Supporting Information

for

Mechanistic insights into the thermal transformations of heterocyclic *o*-distyrylbenzenes: An experimental and computational study

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Additional Figures and Table and Cartesian coordinates with selected energy values

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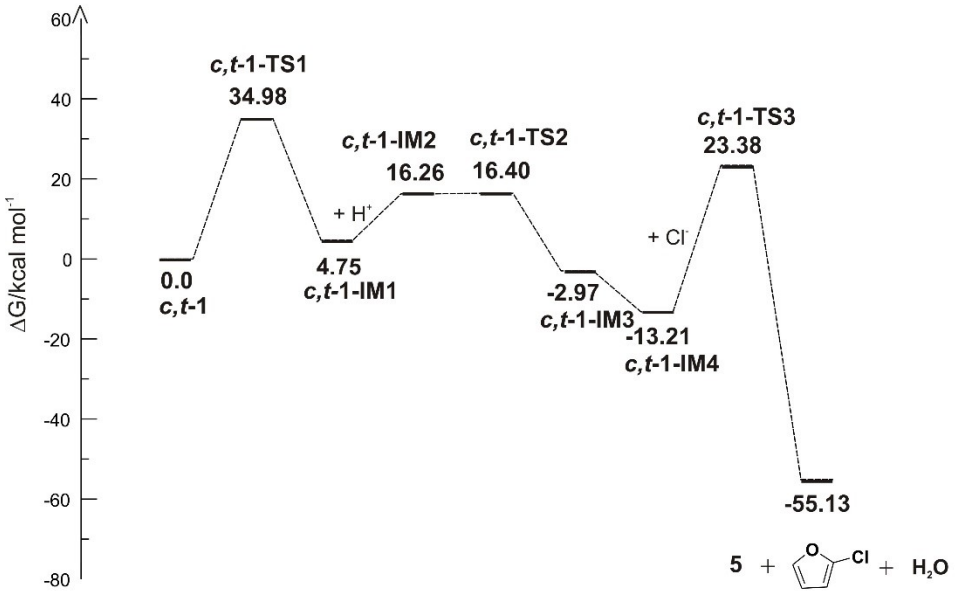


Figure S1 Free energy profile for the possible reaction route of formation of product **5** starting from *cis,trans*-isomer of **1** (***c,t*-1**)

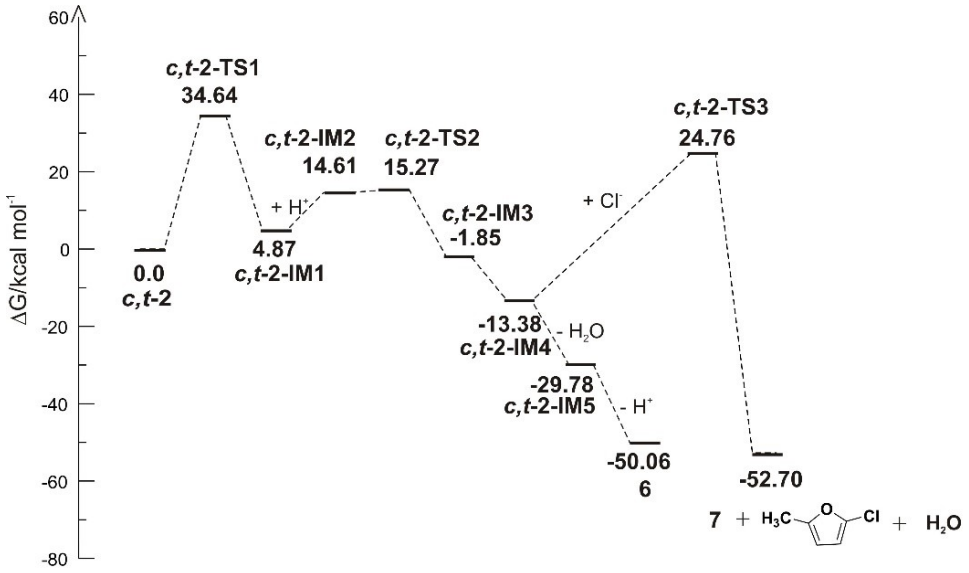


Figure S2 Free energy profiles for the possible reaction routes of formation of products **6** and **7** starting from *cis,trans*-isomer of **2** (***c,t*-2**)

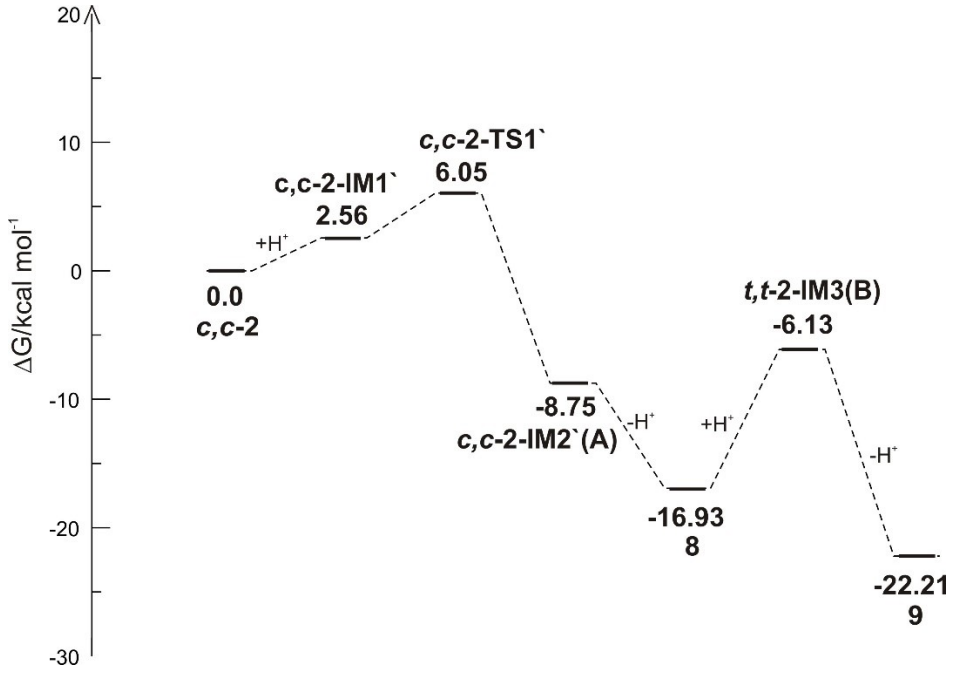


Figure S3 Free energy profile for the possible reaction routes of formation of products **8** and **9** starting from *cis,cis*-isomer of **2** (***c,c*-2**)

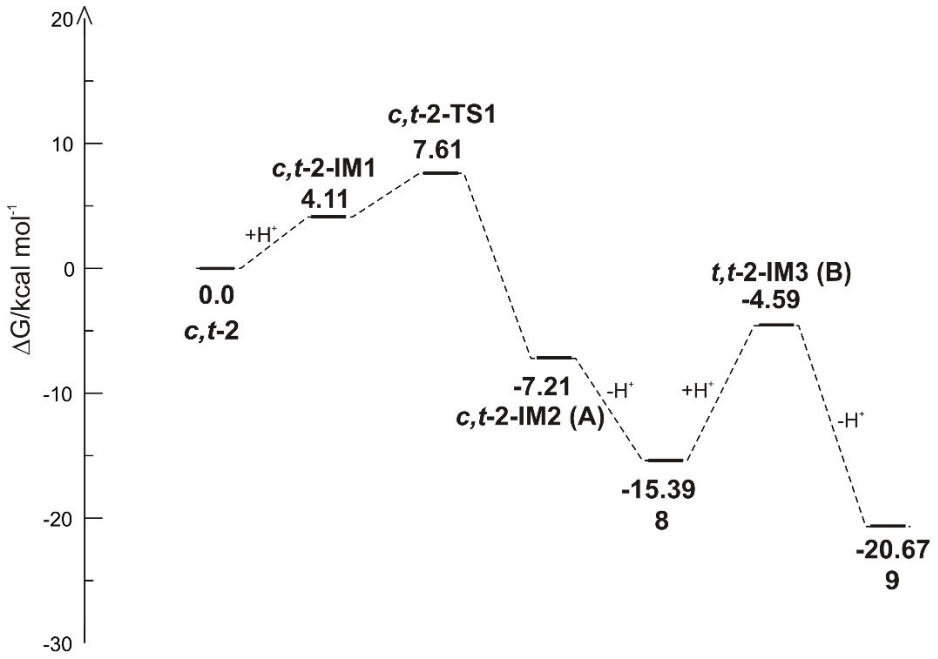


Figure S4 Free energy profile for the possible reaction routes of formation of products **8** and **9** starting from *cis,trans*-isomer of **2** (***c,t*-2**) (protonated at *trans* arm)

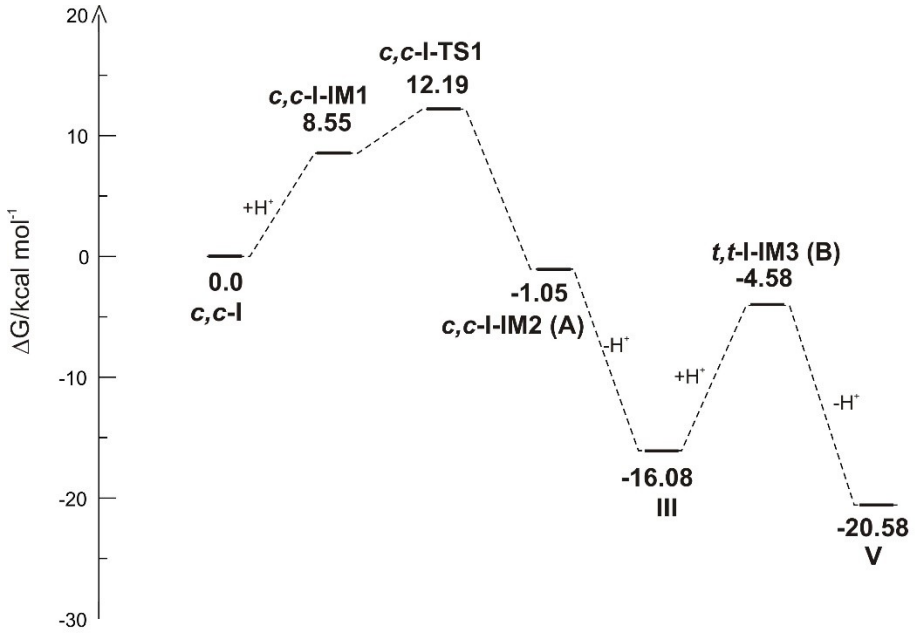


Figure S5 The free energy profiles for the possible reaction routes of formation of products **III** and **V** strating from *cis,cis*-isomer of **I** (***c,c*-I**)

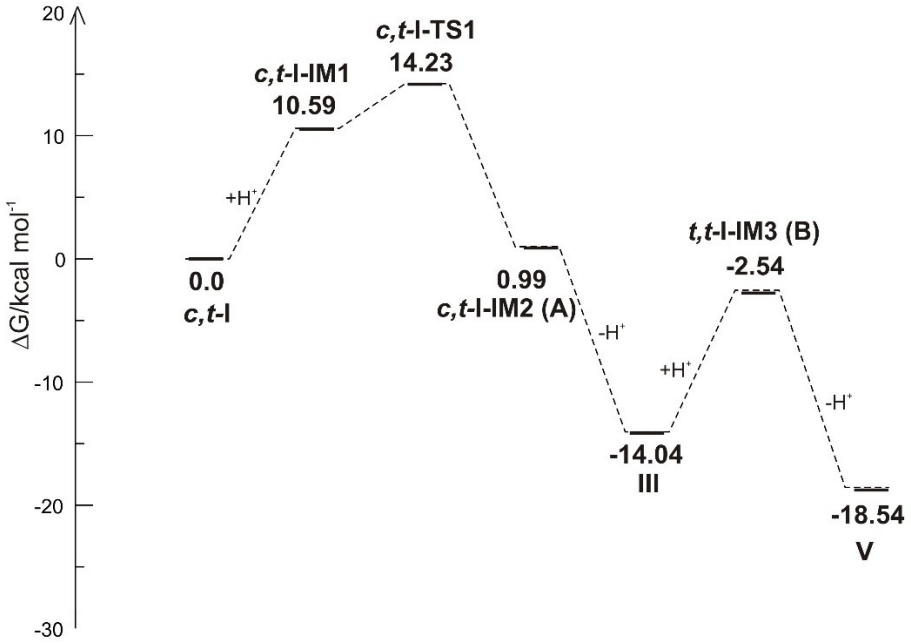


Figure S6 The free energy profiles for the possible reaction routes of formation of products **III** and **V** strating from *cis,trans*-isomer of **I** (***c,t*-I**) (protonated at *trans* arm)

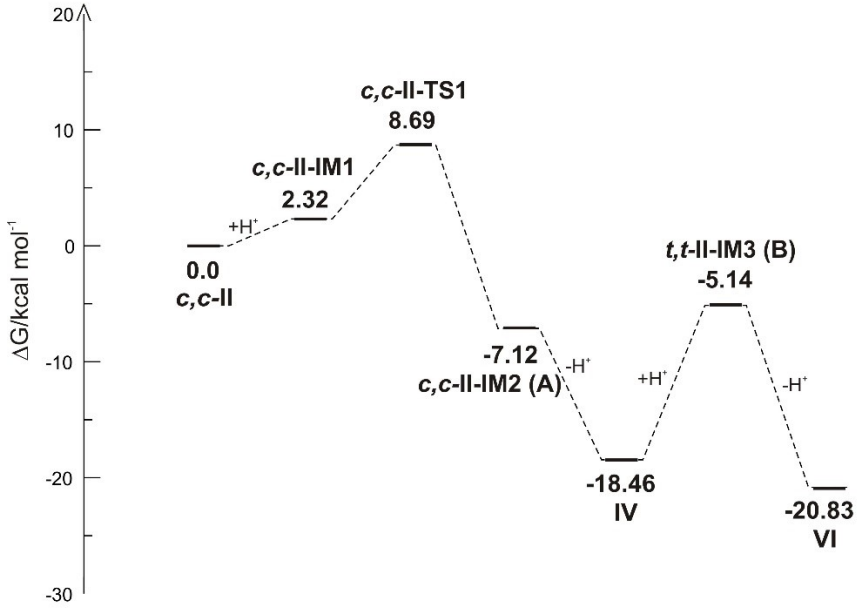


Figure S7 The free energy profiles for the possible reaction routes of formation of products **IV** and **VI** strating from *cis,cis*-isomer of **II (*c,c*-II)**

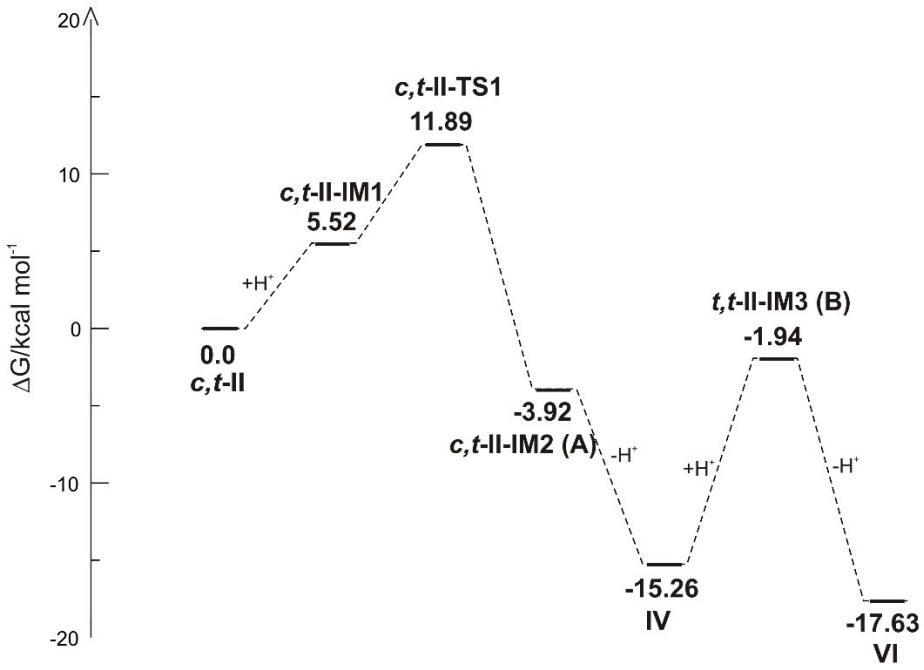


Figure S8 The free energy profiles for the possible reaction routes of formation of products **IV** and **VI** strating from *cis,trans*-isomer of **II** (***c,t*-II**) (protonated at *trans* arm)

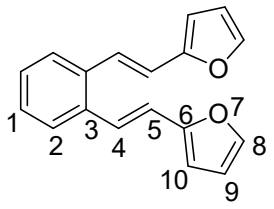
Table S1 Relative Gibbs free energies (in kcal mol^{-1}) of the *trans,trans*-, *cis,trans*- and *cis,cis*-isomers of derivatives **1**, **2**, **I** and **II**

Molecule	***trans,trans*-isomer**	***cis,trans*-isomer**	***cis,cis*-isomer**
1	0.0	1.85	5.04
2	0.0	3.15	6.63
I	0.0	3.01	5.05
II	0.0	3.02	6.10

Table S2 Kinetic barrier $\Delta G^{\ddagger}$ associated with possible intramolecular 6π-cyclization within the ***c,c*-4**, ***c,c*-I** and ***c,c*-II** systems

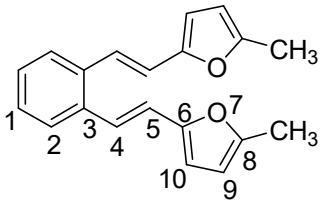
Molecule	$\Delta G^{\ddagger}$/ kcal mol^{-1}
***c,c*-4**	43.81
***c,c*-I**	40.27
***c,c*-II**	40.71

Table S3: 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 ***t,t*-1**, ***t,t*-2**, ***t,t*-3**, ***t,t*-4**, ***t,t*-I**, ***t,t*-II**, ***t,t*-VII** and ***t,t*-VIII**



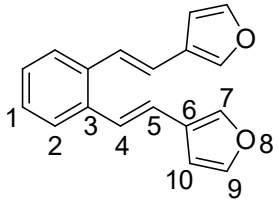
***t,t*-1**

Protonation position	G^*	$G^*_{relat.}$
1	-844.8365467	16.80
2	-844.8336262	18.63
3	-844.8262657	23.25
4	*-844.8537368*	*6.01*
5	-844.8392050	15.13
6	-844.8374307	16.25
7	-844.8092091	33.96
8	**-844.8633212**	**0.00**
9	-844.8357159	17.32
10	-844.8515039	7.41



***t,t*-2**

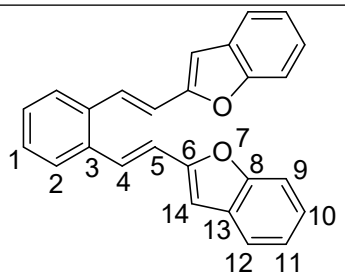
Protonation position	G^*	$G^*_{relat.}$
1	-923.4194813	13.73
2	-923.4167619	15.43
3	-923.4092835	20.13
4	***-923.4413563***	***0.0***
5	-923.4208169	12.89
6	-923.4298060	7.24
7	-923.3948375	29.19
8	-923.4410216	0.21
9	-923.4292491	7.59
10	-923.4351649	3.89



***t,t*-3**

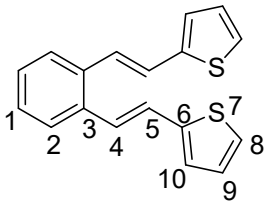
Protonation position	G^*	$G^*_{relat.}$

1	-844.8262632	17.60
2	-844.8237957	19.15
3	-844.8158596	24.13
4	*-844.8391337*	*9.53*
5	-844.8308476	14.73
6	-844.8127738	26.07
7	**-844.8543150**	**0.00**
8	-844.7998621	34.17
9	-844.8391803	9.49
10	-844.8283468	16.30



***t,t*-4**

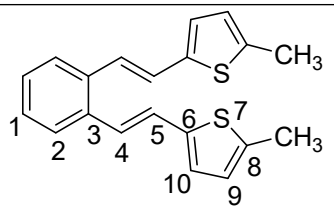
Protonation position	G^*	$G^*_{relat.}$
1	-1152.0269009	14.12
2	-1152.0237974	16.06
3	-1152.0134688	22.55
4	*-1152.0427026*	*4.20*
5	-1152.0305325	11.84
6	-1152.0213066	17.63
7	-1152.0039130	28.54
8	-1152.0136101	22.46
9	-1152.0228444	16.66
10	-1152.0342636	9.50
11	-1152.0275464	13.71
12	-1152.031821	11.03
13	-1152.0034397	28.84
14	**-1152.0493984**	**0.00**



***t,t*-I**

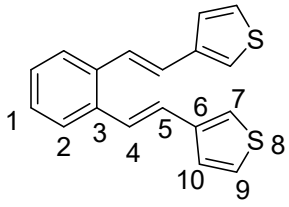
Protonation position	G^*	$G^*_{relat.}$
1	-1490.8024177	10.78
2	-1490.8001415	12.21
3	-1490.7921842	17.20
4	***-1490.8195917***	***0.0***
5	-1490.8065215	8.20
6	-1490.7988417	13.02
7	-1490.7804996	24.53
8	-1490.8172810	1.45

9	-1490.8000069	12.29
10	-1490.8119636	4.79



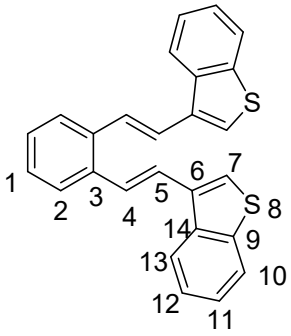
***t,t*-II**

Protonation position	G^*	$G^*_{relat.}$
1	-1569.3746772	12.66
2	-1569.3700643	15.55
3	-1569.3631918	19.86
4	***-1569.3948461***	***0.0***
5	-1569.3763753	11.59
6	-1569.3776035	10.82
7	-1569.3569603	23.77
8	-1569.3907201	2.59
9	-1569.3795992	9.57
10	-1569.3858918	5.62



***t,t*-VII**

Protonation position	G^*	$G^*_{relat.}$
1	-1490.8004242	13.28
2	-1490.7985741	14.44
3	-1490.7883539	20.85
4	*-1490.8127403*	*5.55*
5	-1490.8051796	10.30
6	-1490.7847634	23.11
7	**-1490.8215880**	**0.00**
8	-1490.7799084	26.15
9	-1490.8082904	8.34
10	-1490.8006690	13.13



***t,t*-VIII**

Protonation position	G^*	$G^*_{relat.}$
1	-1797.9852501	12.75

2	-1797.9814356	15.14
3	-1797.9742659	19.64
4	*-1798.0025511*	*1.89*
5	-1797.9930497	7.85
6	-1797.9768226	18.03
7	**-1798.0055613**	**0.00**
8	-1797.9702002	22.19
9	-1797.9609755	27.98
10	-1797.9783050	17.10
11	-1797.9819138	14.84
12	-1797.9793443	16.45
13	-1797.9822530	14.63
14	-1797.9577155	30.02

12. Cartesian coordinates and selected energy values for the calculated structures

12.1. Cartesian coordinates and selected energy values for the calculated structures along the pathway of formation of product **5**

***c,c*-1**
*E*elec.= -844.6713528 a.u.
*G*corr. = 0.226708 a.u.
*E*elec. + *G*corr. = -844.4446448 a.u.

1	6	0	-0.461094	0.539619	2.286292
2	6	0	0.040616	-0.773024	2.424791
3	6	0	0.281510	-1.270930	3.711974
4	6	0	0.026940	-0.505588	4.843681
5	6	0	-0.457615	0.794824	4.705607
6	6	0	-0.685382	1.310112	3.435410
7	1	0	0.692536	-2.270493	3.815223
8	1	0	0.224739	-0.914826	5.829584
9	1	0	-0.646987	1.406191	5.582566
10	1	0	-1.053937	2.326046	3.319262
11	6	0	-0.706192	1.167528	0.970438
12	6	0	0.431995	-1.558637	1.237136
13	6	0	-1.362758	0.669945	-0.092276
14	6	0	0.189091	-2.851891	0.962974
15	6	0	-2.105965	-0.571286	-0.203553
16	6	0	-0.645405	-3.813068	1.656977
17	8	0	-2.544502	-1.204076	0.917983
18	6	0	-3.201536	-2.319623	0.526268
19	6	0	-3.209850	-2.419264	-0.829790
20	6	0	-2.502764	-1.272918	-1.308778
21	1	0	-2.302254	-0.999354	-2.335041
22	1	0	-3.664616	-3.206625	-1.412875
23	1	0	-3.613876	-2.931896	1.315729
24	8	0	-1.363372	-3.454290	2.755513
25	6	0	-2.102466	-4.526443	3.130782
26	6	0	-1.876074	-5.576760	2.297951
27	6	0	-0.926351	-5.114397	1.336149
28	1	0	-0.508563	-5.661769	0.503086
29	1	0	-2.328102	-6.555623	2.363052
30	1	0	-2.724338	-4.391534	4.003422
31	1	0	-0.306876	2.175022	0.864742
32	1	0	0.996581	-1.006647	0.487301
33	1	0	-1.380326	1.266033	-1.001726
34	1	0	0.618761	-3.260945	0.051478

***c,c*-1-TS1**
*E*elec.= -844.6195899 a.u.
*G*corr. = 0.229633 a.u.
*E*elec. + *G*corr. = -844.3899569 a.u.

1	6	0	0.346486	-2.288777	-0.201151
2	6	0	0.545608	-1.181016	0.646877
3	6	0	1.822198	-0.990229	1.191842
4	6	0	2.885437	-1.837405	0.894148
5	6	0	2.689017	-2.916840	0.036346
6	6	0	1.425455	-3.137003	-0.494903
7	1	0	1.978126	-0.151770	1.864397
8	1	0	3.861132	-1.654596	1.333938
9	1	0	3.507470	-3.586913	-0.207141
10	1	0	1.254400	-3.985116	-1.152857
11	6	0	-0.953584	-2.638608	-0.789211
12	6	0	-0.547345	-0.246279	1.092926
13	6	0	-2.058712	-1.889037	-0.790679
14	6	0	-0.376123	1.155751	1.032333
15	6	0	-2.123975	-0.525830	-0.224887
16	6	0	0.666672	1.816767	0.256013
17	8	0	-1.703683	0.488984	-1.057352
18	6	0	-2.001474	1.620887	-0.375179
19	6	0	-3.083048	1.366021	0.494862
20	6	0	-3.178820	-0.001493	0.578413
21	1	0	-3.803140	-0.592221	1.235122
22	1	0	-3.618051	2.114102	1.063659
23	1	0	-1.704647	2.550410	-0.843206
24	8	0	0.904683	3.116028	0.600697
25	6	0	1.824608	3.615390	-0.265374
26	6	0	2.181407	2.667287	-1.167599
27	6	0	1.429058	1.493651	-0.834293
28	1	0	1.448468	0.538268	-1.337037
29	1	0	2.895493	2.782347	-1.970388
30	1	0	2.122139	4.640492	-0.103477
31	1	0	-0.995095	-3.615321	-1.267643
32	1	0	-1.041612	-0.604910	1.993468
33	1	0	-2.964958	-2.272249	-1.253672
34	1	0	-0.743598	1.755889	1.856732

***c,c*-1-IM1**
*E*elec.= - 844.6725872a.u.
*G*corr. = 0.234420a.u.
*E*elec. + *G*corr. = -844.4381672 a.u.

1	6	0	2.636142	0.223434	-0.003040
2	6	0	1.349219	0.653752	0.369575
3	6	0	1.122026	2.021564	0.537508
4	6	0	2.127336	2.954749	0.298198
5	6	0	3.393923	2.527841	-0.099213
6	6	0	3.643620	1.168207	-0.237740
7	1	0	0.140112	2.363694	0.852288
8	1	0	1.920974	4.013204	0.424262
9	1	0	4.181748	3.249389	-0.291697
10	1	0	4.630963	0.820479	-0.530949
11	6	0	2.939743	-1.208519	-0.128193
12	6	0	0.267242	-0.358228	0.678541
13	6	0	2.004210	-2.157812	-0.040777
14	6	0	-1.158901	-0.108858	0.040256
15	6	0	0.568203	-1.799238	0.133658
16	6	0	-1.219235	0.967283	-0.990504
17	8	0	-0.109327	-1.781682	-1.140066
18	6	0	-1.411078	-1.499570	-0.628264
19	6	0	-1.562416	-2.535046	0.472412
20	6	0	-0.331166	-2.731589	0.939111
21	1	0	-0.003143	-3.320509	1.787572
22	1	0	-2.502988	-2.928413	0.837583
23	1	0	-2.154482	-1.487913	-1.424416
24	8	0	-1.828333	2.127946	-0.625686
25	6	0	-1.744496	2.984117	-1.677435
26	6	0	-1.103901	2.389928	-2.715462
27	6	0	-0.760930	1.070363	-2.268041
28	1	0	-0.223081	0.302245	-2.804565
29	1	0	-0.899995	2.832585	-3.679788
30	1	0	-2.191218	3.956497	-1.534428
31	1	0	3.979895	-1.475628	-0.301890
32	1	0	0.163214	-0.399387	1.767657
33	1	0	2.253251	-3.209799	-0.148025
34	1	0	-1.899680	0.112022	0.811829

***c,c*-1-IM2**
*E*elec.= -845.085261 a.u.
*G*corr. = 0.246291 a.u.
*E*elec. + *G*corr. = -844.838970 a.u.

1	6	0	-0.009089	0.046290	-0.090929
2	6	0	0.056880	-0.111989	1.404006
3	6	0	1.523851	-0.043930	1.902215
4	6	0	1.959257	1.417490	1.463005
5	6	0	0.646596	2.024151	0.905744
6	6	0	0.311544	1.304935	-0.378508
7	8	0	-0.416744	1.250920	1.790992
8	6	0	0.415579	3.471004	1.051848
9	6	0	1.150223	4.174807	1.924646
10	6	0	2.240992	3.599248	2.713618
11	6	0	2.647269	2.269573	2.507277
12	6	0	3.748394	1.779298	3.209550
13	6	0	4.406929	2.576294	4.142732
14	6	0	3.982925	3.884582	4.372878
15	6	0	2.912459	4.394887	3.650305
16	6	0	1.569841	-0.286467	3.370874
17	6	0	2.212892	-1.164330	4.177501
18	6	0	1.808969	-0.849829	5.521197
19	6	0	0.946238	0.189001	5.431548
20	8	0	0.784754	0.544016	4.122768
21	1	0	4.096283	0.767538	3.024526
22	1	0	5.256700	2.175829	4.686334
23	1	0	4.494214	4.505721	5.101062
24	1	0	2.585149	5.420219	3.798963
25	1	0	0.412967	1.778927	-1.346540
26	1	0	-0.243840	-0.766029	-0.765215
27	1	0	-0.576990	-0.860614	1.874387
28	1	0	2.898745	-1.935078	3.856559
29	1	0	2.124720	-1.339773	6.430491
30	1	0	0.383928	0.763405	6.151627
31	1	0	0.954794	5.236195	2.057328
32	1	0	2.642500	1.324408	0.613649
33	1	0	-0.382676	3.918584	0.470163
34	1	0	2.124541	-0.804543	1.402987
35	1	0	-0.277836	1.415504	2.757013

***c,c*-1-TS2**
*E*elec.= -845.0833523a.u.
*G*corr. = 0.245576 a.u.
*E*elec. + *G*corr. = -844.8377763 a.u.

1	6	0	3.445975	0.368528	-0.534295
2	6	0	2.304044	1.098083	0.125619
3	6	0	1.060818	1.075175	-0.799047
4	6	0	0.716191	-0.472714	-0.913778
5	6	0	1.771827	-1.196891	-0.085759
6	6	0	3.145956	-0.926069	-0.603509
7	8	0	1.953625	0.150452	1.175720
8	6	0	1.447809	-2.406495	0.620046
9	6	0	0.149394	-2.743136	0.790310
10	6	0	-0.955139	-1.986067	0.228616
11	6	0	-0.705035	-0.886541	-0.613834
12	6	0	-1.782633	-0.253760	-1.234590
13	6	0	-3.087561	-0.659520	-0.971695
14	6	0	-3.338425	-1.722999	-0.101934
15	6	0	-2.274381	-2.392164	0.481821
16	6	0	-0.024716	1.909989	-0.214198
17	6	0	-0.732935	2.981564	-0.648395
18	6	0	-1.631153	3.331242	0.417502
19	6	0	-1.395916	2.452679	1.420520
20	8	0	-0.413749	1.580314	1.053276
21	1	0	-1.601209	0.561956	-1.926653
22	1	0	-3.913579	-0.147554	-1.455091
23	1	0	-4.357692	-2.034396	0.101003
24	1	0	-2.446774	-3.241212	1.137239
25	1	0	3.749440	-1.729447	-1.010151
26	1	0	4.346449	0.857261	-0.882556
27	1	0	2.529293	2.077356	0.546471
28	1	0	-0.634456	3.457373	-1.613546
29	1	0	-2.353766	4.134031	0.428241
30	1	0	-1.809170	2.313316	2.407818
31	1	0	-0.101931	-3.638184	1.354764
32	1	0	0.923708	-0.772070	-1.949637
33	1	0	2.254599	-2.997018	1.038791
34	1	0	1.314636	1.489297	-1.775616
35	1	0	1.096735	0.397731	1.586544

***c,c*-1-IM3**
*E*elec.= -845.1256962 a.u.
*G*corr. = 0.244924 a.u.
*E*elec. + *G*corr. = -844.8807722 a.u.

1	8	0	-0.583408	0.045840	-0.216818
2	6	0	-0.204273	0.136425	1.086580
3	6	0	1.076172	0.592115	1.164243
4	6	0	1.514404	0.795399	-0.187208
5	6	0	0.470213	0.444339	-0.977345
6	6	0	-1.214767	-0.228070	2.129179
7	6	0	-1.899431	1.010790	2.754929
8	6	0	-2.908354	1.619188	1.830337
9	6	0	-3.532964	0.920618	0.860255
10	6	0	-3.214722	-0.459067	0.620161
11	6	0	-2.298582	-1.171945	1.559973
12	6	0	-3.788551	-1.122862	-0.461910
13	6	0	-3.371210	-2.397537	-0.788854
14	6	0	-2.361893	-3.096426	-0.068951
15	6	0	-1.784268	-2.500431	1.078506
16	6	0	-0.790635	-3.197836	1.763354
17	6	0	-0.371067	-4.444099	1.308732
18	6	0	-0.938806	-5.033674	0.171074
19	6	0	-1.932850	-4.364669	-0.512985
20	8	0	-0.965429	1.951561	3.217355
21	1	0	-0.333223	-2.775749	2.651654
22	1	0	0.413045	-4.967194	1.847045
23	1	0	-0.597770	-6.006346	-0.165887
24	1	0	-2.395404	-4.794162	-1.396677
25	1	0	-4.266769	1.389556	0.212634
26	1	0	-3.142952	2.669477	1.988826
27	1	0	-2.446047	0.659465	3.643031
28	1	0	1.639447	0.749382	2.073469
29	1	0	2.480532	1.147809	-0.517374
30	1	0	0.320957	0.413749	-2.046077
31	1	0	-3.804878	-2.889699	-1.656606
32	1	0	-2.964183	-1.403239	2.417565
33	1	0	-4.521524	-0.611603	-1.076384
34	1	0	-0.691199	-0.728306	2.946782
35	1	0	-0.441614	2.248214	2.456274

***c,c*-1-IM4**
*E*elec.= -845.1284695 a.u.
*G*corr. = 0.244321 a.u.
*E*elec. + *G*corr. = -844.8841485 a.u.

1	8	0	2.786256	1.453727	-0.196121
2	6	0	1.556634	0.929448	0.138660
3	6	0	1.221530	1.337114	1.384615
4	6	0	2.304974	2.159876	1.854842
5	6	0	3.229656	2.192600	0.871303
6	6	0	0.906822	0.075066	-0.914545
7	6	0	1.833779	-1.039644	-1.408662
8	6	0	2.109838	-2.077475	-0.369423
9	6	0	1.093122	-2.436740	0.418343
10	6	0	-0.218713	-1.775480	0.332078
11	6	0	-0.343940	-0.563591	-0.327890
12	6	0	-1.349905	-2.373317	0.946651
13	6	0	-2.571376	-1.759303	0.898021
14	6	0	-2.723795	-0.500421	0.259283
15	6	0	-1.593080	0.122284	-0.349896
16	6	0	-1.763554	1.408322	-0.937355
17	6	0	-2.989740	2.023825	-0.933725
18	6	0	-4.114256	1.392998	-0.348296
19	6	0	-3.981092	0.159841	0.235594
20	8	0	3.096639	-0.379502	-1.869960
21	1	0	-0.916344	1.917754	-1.384467
22	1	0	-3.101145	3.005277	-1.383799
23	1	0	-5.077692	1.892592	-0.359793
24	1	0	-4.832576	-0.332573	0.697247
25	1	0	1.205148	-3.248675	1.131209
26	1	0	3.072950	-2.579131	-0.351203
27	1	0	1.437102	-1.477975	-2.328406
28	1	0	0.312509	1.086111	1.911922
29	1	0	2.374500	2.659926	2.809507
30	1	0	4.194166	2.661451	0.751652
31	1	0	-3.441001	-2.218078	1.360083
32	1	0	3.822735	-1.015918	-2.055525
33	1	0	-1.226983	-3.326604	1.452198
34	1	0	0.655221	0.690763	-1.783861
35	1	0	3.379700	0.349418	-1.235621

***c,c*-1-TS3**
*E*elec.= -1229.0129445 a.u.
*G*corr. = 0.214498 a.u.
*E*elec. + *G*corr. = -1228.7984465 a.u.

1	8	0	-2.249851	0.578923	0.808814
2	6	0	-1.883911	-0.410280	-0.044312
3	6	0	-1.456827	-1.520244	0.685692
4	6	0	-1.536845	-1.138804	2.051490
5	6	0	-2.026266	0.130023	2.085272
6	6	0	-0.954978	0.299573	-1.287022
7	6	0	-1.791445	1.338110	-1.869063
8	6	0	-1.635569	2.665632	-1.535020
9	6	0	-0.578012	3.050640	-0.715458
10	6	0	0.417220	2.130296	-0.305978
11	6	0	0.303777	0.773225	-0.657319
12	6	0	1.559925	2.597151	0.423625
13	6	0	2.546628	1.736945	0.784777
14	6	0	2.472010	0.353422	0.430199
15	6	0	1.346275	-0.132499	-0.304089
16	6	0	1.312906	-1.510979	-0.650624
17	6	0	2.328745	-2.359959	-0.271731
18	6	0	3.428294	-1.874166	0.462910
19	6	0	3.499361	-0.540131	0.800555
20	1	0	0.499095	-1.900864	-1.250622
21	1	0	2.287868	-3.407782	-0.551119
22	1	0	4.225962	-2.551599	0.750932
23	1	0	4.349447	-0.153460	1.355684
24	1	0	-0.468639	4.090634	-0.419003
25	1	0	-2.327551	3.410357	-1.912731
26	1	0	-2.614735	1.028697	-2.500360
27	1	0	-1.174670	-2.476829	0.276744
28	1	0	-1.274238	-1.741013	2.910011
29	1	0	-2.262247	0.824957	2.876152
30	1	0	3.411567	2.081901	1.344079
31	1	0	1.613123	3.651644	0.678058
32	1	0	-0.827420	-0.557151	-1.950004
33	17	0	-3.579932	-1.030340	-1.227977

5
*E*elec.= -539.4923589 a.u.
*G*corr. = 0.160640 a.u.
*E*elec. + *G*corr. = -539.3317189 a.u.

1	6	0	-1.217029	-0.121167	3.179776
2	6	0	-1.981272	-1.049408	2.436976

3	6	0	-3.364939	-0.791022	2.263848
4	6	0	-1.796758	1.006902	3.723518
5	6	0	-4.179735	-1.710078	1.514555
6	6	0	-3.646260	-2.827334	0.966331
7	6	0	-2.247812	-3.130626	1.115845
8	6	0	-1.406480	-2.253209	1.846301
9	6	0	-0.038996	-2.588368	1.969210
10	6	0	0.468186	-3.736620	1.396006
11	6	0	-0.370594	-4.603258	0.672658
12	6	0	-1.707770	-4.300450	0.537421
13	6	0	-3.937700	0.369699	2.828981
14	6	0	-3.169391	1.258289	3.548795
15	1	0	0.633400	-1.940649	2.520673
16	1	0	1.522428	-3.971246	1.505119
17	1	0	0.035497	-5.504677	0.224560
18	1	0	-2.370909	-4.958518	-0.018079
19	1	0	-5.000059	0.547707	2.683743
20	1	0	-3.618425	2.147760	3.979454
21	1	0	-1.187547	1.704329	4.289944
22	1	0	-4.262737	-3.520661	0.400635
23	1	0	-5.236095	-1.482164	1.400904
24	1	0	-0.156300	-0.286704	3.332150

2-chloro-furan
*E*elec.= -689.613091 a.u.
*G*corr. = 0.032922 a.u.
*E*elec. + *G*corr. = -689.580169 a.u.

1	6	0	-0.014717	0.000002	-0.066407
2	8	0	-0.001263	-0.000008	1.296834
3	6	0	1.294926	0.000002	1.660913
4	6	0	2.124457	-0.000022	0.590160
5	6	0	1.251595	-0.000009	-0.550231
6	1	0	-0.991763	0.000005	-0.524798
7	1	0	1.541537	-0.000016	-1.590559
8	1	0	3.203727	-0.000039	0.611013
9	17	0	1.605286	0.000008	3.345603

H_2O
*E*elec.= -76.4335538 a.u.
*G*corr. = 0.003975 a.u.
*E*elec. + *G*corr. = -76.4295788 a.u.

1	8	0	-0.025975	0.000000	-0.018367
2	1	0	0.023148	0.000000	0.944813
3	1	0	0.898495	0.000000	-0.293113

3.2. Cartesian coordinates and selected energy values for the calculated structures along the pathway of formation of products **6** and **7**

***c,c*-2**
*E*elec.= -923.3014587 a.u.
*G*corr. = 0.27949 a.u.
*E*elec. + *G*corr. = -923.0219687 a.u.

1	6	0	1.143513	-1.026883	1.079502
2	6	0	-0.088966	-0.438116	1.115815
3	8	0	-0.510365	-0.188182	-0.155901
4	6	0	0.444400	-0.639409	-1.008493
5	6	0	1.482016	-1.171158	-0.301120
6	6	0	-0.936808	-0.076512	2.235683
7	6	0	-2.273767	0.067315	2.264691
8	6	0	-3.280576	-0.215503	1.219121
9	6	0	-3.296946	-1.405041	0.451640
10	6	0	-4.356418	-1.611570	-0.442958
11	6	0	-5.360049	-0.665747	-0.613305
12	6	0	-5.339591	0.508487	0.138202
13	6	0	-4.316501	0.714977	1.055024
14	6	0	-2.292983	-2.458459	0.692084
15	6	0	-1.633646	-3.243527	-0.180563
16	6	0	-1.609642	-3.272816	-1.628811
17	8	0	-2.413398	-2.464874	-2.378219
18	6	0	-2.154323	-2.710536	-3.691439
19	6	0	-1.187541	-3.664553	-3.798293
20	6	0	-0.833659	-4.030843	-2.463514
21	1	0	-4.307339	1.617257	1.661224
22	1	0	-6.125151	1.249008	0.023601
23	1	0	-6.167687	-0.854545	-1.314002
24	1	0	-4.397410	-2.543687	-0.995255
25	1	0	-0.097986	-4.758404	-2.150011
26	1	0	-0.783463	-4.054672	-4.721509
27	6	0	-2.935055	-1.922638	-4.678831
28	1	0	1.722226	-1.332282	1.940045
29	1	0	2.380058	-1.601327	-0.721183
30	6	0	0.206772	-0.415440	-2.457891
31	1	0	-2.033973	-2.601875	1.739722
32	1	0	-2.694313	0.453857	3.191842
33	1	0	-0.941466	-3.967952	0.243601
34	1	0	-0.389550	0.116065	3.155697
35	1	0	0.875216	-1.046220	-3.046966
36	1	0	-0.828150	-0.651380	-2.716576
37	1	0	0.390836	0.629648	-2.730312
38	1	0	-2.655186	-2.222157	-5.689950
39	1	0	-4.009664	-2.085233	-4.549347
40	1	0	-2.743445	-0.850404	-4.566449

***c,c*-2-TS1**
*E*elec.= -923.2506507 a.u.
*G*corr. = 0.281777 a.u.
*E*elec. + *G*corr. = -922.9688737 a.u.

1	6	0	0.015077	-0.055884	0.000829
2	6	0	-0.006106	0.032862	1.365499
3	8	0	1.274206	0.085035	1.832269
4	6	0	2.119997	0.047236	0.762285
5	6	0	1.396333	-0.041786	-0.385772
6	6	0	-1.099449	0.018686	2.323985
7	6	0	-1.077448	0.697908	3.564878
8	6	0	-0.024911	1.733590	3.859245
9	6	0	0.637429	1.843052	5.097847
10	6	0	1.533108	2.901217	5.313205
11	6	0	1.786884	3.848243	4.329734
12	6	0	1.126188	3.750381	3.107241
13	6	0	0.230346	2.708330	2.887495
14	6	0	0.431825	0.896601	6.202447
15	6	0	-0.201787	-0.277646	6.135717
16	6	0	-0.792395	-0.826846	4.895476
17	8	0	0.065946	-1.524438	4.070812
18	6	0	-0.730909	-2.067385	3.116112
19	6	0	-2.036163	-2.205977	3.648468
20	6	0	-2.068037	-1.457996	4.797392
21	1	0	-0.287754	2.640031	1.935064
22	1	0	1.299753	4.485803	2.327485
23	1	0	2.485065	4.657996	4.517140
24	1	0	2.034447	2.970582	6.275282
25	1	0	-2.918591	-1.226757	5.424556
26	1	0	-2.850248	-2.724591	3.159264
27	6	0	-0.067606	-2.883148	2.060432
28	1	0	-0.851661	-0.116924	-0.642002
29	1	0	1.802323	-0.085652	-1.386687
30	6	0	3.573268	0.118961	1.063687
31	1	0	0.858142	1.197431	7.157676
32	1	0	-2.053172	1.007820	3.933846
33	1	0	-0.284623	-0.889720	7.030837
34	1	0	-2.061597	-0.171441	1.861305
35	1	0	4.143424	0.074996	0.134099
36	1	0	3.822716	1.050930	1.581745
37	1	0	3.887750	-0.711906	1.703515
38	1	0	-0.723852	-2.968528	1.190983
39	1	0	0.873880	-2.424853	1.749866
40	1	0	0.142463	-3.891798	2.431652

***c,c*-2-IM1**
*E*elec.= -923.3017985 a.u.
*G*corr. = 0.286032 a.u.
*E*elec. + *G*corr. = -923.0157665 a.u.

1	6	0	1.338699	0.331068	1.516200
2	6	0	0.049923	-0.082771	1.379920
3	8	0	-0.141439	-0.576671	0.126114
4	6	0	1.043221	-0.497032	-0.542442
5	6	0	1.986883	0.057006	0.264397
6	6	0	-1.106460	-0.049103	2.314773
7	6	0	-1.862408	-1.411863	2.552756
8	6	0	-3.289452	-1.039215	2.017014
9	8	0	-2.981804	-0.111792	0.962803
10	6	0	-2.283036	0.845615	1.759765
11	6	0	-4.115694	-2.166830	1.497734
12	6	0	-3.544504	-3.312573	1.116999
13	6	0	-2.103848	-3.568574	1.247961
14	6	0	-1.273937	-2.660417	1.930620
15	6	0	0.071722	-2.987236	2.110619
16	6	0	0.607493	-4.156580	1.576545
17	6	0	-0.208817	-5.037682	0.868474
18	6	0	-1.559366	-4.746332	0.720088
19	6	0	-3.884714	-0.111260	3.072428
20	6	0	-3.247585	1.047654	2.923947
21	1	0	0.713525	-2.310704	2.667466
22	1	0	1.660437	-4.380701	1.718259
23	1	0	0.202121	-5.950529	0.448557
24	1	0	-2.214059	-5.434918	0.191808
25	1	0	-4.586608	-0.419156	3.838769
26	1	0	-3.296718	1.941623	3.535086
27	6	0	-1.893583	2.065116	0.964638
28	1	0	1.771522	0.766869	2.405834
29	1	0	3.018035	0.243134	-0.000757
30	6	0	1.052588	-1.011141	-1.936729
31	1	0	-4.147019	-4.112678	0.692430
32	1	0	-1.921665	-1.593649	3.631337
33	1	0	-5.183832	-2.002256	1.386039
34	1	0	-0.730502	0.358922	3.256145
35	1	0	2.055738	-0.917886	-2.356291
36	1	0	0.758527	-2.065258	-1.966189
37	1	0	0.356782	-0.451996	-2.570377
38	1	0	-2.789027	2.598816	0.635222
39	1	0	-1.293162	2.739463	1.582151
40	1	0	-1.308900	1.782078	0.085880

***c,c*-2-IM2**

*E*elec.= -923.7172816 a.u.
*G*corr. = 0.298403 a.u.
*E*elec. + *G*corr. = -923.4188786 a.u.

1	8	0	-0.002674	-0.077488	0.012584
2	6	0	-0.001922	-0.029077	1.382563
3	6	0	1.272628	0.012597	1.835757
4	6	0	2.117071	-0.026877	0.671560
5	6	0	1.302092	-0.081698	-0.411724
6	6	0	-1.350865	0.002086	2.009879
7	6	0	-2.147821	1.242899	1.499536
8	6	0	-3.496490	1.293915	2.175966
9	6	0	-4.236880	0.286705	1.723914
10	6	0	-3.398896	-0.525989	0.766685
11	6	0	-2.282590	-1.211056	1.597055
12	8	0	-2.615819	0.687990	0.166755
13	6	0	-4.020127	-1.280971	-0.337924
14	6	0	-3.409998	-2.370896	-0.822057
15	6	0	-2.171434	-2.919964	-0.265145
16	6	0	-1.613769	-2.379752	0.906218
17	6	0	-0.489545	-2.986212	1.466002
18	6	0	0.111837	-4.077408	0.843535
19	6	0	-0.418591	-4.590861	-0.339562
20	6	0	-1.563571	-4.020998	-0.880966
21	1	0	-0.077942	-2.600368	2.393852
22	1	0	0.993542	-4.529309	1.287019
23	1	0	0.050130	-5.439553	-0.826851
24	1	0	-2.005509	-4.426709	-1.786974
25	1	0	-5.238357	-0.008238	2.010638
26	1	0	-3.744148	2.039411	2.921145
27	6	0	-1.412686	2.538432	1.312538
28	1	0	1.575845	0.055687	2.872125
29	1	0	3.197138	-0.017774	0.645985
30	6	0	1.519234	-0.151537	-1.877774
31	1	0	-3.849413	-2.904032	-1.661654
32	1	0	-2.760427	-1.594935	2.503418
33	1	0	-4.943598	-0.897900	-0.757968
34	1	0	-1.232877	0.066020	3.092397
35	1	0	-1.844540	0.386505	-0.375985
36	1	0	-0.553429	2.425894	0.647568
37	1	0	-2.087780	3.299733	0.917204
38	1	0	-1.051327	2.861994	2.292816
39	1	0	1.087949	-1.068344	-2.292143
40	1	0	1.055380	0.700403	-2.384580
41	1	0	2.589604	-0.142238	-2.087820

***c,c*-2-TS2**
*E*elec.= -923.7141465 a.u.
*G*corr. = 0.296899 a.u.

*E*elec. + *G*corr. = -923.4172475 a.u.

1	8	0	0.034458	-0.090453	0.101553
2	6	0	-0.011198	-0.054284	1.469289
3	6	0	1.247332	-0.088634	1.969415
4	6	0	2.129570	-0.167619	0.836783
5	6	0	1.349846	-0.166814	-0.274402
6	6	0	-1.366936	0.069886	2.070069
7	6	0	-2.062297	1.370732	1.566530
8	6	0	-3.387018	1.516609	2.282724
9	6	0	-4.218597	0.551074	1.903338
10	6	0	-3.552173	-0.415880	0.985530
11	6	0	-2.368583	-1.093423	1.659485
12	6	0	-4.250784	-1.054740	-0.091268
13	6	0	-3.685479	-2.122319	-0.701946
14	6	0	-2.437832	-2.723132	-0.270731
15	6	0	-1.791278	-2.256413	0.889049
16	6	0	-0.666273	-2.938125	1.353635
17	6	0	-0.147823	-4.014263	0.639634
18	6	0	-0.760663	-4.447096	-0.538902
19	6	0	-1.911280	-3.814055	-0.980568
20	8	0	-2.532005	0.983056	0.234490
21	1	0	-0.187937	-2.622164	2.274927
22	1	0	0.737258	-4.523071	1.008593
23	1	0	-0.350822	-5.285113	-1.092767
24	1	0	-2.424780	-4.156487	-1.874523
25	1	0	-5.245630	0.396504	2.214432
26	1	0	-3.584141	2.318737	2.983809
27	6	0	-1.205689	2.612020	1.520040
28	1	0	1.513496	-0.070484	3.016679
29	1	0	3.208634	-0.221408	0.849522
30	6	0	1.617450	-0.243302	-1.732291
31	1	0	-4.189897	-2.584108	-1.547564
32	1	0	-2.783103	-1.503767	2.590464
33	1	0	-5.193242	-0.635911	-0.424766
34	1	0	-1.249753	0.116000	3.154046
35	1	0	-1.778986	0.648868	-0.298621
36	1	0	-0.347050	2.479792	0.857229
37	1	0	-1.800617	3.458458	1.169947
38	1	0	-0.838034	2.828631	2.526766
39	1	0	1.143458	-1.128456	-2.168303
40	1	0	1.228821	0.638659	-2.250532
41	1	0	2.693276	-0.302375	-1.902810

***c,c*-2-IM3**
*E*elec.= -923.7505429 a.u.
*G*corr. = 0.294686 a.u.

*E*elec. + *G*corr. = -923.4558569 a.u.

1	8	0	-0.483734	0.362958	-0.428165
2	6	0	-0.055889	0.077850	0.832658
3	6	0	1.295267	-0.054827	0.843507
4	6	0	1.731723	0.173975	-0.505339
5	6	0	0.614018	0.419762	-1.238218
6	6	0	-1.090174	-0.057897	1.897320
7	6	0	-1.700450	1.296769	2.358384
8	6	0	-2.755549	1.781828	1.410684
9	6	0	-3.448513	0.979790	0.578960
10	6	0	-3.139068	-0.417447	0.466474
11	6	0	-2.213870	-1.038901	1.455366
12	6	0	-3.727562	-1.179044	-0.542355
13	6	0	-3.326235	-2.484739	-0.744719
14	6	0	-2.323998	-3.123686	0.039856
15	6	0	-1.732524	-2.422052	1.116995
16	6	0	-0.751514	-3.063377	1.871859
17	6	0	-0.358271	-4.358484	1.552893
18	6	0	-0.938947	-5.052861	0.482793
19	6	0	-1.920032	-4.439816	-0.269018
20	8	0	-0.710289	2.305242	2.383430
21	1	0	-0.285185	-2.558860	2.711145
22	1	0	0.414339	-4.837850	2.145991
23	1	0	-0.619218	-6.063152	0.252503
24	1	0	-2.391098	-4.951958	-1.102682
25	1	0	-4.216180	1.382273	-0.074450
26	1	0	-2.969220	2.847906	1.450726
27	6	0	-2.339910	1.157845	3.748856
28	1	0	1.901671	-0.290893	1.706730
29	1	0	2.743498	0.151131	-0.883874
30	6	0	0.364114	0.718343	-2.671677
31	1	0	-3.772186	-3.056082	-1.555656
32	1	0	-2.867842	-1.171602	2.340653
33	1	0	-4.461512	-0.722462	-1.197504
34	1	0	-0.583496	-0.480639	2.770063
35	1	0	-0.032285	2.038042	3.023212
36	1	0	-1.572192	0.848219	4.465747
37	1	0	-2.743576	2.124251	4.060078
38	1	0	-3.148721	0.422904	3.762203
39	1	0	-0.280248	-0.041961	-3.124378
40	1	0	-0.126972	1.689164	-2.790473
41	1	0	1.311834	0.739261	-3.211967

***c,c*-2-IM4**

*E*elec.= -923.7553903 a.u.

*G*corr. = 0.296653 a.u.

*E*elec. + *G*corr. = -923.4587373 a.u.

1	8	0	2.070538	1.051623	-1.577407
2	6	0	1.390093	0.513199	-0.530887
3	6	0	1.522229	1.311932	0.565825
4	6	0	2.334120	2.421546	0.156038
5	6	0	2.638627	2.218408	-1.152727
6	6	0	0.663317	-0.777449	-0.793893
7	6	0	1.549056	-1.956870	-0.345061
8	6	0	0.828212	-3.237419	-0.121925
9	6	0	-0.455641	-3.213344	0.248710
10	6	0	-1.241742	-1.980170	0.318902
11	6	0	-0.755930	-0.805256	-0.233855
12	6	0	-2.543414	-2.036219	0.886565
13	6	0	-3.347593	-0.933670	0.885816
14	6	0	-2.924966	0.258174	0.238738
15	6	0	-1.632033	0.320519	-0.365615
16	6	0	-1.310568	1.491162	-1.114832
17	6	0	-2.188789	2.542007	-1.202350
18	6	0	-3.439755	2.497966	-0.543332
19	6	0	-3.799714	1.373294	0.152398
20	8	0	1.981568	-1.550759	1.123899
21	1	0	-0.376093	1.552863	-1.659250
22	1	0	-1.921466	3.414811	-1.789690
23	1	0	-4.116488	3.343883	-0.609344
24	1	0	-4.769129	1.305152	0.638413
25	1	0	-0.972502	-4.140578	0.482871
26	1	0	1.398544	-4.158070	-0.194340
27	6	0	2.831486	-2.089740	-1.131855
28	1	0	1.050820	1.161582	1.528634
29	1	0	2.644967	3.262816	0.758080
30	6	0	3.433259	2.974024	-2.153523
31	1	0	-4.334057	-0.961372	1.339803
32	1	0	2.556268	-2.242700	1.521056
33	1	0	-2.878269	-2.971136	1.326381
34	1	0	0.598274	-0.891060	-1.886504
35	1	0	2.461191	-0.683897	1.116231
36	1	0	3.381849	-1.147081	-1.176655
37	1	0	3.466982	-2.864798	-0.695173
38	1	0	2.573265	-2.392590	-2.149836
39	1	0	4.278598	2.379355	-2.512745
40	1	0	2.818739	3.243999	-3.017363
41	1	0	3.817516	3.887527	-1.697650

_c,c_-2-IM5

*E*elec.= -847.3299868 a.u.

*G*corr. = 0.268811 a.u.

*E*elec. + *G*corr. = -847.0611758 a.u.

1	8	0	0.012216	0.217228	0.058563
2	6	0	-0.002481	-0.085438	1.382566
3	6	0	1.250406	-0.367512	1.820415
4	6	0	2.105472	-0.214977	0.678866
5	6	0	1.308134	0.139494	-0.364308
6	6	0	-1.357954	-0.125783	2.051601
7	6	0	-1.847652	-1.538188	1.965995
8	6	0	-2.160107	-2.241072	3.105695
9	6	0	-2.031807	-1.629019	4.352622
10	6	0	-1.627572	-0.286213	4.539645
11	6	0	-1.316696	0.496158	3.419399
12	6	0	-1.559898	0.256277	5.862561
13	6	0	-1.194023	1.551899	6.043111
14	6	0	-0.892939	2.384979	4.921885
15	6	0	-0.958517	1.860854	3.594716
16	6	0	-0.673312	2.727229	2.501150
17	6	0	-0.326859	4.036019	2.720570
18	6	0	-0.249047	4.545939	4.037598
19	6	0	-0.529226	3.738455	5.113358
20	1	0	-0.738666	2.360062	1.482596
21	1	0	-0.115242	4.687965	1.879740
22	1	0	0.028293	5.583403	4.194775
23	1	0	-0.479730	4.125090	6.126772
24	1	0	-2.267875	-2.208144	5.243377
25	1	0	-2.497800	-3.269303	3.039318
26	6	0	-1.936473	-2.161028	0.618981
27	1	0	1.526833	-0.640314	2.829323
28	1	0	3.177009	-0.347448	0.639494
29	6	0	1.561178	0.457194	-1.792400
30	1	0	-1.131396	1.981594	7.038192
31	1	0	-1.804347	-0.388096	6.701158
32	1	0	-2.040200	0.469790	1.422260
33	1	0	-2.308082	-1.449759	-0.122934
34	1	0	-0.931617	-2.467792	0.299174
35	1	0	-2.569616	-3.048594	0.645073
36	1	0	1.011332	-0.223012	-2.449755
37	1	0	1.249513	1.479366	-2.027649
38	1	0	2.627174	0.359890	-2.002977

6

*E*elec.= -846.9357753 a.u.
*G*corr. = 0.257605 a.u.

*E*elec. + *G*corr. = -846.6781703 a.u

1	6	0	-0.028055	0.166770	0.054570
2	6	0	0.000418	0.009757	1.457791
3	6	0	1.184421	0.303687	2.188101
4	6	0	2.339124	0.635136	1.436275
5	6	0	2.295330	0.759587	0.061959
6	6	0	1.096105	0.553088	-0.639579
7	6	0	1.160717	0.175594	3.650361
8	6	0	0.032529	-0.455355	4.240948
9	6	0	-1.122302	-0.786329	3.450080
10	6	0	-1.158847	-0.514789	2.126925
11	6	0	2.185199	0.643613	4.525904
12	6	0	2.152879	0.362427	5.893809
13	6	0	1.067286	-0.354976	6.428291
14	6	0	0.015358	-0.724122	5.623521
15	6	0	3.265909	1.537427	4.059352
16	8	0	4.519286	1.010743	3.934620
17	6	0	5.346852	2.002610	3.496803
18	6	0	4.638767	3.154935	3.352982
19	6	0	3.286051	2.854433	3.725195
20	6	0	6.774019	1.640292	3.295617
21	6	0	3.247155	0.851077	6.808095
22	1	0	3.296126	0.758779	1.924354
23	1	0	3.203908	1.006460	-0.478411
24	1	0	1.066474	0.665434	-1.718763
25	1	0	-0.956421	-0.046661	-0.468611
26	1	0	-0.852845	-1.224476	6.044357
27	1	0	1.047924	-0.572434	7.492356
28	1	0	2.435104	3.520838	3.727976
29	1	0	5.037208	4.104774	3.025518
30	1	0	-2.042095	-0.730579	1.532160
31	1	0	-1.973526	-1.233753	3.955654
32	1	0	4.209033	0.394699	6.555787
33	1	0	3.374387	1.935179	6.722691
34	1	0	3.015826	0.611147	7.847813
35	1	0	7.236048	1.318783	4.234324
36	1	0	6.876062	0.824222	2.573857
37	1	0	7.320538	2.506728	2.919573

***c,c*-2-TS3**
*E*elec.= -1384.0788318 a.u.
*G*corr. = 0.288595 a.u.

*E*elec. + *G*corr. = -1383.7902368 a.u

1	6	0	-3.954282	0.575237	0.179538
2	6	0	-2.872905	-0.335583	0.180708
3	6	0	-1.649919	0.019798	-0.461568
4	6	0	-1.577624	1.284450	-1.107134
5	6	0	-2.648574	2.147203	-1.100738
6	6	0	-3.848243	1.795809	-0.445817
7	6	0	-0.566041	-0.919278	-0.453026
8	6	0	-0.755171	-2.190289	0.120789
9	6	0	-1.989237	-2.514243	0.772023
10	6	0	-3.004761	-1.613402	0.811634
11	6	0	0.767527	-0.590163	-0.990762
12	6	0	1.648536	-1.709557	-1.306086
13	6	0	1.424199	-2.944044	-0.717099
14	6	0	0.263274	-3.168891	0.009085
15	6	0	1.630599	0.396885	0.176607
16	8	0	0.853416	1.483493	0.427039
17	6	0	1.643003	2.606455	0.352770
18	6	0	2.924231	2.233908	0.078213
19	6	0	2.945620	0.815863	-0.041773
20	17	0	1.487897	-0.720837	1.962191
21	1	0	-0.667096	1.579792	-1.614986
22	1	0	-2.570201	3.105366	-1.605015
23	1	0	-4.685720	2.486422	-0.443156
24	1	0	-4.874716	0.287130	0.679915
25	1	0	0.091873	-4.141155	0.464024
26	1	0	2.137539	-3.747890	-0.870918
27	6	0	2.767086	-1.462380	-2.245954
28	1	0	3.795900	0.163231	-0.159134
29	1	0	3.761527	2.908160	-0.039173
30	6	0	0.942944	3.902495	0.512484
31	1	0	-3.942509	-1.850855	1.305938
32	1	0	-2.092236	-3.494590	1.228615
33	1	0	0.746108	0.149834	-1.791616
34	1	0	3.260281	-0.508785	-2.005277
35	1	0	3.499239	-2.270304	-2.235157
36	1	0	2.370962	-1.339270	-3.262117
37	1	0	1.661064	4.719560	0.424763
38	1	0	0.173393	4.029826	-0.258415
39	1	0	0.448047	3.970569	1.486814
40	8	0	4.147942	-2.168360	0.531838
41	1	0	4.800783	-1.807252	1.144871
42	1	0	3.300266	-1.945180	0.944360

7

*E*elec.= -578.8026369 a.u

*G*corr. = 0.186879 a.u.

*E*elec. + *G*corr. = -578.6157579 a.u

1	6	0	-0.028055	0.166770	0.054570
2	6	0	0.000418	0.009757	1.457791
3	6	0	1.184421	0.303687	2.188101
4	6	0	2.339124	0.635136	1.436275
5	6	0	2.295330	0.759587	0.061959
6	6	0	1.096105	0.553088	-0.639579
7	6	0	1.160717	0.175594	3.650361
8	6	0	0.032529	-0.455355	4.240948
9	6	0	-1.122302	-0.786329	3.450080
10	6	0	-1.158847	-0.514789	2.126925
11	6	0	2.185199	0.643613	4.525904
12	6	0	2.152879	0.362427	5.893809
13	6	0	1.067286	-0.354976	6.428291
14	6	0	0.015358	-0.724122	5.623521
15	6	0	3.265909	1.537427	4.059352
16	8	0	4.519286	1.010743	3.934620
17	6	0	5.346852	2.002610	3.496803
18	6	0	4.638767	3.154935	3.352982
19	6	0	3.286051	2.854433	3.725195
20	6	0	6.774019	1.640292	3.295617
21	6	0	3.247155	0.851077	6.808095
22	1	0	3.296126	0.758779	1.924354
23	1	0	3.203908	1.006460	-0.478411
24	1	0	1.066474	0.665434	-1.718763
25	1	0	-0.956421	-0.046661	-0.468611
26	1	0	-0.852845	-1.224476	6.044357
27	1	0	1.047924	-0.572434	7.492356
28	1	0	2.435104	3.520838	3.727976
29	1	0	5.037208	4.104774	3.025518
30	1	0	-2.042095	-0.730579	1.532160
31	1	0	-1.973526	-1.233753	3.955654
32	1	0	4.209033	0.394699	6.555787
33	1	0	3.374387	1.935179	6.722691
34	1	0	3.015826	0.611147	7.847813
35	1	0	7.236048	1.318783	4.234324
36	1	0	6.876062	0.824222	2.573857
37	1	0	7.320538	2.506728	2.919573

2-chloro-5-methyl-furan
*E*elec.= -728.9287384 a.u
*G*corr. = 0.058217 a.u.

*E*elec. + *G*corr. = -728.8705154 a.u

1	6	0	0.017861	0.069878	-0.004745
2	6	0	0.010308	-0.000440	1.352194
3	8	0	1.297396	-0.076804	1.813171
4	6	0	2.098878	-0.052982	0.728871
5	6	0	1.392742	0.035635	-0.421684
6	17	0	3.783731	-0.137425	1.034171
7	6	0	-1.061863	-0.010244	2.378883
8	1	0	-0.853648	0.138397	-0.639868
9	1	0	1.794148	0.071422	-1.423115
10	1	0	-2.033136	0.054944	1.886134
11	1	0	-1.031457	-0.929708	2.971168
12	1	0	-0.959528	0.837368	3.063151

Cl^-
*E*elec.= -460.3735973 a.u
*G*corr. = -0.015023 a.u
*E*elec. + *G*corr. = -460.3886203 a..u.

3.3. Cartesian coordinates and selected energy values for the calculated structures along the pathway of formation of products **8** and **9**

***t,t*-2**
*E*elec.= -923.3101957 a.u
*G*corr. = 0.276194 a.u
*E*elec. + *G*corr. = -923.0340017 a..u.

1	6	0	-1.250323	-0.188011	-1.377633
2	6	0	-1.329544	-0.079375	-0.017588
3	8	0	-0.114365	0.293620	0.479338
4	6	0	0.743044	0.424883	-0.567928
5	6	0	0.095154	0.139725	-1.732319
6	6	0	-2.423652	-0.281721	0.902324
7	6	0	-2.350370	-0.090231	2.231616
8	6	0	-3.458781	-0.335951	3.167600
9	6	0	-3.551110	0.381709	4.385057
10	6	0	-4.608837	0.095292	5.261530
11	6	0	-5.553697	-0.877755	4.963383
12	6	0	-5.460948	-1.586952	3.765419
13	6	0	-4.421961	-1.316383	2.884641
14	6	0	-2.580950	1.438988	4.710589
15	6	0	-2.241205	1.797510	5.961624
16	6	0	-1.319225	2.858993	6.289436
17	8	0	-0.772589	3.590433	5.275086
18	6	0	0.056379	4.516315	5.827084
19	6	0	0.048950	4.390673	7.183933
20	6	0	-0.843360	3.315600	7.486458
21	1	0	-4.330812	-1.896305	1.970933
22	1	0	-6.190464	-2.353443	3.523198
23	1	0	-6.364006	-1.076535	5.657831
24	1	0	-4.705453	0.671787	6.176844
25	1	0	-1.103930	2.923602	8.459517
26	1	0	0.615310	4.994559	7.878367
27	6	0	0.758692	5.425670	4.886732
28	1	0	-2.060693	-0.467355	-2.036170
29	1	0	0.530633	0.163872	-2.720981
30	6	0	2.134445	0.828013	-0.242474
31	1	0	-2.118732	1.963173	3.877478
32	1	0	-1.412542	0.263238	2.653549
33	1	0	-2.650253	1.273066	6.822422
34	1	0	-3.353975	-0.596897	0.434885
35	1	0	2.717505	0.908407	-1.161085
36	1	0	2.153178	1.794825	0.270155
37	1	0	2.612827	0.092676	0.412028
38	1	0	1.396872	6.110836	5.446680
39	1	0	1.381170	4.860813	4.185789

40	1	0	0.043973	6.012854	4.301638

***t,t*-2-IM1**

*E*elec.= -923.7317983 a.u
*G*corr. = 0.290442 a.u
*E*elec. + *G*corr. = -923.4413563 a..u.

1	6	0	0.896215	0.106843	3.255904
2	6	0	-0.346442	-0.055317	2.592979
3	8	0	-0.336776	0.750085	1.466928
4	6	0	0.836644	1.362477	1.420778
5	6	0	1.638774	1.002942	2.511813
6	6	0	-1.461860	-0.732412	2.958811
7	6	0	-2.754931	-0.792776	2.216517
8	6	0	-3.931413	-0.660839	3.167950
9	6	0	-3.906518	0.364384	4.133014
10	6	0	-4.946458	0.467451	5.057688
11	6	0	-6.014655	-0.427892	5.016985
12	6	0	-6.046427	-1.430431	4.052199
13	6	0	-5.000843	-1.550593	3.135907
14	6	0	-2.751282	1.285524	4.117754
15	6	0	-1.874912	1.440666	5.127853
16	6	0	-0.676513	2.225275	5.003114
17	6	0	0.447583	2.327222	5.785485
18	6	0	1.318611	3.238134	5.128307
19	6	0	0.676085	3.637795	3.988792
20	8	0	-0.530850	3.022120	3.903028
21	6	0	0.999098	4.642354	2.942887
22	6	0	1.103939	2.232973	0.262055
23	1	0	-4.921241	1.260782	5.799170
24	1	0	-6.822059	-0.337646	5.736945
25	1	0	-6.877256	-2.128118	4.017352
26	1	0	-5.009470	-2.349535	2.399401
27	1	0	1.175686	-0.407547	4.165847
28	1	0	2.637127	1.371962	2.694122
29	1	0	0.611517	1.809027	6.720083
30	1	0	2.294227	3.570913	5.452048
31	1	0	-2.781819	-0.030848	1.430230
32	1	0	-2.573074	1.823385	3.185860
33	1	0	-1.370496	-1.330396	3.863734
34	1	0	-1.990228	0.890347	6.058652
35	1	0	2.080635	4.770550	2.871024
36	1	0	0.607688	4.336531	1.970505
37	1	0	0.554151	5.612265	3.190327
38	1	0	2.006884	2.818671	0.431601
39	1	0	1.243945	1.606661	-0.626605
40	1	0	0.250902	2.891200	0.076463

41	1	0	-2.801005	-1.773536	1.724409

***t,t*-2-TS1**

*E*elec.= -923.7291227 a.u
*G*corr. = 0.292642 a.u
*E*elec. + *G*corr. = -923.4364807 a..u

1	6	0	1.464245	0.600573	-1.628613
2	6	0	0.427652	1.163173	-0.877766
3	8	0	0.976266	1.926975	0.126545
4	6	0	2.305902	1.857648	0.005663
5	6	0	2.661195	1.048282	-1.063034
6	6	0	-0.935856	0.942101	-0.931887
7	6	0	-1.993029	1.741322	-0.225651
8	6	0	-3.145111	0.822554	0.115936
9	6	0	-2.779420	-0.481421	0.487385
10	6	0	-3.759234	-1.433756	0.759206
11	6	0	-5.105977	-1.077375	0.674979
12	6	0	-5.467588	0.220822	0.323684
13	6	0	-4.486876	1.173108	0.036719
14	6	0	-1.321354	-0.718071	0.573859
15	6	0	-0.628160	-1.706242	-0.068078
16	6	0	0.775132	-1.828738	0.059741
17	6	0	1.723584	-2.546836	-0.648234
18	6	0	2.975856	-2.235755	-0.083030
19	6	0	2.732376	-1.346394	0.939498
20	8	0	1.411781	-1.095618	1.027168
21	6	0	3.612920	-0.728426	1.961679
22	6	0	3.113762	2.658212	0.950287
23	1	0	-3.470439	-2.440538	1.046601
24	1	0	-5.872541	-1.816291	0.885881
25	1	0	-6.516622	0.492223	0.258317
26	1	0	-4.768408	2.177932	-0.265660
27	1	0	1.326247	-0.034052	-2.493233
28	1	0	3.672937	0.838172	-1.377310
29	1	0	1.511344	-3.213731	-1.472690
30	1	0	3.946564	-2.609681	-0.373720
31	1	0	-1.579717	2.222967	0.667643
32	1	0	-0.791412	-0.141113	1.332228
33	1	0	-1.265235	0.368694	-1.795758
34	1	0	-1.113603	-2.350530	-0.797090
35	1	0	3.717307	-1.395487	2.824139
36	1	0	4.606370	-0.554021	1.544355
37	1	0	3.194112	0.215619	2.314741
38	1	0	4.165637	2.384895	0.865528
39	1	0	3.003313	3.722704	0.716336
40	1	0	2.771260	2.504313	1.977230
41	1	0	-2.322496	2.534623	-0.908370

***t,t*-2-IM2**
*E*elec.= -923.7475283 a.u
*G*corr. = 0.292472 a.u
*E*elec. + *G*corr. = -923.4550563 a..u.

1	6	0	1.659739	0.883657	-1.613202
2	6	0	0.578034	1.072040	-0.808431
3	8	0	0.945509	1.794163	0.289748
4	6	0	2.275476	2.080664	0.177107
5	6	0	2.761044	1.545136	-0.974995
6	6	0	-0.821088	0.593457	-0.863033
7	6	0	-1.920170	1.664498	-0.674188
8	6	0	-3.083413	0.872749	-0.131907
9	6	0	-2.645847	-0.339061	0.409275
10	6	0	-3.539256	-1.237898	0.978939
11	6	0	-4.896376	-0.909757	0.996030
12	6	0	-5.338028	0.299363	0.458124
13	6	0	-4.433832	1.200934	-0.107692
14	6	0	-1.145275	-0.458135	0.282664
15	6	0	-0.632927	-1.788196	-0.104753
16	6	0	0.655267	-2.151703	0.069456
17	6	0	1.783493	-1.495870	0.646193
18	6	0	2.865070	-2.323769	0.476329
19	6	0	2.384647	-3.469506	-0.187465
20	8	0	1.093931	-3.373864	-0.428478
21	6	0	3.077431	-4.695308	-0.615340
22	6	0	2.878137	2.878570	1.275206
23	1	0	-3.191627	-2.178264	1.398768
24	1	0	-5.612298	-1.602154	1.427938
25	1	0	-6.396809	0.539283	0.474145
26	1	0	-4.782273	2.138116	-0.532468
27	1	0	1.664244	0.338788	-2.546936
28	1	0	3.781018	1.614014	-1.324723
29	1	0	1.755518	-0.530584	1.138179
30	1	0	3.889393	-2.169586	0.781080
31	1	0	-1.591879	2.413043	0.057151
32	1	0	-0.652687	-0.106851	1.198402
33	1	0	-0.969848	0.096125	-1.826824
34	1	0	-1.293852	-2.475101	-0.632482
35	1	0	4.141816	-4.619501	-0.399416
36	1	0	2.652160	-5.554564	-0.085544
37	1	0	2.920068	-4.852724	-1.686805
38	1	0	3.936629	3.043763	1.068734
39	1	0	2.384777	3.850589	1.370521
40	1	0	2.785752	2.359453	2.234252
41	1	0	-2.141241	2.182112	-1.610607

8

*E*elec.= -923.3307512 a.u
*G*corr. = 0.280343 a.u
*E*elec. + *G*corr. = -923.0504082 a..u.

1	6	0	0.713344	-1.281727	-0.713826
2	6	0	0.393755	-0.796074	0.513970
3	8	0	1.214306	-1.344615	1.454582
4	6	0	2.071065	-2.195282	0.818754
5	6	0	1.805637	-2.194022	-0.513764
6	6	0	-0.647046	0.152046	1.025241
7	6	0	-1.812604	-0.598291	1.735557
8	6	0	-2.938130	-0.560975	0.730997
9	6	0	-2.644677	0.320033	-0.318518
10	6	0	-3.568946	0.536443	-1.343487
11	6	0	-4.785569	-0.138622	-1.303857
12	6	0	-5.077223	-1.019217	-0.257450
13	6	0	-4.154723	-1.233599	0.766892
14	6	0	-1.304470	0.891638	-0.129026
15	6	0	-0.765145	1.892002	-0.849298
16	6	0	0.549237	2.469213	-0.679018
17	6	0	1.664656	2.205947	0.075524
18	6	0	2.627174	3.207498	-0.258968
19	6	0	2.046802	4.010966	-1.193778
20	8	0	0.790907	3.571622	-1.454939
21	6	0	2.507221	5.208316	-1.942104
22	6	0	3.063078	-2.903976	1.667902
23	1	0	-3.341056	1.211099	-2.164325
24	1	0	-5.511853	0.014487	-2.096250
25	1	0	-6.028846	-1.541828	-0.244677
26	1	0	-4.383651	-1.917264	1.579903
27	1	0	0.235944	-1.017661	-1.646653
28	1	0	2.327014	-2.772737	-1.263044
29	1	0	1.798386	1.393125	0.773982
30	1	0	3.626453	3.316616	0.137461
31	1	0	-1.532860	-1.615701	2.022143
32	1	0	-0.164311	0.857108	1.712994
33	1	0	-1.357112	2.347908	-1.640579
34	1	0	3.522820	5.463122	-1.635557
35	1	0	2.503806	5.022477	-3.020710
36	1	0	1.857645	6.067518	-1.748424
37	1	0	3.688317	-3.542432	1.041519
38	1	0	3.709076	-2.196086	2.196534
39	1	0	2.568007	-3.529730	2.417145
40	1	0	-2.104539	-0.070660	2.649951

***t,t*-2-IM3**

*E*elec.= -923.7404225 a.u
*G*corr. = 0.292092 a.u
*E*elec. + *G*corr. = -923.4483305 a..u.

1	8	0	0.880979	0.704985	2.155063
2	6	0	0.082256	-0.311931	1.730196
3	6	0	0.823110	-1.258930	1.100602
4	6	0	2.180598	-0.798032	1.152343
5	6	0	2.162691	0.392627	1.809779
6	6	0	-1.372493	-0.184727	2.013271
7	6	0	-1.747438	-0.021613	3.438898
8	6	0	-0.812947	-0.197364	4.595854
9	6	0	-1.731804	-0.210492	5.841564
10	6	0	-3.043813	0.268070	5.315348
11	6	0	-3.023758	0.322054	3.894392
12	6	0	-4.171200	0.692499	3.146283
13	6	0	-5.310162	1.017057	3.842528
14	6	0	-5.316141	0.979348	5.256084
15	6	0	-4.199609	0.614521	6.001736
16	6	0	0.143481	-1.327358	4.445347
17	6	0	1.484922	-1.441598	4.617123
18	6	0	1.807144	-2.803214	4.303009
19	6	0	0.638880	-3.412356	3.961991
20	8	0	-0.387336	-2.520483	4.058165
21	6	0	0.285119	-4.790256	3.534215
22	6	0	3.213534	1.369264	2.194658
23	1	0	-4.139854	0.727804	2.061804
24	1	0	-6.211213	1.310705	3.316270
25	1	0	-6.231733	1.244700	5.776712
26	1	0	-4.237564	0.590021	7.085325
27	1	0	2.157079	-0.651094	4.920146
28	1	0	2.781656	-3.269734	4.321340
29	1	0	0.446633	-2.173287	0.663794
30	1	0	3.058707	-1.289768	0.758863
31	1	0	-1.836949	-1.236167	6.213554
32	1	0	-0.211211	0.727251	4.605567
33	1	0	-1.828325	0.640118	1.447457
34	1	0	4.188890	1.000437	1.873460
35	1	0	3.037914	2.342989	1.726974
36	1	0	3.235642	1.516551	3.278931
37	1	0	1.185097	-5.406345	3.507038
38	1	0	-0.429436	-5.245292	4.227127
39	1	0	-0.167708	-4.787035	2.537842
40	1	0	-1.354808	0.404859	6.661397
41	1	0	-1.883352	-1.093286	1.660661

9

*E*elec.= -923.3354886 a.u
*G*corr. = 0.276800 a.u
*E*elec. + *G*corr. = -923.0586886 a..u.

1	8	0	2.274904	-1.248426	-1.215714
2	6	0	1.136176	-1.384177	-1.953130
3	6	0	0.904323	-2.698707	-2.202056
4	6	0	1.976796	-3.422981	-1.576783
5	6	0	2.778969	-2.495752	-0.990730
6	6	0	0.405490	-0.128963	-2.302050
7	6	0	-0.162548	0.567529	-1.092470
8	6	0	-1.370802	0.376403	-0.501150
9	6	0	-1.544022	1.301452	0.683386
10	6	0	-0.246347	2.063764	0.703831
11	6	0	0.564263	1.605993	-0.350413
12	6	0	1.834642	2.142835	-0.554029
13	6	0	2.277766	3.148240	0.306376
14	6	0	1.469763	3.606133	1.349075
15	6	0	0.197542	3.062752	1.556080
16	6	0	-2.419542	-0.547429	-0.860475
17	6	0	-3.696877	-0.697938	-0.395673
18	6	0	-4.269770	-1.782904	-1.128357
19	6	0	-3.307169	-2.224766	-1.985206
20	8	0	-2.179276	-1.481083	-1.830418
21	6	0	-3.252707	-3.316920	-2.989922
22	6	0	4.032539	-2.576459	-0.196735
23	1	0	2.472284	1.783946	-1.357222
24	1	0	3.264253	3.579498	0.164585
25	1	0	1.833869	4.389144	2.007199
26	1	0	-0.428594	3.419173	2.369658
27	1	0	-4.166820	-0.097917	0.371002
28	1	0	-5.267112	-2.188173	-1.034970
29	1	0	0.067365	-3.097014	-2.757853
30	1	0	2.131851	-4.492584	-1.562080
31	1	0	-2.410815	1.961916	0.557403
32	1	0	1.085290	0.556607	-2.822103
33	1	0	4.326402	-3.621511	-0.084287
34	1	0	4.848750	-2.037363	-0.687840
35	1	0	3.898007	-2.144306	0.799907
36	1	0	-4.239726	-3.771163	-3.091004
37	1	0	-2.941693	-2.934501	-3.967067
38	1	0	-2.542632	-4.094783	-2.690887
39	1	0	-1.707071	0.739075	1.610712
40	1	0	-0.393073	-0.393113	-2.997449

3.4. Cartesian coordinates and selected energy values for the calculated structures along the pathway of formation of products **III** and **V**

***t,t*-I**
*E*elec.= -1490.6367763 a.u
*G*corr. = 0.216141 a.u
*E*elec. + *G*corr. = -1490.4206353 a.u.

1	6	0	0.504655	-2.242201	0.140681
2	6	0	-0.879393	-2.493725	-0.018947
3	6	0	-1.308104	-3.810547	-0.242369
4	6	0	-0.405504	-4.864482	-0.300461
5	6	0	0.958099	-4.616964	-0.140740
6	6	0	1.401182	-3.319374	0.080117
7	1	0	-2.364662	-4.000777	-0.405930
8	1	0	-0.762701	-5.873963	-0.478415
9	1	0	1.672148	-5.433632	-0.179412
10	1	0	2.458917	-3.135165	0.242964
11	6	0	0.994750	-0.880312	0.408590
12	6	0	-1.851549	-1.388731	0.005778
13	6	0	2.210445	-0.427089	0.058499
14	6	0	-3.131916	-1.510987	0.395138
15	6	0	2.737095	0.897468	0.340185
16	6	0	-4.124717	-0.450088	0.396428
17	16	0	1.854295	2.107977	1.230491
18	6	0	3.146112	3.242769	1.074904
19	6	0	4.198225	2.723353	0.380345
20	6	0	3.964160	1.381484	-0.039707
21	1	0	4.671336	0.784732	-0.605315
22	1	0	5.107538	3.275036	0.173853
23	1	0	3.048610	4.228787	1.509886
24	16	0	-3.794827	1.168803	-0.158256
25	6	0	-5.407507	1.676000	0.192124
26	6	0	-6.159730	0.660806	0.704657
27	6	0	-5.425751	-0.555551	0.821240
28	1	0	-5.835031	-1.483211	1.206027
29	1	0	-7.198849	0.773402	0.989958
30	1	0	-5.702474	2.698367	-0.004618
31	1	0	0.313365	-0.212334	0.934140
32	1	0	-1.490873	-0.415529	-0.325094
33	1	0	2.890456	-1.069080	-0.499963
34	1	0	-3.499518	-2.467692	0.763961

***t,t*-I-IM1**

*E*elec.= -1491.0475539 a.u
*G*corr. = 0.229330 a.u
*E*elec. + *G*corr. = -1490.8182239 a.u.

1	16	0	0.050367	0.137215	0.010081
2	6	0	0.025092	0.004864	1.747992
3	6	0	1.304437	-0.046370	2.243589
4	6	0	2.305978	0.021808	1.232422
5	6	0	1.775812	0.125270	-0.019571
6	6	0	-1.197022	-0.030379	2.531874
7	6	0	-2.447308	0.053568	2.046959
8	6	0	-3.664941	0.013067	2.874010
9	6	0	-4.863074	0.610653	2.426977
10	6	0	-6.006162	0.561239	3.228071
11	6	0	-5.992734	-0.085336	4.459487
12	6	0	-4.818514	-0.695469	4.897592
13	6	0	-3.672380	-0.645669	4.113367
14	6	0	-4.952608	1.284203	1.081774
15	6	0	-5.192880	0.416251	-0.093292
16	6	0	-5.437846	-0.923995	-0.160374
17	6	0	-5.661408	-1.609502	-1.390918
18	6	0	-5.899751	-2.958814	-1.231401
19	6	0	-5.868511	-3.324453	0.116014
20	16	0	-5.547825	-2.062998	1.188597
21	1	0	-6.029856	-4.324469	0.505996
22	1	0	2.296182	0.194261	-0.965690
23	1	0	-2.771815	-1.147082	4.453807
24	1	0	-4.796606	-1.217177	5.849203
25	1	0	-6.891083	-0.118207	5.067144
26	1	0	-6.917084	1.035398	2.872211
27	1	0	-5.638399	-1.082828	-2.338821
28	1	0	-6.093288	-3.661739	-2.030523
29	1	0	1.510994	-0.129043	3.305065
30	1	0	3.371281	-0.002158	1.428464
31	1	0	-4.066342	1.889812	0.848796
32	1	0	-2.585157	0.171387	0.972388
33	1	0	-5.188318	0.928877	-1.055300
34	1	0	-1.033315	-0.113590	3.605318
35	1	0	-5.780942	2.010327	1.068161

***t,t*-I-TS1**

*E*elec.= -1491.0479868 a.u
*G*corr. = 0.232772 a.u
*E*elec. + *G*corr. = -1490.8152148 a.u

1	6	0	-2.920104	0.603794	0.025541
2	6	0	-2.466020	-0.679729	-0.315982
3	6	0	-3.373761	-1.727577	-0.457105
4	6	0	-4.735546	-1.489459	-0.269802
5	6	0	-5.185606	-0.212818	0.057780
6	6	0	-4.277362	0.835578	0.212649
7	1	0	-3.016663	-2.718542	-0.721250
8	1	0	-5.444677	-2.303827	-0.380401
9	1	0	-6.245681	-0.032918	0.206527
10	1	0	-4.623286	1.826480	0.492917
11	6	0	-1.849913	1.656678	0.202617
12	6	0	-1.004760	-0.813479	-0.513395
13	6	0	-0.647134	1.053610	0.857590
14	6	0	-0.193869	-1.641096	0.203242
15	6	0	0.677079	1.439742	0.669361
16	6	0	1.221791	-1.727057	0.021178
17	16	0	1.241321	2.465551	-0.633712
18	6	0	2.855491	2.279950	-0.120274
19	6	0	2.993504	1.474177	0.992682
20	6	0	1.758391	0.991976	1.443470
21	1	0	1.613885	0.358298	2.311570
22	1	0	3.948516	1.257612	1.453770
23	1	0	3.647153	2.789384	-0.657551
24	6	0	2.135378	-2.235344	0.930723
25	6	0	3.478045	-2.070046	0.521213
26	6	0	3.576828	-1.443438	-0.695841
27	16	0	2.046556	-1.058985	-1.361571
28	1	0	4.477047	-1.204934	-1.248247
29	1	0	4.337795	-2.391946	1.095487
30	1	0	-2.204998	2.453822	0.870115
31	1	0	-1.588700	2.124045	-0.755240
32	1	0	1.824565	-2.695447	1.862423
33	1	0	-0.604299	-2.193380	1.047887
34	1	0	-0.838115	0.485556	1.767012
35	1	0	-0.589046	-0.276242	-1.369026

***t,t*-I-IM2**

*E*elec.= -1491.0664379 a.u
*G*corr. = 0.233216 a.u
*E*elec. + *G*corr. = -1490.8332219 a.u

1	6	0	-3.122295	1.031106	0.624469
2	6	0	-2.996839	-0.197091	-0.030107

3	6	0	-4.068155	-1.076488	-0.129070
4	6	0	-5.284691	-0.709658	0.449314
5	6	0	-5.416123	0.516115	1.102524
6	6	0	-4.336314	1.397501	1.192654
7	1	0	-3.961283	-2.028365	-0.642345
8	1	0	-6.133364	-1.383793	0.389895
9	1	0	-6.367837	0.786382	1.549614
10	1	0	-4.443499	2.349393	1.704847
11	6	0	-1.823613	1.795077	0.571020
12	6	0	-1.601797	-0.349242	-0.591254
13	6	0	-0.778836	0.692682	0.292309
14	6	0	-0.979718	-1.672440	-0.442803
15	6	0	0.510287	1.100976	-0.334383
16	6	0	0.003072	-2.178389	-1.240339
17	16	0	0.582225	2.201195	-1.680490
18	6	0	2.288682	1.997538	-1.828720
19	6	0	2.779389	1.137824	-0.892446
20	6	0	1.756921	0.620368	-0.039385
21	1	0	1.931259	-0.089676	0.762276
22	1	0	3.828877	0.882153	-0.808061
23	1	0	2.829882	2.546442	-2.588086
24	6	0	0.699882	-3.400033	-1.022463
25	6	0	1.669164	-3.644580	-1.974071
26	6	0	1.723719	-2.624291	-2.929268
27	16	0	0.624539	-1.373296	-2.680269
28	1	0	2.400352	-2.580436	-3.776670
29	1	0	2.315801	-4.511420	-2.002687
30	1	0	-1.592724	2.338900	1.489958
31	1	0	-1.848835	2.522545	-0.251406
32	1	0	0.462315	-4.043437	-0.181938
33	1	0	-1.260466	-2.268753	0.426400
34	1	0	-0.546549	0.194733	1.240449
35	1	0	-1.566400	-0.006438	-1.634518

III

*E*elec.= -1490.6582584 a.u
*G*corr. = 0.220063 a.u
*E*elec. + *G*corr. = -1490.4381954 a.u

1	6	0	-2.642198	0.563347	0.740948
2	6	0	-2.124696	-0.580785	0.119694
3	6	0	-2.927083	-1.350827	-0.726194
4	6	0	-4.246537	-0.961631	-0.938643
5	6	0	-4.760900	0.181532	-0.318661
6	6	0	-3.960450	0.949870	0.526405
7	1	0	-2.529173	-2.231792	-1.222318
8	1	0	-4.879857	-1.546051	-1.599037

9	1	0	-5.790280	0.474642	-0.501039
10	1	0	-4.361283	1.837715	1.007598
11	6	0	-1.605421	1.204346	1.627680
12	6	0	-0.711708	-0.760837	0.497402
13	6	0	-0.270422	0.512354	1.216751
14	6	0	0.009221	-1.866611	0.233622
15	6	0	0.566407	1.411635	0.338684
16	6	0	1.390413	-2.182358	0.547606
17	16	0	0.335324	1.480040	-1.381100
18	6	0	1.521809	2.722049	-1.552496
19	6	0	2.066435	3.062833	-0.350774
20	6	0	1.515834	2.311116	0.733438
21	1	0	1.816212	2.424944	1.769814
22	1	0	2.837003	3.816579	-0.237069
23	1	0	1.753370	3.117283	-2.532538
24	6	0	1.981126	-3.401611	0.301347
25	6	0	3.340962	-3.470578	0.710169
26	6	0	3.777622	-2.301524	1.263127
27	16	0	2.543946	-1.099303	1.284824
28	1	0	4.759448	-2.069371	1.654372
29	1	0	3.966691	-4.348102	0.598517
30	1	0	-1.828029	0.996303	2.680217
31	1	0	-1.554361	2.289913	1.509948
32	1	0	1.439578	-4.220462	-0.159737
33	1	0	-0.497258	-2.681038	-0.283643
34	1	0	0.325466	0.283366	2.106499

***t,t*-I-IM3**

*E*elec.= -1491.0669254 a.u
*G*corr. = 0.231781 a.u
*E*elec. + *G*corr. = -1490.8351444 a.u

1	16	0	0.316123	-2.107188	1.045091
2	6	0	-0.295893	-0.680620	1.807661
3	6	0	0.252903	0.444132	1.258015
4	6	0	1.162514	0.155421	0.196256
5	6	0	1.292790	-1.184137	-0.030538
6	6	0	-1.317846	-0.754677	2.903057
7	6	0	-2.675778	-0.248397	2.573246
8	6	0	-3.678721	-0.016578	3.519303
9	6	0	-4.846023	0.458790	2.860844
10	6	0	-4.640916	0.499977	1.382856
11	6	0	-3.154048	0.116503	1.198544
12	6	0	-3.629932	-0.171771	4.930177
13	6	0	-4.753208	0.157593	5.648058
14	6	0	-5.905751	0.641791	4.985576
15	6	0	-5.966154	0.802652	3.605352
16	6	0	-2.854798	-0.916242	0.146845

17	16	0	-3.371824	-2.563382	0.330726
18	6	0	-2.669796	-3.007084	-1.180851
19	6	0	-2.077943	-1.942912	-1.792422
20	6	0	-2.182318	-0.741172	-1.027559
21	1	0	-2.730295	-0.535683	5.416647
22	1	0	-4.766000	0.055670	6.727186
23	1	0	-6.776836	0.895993	5.582310
24	1	0	-6.865718	1.175545	3.127993
25	1	0	-1.762933	0.213995	-1.325029
26	1	0	-1.582695	-2.009196	-2.753890
27	1	0	-2.742188	-4.029188	-1.528176
28	1	0	1.918072	-1.685574	-0.757335
29	1	0	1.697994	0.909645	-0.368102
30	1	0	-4.870842	1.485178	0.967879
31	1	0	-5.300707	-0.220886	0.888447
32	1	0	0.006172	1.444935	1.596866
33	1	0	-1.455008	-1.784875	3.266108
34	1	0	-2.573055	1.012872	0.925887
35	1	0	-0.972091	-0.199708	3.785943

V

*E*elec.= -1490.6645694 a.u
*G*corr. = 0.219195 a.u
*E*elec. + *G*corr. = -1490.4453744 a.u

1	16	0	0.495283	-1.663751	4.460793
2	6	0	-0.700238	-0.764716	3.576822
3	6	0	-0.464245	0.576476	3.676910
4	6	0	0.687380	0.889243	4.467784
5	6	0	1.306232	-0.220427	4.956245
6	6	0	-1.788361	-1.486235	2.819917
7	6	0	-2.930464	-0.582781	2.460311
8	6	0	-4.019403	-0.302841	3.406250
9	6	0	-4.953802	0.542682	2.785159
10	6	0	-4.476050	0.849916	1.393210
11	6	0	-3.168384	0.087632	1.302253
12	6	0	-4.211895	-0.739695	4.716011
13	6	0	-5.358726	-0.322160	5.392304
14	6	0	-6.290887	0.513335	4.772084
15	6	0	-6.093902	0.952847	3.459179
16	6	0	-2.377956	0.162343	0.083411
17	16	0	-0.692906	-0.281986	-0.013645
18	6	0	-0.611540	0.140767	-1.681019
19	6	0	-1.806323	0.610214	-2.142829
20	6	0	-2.811681	0.629592	-1.135549
21	1	0	-3.486590	-1.386358	5.203148
22	1	0	-5.529694	-0.650669	6.413026

23	1	0	-7.176840	0.825692	5.316432
24	1	0	-6.820999	1.603674	2.981336
25	1	0	-3.826998	0.970853	-1.303426
26	1	0	-1.965700	0.931475	-3.165277
27	1	0	0.317143	0.016819	-2.222246
28	1	0	2.187664	-0.280676	5.580730
29	1	0	1.031497	1.898312	4.662906
30	1	0	-4.322450	1.923692	1.232867
31	1	0	-5.190196	0.515425	0.630437
32	1	0	-1.094612	1.320265	3.201317
33	1	0	-1.368749	-1.955266	1.923105
34	1	0	-2.175107	-2.306476	3.436638

3.5. Cartesian coordinates and selected energy values for the calculated structures along the pathway of formation of products **IV** and **VI**

***t,t*-II**
*E*elec.= -1569.2585143 a.u
*G*corr. = 0.266175 a.u
*E*elec. + *G*corr. = -1568.9923393 a.u.

1	6	0	0.926623	0.271482	1.972280
2	6	0	-0.313393	0.319218	1.389473
3	16	0	-0.191948	-0.017074	-0.319190
4	6	0	1.533129	-0.223376	-0.225109
5	6	0	1.972703	-0.038232	1.054572
6	6	0	-1.568887	0.605226	2.060865
7	6	0	-2.783995	0.601146	1.483584
8	6	0	-4.076475	0.850345	2.140227
9	6	0	-4.261437	1.727439	3.237033
10	6	0	-5.540212	1.832375	3.807227
11	6	0	-6.616270	1.101420	3.321740
12	6	0	-6.441233	0.261493	2.221642
13	6	0	-5.186773	0.152250	1.638191
14	6	0	-3.168161	2.575451	3.733663
15	6	0	-3.027856	2.986781	5.005415
16	6	0	-1.966580	3.846417	5.499468
17	16	0	-0.674240	4.441655	4.485717
18	6	0	0.065000	5.293685	5.812004
19	6	0	-0.654330	5.117317	6.958890
20	6	0	-1.806485	4.294909	6.784607
21	1	0	-5.043608	-0.502699	0.782647
22	1	0	-7.279331	-0.298055	1.818244
23	1	0	-7.594033	1.208122	3.780891
24	1	0	-5.692100	2.531520	4.624442
25	1	0	-2.499216	4.038230	7.578888
26	1	0	-0.364107	5.565182	7.903141
27	6	0	1.318419	6.085116	5.611905
28	1	0	1.075974	0.455400	3.030943
29	1	0	3.018759	-0.121792	1.328260
30	6	0	2.331712	-0.553144	-1.445813
31	1	0	-2.430477	2.882314	2.992896
32	1	0	-2.861067	0.319550	0.432292
33	1	0	-3.732578	2.656337	5.767604
34	1	0	-1.464643	0.812486	3.124316
35	1	0	1.619983	6.532172	6.561804
36	1	0	2.138668	5.456206	5.252399
37	1	0	1.174113	6.889612	4.884098
38	1	0	3.384209	-0.660007	-1.173941
39	1	0	1.999012	-1.489404	-1.904323
40	1	0	2.251341	0.233472	-2.202556

***t,t*-II-IM1**
*E*elec.= -1569.6771136 a.u
*G*corr. = 0.279628 a.u
*E*elec. + *G*corr. = -1569.3974856 a.u.

1	6	0	-2.439415	-1.049266	-0.134462
2	6	0	-3.446849	-0.561413	0.757972
3	16	0	-3.878041	-1.835108	1.909880
4	6	0	-2.764267	-2.903888	1.202198
5	6	0	-2.062725	-2.343330	0.115912
6	6	0	-3.963361	0.692552	0.680045
7	6	0	-5.006372	1.348916	1.507608
8	6	0	-5.515039	0.587711	2.705547
9	6	0	-4.812034	0.589222	3.930064
10	6	0	-5.329386	-0.162382	4.996375
11	6	0	-6.512311	-0.880024	4.866464
12	6	0	-7.208848	-0.866564	3.659146
13	6	0	-6.705765	-0.132909	2.589714
14	6	0	-3.547453	1.329122	4.072296
15	6	0	-3.065163	1.798805	5.236085
16	6	0	-1.808851	2.502752	5.412362
17	6	0	-1.335675	3.042536	6.580351
18	6	0	-0.066532	3.675373	6.438987
19	6	0	0.429144	3.618104	5.167742
20	16	0	-0.669953	2.773129	4.115644
21	6	0	1.719475	4.165535	4.646533
22	6	0	-2.583180	-4.284290	1.715953
23	1	0	-4.780023	-0.203940	5.931915
24	1	0	-6.885398	-1.459218	5.705372
25	1	0	-8.132291	-1.425995	3.550168
26	1	0	-7.239166	-0.116611	1.642824
27	1	0	-2.040275	-0.418294	-0.921601
28	1	0	-1.318129	-2.902054	-0.437525
29	1	0	-1.889218	2.984654	7.511412
30	1	0	0.466737	4.158679	7.250230
31	1	0	-4.617723	2.339349	1.778958
32	1	0	-2.974754	1.503914	3.161783
33	1	0	-3.558902	1.305110	-0.125674
34	1	0	-3.639475	1.675143	6.153282
35	1	0	-2.760933	-4.992543	0.900327
36	1	0	-1.543327	-4.409008	2.036007
37	1	0	-3.247610	-4.515028	2.548856
38	1	0	2.261113	4.654259	5.459399
39	1	0	2.354912	3.374055	4.237414
40	1	0	1.553087	4.900487	3.853107
41	1	0	-5.832440	1.563198	0.812382

***t,t*-II-TS1**
*E*elec.= -1569.6663314 a.u
*G*corr. = 0.280485 a.u
*E*elec. + *G*corr. = -1569.3858464 a.u

1	6	0	-0.583811	-2.292090	-0.058135
2	6	0	-1.153479	-1.058350	-0.380684
3	16	0	-2.622781	-0.804284	0.536665
4	6	0	-2.460628	-2.337616	1.305392
5	6	0	-1.325095	-3.009883	0.886653
6	6	0	-0.628808	-0.143482	-1.305232
7	6	0	-1.436141	0.969440	-1.914620
8	6	0	-1.774367	2.021449	-0.881322
9	6	0	-0.861368	2.180583	0.170966
10	6	0	-1.131929	3.091967	1.193129
11	6	0	-2.290982	3.862845	1.146432
12	6	0	-3.187706	3.715869	0.089158
13	6	0	-2.933824	2.790845	-0.921897
14	6	0	0.346869	1.322823	0.182875
15	6	0	1.353724	1.432707	-0.736707
16	6	0	2.588671	0.709520	-0.719211
17	6	0	3.560768	0.749665	-1.696361
18	6	0	4.672489	-0.078051	-1.409860
19	6	0	4.553169	-0.752477	-0.220391
20	16	0	3.058928	-0.371757	0.568146
21	6	0	5.526424	-1.699982	0.402152
22	6	0	-3.471289	-2.809905	2.294926
23	1	0	-0.432584	3.199399	2.016893
24	1	0	-2.497731	4.573010	1.940629
25	1	0	-4.096284	4.308953	0.060282
26	1	0	-3.643844	2.652773	-1.732219
27	1	0	0.332637	-2.638716	-0.523986
28	1	0	-1.062745	-3.992621	1.259284
29	1	0	3.460952	1.362203	-2.585871
30	1	0	5.539912	-0.181600	-2.051478
31	1	0	-0.872652	1.405656	-2.743962
32	1	0	0.503842	0.703817	1.066779
33	1	0	0.236442	-0.509391	-1.854188
34	1	0	1.218429	2.097009	-1.590704
35	1	0	-3.208719	-3.812309	2.636345
36	1	0	-3.509347	-2.141850	3.160867
37	1	0	-4.471260	-2.836886	1.852046
38	1	0	6.392590	-1.812825	-0.252908
39	1	0	5.871677	-1.332534	1.373184
40	1	0	5.078973	-2.686106	0.557903
41	1	0	-2.352785	0.534655	-2.332082

***t,t*-II-IM2**

*E*elec.= -1569.6916451 a.u
*G*corr. = 0.282508 a.u
*E*elec. + *G*corr. = -1569.4091371 a.u

1	6	0	-0.754211	-2.283461	0.124075
2	6	0	-1.252699	-1.022362	-0.020811
3	16	0	-2.777217	-0.871218	0.815502
4	6	0	-2.725543	-2.526734	1.352450
5	6	0	-1.593606	-3.140230	0.904273
6	6	0	-0.636809	0.113278	-0.782903
7	6	0	-1.587723	0.714738	-1.851305
8	6	0	-2.277934	1.836775	-1.117921
9	6	0	-1.564434	2.192295	0.029594
10	6	0	-1.987919	3.220953	0.863225
11	6	0	-3.174099	3.882826	0.544604
12	6	0	-3.901254	3.524200	-0.592634
13	6	0	-3.458087	2.501461	-1.432881
14	6	0	-0.320488	1.319728	0.171627
15	6	0	0.823982	2.112503	-0.336277
16	6	0	1.877378	2.572569	0.387654
17	6	0	2.957286	3.352807	-0.121176
18	6	0	3.897445	3.664080	0.831007
19	6	0	3.576735	3.145398	2.100146
20	16	0	2.117884	2.270720	2.109620
21	6	0	4.373723	3.340874	3.336690
22	6	0	-3.829498	-3.097378	2.186411
23	1	0	-1.417366	3.492623	1.747415
24	1	0	-3.537070	4.679023	1.186731
25	1	0	-4.825570	4.044824	-0.823628
26	1	0	-4.029179	2.224846	-2.314418
27	1	0	0.186228	-2.591890	-0.320142
28	1	0	-1.366585	-4.177898	1.123856
29	1	0	2.995651	3.645424	-1.165076
30	1	0	4.798776	4.239775	0.660704
31	1	0	-1.008329	1.112453	-2.692983
32	1	0	-0.153898	0.989305	1.201788
33	1	0	0.282049	-0.269118	-1.235841
34	1	0	0.811551	2.378219	-1.394907
35	1	0	-3.617492	-4.147255	2.401538
36	1	0	-3.930685	-2.566440	3.137912
37	1	0	-4.793103	-3.041003	1.670972
38	1	0	5.437755	3.327814	3.090535
39	1	0	4.137764	4.329645	3.748328
40	1	0	4.157470	2.588597	4.096173
41	1	0	-2.277882	-0.032578	-2.250876

IV

*E*elec.= -1569.2798276 a.u
*G*corr. = 0.267811 a.u
*E*elec. + *G*corr. = -1569.0120166 a.u

1	6	0	1.781949	1.645129	-1.995983
2	6	0	1.365684	0.640661	-1.173168
3	16	0	1.855743	0.955948	0.468548
4	6	0	2.624362	2.454716	0.027856
5	6	0	2.497480	2.678285	-1.311345
6	6	0	0.657920	-0.634872	-1.558144
7	6	0	1.664911	-1.807917	-1.754925
8	6	0	1.527672	-2.628965	-0.498194
9	6	0	0.386493	-2.247331	0.219702
10	6	0	0.046116	-2.900542	1.407284
11	6	0	0.858545	-3.935846	1.861228
12	6	0	1.997095	-4.315464	1.143823
13	6	0	2.337276	-3.663384	-0.041809
14	6	0	-0.289266	-1.132764	-0.467445
15	6	0	-1.520737	-0.687253	-0.156126
16	6	0	-2.314927	0.373793	-0.744163
17	6	0	-3.614643	0.652227	-0.391806
18	6	0	-4.186196	1.732408	-1.118925
19	6	0	-3.327829	2.286223	-2.027185
20	16	0	-1.789371	1.481909	-1.989742
21	6	0	-3.574101	3.428132	-2.962320
22	6	0	3.289728	3.311947	1.058659
23	1	0	-0.829054	-2.602395	1.978013
24	1	0	0.610969	-4.447104	2.786384
25	1	0	2.623279	-5.120586	1.515907
26	1	0	3.222496	-3.957598	-0.598982
27	1	0	1.576230	1.648956	-3.061489
28	1	0	2.897170	3.563561	-1.794769
29	1	0	-4.136715	0.084137	0.370796
30	1	0	-5.198403	2.094978	-0.976365
31	1	0	1.380897	-2.405307	-2.628620
32	1	0	0.121628	-0.435991	-2.491901
33	1	0	-2.042710	-1.196343	0.654111
34	1	0	3.700922	4.203335	0.579086
35	1	0	2.584695	3.634191	1.831283
36	1	0	4.107923	2.783264	1.557385
37	1	0	-4.582013	3.817171	-2.800892
38	1	0	-2.862166	4.243280	-2.800758
39	1	0	-3.490754	3.116666	-4.008271
40	1	0	2.683183	-1.446357	-1.920832

***t,t*-II-IM3**
*E*elec.= -1569.6893342 a.u
*G*corr. = 0.283267 a.u
*E*elec. + *G*corr. = -1569.4060672 a.u

1	16	0	0.628026	-1.565430	1.238484
2	6	0	-0.354229	-0.273560	1.844495
3	6	0	-0.031861	0.906374	1.238958
4	6	0	1.011788	0.769296	0.273308
5	6	0	1.479215	-0.508656	0.155868
6	6	0	-1.391737	-0.503636	2.907644
7	6	0	-2.770723	-0.118318	2.522658
8	6	0	-3.284627	-0.138038	1.115192
9	6	0	-4.811663	0.070574	1.250653
10	6	0	-4.990188	0.460105	2.680701
11	6	0	-3.776046	0.290496	3.403910
12	6	0	-3.698141	0.551597	4.797143
13	6	0	-4.837778	0.982987	5.431957
14	6	0	-6.035129	1.163071	4.702257
15	6	0	-6.125871	0.914391	3.336000
16	6	0	-2.833479	-1.339807	0.333293
17	6	0	-2.943166	-2.652339	0.693446
18	6	0	-2.415598	-3.541831	-0.291329
19	6	0	-1.913464	-2.901947	-1.389096
20	16	0	-2.082096	-1.183017	-1.218623
21	6	0	-1.291283	-3.501764	-2.611041
22	6	0	2.559686	-1.025300	-0.741933
23	1	0	-2.765454	0.424066	5.337118
24	1	0	-4.826188	1.199485	6.494002
25	1	0	-6.917117	1.510438	5.232595
26	1	0	-7.059974	1.060494	2.804587
27	1	0	-3.387713	-2.972754	1.631171
28	1	0	-2.408418	-4.621998	-0.193587
29	1	0	-0.525073	1.843892	1.475715
30	1	0	1.408001	1.590925	-0.313419
31	1	0	-5.206138	0.820314	0.560567
32	1	0	-2.851664	0.769332	0.662322
33	1	0	-1.118866	-0.006734	3.844343
34	1	0	-1.269594	-4.589145	-2.509343
35	1	0	-1.856017	-3.253542	-3.514665
36	1	0	-0.264758	-3.150516	-2.752846
37	1	0	2.961291	-0.201067	-1.335676
38	1	0	3.381587	-1.468269	-0.171353
39	1	0	2.181725	-1.788903	-1.428662
40	1	0	-5.336393	-0.870691	1.055186
41	1	0	-1.465427	-1.575257	3.155705

VI

*E*elec.= -1569.2864606 a.u
*G*corr. = 0.270664 a.u
*E*elec. + *G*corr. = -1569.0157966 a.u

1	16	0	1.412979	1.014364	1.757626
2	6	0	-0.199322	0.404258	1.510091
3	6	0	-0.183111	-0.956195	1.418112
4	6	0	1.129032	-1.516888	1.546397
5	6	0	2.104298	-0.584199	1.734713
6	6	0	-1.367924	1.351075	1.396734
7	6	0	-2.685864	0.642440	1.469752
8	6	0	-3.491446	0.253080	0.447662
9	6	0	-4.762411	-0.374236	0.981936
10	6	0	-4.565286	-0.320461	2.472067
11	6	0	-3.322483	0.277834	2.741542
12	6	0	-2.879906	0.445541	4.052635
13	6	0	-3.704279	0.011156	5.091168
14	6	0	-4.942220	-0.578254	4.823407
15	6	0	-5.382845	-0.748422	3.507226
16	6	0	-3.228276	0.375300	-0.977111
17	6	0	-2.030107	0.400184	-1.646459
18	6	0	-2.176645	0.522167	-3.059550
19	6	0	-3.477384	0.579918	-3.472771
20	16	0	-4.552288	0.485920	-2.112388
21	6	0	-4.005930	0.705168	-4.866634
22	6	0	3.575455	-0.791822	1.915148
23	1	0	-1.914740	0.899419	4.262868
24	1	0	-3.379762	0.129294	6.120678
25	1	0	-5.567561	-0.909366	5.646868
26	1	0	-6.345754	-1.208648	3.303111
27	1	0	-1.074953	0.293107	-1.143336
28	1	0	-1.343872	0.555510	-3.753721
29	1	0	-1.082117	-1.543870	1.264572
30	1	0	1.340729	-2.579979	1.502218
31	1	0	-5.655058	0.183100	0.666970
32	1	0	-1.300419	1.909493	0.455281
33	1	0	-3.170307	0.736286	-5.569500
34	1	0	-4.645876	-0.141944	-5.131942
35	1	0	-4.594099	1.619181	-4.994333
36	1	0	3.803330	-1.857723	1.840781
37	1	0	4.154965	-0.264021	1.151447
38	1	0	3.915521	-0.437356	2.893149
39	1	0	-4.886136	-1.400778	0.615433
40	1	0	-1.318716	2.088617	2.207525