Supplementary Material (ESI) for *PCCP*

Second-order Perturbation Theory with Complete and Restricted Active Space Reference Functions Applied to Oligomeric Unsaturated Hydrocarbons

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Supporting Information

Supplementary Material (ESI) for *PCCP*

Cartesian Coordinates of the systems in study :

Ethene Oligomers :

Monomer

C	-0.671081	0.000000	0.000000
C	0.671081	0.000000	0.000000
H	-1.251970	0.940593	0.000000
H	1.251970	0.940593	0.000000
H	-1.251970	-0.940593	0.000000
H	1.251970	-0.940593	0.000000

DIMER

C	-1.753076	-0.639740	0.000000
C	1.753076	0.639740	0.000000
C	-0.399654	-0.609577	0.000000
C	0.399654	0.609577	0.000000
H	-2.346301	0.293341	0.000000

H	2.346301	-0.293341	0.000000
H	-2.311065	-1.591707	0.000000
H	2.311065	1.591707	0.000000
H	0.162215	-1.563801	0.000000
H	-0.162215	1.563801	0.000000

TRIMER

C	-2.824392	-1.283823	0.000000
C	2.824392	1.283823	0.000000
C	-1.468084	-1.238958	0.000000
C	1.468084	1.238958	0.000000
H	-3.427301	-0.357265	0.000000
H	3.427301	0.357265	0.000000
H	-3.370938	-2.242158	0.000000
H	3.370938	2.242158	0.000000
H	-0.899808	-2.189302	0.000000
H	0.899808	2.189302	0.000000

C	-0.683520	-0.020769	0.000000
C	0.683520	0.020769	0.000000
H	-1.243323	0.934950	0.000000
H	1.243323	-0.934950	0.000000

TETRAMER

C	-1.758680	-0.655031	0.000000
C	1.758680	0.655031	0.000000
C	-0.387619	-0.606079	0.000000
C	0.387619	0.606079	0.000000
H	-2.322251	0.298249	0.000000
H	2.322251	-0.298249	0.000000
H	0.173405	-1.561007	0.000000
H	-0.173405	1.561007	0.000000
C	2.534726	1.875578	0.000000
C	-2.534726	-1.875578	0.000000
C	3.892056	1.929500	0.000000

C	-3.892056	-1.929500	0.000000
H	1.961281	2.822871	0.000000
H	-1.961281	-2.822871	0.000000
H	4.432035	2.891484	0.000000
H	-4.432035	-2.891484	0.000000
H	4.500991	1.006992	0.000000
H	-4.500991	-1.006992	0.000000

PENTAMER :

C	-0.687972	-0.026402	0.000000
C	0.687972	0.026402	0.000000
H	-1.249994	0.927744	0.000000
H	1.249994	-0.927744	0.000000
C	1.457201	1.237868	0.000000
C	-1.457201	-1.237868	0.000000
C	2.830172	1.292306	0.000000
C	-2.830172	-1.292306	0.000000

H	0.893894	2.191518	0.000000
H	-0.893894	-2.191518	0.000000
H	3.396713	0.340853	0.000000
H	-3.396713	-0.340853	0.000000
C	3.600331	2.514851	0.000000
C	-3.600331	-2.514851	0.000000
C	4.958134	2.575512	0.000000
C	-4.958134	-2.575512	0.000000
H	3.023118	3.459899	0.000000
H	-3.023118	-3.459899	0.000000
H	5.493296	3.540142	0.000000
H	-5.493296	-3.540142	0.000000
H	5.571492	1.655989	0.000000
H	-5.571492	-1.655989	0.000000

HEXAMER

C	0.382191	0.604652	0.000000
C	-0.382191	-0.604652	0.000000

C	1.760542	0.661229	0.000000
C	-1.760542	-0.661229	0.000000
H	-0.180938	1.558226	0.000000
H	0.180938	-1.558226	0.000000
H	2.324218	-0.291906	0.000000
H	-2.324218	0.291906	0.000000
C	2.525477	1.872920	0.000000
C	-2.525477	-1.872920	0.000000
C	3.899512	1.931573	0.000000
C	-3.899512	-1.931573	0.000000
H	1.960116	2.825387	0.000000
H	-1.960116	-2.825387	0.000000
H	4.468586	0.981638	0.000000
H	-4.468586	-0.981638	0.000000
C	4.665273	3.155770	0.000000
C	-4.665273	-3.155770	0.000000
C	6.023272	3.221350	0.000000

C	-6.023272	-3.221350	0.000000
H	4.085075	4.098992	0.000000
H	-4.085075	-4.098992	0.000000
H	6.555406	4.187618	0.000000
H	-6.555406	-4.187618	0.000000
H	6.639886	2.303984	0.000000
H	-6.639886	-2.303984	0.000000

SEPTAMER

C	-0.690384	-0.029329	0.000000
C	0.690384	0.029329	0.000000
H	-1.254054	0.923866	0.000000
H	1.254054	-0.923866	0.000000
C	1.451936	1.238238	0.000000
C	-1.451936	-1.238238	0.000000
C	2.831419	1.297321	0.000000
C	-2.831419	-1.297321	0.000000

H	0.887835	2.191256	0.000000
H	-0.887835	-2.191256	0.000000
H	3.396440	0.345028	0.000000
H	-3.396440	-0.345028	0.000000
C	3.593469	2.509889	0.000000
C	-3.593469	-2.509889	0.000000
C	4.967953	2.571732	0.000000
C	-4.967953	-2.571732	0.000000
H	3.026341	3.461315	0.000000
H	-3.026341	-3.461315	0.000000
H	5.539160	1.623120	0.000000
H	-5.539160	-1.623120	0.000000
C	-5.730379	-3.797723	0.000000
C	5.730379	3.797723	0.000000
C	-7.088424	-3.867312	0.000000
C	7.088424	3.867312	0.000000
H	-5.147640	-4.739399	0.000000

H	5.147640	4.739399	0.000000
H	-7.617292	-4.835387	0.000000
H	7.617292	4.835387	0.000000
H	-7.707947	-2.951940	0.000000
H	7.707947	2.951940	0.000000

OCTAMER

C	0.379491	0.604069	0.000000
C	-0.379491	-0.604069	0.000000
C	1.761511	0.664821	0.000000
C	-1.761511	-0.664821	0.000000
H	-0.184875	1.556877	0.000000
H	0.184875	-1.556877	0.000000
H	2.326165	-0.287762	0.000000
H	-2.326165	0.287762	0.000000
C	2.520702	1.874052	0.000000
C	-2.520702	-1.874052	0.000000

C	3.900778	1.935442	0.000000
C	-3.900778	-1.935442	0.000000
H	1.955412	2.826378	0.000000
H	-1.955412	-2.826378	0.000000
H	4.467174	0.983984	0.000000
H	-4.467174	-0.983984	0.000000
C	4.660551	3.148924	0.000000
C	-4.660551	-3.148924	0.000000
C	6.035252	3.213232	0.000000
C	-6.035252	-3.213232	0.000000
H	4.091916	4.099452	0.000000
H	-4.091916	-4.099452	0.000000
H	6.608066	2.265603	0.000000
H	-6.608066	-2.265603	0.000000
C	6.795415	4.440463	0.000000
C	-6.795415	-4.440463	0.000000
C	8.153455	4.512486	0.000000

C	-8.153455	-4.512486	0.000000
H	6.211029	5.381118	0.000000
H	-6.211029	-5.381118	0.000000
H	8.680634	5.481480	0.000000
H	-8.680634	-5.481480	0.000000
H	8.774546	3.598179	0.000000
H	-8.774546	-3.598179	0.000000

NONAMER

C	-0.691719	-0.031287	0.000000
C	0.691719	0.031287	0.000000
H	-1.256683	0.921138	0.000000
H	1.256683	-0.921138	0.000000
C	1.448538	1.239253	0.000000
C	-1.448538	-1.239253	0.000000
C	2.831323	1.301867	0.000000
C	-2.831323	-1.301867	0.000000

H	0.883428	2.191630	0.000000
H	-0.883428	-2.191630	0.000000
H	3.396802	0.349794	0.000000
H	-3.396802	-0.349794	0.000000
C	3.588686	2.511384	0.000000
C	-3.588686	-2.511384	0.000000
C	4.969162	2.574471	0.000000
C	-4.969162	-2.574471	0.000000
H	3.022541	3.463203	0.000000
H	-3.022541	-3.463203	0.000000
H	5.536447	1.623561	0.000000
H	-5.536447	-1.623561	0.000000
C	-5.727311	-3.788499	0.000000
C	5.727311	3.788499	0.000000
C	-7.102175	-3.854628	0.000000
C	7.102175	3.854628	0.000000

H	-5.157691	-4.738442	0.000000
H	5.157691	4.738442	0.000000
H	-7.676128	-2.907708	0.000000
H	7.676128	2.907708	0.000000
C	-7.860371	-5.082837	0.000000
C	7.860371	5.082837	0.000000
C	-9.218378	-5.157425	0.000000
C	9.218378	5.157425	0.000000
H	-7.274530	-6.022601	0.000000
H	7.274530	6.022601	0.000000
H	-9.743381	-6.127597	0.000000
H	9.743381	6.127597	0.000000
H	-9.841270	-4.244372	0.000000
H	9.841270	4.244372	0.000000

DECAMER

C	-1.762226	-0.666914	0.000000
C	1.762226	0.666914	0.000000

C	-0.377742	-0.603513	0.000000
C	0.377742	0.603513	0.000000
H	-2.327389	0.285382	0.000000
H	2.327389	-0.285382	0.000000
H	0.187228	-1.555955	0.000000
H	-0.187228	1.555955	0.000000
C	2.517757	1.874579	0.000000
C	-2.517757	-1.874579	0.000000
C	3.901182	1.938463	0.000000
C	-3.901182	-1.938463	0.000000
H	1.952215	2.826713	0.000000
H	-1.952215	-2.826713	0.000000
H	4.467379	0.986826	0.000000
H	-4.467379	-0.986826	0.000000
C	-4.656875	-3.148327	0.000000
C	4.656875	3.148327	0.000000

C	-6.037701	-3.213361	0.000000
C	6.037701	3.213361	0.000000
H	-4.089726	-4.099556	0.000000
H	4.089726	4.099556	0.000000
H	-6.606245	-2.263209	0.000000
H	6.606245	2.263209	0.000000
C	-6.793755	-4.428281	0.000000
C	6.793755	4.428281	0.000000
C	-8.168751	-4.496756	0.000000
C	8.168751	4.496756	0.000000
H	-6.222703	-5.377367	0.000000
H	6.222703	5.377367	0.000000
H	-8.744222	-3.550761	0.000000
H	8.744222	3.550761	0.000000
C	-8.924798	-5.726090	0.000000
C	8.924798	5.726090	0.000000
C	-10.282773	-5.802906	0.000000

C	10.282773	5.802906	0.000000
H	-8.337452	-6.664913	0.000000
H	8.337452	6.664913	0.000000
H	-10.806359	-6.773837	0.000000
H	10.806359	6.773837	0.000000
H	-10.907085	-4.890816	0.000000
H	10.907085	4.890816	0.000000

Acetylene Oligomers :

MONOMER

C	0.000000	0.000000	-0.609835
C	0.000000	0.000000	0.609835
H	0.000000	0.000000	-1.693089
H	0.000000	0.000000	1.693089

DIMER

C	-1.897933	0.000000	0.000000
C	1.897933	0.000000	0.000000

C	-0.680607	0.000000	0.000000
C	0.680607	0.000000	0.000000
H	-2.967885	0.000000	0.000000
H	2.967885	0.000000	0.000000

TRIMER

C	0.000000	0.000000	-0.615404
C	0.000000	0.000000	0.615404
C	0.000000	0.000000	1.965386
C	0.000000	0.000000	-1.965386
C	0.000000	0.000000	3.186011
C	0.000000	0.000000	-3.186011
H	0.000000	0.000000	4.255850
H	0.000000	0.000000	-4.255850

TETRAMER

C	0.000000	0.000000	0.668876

C	0.000000	0.000000	-0.668876
C	0.000000	0.000000	1.904640
C	0.000000	0.000000	-1.904640
C	0.000000	0.000000	3.252015
C	0.000000	0.000000	-3.252015
C	0.000000	0.000000	4.474504
C	0.000000	0.000000	-4.474504
H	0.000000	0.000000	5.544598
H	0.000000	0.000000	-5.544598

PENTAMER

C	0.000000	0.000000	1.947804
C	0.000000	0.000000	-1.947804
C	0.000000	0.000000	3.183947
C	0.000000	0.000000	-3.183947
C	0.000000	0.000000	4.526629
C	0.000000	0.000000	-4.526629

C	0.000000	0.000000	5.749269
C	0.000000	0.000000	-5.749269
C	0.000000	0.000000	0.619532
C	0.000000	0.000000	-0.619532
H	0.000000	0.000000	6.818625
H	0.000000	0.000000	-6.818625

Phenylene Oligomers :

MONOMER

C	1.209918	-0.698488	0.000000
C	-1.209918	-0.698488	0.000000
C	1.209918	0.698488	0.000000
C	-1.209918	0.698488	0.000000
C	0.000000	-1.396832	0.000000
C	0.000000	1.396832	0.000000
H	0.000000	-2.487835	0.000000
H	0.000000	2.487835	0.000000
H	2.154726	-1.244157	0.000000

H	-2.154726	-1.244157	0.000000
H	2.154726	1.244157	0.000000
H	-2.154726	1.244157	0.000000

DIMER

C	1.150756	0.380265	-1.473857
C	-1.150756	-0.380265	-1.473857
C	-1.150756	0.380265	1.473857
C	1.150756	-0.380265	1.473857
C	0.000000	0.000000	-0.743906
C	0.000000	0.000000	0.743906
C	-1.151159	-0.381139	-2.876312
C	1.151159	0.381139	-2.876312
C	1.151159	-0.381139	2.876312
C	-1.151159	0.381139	2.876312
C	0.000000	0.000000	-3.585130
C	0.000000	0.000000	3.585130

H	-2.058374	-0.691306	-3.421080
H	2.058374	0.691306	-3.421080
H	2.058374	-0.691306	3.421080
H	-2.058374	0.691306	3.421080
H	2.052276	0.708028	-0.930702
H	-2.052276	-0.708028	-0.930702
H	-2.052276	0.708028	0.930702
H	2.052276	-0.708028	0.930702
H	0.000000	0.000000	-4.687516
H	0.000000	0.000000	4.687516

TRIMER

C	0.000000	2.922319	0.000000
C	0.000000	-2.922319	0.000000
C	0.986876	3.652825	-0.703561
C	-0.986876	-3.652825	-0.703561
C	-0.986876	3.652825	0.703561

C	0.986876	-3.652825	0.703561
C	0.987277	5.055078	-0.704038
C	-0.987277	-5.055078	-0.704038
C	-0.987277	5.055078	0.704038
C	0.987277	-5.055078	0.704038
C	0.000000	5.763876	0.000000
C	0.000000	-5.763876	0.000000
H	1.751538	3.110719	-1.283494
H	-1.751538	-3.110719	-1.283494
H	-1.751538	3.110719	1.283494
H	1.751538	-3.110719	1.283494
H	1.762212	5.599739	-1.268487
H	-1.762212	-5.599739	-1.268487
H	-1.762212	5.599739	1.268487
H	1.762212	-5.599739	1.268487
H	0.000000	6.866273	0.000000

H	0.000000	-6.866273	0.000000
C	0.000000	1.436615	0.000000
C	0.000000	-1.436615	0.000000
C	1.207339	0.699668	-0.000351
C	-1.207339	-0.699668	-0.000351
C	-1.207339	0.699668	0.000351
C	1.207339	-0.699668	0.000351
H	2.170799	1.235110	0.017871
H	-2.170799	-1.235110	0.017871
H	-2.170799	1.235110	-0.017871
H	2.170799	-1.235110	-0.017871

Supplementary Material (ESI) for *PCCP*

Total Energies and Weights

CASPT2/RASPT2 , CASSCF/RASSCF energies and weights for the various oligomers in study.

CASPT2 & RASPT2 Total Energies (in a.u) :

Acetylene		CASPT2	RASPT2		
			(ae,ao)/2	(ae,ao)/3	(ae,ao)/4
one	Neutral	-77.15084	-77.14952	-77.14952	-77.15086
	Cation	-76.73593	-76.73593	-76.73593	-76.73593
	Exc.state	-76.88169	-76.88077	-76.88173	-76.88173
two	Neutral	-153.13734	-153.13027	-153.13973	-153.13729
	Cation	-152.76913	-152.76324	-152.77424	-152.76930
	Exc.state	-152.93576	-152.91489	-152.93428	-152.94039
three	Neutral	-229.12494	-229.10868	-229.11949	-229.12421
	Cation	-228.78234	-228.76524	-228.77874	-228.78199
	Exc.state	-228.96013	-228.89951	-228.95305	-228.96183
four	Neutral	-305.11365	-305.08541	-305.09862	-305.11175
	Cation	-304.78792	-304.75706	-304.77648	-304.78648
	Exc.state	-304.97215	-304.87821	-304.95447	-304.97160
five	Neutral	NP	-381.07742	-381.09501	-381.10675

	Cation	NP	-380.76031	-380.78223	-380.79020
	Exc.state	NP	-380.86787	-380.96490	-380.98191

CASSCF & RASSCF Total Energies (in a.u)

Acetylene		CASSCF	RASSCF		
			(ae,ao)/2	(ae,ao)/3	(ae,ao)/4
one	Neutral	-76.91838	-76.91558	-76.91558	-76.91839
	Cation	-76.53540	-76.53540	-76.53540	-76.53540
	Exc.state	-76.62167	-76.61806	-76.62169	-76.62169
two	Neutral	-152.69358	-152.68094	-152.68649	-152.69305
	Cation	-152.34913	-152.33803	-152.34651	-152.34890
	Exc.state	-152.45382	-152.32067	-152.44989	-152.45306
three	Neutral	-228.46763	-228.43893	-228.44734	-228.46525
	Cation	-228.14629	-228.11652	-228.13043	-228.14417
	Exc.state	-228.26589	-228.16314	-228.24943	-228.25857
four	Neutral	-304.24174	-304.19225	-304.20321	-304.23573
	Cation	-303.93556	-303.88307	-303.90328	-303.92941
	Exc.state	-304.06355	-303.89872	-304.02867	-304.04525
five	Neutral	NP	-379.90083	-379.90926	-379.94200

	Cation	NP	-379.60334	-379.62351	-379.65312
	Exc.state	NP	-379.61221	-379.75772	-379.77790

CASSCF & RASSCF Weights :

Acetylene		CASSCF	RASSCF		
			(ae,ao)/2	(ae,ao)/3	(ae,ao)/4
one	Neutral	0.92909	0.92862	0.92862	0.92908
	Cation	0.93978	0.93978	0.93978	0.93978
	Exc.state	0.91449	0.91340	0.91449	0.91449
two	Neutral	0.87459	0.87262	0.86781	0.87
	Cation	0.88047	0.87821	0.87457	0.88024
	Exc.state	0.83429	0.54385	0.84450	0.84854
three	Neutral	0.82491	0.82042	0.81744	0.82425
	Cation	0.82378	0.82427	0.82291	0.82854
	Exc.state	0.79939	0.76057	0.77232	0.80050
four	Neutral	0.78010	0.77269	0.76925	0.77845

	Cation	0.78371	0.77556	0.77384	0.78155
	Exc.state	0.75946	0.76087	0.60492	0.76548
five	Neutral	NP	0.70751	0.70321	0.71341
	Cation	NP	0.71346	0.68885	0.71346
	Exc.state	NP	0.65392	0.69550	0.70692

Phenylene		CASPT2	RASPT2		
			(ae,ao)/2	(ae,ao)/3	(ae,ao)/4
one	Neutral	-231.72045	-231.72014	-231.72048	-231.72048
	Cation	-231.37224	-231.37166	-231.37787	-231.37223
	Exc.state	-231.53918	-231.52957	-231.53906	-231.53934
two	Neutral	-462.26953	-462.26946	-462.27755	-462.27075
	Cation	-461.95929	-461.95877	-461.96517	-461.96026
	Exc.state	-462.10869	-462.06312	-462.09896	-462.10270
.	Neutral	NP	-692.82957	-692.83762	-692.83120

	Cation	NP	-692.53638	-692.54563	-692.53816
	Exc.state	NP	-692.61868	-692.66201	-692.66677

Phenylene		CASSCF	RASSCF		
			(ae,ao)/2	(ae,ao)/3	(ae,ao)/4
one	Neutral	-230.86008	-230.85495	-230.85607	-230.86004
	Cation	-230.54844	-230.54496	-230.54800	-230.54844
	Exc.state	-230.67748	-230.65263	-230.67254	-230.67723
two	Neutral	-460.55589	-460.53384	-460.53954	-460.55402
	Cation	-460.27140	-460.25056	-460.26019	-460.26994

	Exc.state	-460.37977	-460.28463	-460.35028	-460.37085
three	Neutral	NP	-690.17888	-690.18439	-690.20427
	Cation	NP	-689.92904	-689.93723	-689.96044
	Exc.state	NP	-689.87858	-689.96858	-689.97763

CASSCF & RASSCF Weights :

Phenylene		CASSCF	RASSCF		
			(ae,ao)/2	(ae,ao)/3	(ae,ao)/4
one	Neutral	0.78099	0.77942	0.77960	0.78096
	Cation	0.79116	0.79004	0.78710	0.79117
	Exc.state	0.77074	0.76994	0.77006	0.77073

two	Neutral	0.63935	0.63367	0.63113	0.63849
	Cation	0.64197	0.63624	0.63585	0.64119
	Exc.state	0.61123	0.55179	0.62527	0.62846
three	Neutral	NP	0.52453	0.52273	0.52951
	Cation	NP	0.52794	0.52900	0.53458
	Exc.state	NP	0.50513	0.50762	0.51177

CASPT2 & RASPT2 Total Energies (in a.u) :

Ethylene		CASPT2	RASPT2		
			(ae,ao)/2	(ae,ao)/3	(ae,ao)/4
one	Neutral	-78.39535	-78.39535	CND	CND
	Cation	-78.01017	CND	CND	CND
	Exc.state	-78.09293	-78.09293	CND	CND

two	Neutral	-155.62565	-155.62883	-155.63727	-155.62565
	Cation	-155.28845	-155.28843	-155.28843	-155.28843
	Exc.state	-155.39444	-155.40024	-155.40154	-155.39381
three	Neutral	-232.85370	-232.85368	-232.86622	-232.85375
	Cation	-232.55301	-232.56098	-232.56118	-232.55325
	Exc.state	-232.66299	-232.66147	-232.66839	-232.66579
four	Neutral	-310.08664	-310.08435	-310.09568	-310.08688
	Cation	-309.80427	-309.80355	-309.81123	-309.80423
	Exc.state	-309.92876	-309.91016	-309.92764	-309.93138
Five	Neutral	-387.31590	-387.31432	-387.32503	-387.31641
	Cation	-387.04711	-387.04657	-387.05448	-387.04707
	Exc.state	-387.18203	-387.15877	-387.17904	-387.18271
Six	Neutral	-464.54852	-464.54309	-464.55096	-464.54982
	Cation	-464.28980	-464.28718	-464.29470	-464.29094
	Exc.state	-464.42826	-464.38287	-464.41070	-464.43059
Seven	Neutral	-541.77941	-541.77416	-541.78397	-541.78084
	Cation	-541.52677	-541.52499	-541.53244	-541.52902
	Exc.state	-464.42826	-541.62027	-541.65499	-541.62027
Eight	Neutral	NP	-619.00122	-619.00923	-619.01384

	Cation	NP	-618.76035	-618.76942	-618.76901
	Exc.state	NP	-618.83889	-618.88151	-618.91226
Nine	Neutral	NP	-696.23241	-696.24240	-696.24493
	Cation	NP	-695.99555	-696.00534	-696.00408
	Exc.state	NP	-696.07487	-696.12257	-696.15620
Ten	Neutral	NP	-773.45863	-773.46686	-773.47829
	Cation	NP	-773.18141	-773.19422	-773.20670
	Exc.state	NP	-773.28607	-773.34976	-773.38751

Ethylene		CASSCF	RASSCF		
			(ae,ao)/2	(ae,ao)/3	(ae,ao)/4
one	Neutral	-78.09233	-78.09233	CND	CND
	Cation	-77.73326	CND	CND	CND
	Exc.state	-77.76910	-77.76910	CND	CND
two	Neutral	-155.03486	-155.03315	-155.03486	-155.03486
	Cation	-154.72353	-154.72353	-154.72353	-154.72353
	Exc.state	-154.74988	-154.74988	-154.74988	-154.74988

three	Neutral	-231.95208	-231.94948	-231.951753	-231.95207
	Cation	-231.69052	-231.68959	-231.69167	-231.69173
	Exc.state	-231.73451	-231.72743	-231.73427	-231.73451
four	Neutral	-308.92010	-308.90769	-308.91215	-308.91955
	Cation	-308.65811	-308.65023	-308.65570	-308.65793
	Exc.state	-308.75021	-308.69874	-308.72944	-308.74840
Five	Neutral	-385.83643	-385.82370	-385.82789	-385.83581
	Cation	-385.59997	-385.58769	-385.59500	-385.59945
	Exc.state	-385.67752	-385.62106	-385.65585	-385.67525
Six	Neutral	-462.80492	-462.77639	-462.78162	-462.80211
	Cation	-462.56251	-462.54102	-462.55154	-462.56102
	Exc.state	-462.67301	-462.56466	-462.61988	-462.66235
Seven	Neutral	-539.71938	-539.69122	-539.69657	-539.71659
	Cation	-539.49667	-539.46979	-539.48135	-539.49419
	Exc.state	-539.59312	-539.48086	-539.54041	-539.58170
Eight	Neutral	NP	-616.64095	-616.64711	-619.01384
	Cation	NP	-616.41816	-616.43179	-616.45295
	Exc.state	NP	-616.41321	-616.49411	-616.55320
Nine	Neutral	NP	-693.55562	-693.56210	-693.59632

	Cation	NP	-696.00408	-693.35690	-693.37998
	Exc.state	NP	-693.32645	-693.41135	-693.46863
Ten	Neutral	NP	-770.50216	-770.50905	-770.55939
	Cation	NP	-770.23332	-770.25147	-770.29513
	Exc.state	NP	-770.25342	-770.35953	-770.43110

Ethylene		CASSCF	RASSCF		
			(ae,ao)/2	(ae,ao)/3	(ae,ao)/4
one	Neutral	0.91078	0.91078	CND	CND
	Cation	0.91758	CND	CND	CND
	Exc.state	0.89242	0.89242	CND	CND
two	Neutral	0.83754	0.83439	0.82780	0.83754
	Cation	0.84440	0.84441	0.84441	0.84441
	Exc.state	0.80372	0.79706	0.79268	0.80563
three	Neutral	0.76648	0.76543	0.75698	0.76642
	Cation	0.77762	0.77086	0.77108	0.77779
	Exc.state	0.74552	0.73086	0.73938	0.73779

four	Neutral	0.72217	0.71913	0.71300	0.72191
	Cation	0.72613	0.72364	0.72098	0.72616
	Exc.state	0.69126	0.69829	0.68300	0.69157
Five	Neutral	0.66799	0.66463	0.65950	0.66759
	Cation	0.67498	0.67133	0.66963	0.67495
	Exc.state	0.64685	0.64393	0.64243	0.67211
Six	Neutral	0.63440	0.62865	0.62643	0.63322
	Cation	0.63669	0.63139	0.63113	0.63585
	Exc.state	0.62009	0.58860	0.54204	0.61923
Seven	Neutral	0.59149	0.58618	0.58284	0.59031
	Cation	0.59650	0.59010	0.59013	0.59514
	Exc.state	0.56853	0.59447	0.53309	0.59653
Eight	Neutral	NP	0.55741	0.55591	0.56292
	Cation	NP	0.55898	0.55916	0.56465
	Exc.state	NP	0.54616	0.57038	0.56569
Nine	Neutral	NP	0.52360	0.52099	0.52857
	Cation	NP	0.52586	0.52611	0.53137
	Exc.state	NP	0.50304	0.51168	0.50055
Ten	Neutral	NP	0.50003	0.49894	0.50585

	Cation	NP	0.49858	0.49892	0.50542
	Exc.state	NP	0.48878	0.49248	0.47229

DFT Total Energies (in a.u) :

Ethene	Neutral	Cation
One	-78.49894	-78.11964
Two	-155.82611	-155.49986
Three	-233.15547	-232.60459
Four	-310.48571	-310.22019
Five	-387.81637	-387.56610
Six	-465.14727	-464.90844
Seven	-542.47830	-542.24847
Eight	-619.80943	-619.58688
Nine	-697.14064	-696.92398
Ten	-774.47188	-774.26040

Acetylene	Neutral	Cation
One	-77.25010	-76.83684
Two	-153.34006	-152.98026
Three	-229.43115	-229.10288
Four	-305.52825	-305.21746
Five	-381.62388	-381.32847

Phenylene	Neutral	Cation
One	-232.01475	-231.68029
Two	-462.84638	-462.56088

Three	-693.67915	-693.41621