0.789680
H	-3.821737	-4.551653	1.420099
H	-0.935237	0.895025	3.112160
H	-2.525815	2.861981	2.363865
H	0.993243	0.550572	1.360037
H	3.303195	1.754863	1.545282
H	0.024147	-1.320381	2.187354
H	1.040652	-2.299391	-1.409431
H	6.201642	-1.066264	-0.828996
H	5.079981	2.852520	0.549945
H	8.521563	-0.301697	-1.113549

H	7.417587	3.599598	0.308032
H	9.153015	2.032678	-0.534504
H	-5.015959	0.964079	-1.114076
H	-3.170721	4.384513	0.730652
H	-6.586145	2.448629	-2.291946
H	-4.779993	5.863241	-0.412691
H	-6.493379	4.906764	-1.938418
H	-2.635148	-2.166058	2.529708
H	-1.245778	-3.240757	2.721672

11-IM3
*E*elec.= -1953.1497795 a.u.
*G*corr. = 0.383838 a.u.
*E*elec. + *G*corr. = -1952.7659415 a.u.

C	3.676278	-0.721630	1.699511
C	4.731659	-0.636770	0.648165
C	4.311750	0.198735	-0.422944
C	3.055802	0.738413	-0.127849
C	2.580083	0.255401	1.216048
C	5.138778	0.432240	-1.553984
C	6.369504	-0.175500	-1.581266
C	6.782290	-0.997905	-0.506432
C	5.984992	-1.232354	0.608533
C	2.378451	1.749105	-0.987745
C	1.002500	2.183860	-0.585147
S	-0.404491	1.423895	-1.242340
C	-1.459936	2.338147	-0.214542
C	-0.741969	3.208511	0.564716
C	0.663413	3.125609	0.345164
C	1.171350	-0.271476	1.238381
S	0.672913	-1.609281	0.245222
C	-0.975566	-1.468746	0.788726
C	-1.095867	-0.467666	1.714807
C	0.127174	0.213017	1.969969
C	-2.049552	-2.299135	0.224053
C	-1.810145	-3.588729	-0.266176
C	-2.848266	-4.339839	-0.809327
C	-4.139127	-3.817264	-0.865346
C	-4.385828	-2.533962	-0.378907
C	-3.350069	-1.776478	0.156283
C	-2.902286	2.048528	-0.190093
C	-3.581359	1.604363	-1.332386
C	-4.931478	1.271823	-1.267222
C	-5.625189	1.384480	-0.063480
C	-4.959533	1.834305	1.076663
C	-3.607507	2.158299	1.017220
H	4.803201	1.070963	-2.364668
H	7.037516	-0.029362	-2.422330

H	7.762185	-1.463312	-0.559740
H	6.330851	-1.866501	1.417384
H	0.228814	1.051306	2.650553
H	-2.035711	-0.225930	2.199061
H	1.400119	3.721831	0.873266
H	-1.206726	3.883547	1.274837
H	2.574962	1.157107	1.850535
H	-3.054826	1.527115	-2.280316
H	-3.084007	2.476065	1.914588
H	-5.442617	0.926856	-2.160814
H	-5.490568	1.921072	2.019631
H	-6.677752	1.123560	-0.014068
H	-0.811091	-4.013796	-0.209382
H	-3.541247	-0.764886	0.507535
H	-2.648408	-5.338868	-1.184134
H	-5.385685	-2.112869	-0.428792
H	-4.947116	-4.404632	-1.290012
H	3.295192	-1.745056	1.777872
H	4.065116	-0.447470	2.684299
H	2.418702	1.394197	-2.025545
H	3.052253	2.621019	-0.968301

17

*E*elec.= -1952.7467902 a.u.
*G*corr. = 0.369481 a.u.
*E*elec. + *G*corr. = -1952.3773092 a.u.

C	4.085107	-1.065941	0.707483
C	4.737655	0.258411	0.428499
C	3.863336	1.040437	-0.345687
C	2.640719	0.267902	-0.603536
C	2.743150	-0.939668	0.014344
C	4.219184	2.331219	-0.736008
C	5.465602	2.822355	-0.346073
C	6.336691	2.041256	0.417119
C	5.976418	0.748712	0.811052
C	1.506920	0.805944	-1.426517
C	0.469588	1.510610	-0.588452
S	-1.025037	2.031586	-1.302904
C	-1.597766	2.694791	0.205947
C	-0.664704	2.507970	1.189235
C	0.509155	1.833570	0.737471
C	1.788551	-2.030447	0.093488
S	0.097035	-1.869665	-0.299944
C	-0.228861	-3.530387	0.097938
C	0.914255	-4.155584	0.529739
C	2.051166	-3.308555	0.532418
C	-1.579917	-4.095122	-0.029961
C	-2.517922	-3.556686	-0.922136

C	-3.789739	-4.110123	-1.031804
C	-4.144502	-5.214651	-0.259937
C	-3.218100	-5.758045	0.629693
C	-1.949724	-5.201443	0.749851
C	-2.918511	3.333822	0.312085
C	-3.541380	3.920137	-0.798203
C	-4.788596	4.525135	-0.674009
C	-5.431210	4.562516	0.561463
C	-4.819446	3.982485	1.672221
C	-3.578713	3.366957	1.549243
H	3.543981	2.945397	-1.326034
H	5.761898	3.825350	-0.637944
H	7.301541	2.443112	0.711026
H	6.654050	0.144545	1.407978
H	3.040579	-3.630782	0.836845
H	0.941839	-5.200773	0.816558
H	1.354340	1.596290	1.374180
H	-0.802609	2.857867	2.206346
H	-3.042409	3.919245	-1.763846
H	-3.121544	2.893969	2.413055
H	-5.254322	4.975315	-1.545192
H	-5.315918	3.999050	2.637663
H	-6.402620	5.036885	0.658787
H	-2.248826	-2.709652	-1.547741
H	-1.243041	-5.614514	1.463168
H	-4.501894	-3.681562	-1.730031
H	-3.487225	-6.614324	1.240338
H	-5.135424	-5.648269	-0.349867
H	4.668049	-1.903667	0.304467
H	3.963067	-1.252465	1.781092
H	1.035318	-0.002381	-1.997024
H	1.908798	1.505129	-2.170040

Cartesian coordinates and selected energy values for the calculated structures along the pathway of formation of products **18** and **12-indene**

12
*E*elec.= -1952.7174576 a.u.
*G*corr. = 0.365914 a.u.
*E*elec. + *G*corr. = -1952.3515436 a.u.

C	7.465876	-0.917251	0.968042
C	6.659921	-1.525350	-0.003046
C	7.198464	-2.570451	-0.765784
C	8.504132	-3.002131	-0.555147
C	9.298113	-2.391193	0.414595
C	8.774386	-1.346241	1.173404
C	5.267632	-1.074126	-0.214007
C	4.801535	0.256100	0.044412
C	3.471348	0.439159	-0.226878
S	2.758212	-1.041846	-0.806850
C	4.259074	-1.877237	-0.677798
C	2.724617	1.676926	-0.077808
C	1.415163	1.835516	-0.333364
C	0.686656	3.107651	-0.205543
C	-0.700690	3.118491	0.075878
C	-1.366473	4.350190	0.162059
C	-0.694619	5.549697	-0.035154
C	0.671481	5.538932	-0.317822
C	1.347887	4.328921	-0.404144
C	-1.430383	1.862477	0.313748
C	-2.731806	1.678999	0.035142
C	-3.490106	0.465229	0.287526
C	-4.793419	0.234991	-0.065528
C	-5.268682	-1.069137	0.290886
C	-4.296722	-1.801098	0.921039
S	-2.819508	-0.930926	1.086657
C	-6.635731	-1.562122	0.016560
C	-7.708731	-0.667064	-0.084375
C	-8.997626	-1.130403	-0.334243
C	-9.236636	-2.494947	-0.484557
C	-8.175120	-3.393757	-0.387309
C	-6.885626	-2.931792	-0.143985
H	4.308515	-2.929135	-0.928401
H	-4.375300	-2.801660	1.326498
H	2.402865	4.322494	-0.661209
H	1.205530	6.470002	-0.478930
H	-1.231953	6.489740	0.039735
H	-2.421790	4.361943	0.417628
H	-5.387515	0.974397	-0.591919
H	5.435111	1.062839	0.397519
H	-0.859842	1.041418	0.746000
H	0.834205	0.975722	-0.664212

H	-3.305164	2.476115	-0.435817
H	3.316041	2.514990	0.287861
H	-7.537096	0.396960	0.049887
H	-9.817733	-0.422612	-0.405911
H	-10.241846	-2.855573	-0.678646
H	-8.349756	-4.458108	-0.511290
H	-6.060412	-3.636541	-0.094852
H	6.594902	-3.034743	-1.540500
H	8.905817	-3.811470	-1.157086
H	10.318249	-2.725369	0.575243
H	9.383686	-0.865871	1.932787
H	7.060699	-0.114950	1.577823

12-IM1
*E*elec.= -1953.1326228 a.u.
*G*corr. = 0.382759 a.u.
*E*elec. + *G*corr. = -1952.7498638 a.u

C	3.599674	1.226152	0.627946
C	2.389330	1.900786	0.423254
C	2.380378	3.052416	-0.374181
C	3.556149	3.516564	-0.954859
C	4.756733	2.839435	-0.747438
C	4.774110	1.694646	0.046725
C	1.131207	1.387412	1.007684
C	-0.157461	1.722615	0.578309
C	-1.183984	1.042870	1.264813
S	-0.499600	-0.017869	2.482230
C	1.065922	0.466285	2.057228
C	-2.515874	1.107311	0.931624
C	-3.630090	0.369829	1.577974
C	-4.780711	0.049330	0.638070
C	-4.574437	-0.233956	-0.726222
C	-5.682706	-0.447080	-1.555497
C	-6.973867	-0.435700	-1.040677
C	-7.174015	-0.187322	0.315853
C	-6.082791	0.063917	1.141822
C	-3.214057	-0.275984	-1.302883
C	-2.225017	-1.035297	-0.791767
C	-0.829046	-1.001336	-1.172254
C	0.178067	-1.677189	-0.533889
C	1.487543	-1.338608	-0.998271
C	1.432221	-0.406833	-2.005258
S	-0.175721	0.064230	-2.388051
C	2.741984	-1.853316	-0.410977
C	2.755493	-2.357087	0.896644
C	3.948699	-2.764168	1.488286
C	5.147360	-2.676157	0.782810
C	5.141531	-2.191120	-0.524841

C	3.949752	-1.787207	-1.118025
H	2.258734	0.060144	-2.526279
H	1.905745	0.065934	2.615960
H	-5.517686	-0.640166	-2.611664
H	-7.820002	-0.615576	-1.695960
H	-8.178166	-0.168871	0.727063
H	-6.239338	0.289728	2.193041
H	-0.389814	2.420834	-0.218432
H	-0.025651	-2.397930	0.250940
H	-3.265991	-0.526698	2.093102
H	-3.029723	0.349414	-2.177120
H	-2.443353	-1.697147	0.046892
H	1.455276	3.597131	-0.536343
H	3.533627	4.411361	-1.568618
H	5.672824	3.201819	-1.202746
H	5.702107	1.155274	0.209116
H	3.626833	0.317483	1.222670
H	3.956217	-1.419073	-2.139857
H	6.068330	-2.129672	-1.086868
H	6.077940	-2.989248	1.245393
H	3.941113	-3.145066	2.504842
H	1.832348	-2.412843	1.466495
H	-2.779947	1.858974	0.188187
H	-4.008876	1.045250	2.361299

12-TS1
*E*elec.= -1953.1288873 a.u.
*G*corr. = 0.383456 a.u.
*E*elec. + *G*corr. = -1952.7454313 a.u

C	-3.569808	1.250911	-0.594332
C	-2.365448	1.949225	-0.431214
C	-2.368567	3.139791	0.306157
C	-3.547756	3.619414	0.868985
C	-4.740733	2.918308	0.703275
C	-4.747444	1.734186	-0.032358
C	-1.104920	1.418152	-0.993873
C	0.187002	1.714024	-0.490109
C	1.208847	1.037483	-1.137868
S	0.564310	0.027446	-2.407736
C	-1.027952	0.532054	-2.051530
C	2.571875	1.054231	-0.752423
C	3.673365	0.456070	-1.574933
C	4.829819	0.080565	-0.681224
C	4.529841	-0.148801	0.666867
C	5.547275	-0.467190	1.567848
C	6.858835	-0.580408	1.114094
C	7.155369	-0.366556	-0.231954
C	6.143893	-0.031122	-1.128881

C	3.107483	-0.031908	1.081291
C	2.179512	-0.994184	0.763939
C	0.809451	-0.983724	1.148133
C	-0.188478	-1.695531	0.511515
C	-1.494387	-1.372681	0.962182
C	-1.451134	-0.430525	1.970916
S	0.132355	0.073462	2.361047
C	-2.743200	-1.911033	0.384717
C	-2.757321	-2.391644	-0.930971
C	-3.944577	-2.831326	-1.510072
C	-5.133642	-2.796798	-0.783744
C	-5.125800	-2.329905	0.530104
C	-3.939844	-1.892739	1.111872
H	-2.290680	0.011817	2.493922
H	-1.846052	0.169603	-2.662898
H	5.309602	-0.633098	2.614217
H	7.650685	-0.832470	1.811930
H	8.179590	-0.449102	-0.581346
H	6.374734	0.155029	-2.173803
H	0.387876	2.387226	0.336614
H	0.032996	-2.419348	-0.265777
H	3.317822	-0.410580	-2.144795
H	2.859375	0.715764	1.835001
H	2.462282	-1.779122	0.061495
H	-1.448103	3.702420	0.430006
H	-3.533605	4.544687	1.436299
H	-5.658905	3.291581	1.145544
H	-5.669867	1.176312	-0.161537
H	-3.584072	0.313437	-1.143679
H	-3.942885	-1.540717	2.139419
H	-6.045516	-2.308885	1.106269
H	-6.059820	-3.135598	-1.236870
H	-3.940847	-3.194586	-2.532940
H	-1.840933	-2.400486	-1.514212
H	2.846660	1.913833	-0.141523
H	3.983700	1.217632	-2.302673

12-IM2

*E*elec.= -1953.1421846 a.u
*G*corr. = 0.381143 a.u.
*E*elec. + *G*corr. = -1952.7610416 a.u

C	-1.597582	4.964407	0.279715
C	-1.061640	3.759179	-0.193243
C	-1.600920	3.193426	-1.356010
C	-2.650465	3.815941	-2.026336
C	-3.180121	5.011481	-1.544432
C	-2.650178	5.582335	-0.387991
C	0.043037	3.088284	0.525133

C	1.028802	2.257184	-0.109712
C	1.947469	1.739468	0.757527
S	1.613434	2.255901	2.380502
C	0.247093	3.173085	1.876010
C	3.058473	0.762924	0.496488
C	2.591564	-0.731800	0.565286
C	3.640571	-1.432437	-0.287831
C	4.305239	-0.504779	-1.095625
C	3.768768	0.887562	-0.869079
C	5.301318	-0.936626	-1.963813
C	5.610307	-2.297959	-2.013995
C	4.930222	-3.218333	-1.214323
C	3.925860	-2.790919	-0.344858
C	1.291464	-0.906908	-0.124487
C	0.180568	-1.521126	0.371653
C	-1.048725	-1.687608	-0.316330
C	-2.025001	-2.327970	0.435483
C	-1.527459	-2.655548	1.708915
S	0.068371	-2.201339	1.992504
C	-3.399861	-2.630062	-0.011883
C	-4.032072	-1.796436	-0.941777
C	-5.324356	-2.081366	-1.370566
C	-5.997244	-3.196671	-0.874269
C	-5.372255	-4.028530	0.053064
C	-4.078955	-3.748992	0.483182
H	-2.085814	-3.147270	2.499610
H	-0.343482	3.709722	2.607199
H	3.387498	-3.498576	0.279664
H	5.184904	-4.271891	-1.268092
H	6.391820	-2.645052	-2.682790
H	5.835266	-0.227269	-2.589294
H	1.053633	2.077646	-1.179433
H	-1.172594	-1.344076	-1.338530
H	3.060901	1.149880	-1.664557
H	2.557522	-1.095963	1.596049
H	1.217528	-0.522871	-1.143554
H	-1.208151	2.251105	-1.727906
H	-3.058856	3.362037	-2.924023
H	-3.998363	5.496454	-2.067249
H	-3.051346	6.517399	-0.009434
H	-1.174033	5.427014	1.166697
H	-3.589531	-4.412627	1.190133
H	-5.889244	-4.901311	0.438559
H	-7.006037	-3.416527	-1.208783
H	-5.808403	-1.426962	-2.088288
H	-3.519559	-0.914885	-1.316118
H	3.820532	0.856475	1.277236
H	4.543601	1.657294	-0.850745

12-indane
*E*elec.= -1952.7391285 a.u
*G*corr. = 0.369894 a.u.
*E*elec. + *G*corr. = -1952.3692345 a.u

C	-3.536277	3.862455	1.265325
C	-3.587863	2.886249	0.260795
C	-4.289315	3.173289	-0.917621
C	-4.924591	4.400933	-1.084742
C	-4.872338	5.361823	-0.076914
C	-4.176491	5.086469	1.099624
C	-2.920372	1.578878	0.439604
C	-2.421262	0.771897	-0.638783
C	-1.833819	-0.388368	-0.228189
S	-1.886471	-0.524036	1.501824
C	-2.696299	0.987575	1.654515
C	-1.252052	-1.477045	-1.098583
C	-0.237486	-2.344800	-0.357088
C	-0.891609	-3.630266	-0.059098
C	-2.120019	-3.707986	-0.727559
C	-2.350625	-2.478826	-1.568730
C	-2.928003	-4.831945	-0.592306
C	-2.496631	-5.880512	0.220114
C	-1.269628	-5.804498	0.887236
C	-0.459133	-4.680963	0.754697
C	1.029190	-2.041631	-0.017244
C	1.796394	-0.831973	-0.249110
C	3.128076	-0.692920	0.060265
C	3.680143	0.577707	-0.289683
C	2.736394	1.391711	-0.862435
S	1.194343	0.639616	-0.969123
C	5.087656	0.968108	-0.058336
C	5.819201	0.402492	0.994058
C	7.142125	0.773745	1.218250
C	7.755286	1.717856	0.396888
C	7.035855	2.286230	-0.653563
C	5.715529	1.911918	-0.882297
H	2.855250	2.414936	-1.195266
H	-2.978660	1.350598	2.634088
H	0.486385	-4.622407	1.286530
H	-0.950264	-6.626422	1.520341
H	-3.119270	-6.761812	0.339208
H	-3.880800	-4.892347	-1.110725
H	-2.468165	1.062058	-1.683577
H	3.700554	-1.500869	0.503430
H	-3.355265	-2.064691	-1.451528
H	1.603612	-2.807014	0.503245
H	-4.352015	2.424629	-1.702025
H	-5.466035	4.604470	-2.003552

H	-5.367570	6.318790	-0.207857
H	-4.122782	5.831457	1.887617
H	-2.975120	3.665401	2.174339
H	5.169639	2.341596	-1.717458
H	7.507176	3.016915	-1.303685
H	8.786709	2.007047	0.572108
H	7.692651	0.327573	2.040755
H	5.344239	-0.319666	1.651723
H	-0.794608	-0.989375	-1.966060
H	-2.213843	-2.715735	-2.629507

12-IM3

*E*elec.= -1953.152692 a.u
*G*corr. = 0.385206 a.u.
*E*elec. + *G*corr. = -1952.767486 a.u

C	-3.838255	2.409391	-0.094643
C	-2.776016	1.727796	0.513683
C	-3.064123	0.780938	1.505087
C	-4.381714	0.497570	1.852867
C	-5.432736	1.165111	1.225770
C	-5.154950	2.128550	0.256810
C	-1.383959	1.933822	0.060199
C	-0.214665	1.666447	0.850494
C	0.951914	1.858162	0.174245
S	0.651162	2.404543	-1.445075
C	-1.051641	2.333598	-1.207660
C	2.346744	1.619710	0.667457
C	3.093846	0.491586	0.047241
C	2.488197	-0.594534	-0.798377
C	3.635735	-1.606494	-1.023262
C	4.839243	-0.911663	-0.480959
C	4.471055	0.297284	0.174398
C	6.173169	-1.290773	-0.531327
C	7.106856	-0.472434	0.096301
C	6.748655	0.721848	0.765618
C	5.436569	1.123028	0.810742
C	1.192283	-1.139532	-0.269928
C	-0.015026	-1.195097	-0.898936
C	-1.063327	-1.720509	-0.069081
C	-0.600155	-2.048329	1.178370
S	1.083632	-1.743692	1.353929
C	-2.484961	-1.828753	-0.461869
C	-3.334300	-2.748591	0.167003
C	-4.694131	-2.774769	-0.127533
C	-5.227585	-1.885898	-1.059614
C	-4.387202	-0.979542	-1.704737
C	-3.026422	-0.954042	-1.412686
H	-1.715998	2.577739	-2.026488

H	-1.162756	-2.440613	2.015721
H	5.141871	2.041941	1.307065
H	7.522871	1.318667	1.233672
H	8.154330	-0.757975	0.074710
H	6.479597	-2.201258	-1.034127
H	-0.157193	-0.859351	-1.921205
H	-0.242341	1.329035	1.881563
H	3.452990	-2.530641	-0.463732
H	2.966863	2.521703	0.592582
H	-2.386090	-0.219784	-1.894475
H	-4.793603	-0.280568	-2.429610
H	-6.289577	-1.901314	-1.283835
H	-5.338076	-3.492561	0.371333
H	-2.925519	-3.450015	0.888835
H	-3.632316	3.166532	-0.845851
H	-5.966120	2.663329	-0.227683
H	-6.460377	0.939016	1.492716
H	-4.587307	-0.255677	2.607519
H	-2.253691	0.229643	1.974220
H	2.255629	-0.105740	-1.759467
H	3.754710	-1.881374	-2.074243
H	2.306821	1.392395	1.744977

18

*E*elec.= -1952.7454483 a.u
*G*corr. = 0.368843 a.u.
*E*elec. + *G*corr. = -1952.3766053 a.u

C	5.102698	2.705735	0.537817
C	3.798071	2.193977	0.511396
C	2.935429	2.500129	1.572163
C	3.364763	3.299449	2.628193
C	4.661806	3.808786	2.641115
C	5.528483	3.509474	1.590537
C	3.335250	1.353024	-0.613231
C	2.304997	0.354778	-0.501687
C	2.042808	-0.293470	-1.670975
S	3.056112	0.310360	-2.947197
C	3.826841	1.431114	-1.887203
C	1.035281	-1.382011	-1.944889
C	0.455447	-1.955014	-0.685740
C	-0.697659	-1.628225	-0.046481
C	-0.897545	-2.511749	1.169134
C	0.328697	-3.381752	1.161696
C	1.123606	-3.031517	0.057400
C	0.729186	-4.385884	2.030220
C	1.943715	-5.035825	1.788614
C	2.737379	-4.682778	0.694487
C	2.335806	-3.675994	-0.184228

C	-1.677704	-0.601053	-0.363988
C	-2.963552	-0.532790	0.110460
C	-3.683781	0.624373	-0.325630
C	-2.910497	1.426231	-1.124834
S	-1.327340	0.795925	-1.349334
C	-5.088162	0.915430	0.035663
C	-5.557689	2.234908	0.088391
C	-6.883087	2.503431	0.415310
C	-7.760974	1.459327	0.704092
C	-7.302556	0.144156	0.660686
C	-5.978119	-0.126392	0.327678
H	4.581952	2.104706	-2.271001
H	-3.195659	2.346431	-1.618303
H	2.957479	-3.399911	-1.031951
H	3.678879	-5.197127	0.527717
H	2.275250	-5.821790	2.460080
H	0.116623	-4.661938	2.883952
H	-3.380639	-1.285322	0.770767
H	1.795481	0.115614	0.425824
H	-0.980441	-1.914606	2.084913
H	0.240321	-0.995458	-2.592361
H	-5.635982	-1.155965	0.277917
H	-7.978820	-0.676132	0.880800
H	-8.793795	1.669907	0.963109
H	-7.228773	3.531837	0.454085
H	-4.874517	3.055586	-0.111173
H	5.791623	2.456517	-0.264251
H	6.543501	3.894770	1.595586
H	4.996291	4.431893	3.464556
H	2.681488	3.528788	3.440116
H	1.916572	2.123709	1.561861
H	-1.820158	-3.100376	1.090418
H	1.519364	-2.190973	-2.505236

Cartesian coordinates and selected energy values for the calculated structures of **13** and **14**

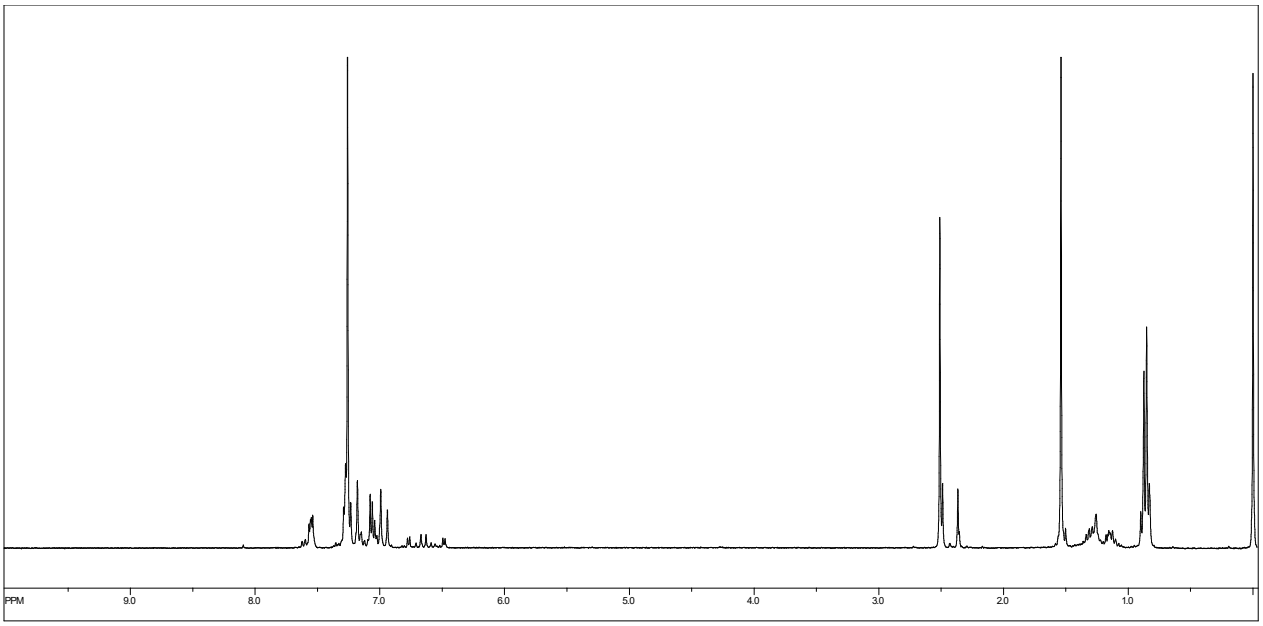
13
*E*elec.= -1899.6401972 a.u
*G*corr. = 0.214280 a.u
*E*elec. + *G*corr. = -1899.4259172 a.u.

C	-2.741457	-0.242415	-4.085704
C	-2.530941	0.152377	-2.780079
S	-3.926703	0.946611	-2.113961
C	-4.761223	0.721093	-3.608340
C	-4.028955	0.082617	-4.569310
C	-1.310278	-0.054556	-2.022573
C	-1.132483	0.278412	-0.732634
C	0.123826	0.089659	0.007255
C	0.115902	-0.102394	1.409616
C	1.337533	-0.254110	2.081758
C	2.545634	-0.205769	1.398863
C	2.553802	-0.007819	0.017960
C	1.353797	0.140051	-0.664911
C	-1.151682	-0.186833	2.149531
C	-1.301368	0.159686	3.439469
C	-2.534926	0.054190	4.197005
C	-2.712127	0.465043	5.502620
C	-4.022041	0.247356	5.986259
C	-4.804509	-0.328557	5.025322
S	-3.991470	-0.622204	3.530937
N	-6.177909	-0.689099	5.166746
O	-6.718742	-0.470420	6.239869
N	-6.100198	1.193718	-3.749724
O	-6.657247	1.020441	-4.822844
O	-6.610276	1.746522	-2.782569
O	-6.731875	-1.197968	4.199618
H	1.365493	0.330299	-1.733631
H	3.492990	0.038435	-0.523709
H	3.477813	-0.329367	1.940514
H	1.333510	-0.444675	3.150478
H	-2.013091	-0.561334	1.597813
H	-1.960041	0.722708	-0.180893
H	-0.467073	0.574465	4.001698
H	-0.513065	-0.536753	-2.584826
H	-1.982411	-0.752276	-4.666731
H	-4.406228	-0.134569	-5.560581
H	-1.913592	0.910559	6.083618
H	-4.380091	0.494959	6.977530

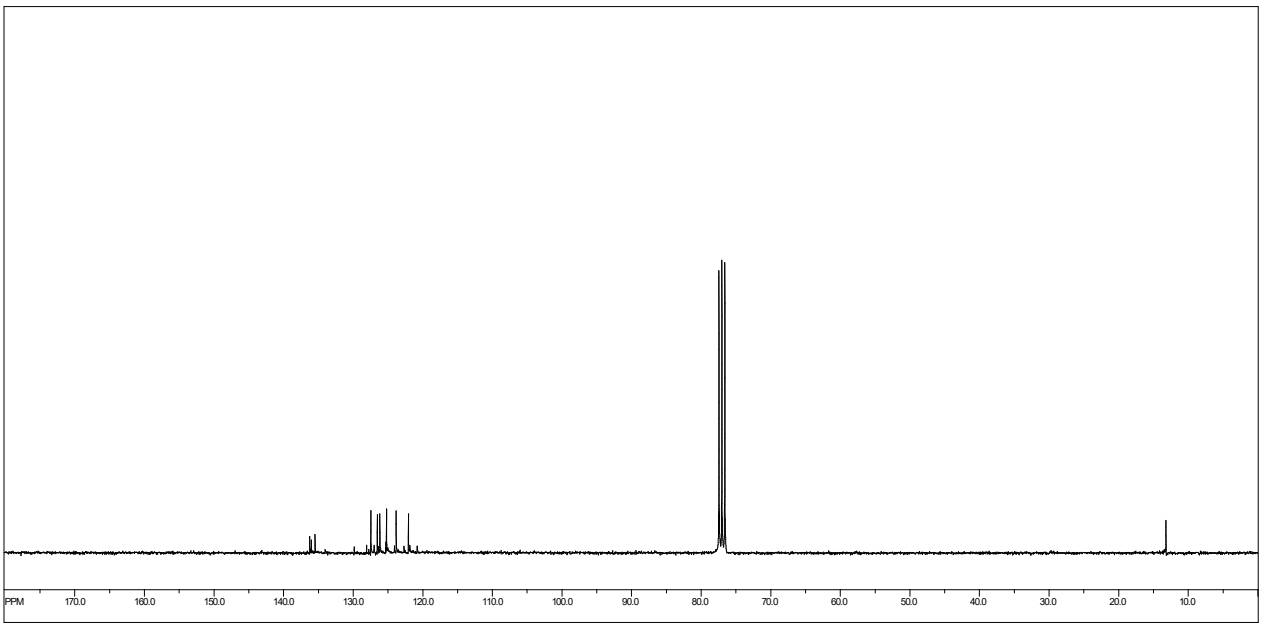
14

*E*elec.= -849.0903098 a.u
*G*corr. = 0.284545 a.u
*E*elec. + *G*corr. = -848.8057648 a.u.

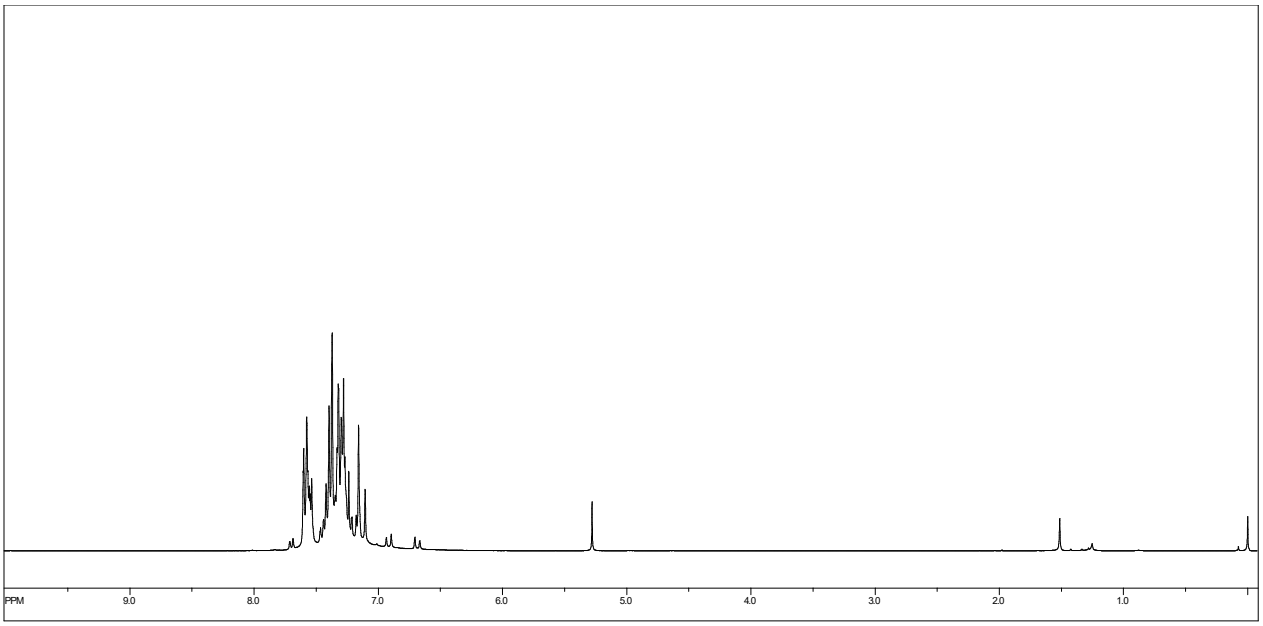
C	-5.137104	-2.946030	-0.386103
C	-3.995716	-2.887709	0.415110
C	-3.189883	-1.755108	0.411421
C	-3.506752	-0.655715	-0.402677
C	-4.661544	-0.724317	-1.194826
C	-5.468624	-1.858211	-1.190453
C	-2.689834	0.566293	-0.456851
C	-1.462500	0.725683	0.063555
C	-0.708062	1.991613	0.019285
C	0.706903	1.992095	-0.004999
C	1.384297	3.220239	-0.020634
C	0.695889	4.426658	0.000509
C	-0.698412	4.426162	0.030737
C	-1.386145	3.219238	0.043474
C	1.462050	0.726927	-0.058087
C	2.689482	0.564603	0.461179
C	3.507078	-0.656543	0.398485
C	3.190820	-1.750404	-0.423267
C	3.997280	-2.882505	-0.434855
C	5.138699	-2.945785	0.365938
C	5.469616	-1.863420	1.177859
C	4.661908	-0.730031	1.190141
H	-2.470274	3.220946	0.106051
H	-1.246985	5.362645	0.053332
H	1.243936	5.363584	-0.015561
H	2.468424	3.222991	-0.083195
H	0.974032	-0.109824	-0.553534
H	-0.974020	-0.114222	0.553176
H	3.142173	1.391053	1.008376
H	-3.142978	1.396282	-0.998287
H	2.316772	-1.712431	-1.066586
H	4.921163	0.114599	1.823316
H	3.739443	-3.718757	-1.077693
H	6.357821	-1.900026	1.801212
H	5.766594	-3.831252	0.352107
H	-2.315851	-1.721142	1.054986
H	-4.921268	0.124567	-1.822092
H	-3.737413	-3.728284	1.052096
H	-6.356811	-1.890958	-1.814045
H	-5.764508	-3.831921	-0.378451



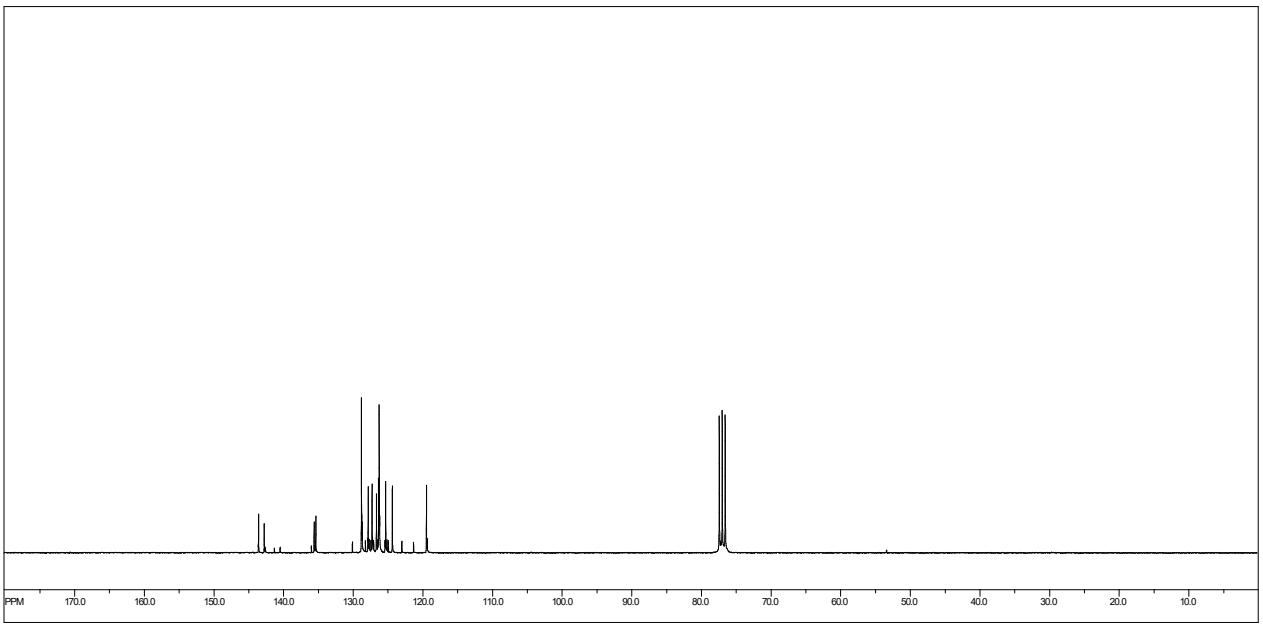
^{1}H NMR spectrum of ***tt*-9** ($CDCl_3$; 75 MHz)



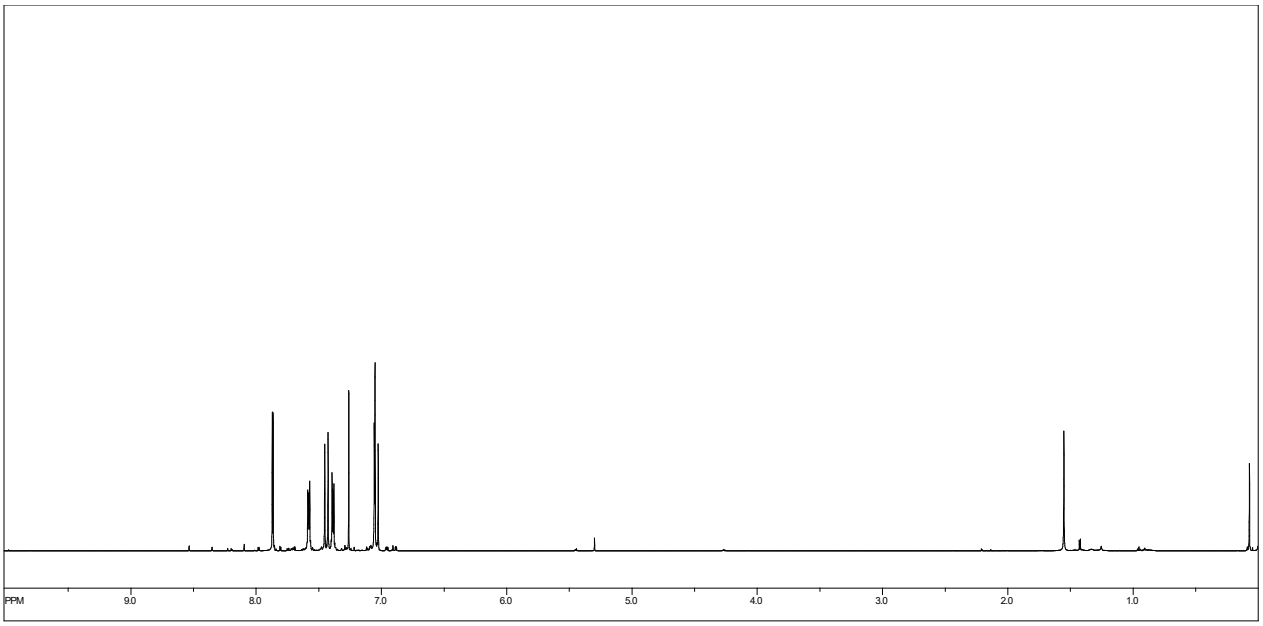
^{13}C NMR spectrum of ***tt*-9** ($CDCl_3$; 75 MHz)



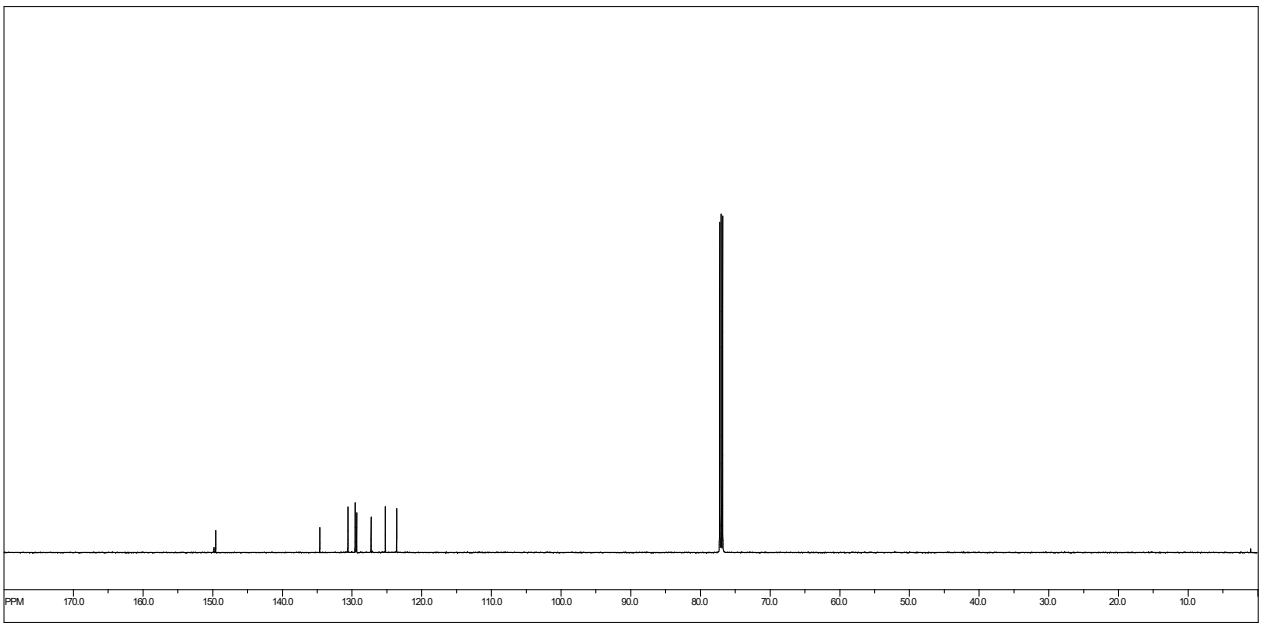
^{1}H NMR spectrum of ***tt*-12** ($CDCl_3$; 75 MHz)



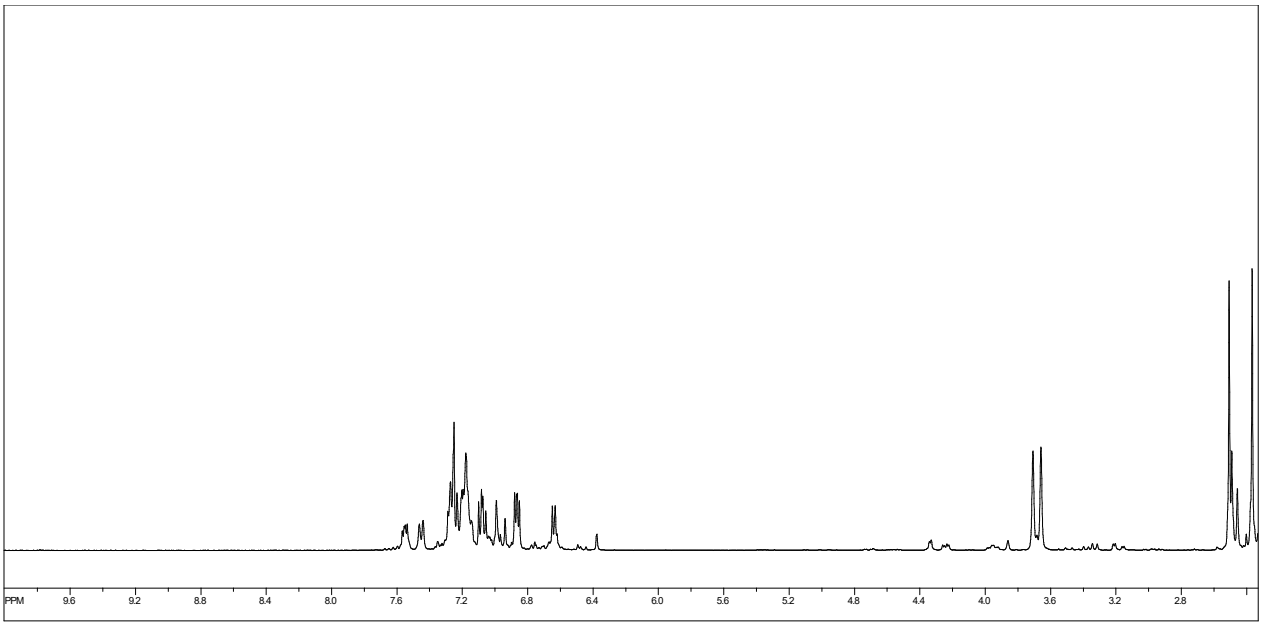
^{13}C NMR spectrum of ***tt*-12** ($CDCl_3$; 75 MHz)



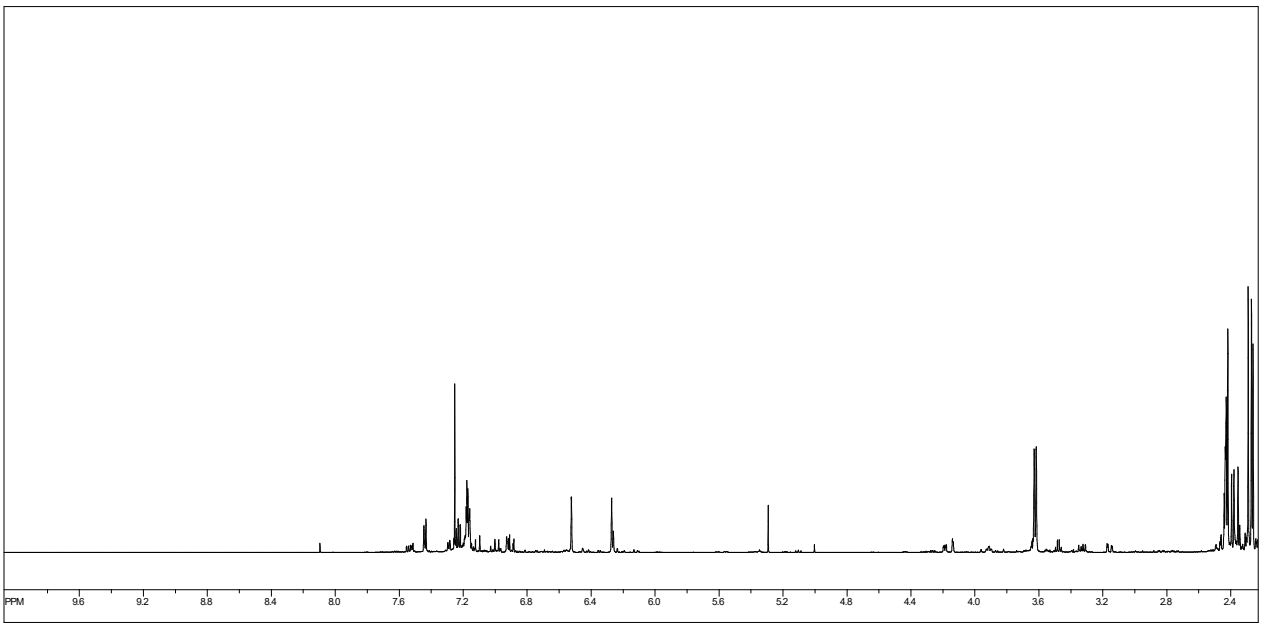
^{1}H NMR spectrum of ***tt*-13** ($CDCl_3$; 75 MHz)



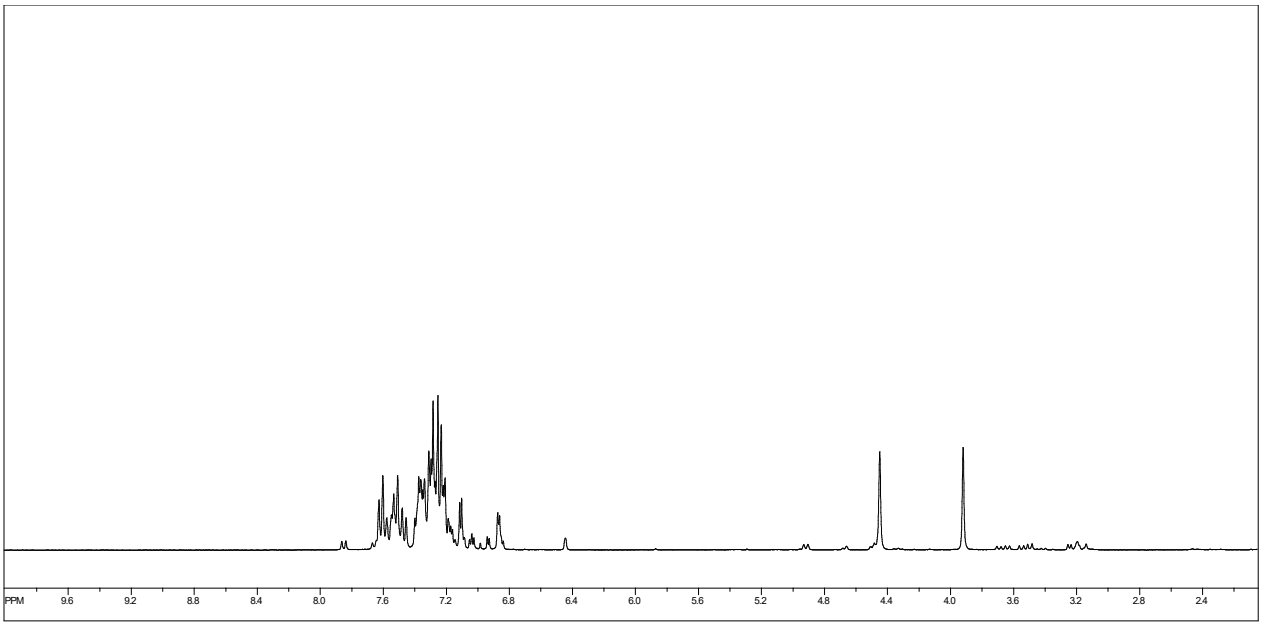
^{13}C NMR spectrum of ***tt*-13** ($CDCl_3$; 75 MHz)



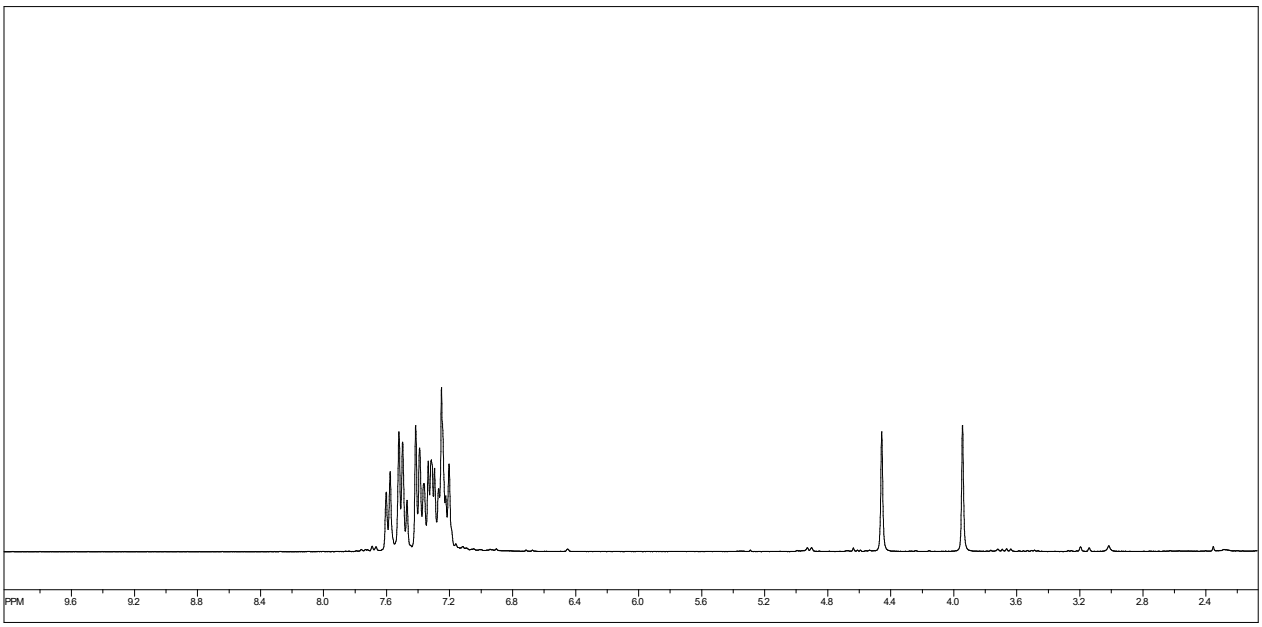
^{1}H NMR spectrum of **15** ($CDCl_3$; 75 MHz)



^{1}H NMR spectrum of **16** with 10% of indane derivatives ($CDCl_3$; 75 MHz)



^{1}H NMR spectrum of **17** ($CDCl_3$; 75 MHz)



^{1}H NMR spectrum of **18** ($CDCl_3$; 75 MHz)