Supporting Information

Vibrationally Mediated Stabilization of Electron in Non-Polar Matter

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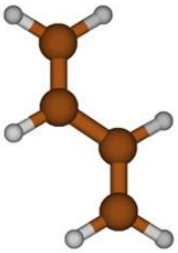
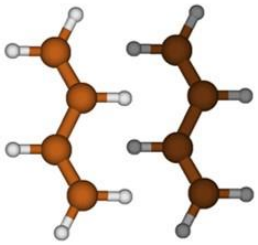
Section S1: Structure and energetics of butadiene clusters

For each cluster size, we show figure of the optimized butadiene cluster in the minimum of the neutral state. For these structures, we calculate vertical electron affinity according to ΔKS approach as well as using the simple technique by Tozer and De Proft[1] (T-DP). In the latter case, even the negative EAs should correspond to the true energies of resonances. We also present adiabatic electron affinity, including the electron affinity calculated for a cluster embedded in a polarizable continuum mimicking benzene. The VEA calculations were performed at the LC-ωPBE/6-31+g* level, while the resonance energy calculations were done with BLYP functional and consistent basis 6-31+g*. All the calculations were performed with the Gaussian 09 code (revision D.01)[2].

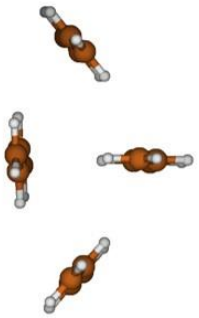
Table S1: Vertical electron affinities calculated with ΔKS approach (VEA), with Tozer's and De Proft's approach (VEA T-DP), adiabatic electron affinities in gas phase (AEA) and in PCM simulated benzene solvent (AEA in PCM) and reorganization energy of the PCM solvent upon ionization (Solvent shift) for clusters of various sizes (*n*). Shown structures represent neutral ground state minima. All values are in eV.



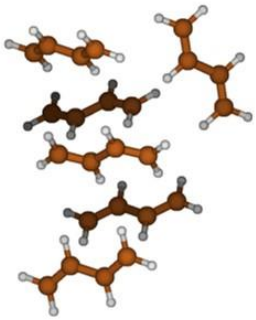
n	1
VEA	-1.01
VEA T-DP	-1.30
AEA	-0.70
AEA in PCM	-0.58
Solvent shift	0.25



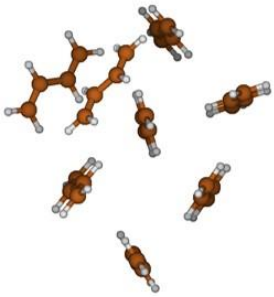
n	2
VEA	-1.07
VEA T-DP	-0.32
AEA	-0.46
AEA in PCM	-0.66
Solvent shift	-0.05



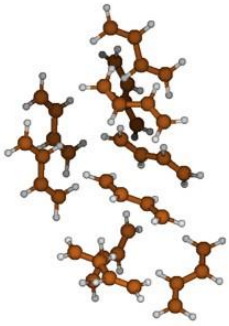
n	4
VEA	-0.88
VEA T-DP	0.22
AEA	-0.31
AEA in PCM	-0.69
Solvent shift	-0.19



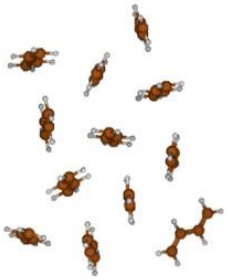
n	6
VEA	-0.97
VEA T-DP	0.49
AEA	0.02
AEA in PCM	-0.84
Solvent shift	-0.22



n	8
VEA	-0.66
VEA T-DP	0.59
AEA	-0.20
AEA in PCM	0.64
Solvent shift	-0.02



n	10
VEA	-0.79
VEA T-DP	0.64
AEA	0.09
AEA in PCM	0.83
Solvent shift	-0.02



n	12
VEA	-0.91
VEA T-DP	0.71
AEA	0.03
AEA in PCM	0.70
Solvent shift	-0.10

VEA – vertical electron affinity in eV calculated on LC-ωPBE level of theory with 6-31+g* basis set

VEA T-DP – vertical electron affinity in eV calc. on BLYP/6-31+g* level of theory based on Tozer's and De Proft's approach

AEA – adiabatic electron affinity calculated in eV on LC-ωPBE/6-31+g*

AEA in PCM – adiabatic electron affinity in eV calculated on LC-ωPBE/6-31+g* in benzene solvent via polarized continuum model

Solvent shift – non equilibrium solvent reorganization energy in eV

Section S2: Electron densities of unpaired electron in anionic $(But)_8$ clusters

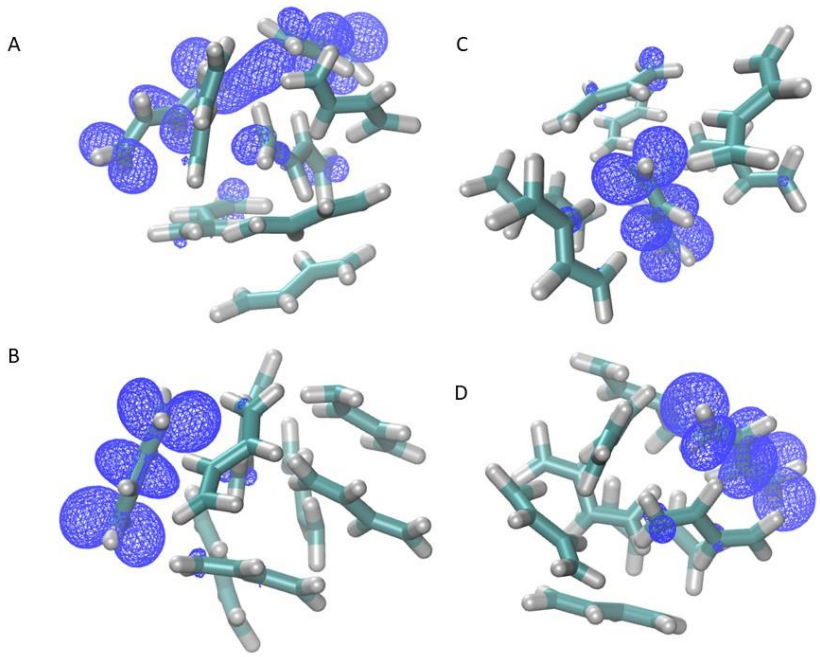


Figure S1: Electron densities of the unpaired electron in the anionic $(But)_8$ clusters. Four representative structures were taken from the Pi+GLE MD simulation at 300 K. Molecular orbitals were recalculated at the LC-ωPBE 6-31+g* level. Visualized is the electron density covering 99.9% probability of finding the electron.

Table S2: Electron affinities and radius of gyration for structures in Figure S1.

	Vertical el. affinity (eV)	Gyration radius (Å)
A	-0.62	3.8
B	-0.28	2.18
C	-0.32	2.44
D	0.3	2.44

Section S3: Vertical electron affinity along normal modes.

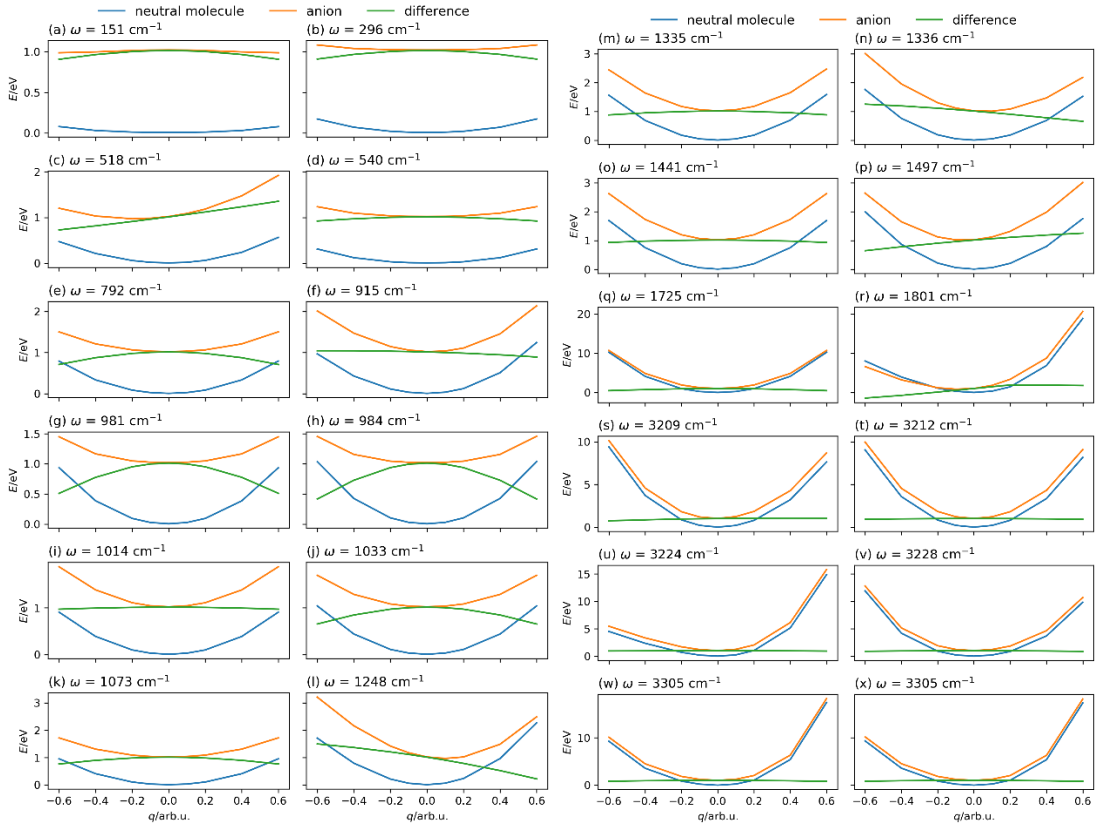


Figure S2. Electron energies for the ground state (blue curve), anionic state (orange curve) and electron affinity (green curve) along normal modes for butadiene molecule.

Section S4: Cartesian coordinates of the optimized structures of butadiene clusters with *n* units. Optimized in the neutral ground state on the LC-ωPBE/6-31+g* level of theory

These structures were used to calculate VEAs and Solvent shifts, as well as for neutral part of AEAs in gas phase and in PCM. These structures were used as initial structures for optimization on BLYP/6-31+g* level of theory for VEA T-DP calculations.

***n*=1**

C 1.840281 0.111202 0.000188
C 0.611662 -0.402706 -0.000341
C -0.611695 0.402810 -0.000242
C -1.840229 -0.111295 0.000253
H 0.478741 -1.484088 -0.000547
H 2.722650 -0.521365 0.000562
H 2.006240 1.186154 0.000641
H -0.478912 1.484183 -0.000603
H -2.722573 0.521257 0.000218
H -2.006257 -1.186200 0.000585

***n*=2**

C 2.434911 0.687982 -0.172106
C 1.953891 1.889032 0.144969
H 3.297727 0.608179 -0.832822
H 2.402033 2.800704 -0.238609
H 1.093472 1.999942 0.801013
C 1.872496 -0.572204 0.319634
C 2.353415 -1.773187 0.002034
H 1.010150 -0.493256 0.980845
H 1.908803 -2.684674 0.390021
H 3.212788 -1.886225 -0.655267
C -2.437688 -0.688270 0.168182
C -1.954848 -1.889075 -0.147074
H -3.306430 -0.609118 0.821166
H -2.407298 -2.801129 0.230487
H -1.088578 -1.999307 -0.795465
C -1.869720 0.572481 -0.315715
C -2.352457 1.773212 0.000077

H	-1.001465	0.494302	-0.969245
H	-1.903550	2.685117	-0.381943
H	-3.217651	1.885643	0.649807

***n*=4**

C	-0.309433	-2.769007	-0.415486
C	-0.565610	-2.811329	0.891545
H	-0.323971	-3.687945	-1.000986
H	-0.790905	-3.745696	1.397030
H	-0.557487	-1.908001	1.498023
C	0.000651	-1.534507	-1.141173
C	0.257097	-1.484729	-2.447772
H	0.016584	-0.616747	-0.554117
H	0.483037	-0.545621	-2.944449
H	0.250442	-2.380544	-3.065147
C	3.984302	0.131959	-0.524266
C	4.778675	0.994783	-1.156062
H	3.160990	-0.340169	-1.059388
H	4.631398	1.243252	-2.202764
H	5.608668	1.481059	-0.647958
C	4.141809	-0.240470	0.883912
C	3.346259	-1.102238	1.515937
H	4.967268	0.227795	1.419758
H	3.499884	-1.355332	2.560873
H	2.516527	-1.589104	1.008253
C	-4.112069	0.834915	-0.733419
C	-3.421067	0.946216	-1.867100
H	-4.908792	1.545039	-0.512766
H	-3.633094	1.731500	-2.586799
H	-2.622197	0.250554	-2.114488
C	-3.872376	-0.207661	0.267693
C	-4.558398	-0.314318	1.404609
H	-3.082248	-0.923461	0.043295
H	-4.352564	-1.104107	2.120749
H	-5.354017	0.383465	1.656917
C	0.610385	2.102985	0.369382

C	0.373508	2.635435	-0.828915
H	1.637241	1.957370	0.702940
H	1.184634	2.936998	-1.484974
H	-0.641005	2.790070	-1.190066
C	-0.445108	1.679006	1.293114
C	-0.209092	1.139890	2.488666
H	-1.471824	1.818897	0.956351
H	-1.020822	0.840174	3.145007
H	0.805052	0.984980	2.850709

***n*=6**

C	0.601722	-2.392659	2.555908
C	0.526997	-3.459355	3.351596
H	-0.063288	-2.309250	1.696838
H	-0.185478	-4.257994	3.167676
H	1.177779	-3.571336	4.216177
C	1.544816	-1.289952	2.758296
C	1.617931	-0.222262	1.964962
H	2.214247	-1.374881	3.614268
H	2.333242	0.574458	2.147721
H	0.963025	-0.109237	1.102579
C	-2.449803	0.247271	2.471320
C	-3.369657	-0.712433	2.378343
H	-1.566600	0.093155	3.090360
H	-3.262118	-1.650878	2.914548
H	-4.260268	-0.589205	1.765744
C	-2.543083	1.532766	1.774251
C	-1.623883	2.492891	1.866289
H	-3.423683	1.684558	1.150235
H	-1.733492	3.436173	1.339091
H	-0.733575	2.369715	2.479448
C	-1.115110	-0.930014	-1.130677
C	-1.320115	-2.243225	-1.220533
H	-1.698456	-0.339117	-0.426576
H	-2.064596	-2.743389	-0.607332
H	-0.746957	-2.862367	-1.907185

C	-0.125354	-0.203283	-1.931333
C	0.066571	1.116438	-1.853006
H	0.476400	-0.797226	-2.618110
H	0.805741	1.619720	-2.463295
H	-0.519359	1.727798	-1.168736
C	-5.117289	1.300423	-1.814707
C	-4.036496	1.843618	-2.369627
H	-5.979512	1.925206	-1.583306
H	-3.988725	2.903631	-2.604784
H	-3.163645	1.246601	-2.610684
C	-5.236997	-0.122631	-1.487276
C	-6.318292	-0.667467	-0.931496
H	-4.376375	-0.747032	-1.725424
H	-6.370622	-1.728839	-0.708146
H	-7.193401	-0.070032	-0.684871
C	3.591651	-1.283847	-1.997375
C	4.182061	-0.568118	-2.953548
H	3.270902	-0.800844	-1.074895
H	4.359632	0.497428	-2.842302
H	4.511276	-1.025614	-3.884391
C	3.325971	-2.721041	-2.095043
C	2.719019	-3.425045	-1.141150
H	3.654953	-3.215102	-3.009067
H	2.541042	-4.491962	-1.247916
H	2.383481	-2.961174	-0.217287
C	3.518220	3.538997	0.768627
C	2.237852	3.905821	0.749810
H	4.248028	4.146774	1.303012
H	1.893432	4.799021	1.262030
H	1.488655	3.314004	0.228498
C	4.027462	2.329327	0.118472
C	5.300249	1.938947	0.161543
H	3.294241	1.729816	-0.420613
H	5.634701	1.030271	-0.329742
H	6.052729	2.516153	0.694548

***n*=8**

C	4.783268	-1.753361	-2.140892
C	4.183848	-2.425390	-3.122731
H	5.591910	-1.061099	-2.375380
H	4.479906	-2.303219	-4.160276
H	3.377236	-3.125725	-2.917354
C	4.423871	-1.883555	-0.726553
C	5.011012	-1.199030	0.253973
H	3.628836	-2.589967	-0.490512
H	4.714286	-1.327507	1.290413
H	5.812570	-0.490923	0.053183
C	2.272074	4.473598	-1.639086
C	1.082430	5.071709	-1.599179
H	3.181356	5.073540	-1.609368
H	0.993039	6.152210	-1.538084
H	0.156217	4.502023	-1.627971
C	2.451948	3.021830	-1.718206
C	3.640519	2.420317	-1.744830
H	1.542131	2.422926	-1.752407
H	3.732870	1.339729	-1.803359
H	4.565773	2.992202	-1.713213
C	-2.303098	3.002931	0.131747
C	-2.848801	3.721242	1.112370
H	-1.458361	2.348502	0.345137
H	-2.471248	3.672133	2.129252
H	-3.692059	4.384469	0.930729
C	-2.772307	3.032032	-1.256117
C	-2.240154	2.300975	-2.235116
H	-3.606632	3.699407	-1.471893
H	-2.616897	2.354751	-3.252307
H	-1.410063	1.621633	-2.053457
C	0.648830	-0.806637	-1.618464
C	-0.069509	-1.382727	-2.582269
H	1.685707	-0.531521	-1.810441
H	0.353345	-1.580532	-3.562944
H	-1.103890	-1.677732	-2.418247

C	0.129476	-0.512727	-0.279866
C	0.844721	0.081073	0.675436
H	-0.899641	-0.810379	-0.080165
H	0.425806	0.284605	1.656716
H	1.876979	0.382313	0.511335
C	1.954546	3.482302	2.412740
C	0.963045	4.194799	2.945432
H	2.090531	3.472279	1.332050
H	0.282574	4.769300	2.324280
H	0.802241	4.231036	4.021055
C	2.907425	2.694989	3.198906
C	3.908133	1.995620	2.665727
H	2.769186	2.703357	4.279961
H	4.598105	1.427628	3.282816
H	4.071119	1.971500	1.590366
C	-5.740129	-0.103736	-1.084723
C	-6.216609	-0.836708	-2.090151
H	-4.830214	0.479599	-1.223246
H	-5.719971	-0.870107	-3.055218
H	-7.124516	-1.426719	-1.983839
C	-6.373283	-0.020175	0.233907
C	-5.896017	0.711837	1.239646
H	-7.285817	-0.599828	0.371289
H	-6.397087	0.747855	2.202507
H	-4.988686	1.302512	1.132574
C	-2.982937	-2.407188	1.556756
C	-2.351062	-2.172703	2.706246
H	-3.874237	-1.834188	1.301948
H	-2.704510	-1.419937	3.404740
H	-1.460192	-2.729963	2.988404
C	-2.549944	-3.412406	0.582528
C	-3.172113	-3.637729	-0.574127
H	-1.665819	-3.993604	0.843339
H	-2.819921	-4.395858	-1.267677
H	-4.056338	-3.073578	-0.863436
C	1.582156	-4.976826	0.705527
C	1.177415	-4.890099	-0.561202

H	1.944941	-5.928150	1.094003
H	1.199420	-5.750953	-1.223144
H	0.809118	-3.954590	-0.977599
C	1.574467	-3.849671	1.641782
H	1.217753	-2.896532	1.251941
C	1.975024	-3.936888	2.909544
H	1.955613	-3.076386	3.571775
H	2.338064	-4.872703	3.329191

***n*=10**

C	1.452081	0.826367	3.861489
C	2.609781	1.479389	3.767162
H	0.516604	1.344643	3.653472
H	2.648097	2.528848	3.490227
H	3.558726	0.986361	3.966735
C	1.341676	-0.586162	4.234538
C	0.182470	-1.237036	4.327769
H	2.276281	-1.107334	4.439635
H	0.140993	-2.284890	4.610642
H	-0.765155	-0.744076	4.121982
C	6.387003	-1.801909	-1.665636
C	7.410675	-1.142629	-1.124874
H	5.600125	-2.193614	-1.022003
H	7.481436	-0.986390	-0.052635
H	8.215212	-0.741347	-1.737921
C	6.242723	-2.048040	-3.102556
C	5.223422	-2.713146	-3.644413
H	7.031799	-1.654687	-3.743191
H	5.154989	-2.878213	-4.715470
H	4.422702	-3.120004	-3.030683
C	0.619273	-2.390909	0.396722
C	0.000125	-3.503163	0.002559
H	0.571329	-2.084812	1.441698
H	-0.557184	-4.121326	0.700119
H	0.032540	-3.836585	-1.032698
C	1.387780	-1.521687	-0.498613

C	2.002651	-0.408051	-0.100493
H	1.445596	-1.825406	-1.544013
H	2.564630	0.207980	-0.796666
H	1.963065	-0.078639	0.936271
C	-3.064143	-0.391948	-3.109069
C	-1.967856	-0.956329	-2.604317
H	-3.444332	-0.721650	-4.075828
H	-1.438444	-1.741856	-3.135869
H	-1.560573	-0.652782	-1.642585
C	-3.823678	0.666476	-2.438425
C	-4.927246	1.215784	-2.944463
H	-3.443709	0.999937	-1.472663
H	-5.470060	1.994103	-2.416712
H	-5.327046	0.900465	-3.906177
C	-5.420956	-3.955023	-0.742485
C	-4.110907	-4.173732	-0.638467
H	-6.123500	-4.753187	-0.503126
H	-3.718933	-5.135115	-0.319238
H	-3.387025	-3.397297	-0.876386
C	-6.002433	-2.681667	-1.174262
C	-7.311768	-2.471056	-1.301239
H	-5.301301	-1.880005	-1.402601
H	-7.703181	-1.513158	-1.630544
H	-8.037933	-3.251634	-1.083431
C	6.249839	-0.889071	2.996360
C	6.775960	0.334909	2.980683
H	6.680005	-1.653290	3.643237
H	7.628297	0.597264	3.600185
H	6.368877	1.118395	2.345072
C	5.101004	-1.294575	2.182453
C	4.569270	-2.515891	2.202811
H	4.673294	-0.532272	1.532016
H	3.713592	-2.771615	1.584863
H	4.973293	-3.300444	2.839280
C	-0.073163	3.787789	-1.441065
C	-0.337793	2.694940	-2.155384
H	-0.621194	4.709147	-1.637175

H	-1.094806	2.690866	-2.933788
H	0.194398	1.761803	-1.983445
C	0.933210	3.841120	-0.377551
C	1.201557	4.932129	0.338767
H	1.479440	2.918486	-0.181643
H	1.954401	4.928326	1.121322
H	0.673424	5.867937	0.168787
C	-3.143169	-0.643033	1.688737
C	-4.269667	-1.142978	2.195291
H	-2.470826	-1.290453	1.125731
H	-4.542255	-2.184397	2.053831
H	-4.961761	-0.521980	2.760454
C	-2.735570	0.757232	1.832343
C	-1.612520	1.260834	1.320993
H	-3.415178	1.404535	2.386035
H	-1.350166	2.308322	1.437219
H	-0.913247	0.641802	0.762376
C	-6.253838	2.058690	0.758964
C	-5.684229	3.258309	0.651595
H	-5.703593	1.169056	0.453975
H	-4.675795	3.375421	0.265259
H	-6.207329	4.165377	0.947069
C	-7.606214	1.838010	1.277278
H	-8.158046	2.724553	1.588965
C	3.650408	2.222417	-2.809743
C	3.409915	1.230428	-3.666520
H	2.996419	3.093830	-2.794163
H	2.573470	1.270961	-4.358143
H	4.043246	0.346518	-3.706729
C	4.762934	2.221495	-1.856023
C	5.002221	3.212445	-0.997738
H	5.416107	1.349125	-1.871920
H	5.842792	3.177911	-0.310833
H	4.367386	4.094987	-0.957912
C	-8.169514	0.635427	1.384031
H	-9.174218	0.511392	1.777195
H	-7.643659	-0.266828	1.079287

***n*=12**

C	6.003853	4.157058	2.042350
C	6.859229	4.226003	1.023370
C	6.500368	4.722328	-0.307612
C	7.351134	4.788234	-1.330643
C	6.849846	-1.301047	0.771635
C	6.707427	0.097056	0.357666
C	6.444378	0.474052	-0.892968
C	7.120026	-1.682485	2.019399
C	1.964443	3.688997	0.352731
C	2.849516	3.221047	-0.527196
C	1.884854	3.238080	1.744908
C	0.998914	3.707437	2.622601
C	2.683938	-0.642551	1.070558
C	2.223726	-1.127057	2.223411
C	3.065969	-1.781537	3.227393
C	2.603658	-2.283297	4.371981
C	6.120320	-5.292148	-0.680043
C	6.416508	-4.604532	-1.782047
C	5.458022	-3.754435	-2.492415
C	5.757399	-3.051769	-3.584057
C	1.296195	-3.787892	-1.306212
C	1.063837	-3.737586	-2.617320
C	1.646269	-5.016174	-0.587822
C	1.920691	-5.058852	0.715426
C	-0.862344	0.664833	0.283458
C	-0.853746	0.139082	-1.084895
C	-0.118108	0.657240	-2.068394
C	-1.577665	0.129859	1.272545
C	-3.107905	-3.258300	-1.822832
C	-3.523228	-3.190594	-0.558446
C	-2.893622	-3.918275	0.546622
C	-3.325597	-3.860731	1.805956
C	-5.621363	-0.006704	0.878995
C	-5.734063	0.097023	-0.578454

C	-4.895252	0.802884	-1.335655
C	-6.427494	-0.751540	1.634981
C	-7.271333	-4.661512	0.556061
C	-7.772217	-5.000579	1.742855
C	-8.068021	-4.088195	-0.531579
C	-7.565287	-3.741746	-1.715811
C	-7.142651	3.875867	0.863358
C	-6.425607	4.566599	-0.021591
C	-6.419043	6.029275	-0.103339
C	-5.701008	6.721985	-0.986153
C	-1.871581	4.342389	-0.896740
C	-1.373881	5.457986	-1.706245
C	-0.646383	5.304364	-2.811952
C	-2.599850	4.495979	0.207852
H	7.891947	3.905205	1.158820
H	6.308385	3.787553	3.017105
H	4.967563	4.470041	1.936201
H	5.469570	5.050012	-0.437252
H	7.045822	5.166526	-2.301565
H	8.385960	4.468008	-1.231333
H	6.722459	-2.053790	-0.005870
H	7.219998	-2.731379	2.282506
H	7.256048	-0.957886	2.819687
H	6.823659	0.852121	1.134696
H	6.348290	1.522534	-1.160757
H	6.320731	-0.257215	-1.689209
H	2.595314	2.470211	2.049185
H	0.969495	3.347263	3.646685
H	0.271252	4.466505	2.343876
H	1.245058	4.447520	0.044838
H	2.875448	3.584249	-1.550842
H	3.583031	2.464741	-0.254147
H	7.421167	-4.658340	-2.201109
H	6.858869	-5.913404	-0.182104
H	5.125515	-5.256720	-0.241312
H	4.448451	-3.716599	-2.084586
H	5.015841	-2.435730	-4.083712

H	6.754612	-3.072228	-4.018817
H	4.128132	-1.849911	2.994059
H	3.260873	-2.763792	5.090615
H	1.548223	-2.229158	4.630443
H	1.160465	-1.045955	2.448273
H	2.017985	-0.169393	0.355000
H	3.736594	-0.699005	0.800900
H	-1.615417	3.341660	-1.243483
H	-2.951167	3.643516	0.781144
H	-2.881645	5.481412	0.572515
H	-1.627176	6.459906	-1.360193
H	-0.294588	6.155457	-3.387112
H	-0.382229	4.315581	-3.180856
H	-0.242466	1.540498	0.474323
H	-1.555673	0.547586	2.275423
H	-2.197963	-0.749539	1.113258
H	-1.491891	-0.722939	-1.277117
H	-0.137355	0.242188	-3.072058
H	0.533634	1.511996	-1.898359
H	-4.819952	0.567975	1.342793
H	-6.310328	-0.800576	2.713584
H	-7.230391	-1.342506	1.200163
H	-6.557641	-0.448226	-1.040196
H	-5.009843	0.857206	-2.414247
H	-4.058510	1.345422	-0.901101
H	1.681542	-5.930970	-1.179627
H	2.176881	-5.990909	1.210925
H	1.904529	-4.161372	1.329664
H	1.233372	-2.878148	-0.710052
H	-2.024829	-4.526973	0.297320
H	-2.832703	-4.411963	2.601295
H	-4.189091	-3.258368	2.080902
H	-4.373904	-2.559906	-0.301028
H	-3.601566	-2.696804	-2.610910
H	-2.255376	-3.870235	-2.109460
H	0.810533	-2.804582	-3.111704
H	1.121960	-4.627273	-3.241208

H -7.051416 6.556558 0.610690
H -5.729356 7.807169 -1.016942
H -5.059858 6.223955 -1.710110
H -5.800746 4.037287 -0.739904
H -7.122127 2.790579 0.888229
H -7.777244 4.375136 1.592736
H -9.131119 -3.951042 -0.334333
H -8.190822 -3.323957 -2.499173
H -6.509278 -3.871472 -1.942310
H -6.210687 -4.807766 0.355031
H -7.147272 -5.424648 2.522899
H -8.827194 -4.869613 1.974198

Section S3: Cartesian coordinates of the optimized structures of anion butadiene clusters with *n* units. Optimized in the anion ground state on the LC-ωPBE/6-31+g* level of theory:

These structures were used to calculated anion parts of AEAs in gas phase and in PCM.

***n*=1**

C -1.909519 0.099222 0.000380
C -0.594595 -0.373748 -0.000098
C 0.594573 0.373675 -0.000069
C 1.909525 -0.099158 -0.000299
H -0.467449 -1.461687 -0.000279
H -2.757183 -0.582169 -0.001100
H -2.130603 1.166387 0.000062
H 0.467349 1.461718 -0.000205
H 2.757267 0.582129 0.000623
H 2.130714 -1.166323 0.001417

***n*=2**

C -2.069618 -1.157707 0.040001
C -0.986254 -1.934410 0.072891
H -3.065717 -1.604675 0.069783
H -1.077747 -3.016940 0.129019
H 0.023971 -1.524880 0.039314
C -2.012563 0.305011 -0.036578

C	-3.098500	1.078388	-0.086284
H	-1.018062	0.757898	-0.047700
H	-3.016295	2.160297	-0.141291
H	-4.103774	0.657685	-0.073564
C	1.788775	0.944772	0.405720
C	1.284111	2.182612	-0.002236
H	1.808078	0.756406	1.484524
H	0.959560	2.927222	0.720771
H	1.253966	2.465738	-1.054146
C	2.285113	-0.094348	-0.400366
C	2.795315	-1.329536	0.007318
H	2.268314	0.095571	-1.478834
H	3.176328	-2.049906	-0.712579
H	2.873106	-1.593103	1.061909

***n*=4**

C	-0.677580	1.687430	-1.200136
C	-0.522381	0.928676	-2.286029
H	-1.137011	2.674329	-1.284759
H	-0.846459	1.276270	-3.264402
H	-0.063030	-0.058275	-2.230329
C	-0.260679	1.275389	0.143889
C	-0.435041	2.028616	1.229597
H	0.212563	0.296724	0.236278
H	-0.108284	1.683088	2.205815
H	-0.903093	3.011093	1.176916
C	3.821401	0.757825	0.876981
C	4.537508	1.331131	1.845065
H	2.991506	0.095484	1.127805
H	4.314247	1.155612	2.893619
H	5.370086	1.997243	1.621944
C	4.081392	0.965092	-0.550371
C	3.381474	0.376254	-1.519946
H	4.897827	1.644851	-0.801106
H	3.607616	0.561549	-2.567001
H	2.563974	-0.311465	-1.308829

C	-4.571983	-0.543685	0.987057
C	-3.536015	-1.233193	1.461871
H	-5.573319	-0.725410	1.379014
H	-3.660708	-1.983168	2.237652
H	-2.524624	-1.077724	1.093986
C	-4.455591	0.471906	-0.062001
C	-5.488134	1.158491	-0.550656
H	-3.452028	0.650840	-0.445703
H	-5.357684	1.901806	-1.331671
H	-6.501415	0.998517	-0.186487
C	1.438255	-2.237870	0.475561
C	1.056416	-1.902547	1.777491
H	2.504681	-2.427469	0.313498
H	1.771428	-1.920863	2.596606
H	0.010548	-1.748037	2.042480
C	0.622171	-2.361910	-0.663094
C	1.010266	-2.668310	-1.970186
H	-0.449200	-2.202293	-0.499022
H	0.274669	-2.807297	-2.758877
H	2.048829	-2.885194	-2.217989

***n*=6**

C	0.634445	-2.286096	2.288392
C	0.629134	-3.469436	2.958838
H	-0.119036	-2.138007	1.514851
H	-0.102118	-4.239079	2.731115
H	1.350704	-3.680483	3.746804
C	1.549491	-1.201124	2.493350
C	1.564149	-0.028876	1.798409
H	2.302405	-1.341473	3.273835
H	2.312035	0.728235	2.017383
H	0.821022	0.175092	1.032273
C	-2.359022	-0.063876	2.547263
C	-3.367184	-0.930828	2.307193
H	-1.530127	-0.395248	3.172654
H	-3.336497	-1.936985	2.713547

H	-4.198974	-0.675010	1.653485
C	-2.218746	1.267314	2.012978
C	-1.165316	2.075974	2.280158
H	-2.995798	1.627439	1.335595
H	-1.086704	3.065463	1.837972
H	-0.366163	1.757451	2.944740
C	-0.958116	-0.497226	-1.180755
C	-1.009882	-1.796666	-1.546901
H	-1.538814	-0.179205	-0.317517
H	-1.626541	-2.497779	-0.992474
H	-0.410372	-2.184754	-2.367978
C	-0.187061	0.545365	-1.808335
C	-0.206253	1.842121	-1.414194
H	0.420293	0.264739	-2.671593
H	0.388501	2.594550	-1.925334
H	-0.788609	2.156836	-0.550604
C	-5.306378	1.206557	-1.524294
C	-4.282186	2.011762	-1.803688
H	-6.265126	1.629350	-1.222530
H	-4.377088	3.091913	-1.733945
H	-3.310985	1.623502	-2.102780
C	-5.227667	-0.254936	-1.582841
C	-6.255977	-1.063420	-1.328949
H	-4.255615	-0.673432	-1.838408
H	-6.151290	-2.143509	-1.368101
H	-7.234571	-0.671001	-1.058722
C	3.190094	-1.551766	-1.931712
C	3.586411	-0.862042	-3.001997
H	2.659076	-1.042435	-1.126347
H	3.412886	0.207155	-3.089007
H	4.114976	-1.343426	-3.823539
C	3.428005	-2.987319	-1.760766
C	3.038236	-3.677094	-0.689805
H	3.958704	-3.489475	-2.571085
H	3.236278	-4.742520	-0.604007
H	2.507489	-3.209560	0.136036
C	3.579217	3.533367	0.602196

C	2.365905	3.878287	1.029708
H	4.441368	4.149647	0.860662
H	2.213682	4.766606	1.637171
H	1.487957	3.278303	0.800585
C	3.859328	2.338091	-0.199824
C	5.090491	1.984522	-0.566718
H	3.003918	1.725702	-0.487884
H	5.281235	1.082578	-1.139753
H	5.955184	2.582889	-0.283337

***n*=8**

C	7.099505	0.567619	2.030074
C	7.794746	-0.568708	1.973679
H	7.606876	1.491926	2.310841
H	8.856981	-0.598949	2.200798
H	7.321315	-1.506279	1.691804
C	5.668634	0.683301	1.737900
C	4.999109	1.834606	1.785123
H	5.132739	-0.226856	1.469615
H	3.934707	1.878394	1.566175
H	5.499038	2.766285	2.049941
C	2.308942	3.808443	-2.713489
C	3.145262	3.538848	-1.711643
H	2.654471	4.377944	-3.577221
H	4.178411	3.874935	-1.734564
H	2.829379	2.971897	-0.837805
C	0.911059	3.370821	-2.740821
C	0.068684	3.625462	-3.741727
H	0.567167	2.798843	-1.880166
H	-0.958521	3.273288	-3.723290
H	0.382359	4.190826	-4.617934
C	-2.852051	2.418107	-1.170978
C	-2.154518	1.531159	-0.462317
H	-2.567538	3.470329	-1.152751
H	-1.296962	1.812429	0.144249
H	-2.410733	0.473653	-0.466314

C	-4.005859	2.065801	-2.001710
C	-4.696637	2.933448	-2.741390
H	-4.297657	1.015562	-1.992629
H	-5.547234	2.621476	-3.340503
H	-4.433185	3.988823	-2.770239
C	-3.046875	-3.188287	-1.439394
C	-3.608283	-3.202318	-2.649027
H	-3.538501	-3.707749	-0.615802
H	-4.543437	-3.721763	-2.838741
H	-3.146377	-2.694756	-3.493035
C	-1.787769	-2.514962	-1.113854
C	-1.254923	-2.492149	0.107878
H	-1.276409	-2.011181	-1.933919
H	-0.309627	-1.996295	0.323881
H	-1.753718	-2.986113	0.940659
C	1.441128	0.887705	0.767659
C	1.140768	2.078921	1.437573
H	1.256404	0.861326	-0.311514
H	0.778786	2.957746	0.908675
H	1.323730	2.192432	2.505488
C	1.963405	-0.293499	1.323705
C	2.295474	-1.477919	0.665615
H	2.140319	-0.269598	2.403957
H	2.682224	-2.335031	1.212404
H	2.168653	-1.579759	-0.411870
C	-6.983903	-1.945675	-0.026192
C	-8.255518	-2.337426	-0.101461
H	-6.264515	-2.302278	-0.763012
H	-8.599972	-3.009079	-0.882350
H	-8.997716	-1.996813	0.617560
C	-6.456890	-1.041906	0.999129
C	-5.179546	-0.669803	1.065003
H	-7.171022	-0.667398	1.732365
H	-4.813695	0.005859	1.832225
H	-4.448876	-1.028895	0.343372
C	-2.681507	1.475820	3.683534
C	-3.757465	1.996578	4.274590

H	-2.089631	2.080281	2.996555
H	-4.069478	3.020276	4.088955
H	-4.363827	1.414321	4.966491
C	-2.211703	0.103260	3.887285
C	-1.143289	-0.397432	3.267131
H	-2.787279	-0.510351	4.581487
H	-0.817061	-1.419645	3.438150
H	-0.552512	0.194330	2.568823
C	5.505012	-2.522428	-1.381032
C	6.702376	-1.997006	-1.638448
H	4.766705	-1.949086	-0.819053
H	6.968831	-1.001935	-1.295001
H	7.457510	-2.546778	-2.198640
C	5.101759	-3.862381	-1.816834
H	5.837934	-4.427133	-2.390695
C	3.913315	-4.403537	-1.550902
H	3.655472	-5.401469	-1.895097
H	3.160817	-3.864789	-0.980270

***n*=10**

C	-4.735624	0.747309	-2.744125
C	-4.518921	1.968350	-2.255456
H	-3.934720	0.009142	-2.695725
H	-3.560285	2.238990	-1.817588
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H	-8.281328	-1.117996	0.373413
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