Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Organic photovoltaics without p-n junctions: Computational study of ferroelectric columnar molecular clusters

A.L. Sobolewski

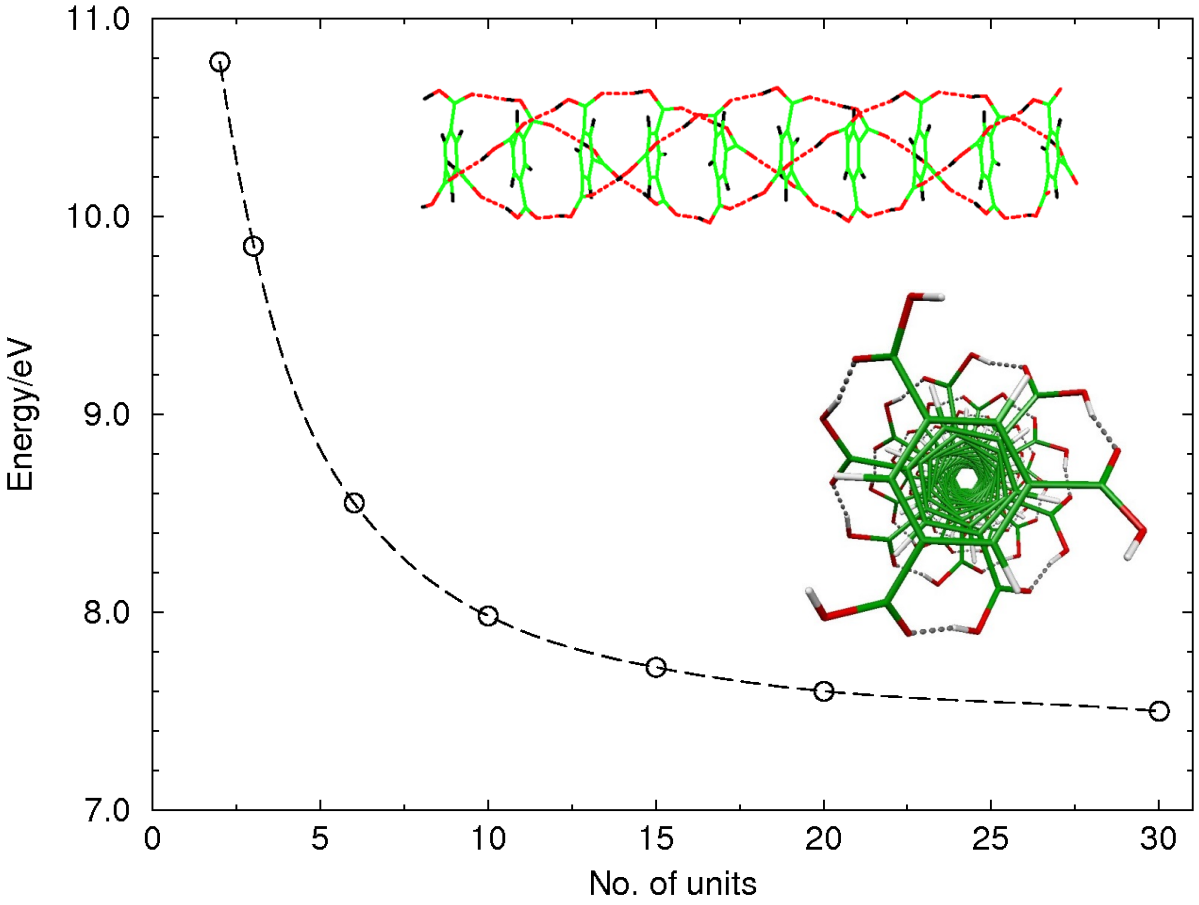


Fig. S1. HOMO-LUMO gap variation vs. the $(B3CA)_n$ cluster size computed at the HF/def-SV(P) level.

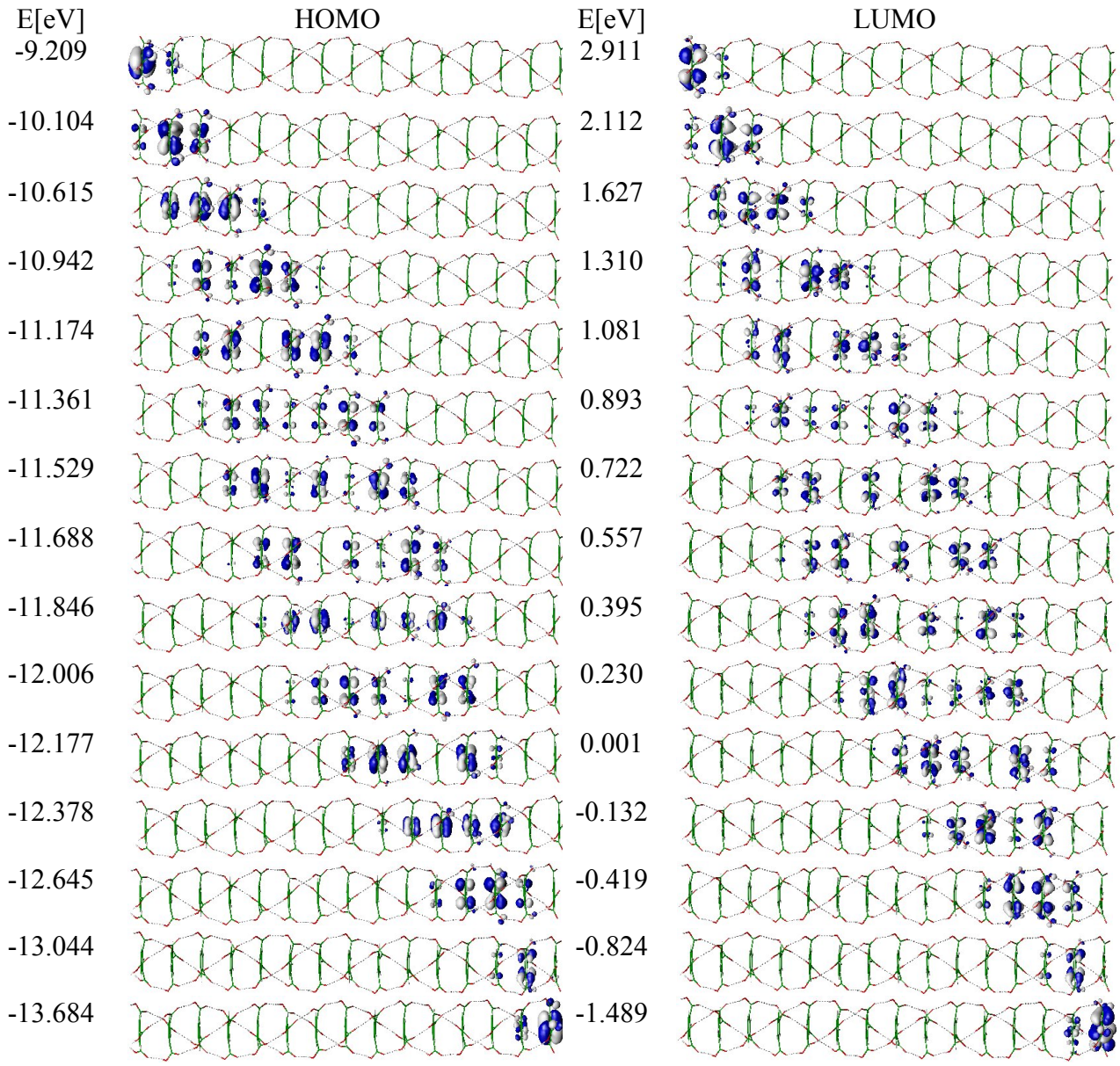


Fig. S2. Frontier HOMOs and LUMOs of the columnar $(B3CA)_{15}$ cluster computed at the HF/def-SV(P) level. Numbers denote orbital energy.

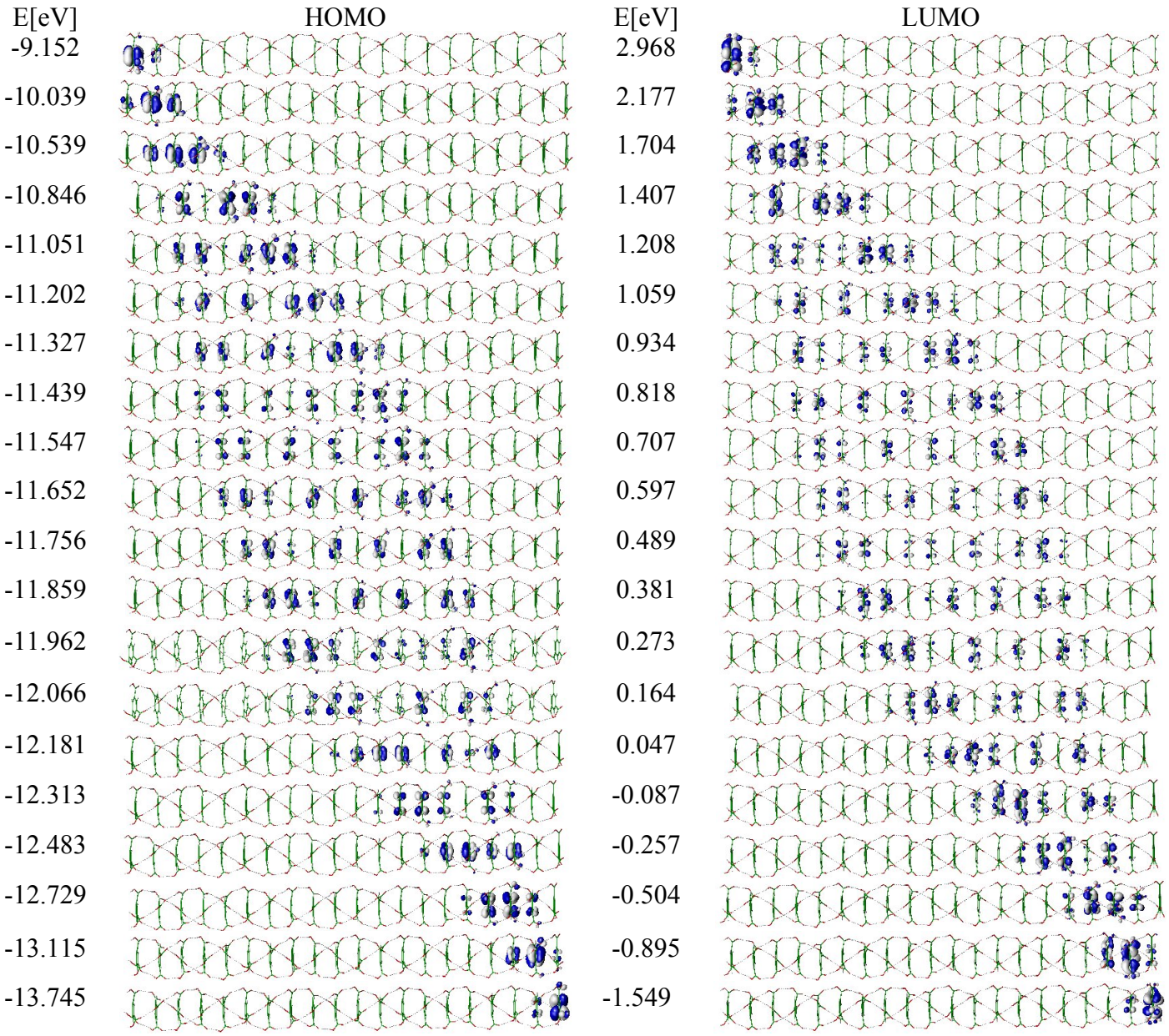


Fig. S3. Frontier HOMOs and LUMOs of the columnar $(B3CA)_{20}$ cluster computed at the HF/def-SV(P) level. Numbers denote orbital energy.

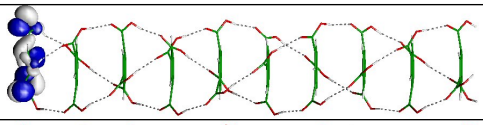
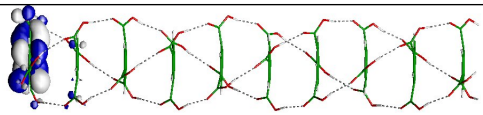
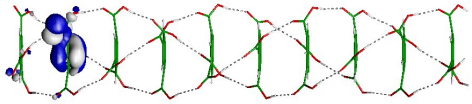
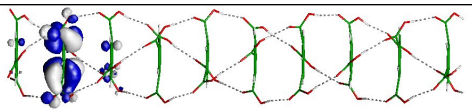
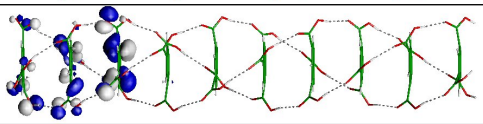
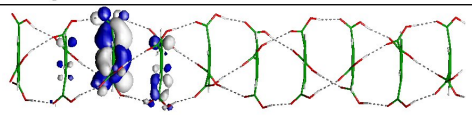
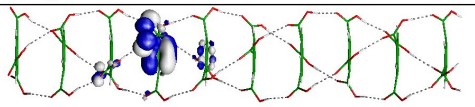
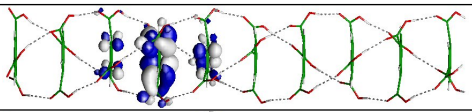
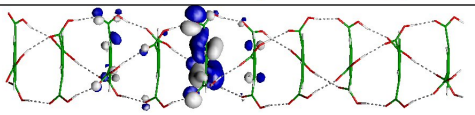
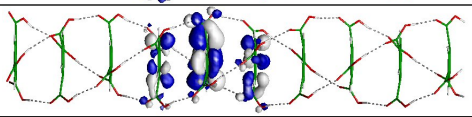
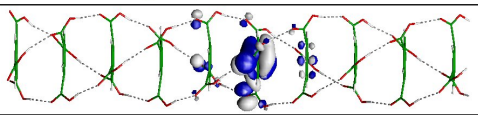
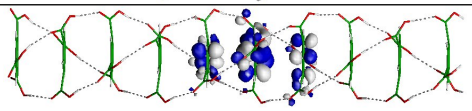
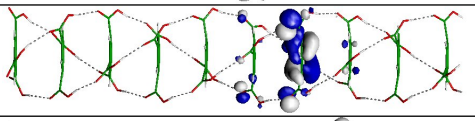
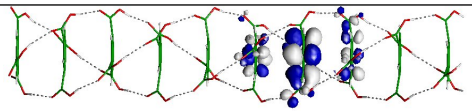
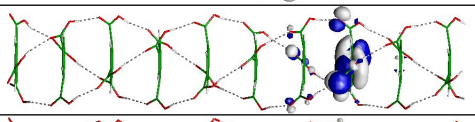
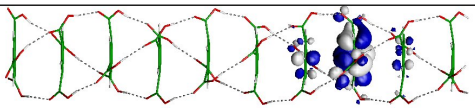
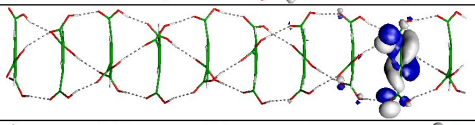
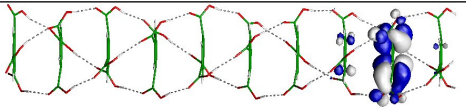
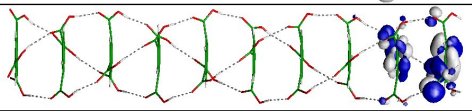
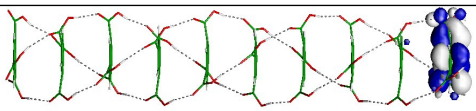
E[eV]	HOMO	E[eV]	LUMO
-6.254		-0.591	
-7.149		-1.324	
-7.666		-1.858	
-8.081		-2.232	
--8.383		-2.529	
--8.642		-2.798	
-8.914		-3.080	
-9.237		-3.417	
--9.683		-3.880	
-10.422		-4.587	

Fig. S4. Frontier HOMOs and LUMOs of the columnar $(B3CA)_{10}$ cluster computed with the DFT/B3-LYP/def-SV(P) method at the HF/def-SV(P) equilibrium geometry of the ground state. Numbers denote orbital energy.

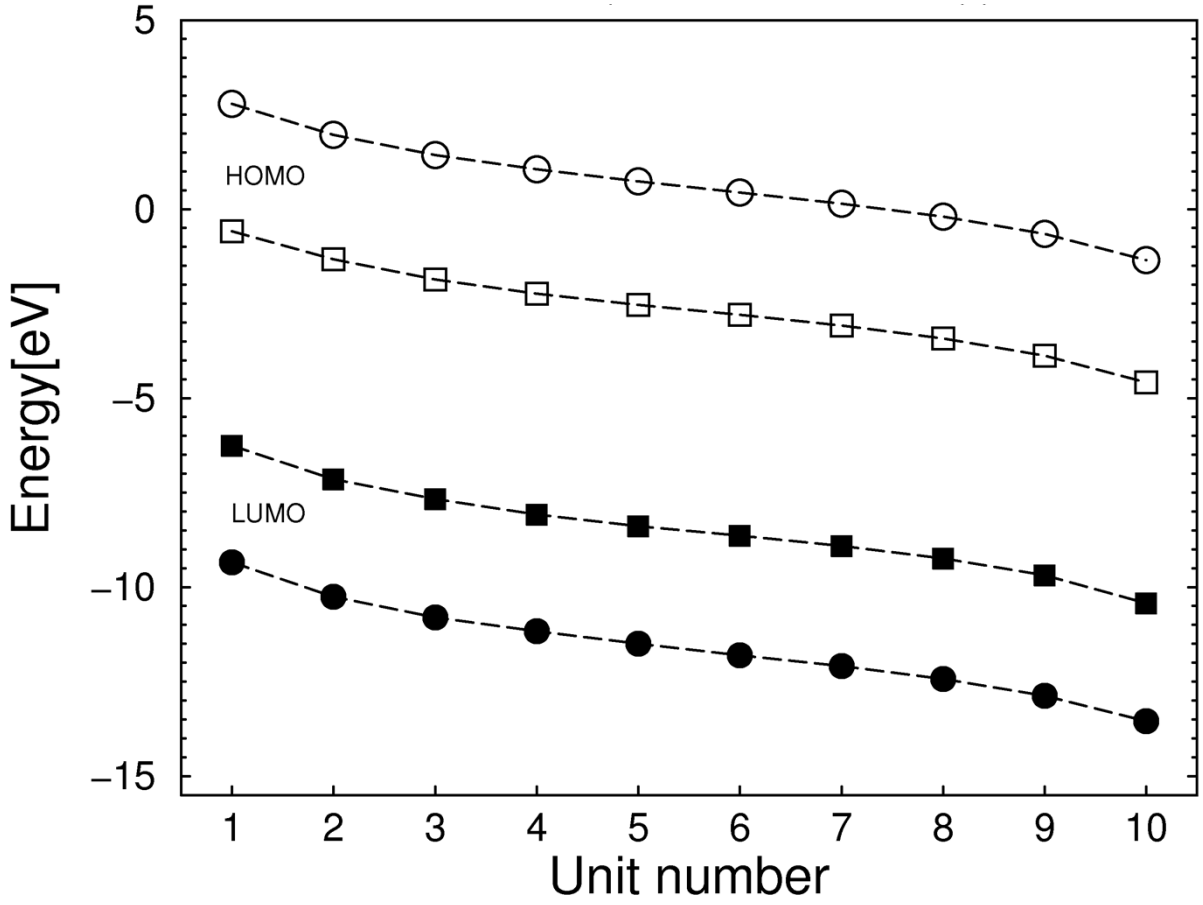


Fig. S5. Energy of frontier HOMOs (full symbols) and LUMOs (empty symbols) of the columnar $(B3CA)_{10}$ cluster computed at the HF/def-SV(P) level (circles) and DFT/B3-LYP/def-SV(P) level (squares) and plotted vs. their localization on successive molecular units.

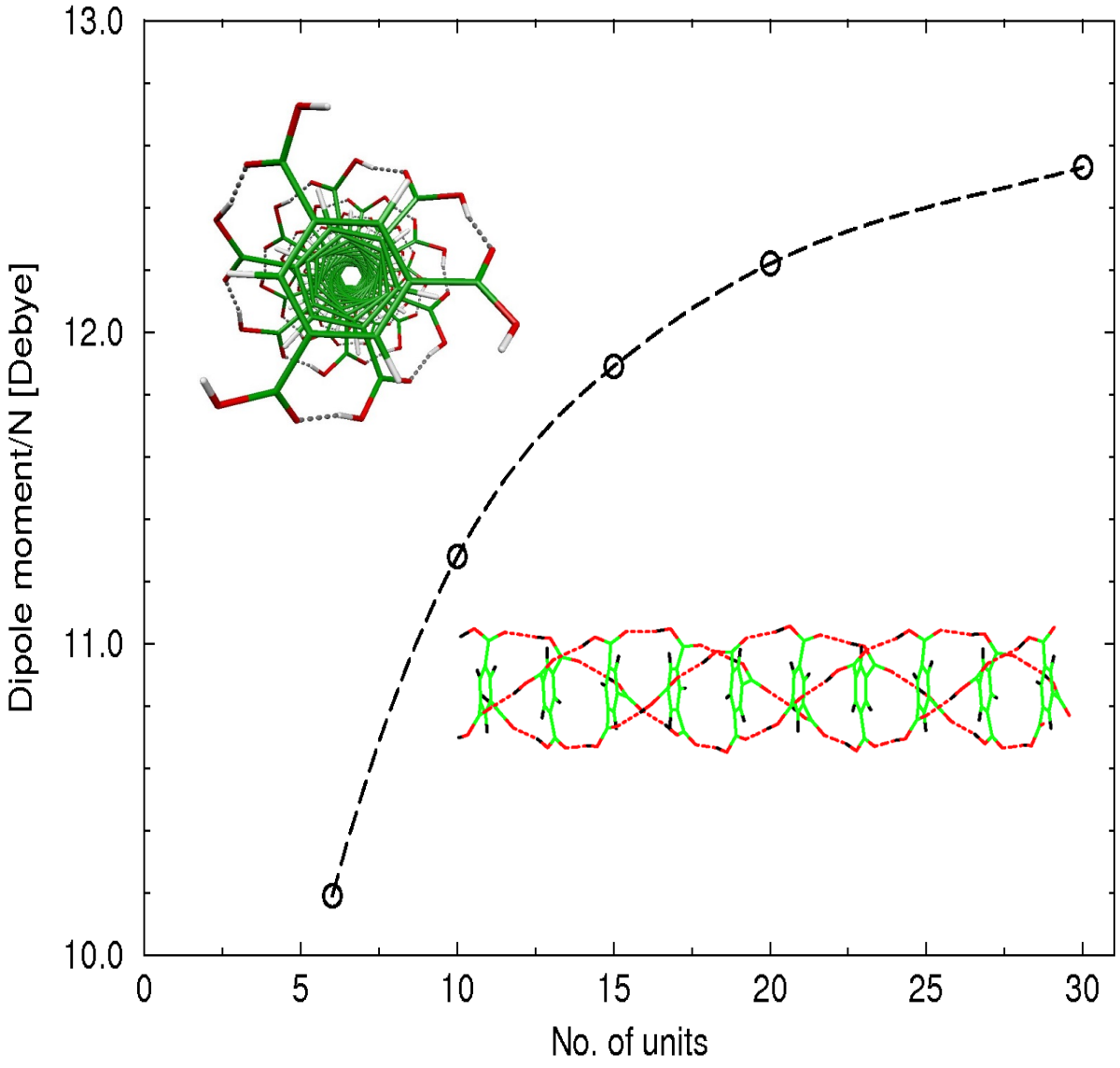


Fig. S6. Average dipole moment per molecular unit plotted vs. the $(B3CA)_n$ cluster size computed at the HF/def-SV(P) level.

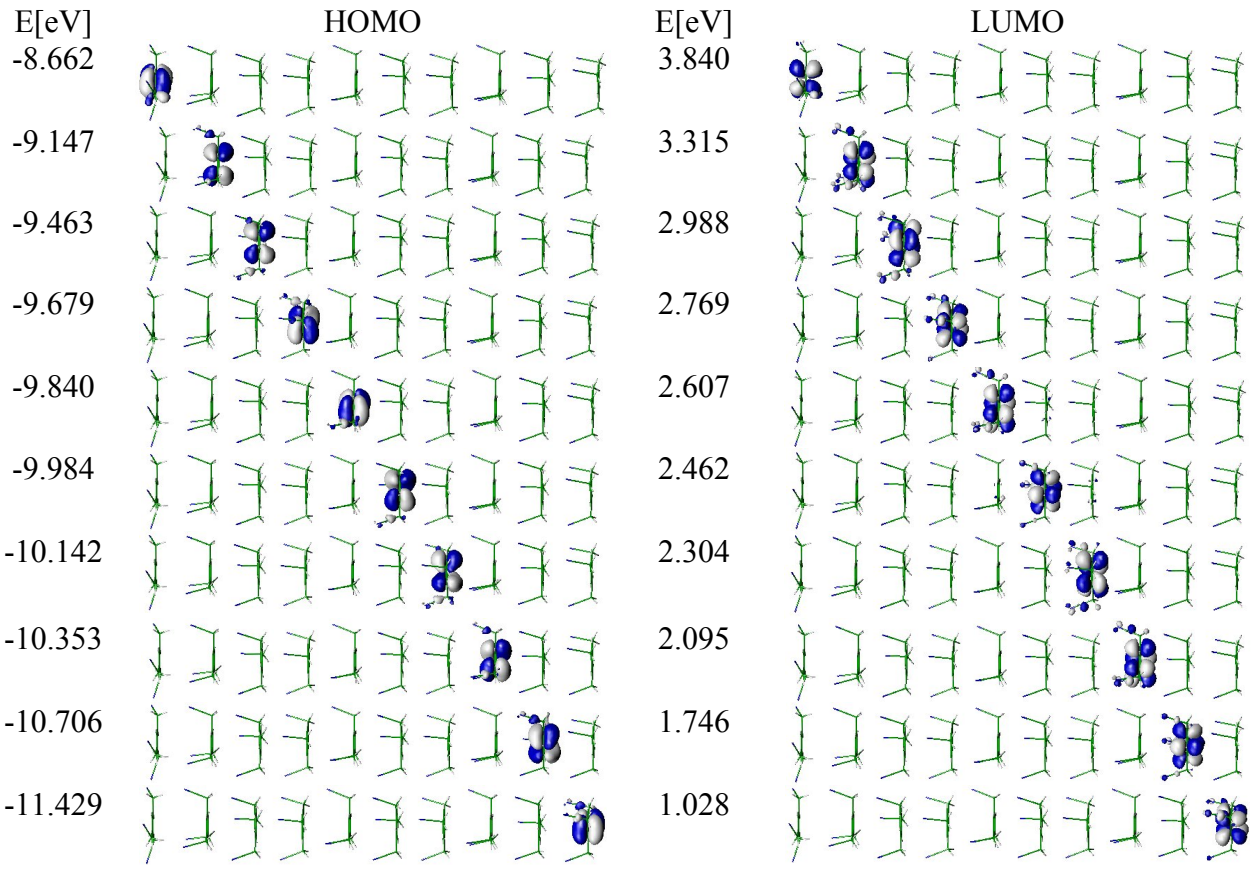


Fig. S7. Frontier HOMOs and LUMOs of the columnar $(B3CN)_{10}$ cluster computed at the HF/def-SV(P) level. Numbers denote orbital energy.

Fig. S8. Singly-occupied natural molecular orbitals of the lowest excited triplet state of the columnar $(B3CN)_{10}$ cluster computed at the UHF/def-SV(P) level.

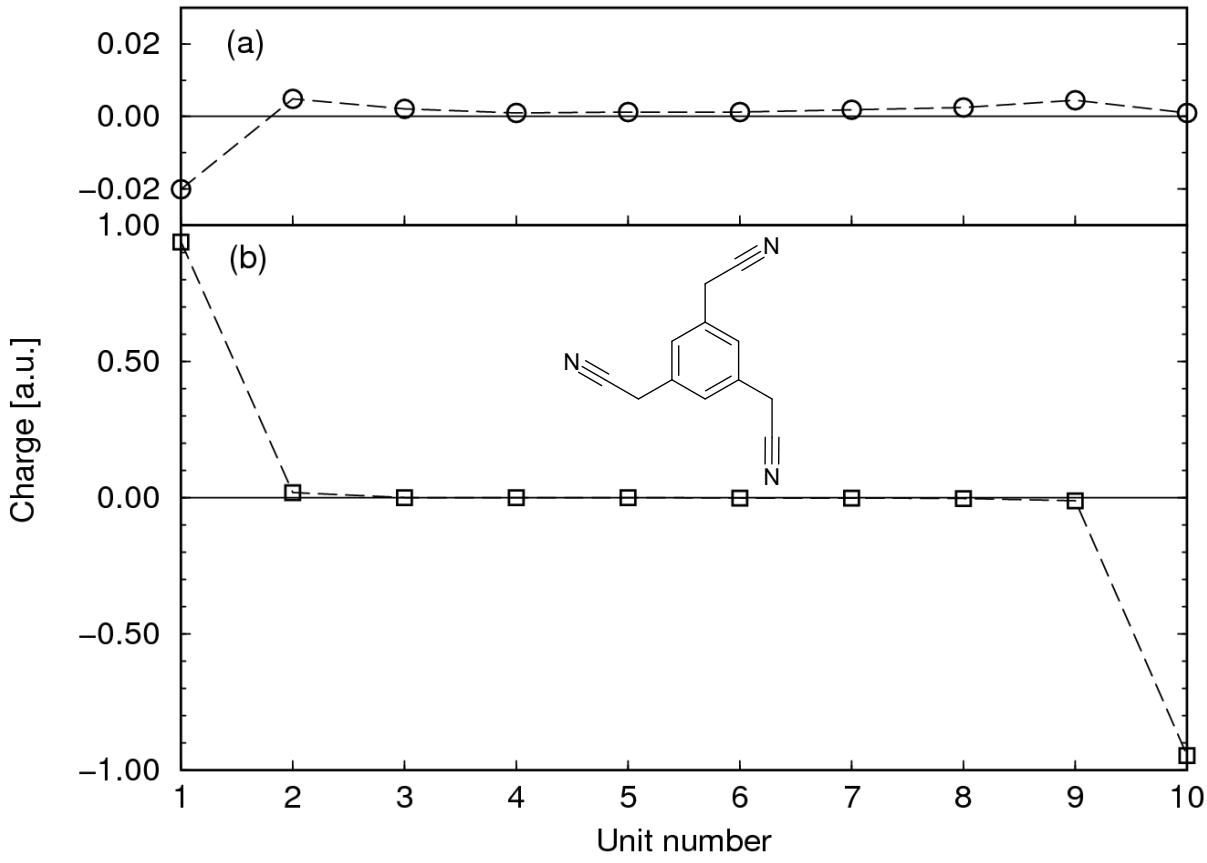
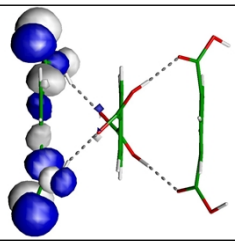
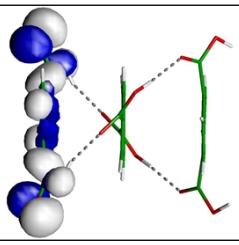
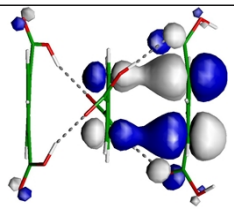
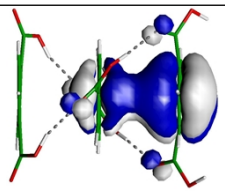
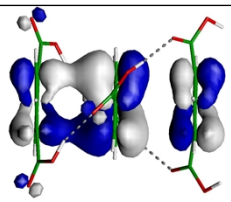
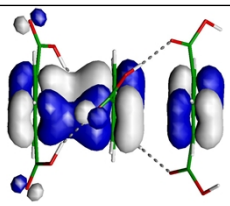
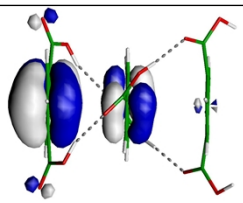
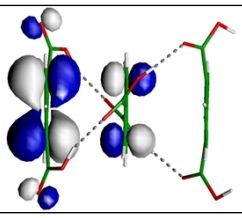
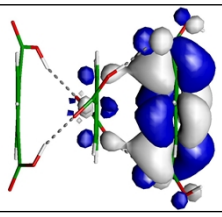
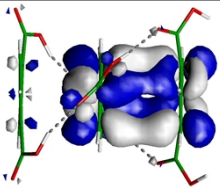
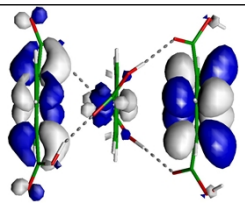
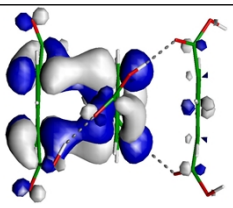


Fig. S9. Population of charge on particular molecular units of the columnar $(B3CN)_{10}$ cluster in the ground state (a) and in the lowest excited triplet state (b).

Table S1. Vertical excitation energy (ΔE), oscillator strength (f), dipole moment (μ), and the electronic character of the lowest excited singlet and triplet states of the $(B2CA)_3$ hydrogen-bonded complex, determined with the ADC(2)/cc-pVDZ method at the MP2/cc-pVDZ equilibrium geometry of the ground state.

State	ΔE/eV	f	μ/Debye	Electronic Configuration
S_0	-	-	15.18	$(63a)^2(66b)^2$
$S_1(\pi\pi^*)$	4.14	0.0023	9.56	0.57(66b-65a)+0.39(66b-64a)-0.33(65b-64a)
$S_2(n\pi^*)$	4.38	0.0023	11.38	0.39(60b-65a)+0.38(60b-67a)-0.36(60b-66a)
$S_3(\pi\pi^*)$	4.49	0.0017	12.50	0.50(63a-65a)-0.47(63a-66a)+0.47(63a-67a)
$S_4(\pi\pi^*)$	4.51	0.0102	10.50	0.37(65b-64a)-0.34(64b-64a)
$T_1(\pi\pi^*)$	3.51	-	13.81	0.49(65b-65a)-0.36(66b-67a)-0.33(64b-65a)
$T_2(\pi\pi^*)$	3.67	-	14.10	0.34(66b-67a)-0.32(66b-66a)-0.31(64b-65a)
$T_3(\pi\pi^*)$	3.80	-	14.23	0.42(62b-64a)-0.41(61b-64a)-0.35(63b-64a)

Table S2. Hartree-Fock molecular orbitals involved into the lowest electronic excitations (Table S1) of the $(B2CA)_3$ complex computed at the MP2/cc-pVDZ equilibrium geometry of the ground state. Numbers denote symmetry labels in the C_2 point group of symmetry.

HOMO			
60b	*63a*	*61b*	*62b*
			
63b	*64b*	*65b*	*66b*
			
LUMO			
64a	*65a*	*66a*	*67a*
			

$(B3CA)_{10}$

HF/def-SV(P) geometry of the S_0 state (μ= 112.8 Debye).

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  210
FINAL HEAT OF FORMATION = -7929.082020
 O     2.458082    -2.390794    16.099789
 O    -3.299529    -0.933365    16.099789
 O     0.841447     3.324158    16.099789
 C     1.386988     0.068642    17.130935
 C     0.746731    -1.173679    17.129164
 C    -0.634048    -1.235487    17.130935
 C    -1.389802    -0.059848    17.129164
 C    -0.752939     1.166846    17.130935
 C     0.643071     1.233528    17.129164
 C     1.575343    -2.403497    16.889432
 C    -2.869161    -0.162538    16.889432
 C     1.293818     2.566035    16.889432
 H    -1.318937     2.087037    17.062993
 H     2.466896     0.098715    17.062993
 H    -1.147958    -2.185752    17.062993
 O     1.256185    -3.495227    17.539578
 O     2.398863     2.835501    17.539578
 O    -3.655047     0.659725    17.539578
 H     0.628051    -3.369177    18.244447
 H    -3.231818     1.140680    18.244447
 H     2.603767     2.228497    18.244447
 O    -1.390058    -3.129783    12.227096
 O     3.405501     0.361066    12.227096
 O    -2.015443     2.768717    12.227096
 C    -1.379307     0.162560    13.263645
 C    -0.838079    -1.111068    13.262507
 C     0.548873    -1.275795    13.263645
 C     1.381253    -0.170264    13.262507
 C     0.830434     1.113235    13.263645
 C    -0.543174     1.281332    13.262507
 C    -1.703650    -2.321146    13.040041
 C     2.861997    -0.314832    13.040041
 C    -1.158346     2.635978    13.040041
 H     1.489406     1.969736    13.206680
 H     0.961139    -2.274732    13.206680
 H    -2.450545     0.304996    13.206680
 O    -2.805727    -2.432342    13.722421
 O     3.509334    -1.213660    13.722421
 O    -0.703607     3.646002    13.722421
 H    -2.924993    -1.824850    14.458186
 H    -0.117870     3.445543    14.458186
 H     3.042863    -1.620693    14.458186
 O     1.510792    -3.074756     8.394016
 O    -3.418213     0.228993     8.394016
 O     1.907421     2.845763     8.394016
 C     1.331643    -0.394125     9.431290
 C     0.318227    -1.354501     9.429662
 C    -1.007144    -0.956174     9.431290
 C    -1.332146     0.401658     9.429662
 C    -0.324499     1.350299     9.431290
 C     1.013919     0.952843     9.429662
 C     0.693150    -2.794561     9.211936
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C	-2.766736	0.796995	9.211936
C	2.073586	1.997566	9.211936
H	-0.562238	2.404611	9.379069
H	2.363573	-0.715393	9.379069
H	-1.801335	-1.689218	9.379069
O	0.078035	-3.708600	9.900830
O	3.172724	1.921880	9.900830
O	-3.250759	1.786720	9.900830
H	-0.460857	-3.409165	10.641459
H	-2.721995	2.103697	10.641459
H	3.182852	1.305469	10.641459
O	-2.367084	-2.478102	4.579915
O	3.329641	-0.810904	4.579915
O	-0.962557	3.289006	4.579915
C	-1.244903	0.615312	5.616057
C	-1.161333	-0.766096	5.614378
C	0.089576	-1.385773	5.616057
C	1.244126	-0.622696	5.614378
C	1.155327	0.770461	5.616057
C	-0.082792	1.388792	5.614378
C	-2.384040	-1.614635	5.399403
C	2.590335	-1.257321	5.399403
C	-0.206295	2.871957	5.399403
H	2.062681	1.357730	5.565925
H	0.144488	-2.465199	5.565925
H	-2.207169	1.107469	5.565925
O	-3.451919	-1.353579	6.090818
O	2.898193	-2.312660	6.090818
O	0.553726	3.666239	6.090818
H	-3.355736	-0.745784	6.833693
H	1.032000	3.279045	6.833693
H	2.323736	-2.533261	6.833693
C	0.146244	1.380900	1.810944
C	1.274156	0.558512	1.809133
C	1.122773	-0.817101	1.810944
C	-0.153393	-1.382708	1.809133
C	-1.269016	-0.563799	1.810944
C	-1.120764	0.824196	1.809133
C	2.622982	1.187917	1.596193
O	3.630438	0.749018	2.287991
C	-0.282725	-2.865527	1.596193
O	-1.166551	-3.518560	2.287991
C	-2.340257	1.677611	1.596193
O	-2.463887	2.769542	2.287991
O	2.753471	2.043019	0.777850
O	0.392571	-3.406086	0.777850
O	-3.146042	1.363066	0.777850
O	-3.703772	-0.129138	-1.509703
C	-2.785066	-0.732382	-2.201694
O	-3.058296	-1.555714	-3.017288
C	-1.349681	-0.337288	-1.991266
C	-0.375406	-1.336861	-1.989605
C	0.966941	-1.000214	-1.991266
C	1.345459	0.343320	-1.989605
C	0.382740	1.337502	-1.991266
C	-0.970053	0.993542	-1.989605
C	2.026795	-2.045747	-2.201694
O	1.963723	-3.142991	-1.509703

C	0.758272	2.778129	-2.201694
O	1.740049	3.272129	-1.509703
O	2.876436	-1.870705	-3.017288
O	0.181860	3.426419	-3.017288
O	-2.254227	-2.940005	-5.305124
C	-1.203143	-2.617089	-5.997881
O	-0.739522	-3.355571	-6.808082
C	-0.596906	-1.256685	-5.791727
C	-1.383489	-0.117999	-5.790433
C	-0.789868	1.145279	-5.791727
C	0.589554	1.257136	-5.790433
C	1.386775	0.111407	-5.791727
C	0.793935	-1.139137	-5.790433
C	2.868037	0.266592	-5.997881
O	3.673232	-0.482215	-5.305124
C	-1.664894	2.350497	-5.997881
O	-1.419005	3.422220	-5.305124
O	3.275771	1.037341	-6.808082
O	-2.536249	2.318230	-6.808082
O	2.688486	2.545796	-9.098106
C	1.595620	2.399419	-9.789352
O	1.249422	3.211446	-10.586402
C	0.785613	1.148332	-9.591063
C	1.384854	-0.099202	-9.590356
C	0.601678	-1.254527	-9.591063
C	-0.778338	-1.149717	-9.590356
C	-1.387291	0.106195	-9.591063
C	-0.606515	1.248919	-9.590356
C	1.280148	-2.581557	-9.789352
O	0.860481	-3.601195	-9.098106
C	-2.875768	0.182138	-9.789352
O	-3.548967	1.055399	-9.098106
O	2.156483	-2.687754	-10.586402
O	-3.405905	-0.523692	-10.586402
O	-0.334355	3.683836	-12.884197
C	-0.908202	2.737738	-13.575843
C	-0.419460	1.327163	-13.391546
C	0.932300	1.028685	-13.391852
C	1.359087	-0.300318	-13.391546
C	0.424718	-1.321738	-13.391852
C	-0.939627	-1.026845	-13.391546
C	-1.357018	0.293053	-13.391852
C	2.825052	-0.582343	-13.575843
O	3.357473	-1.552358	-12.884197
C	-1.916850	-2.155395	-13.575843
O	-3.023118	-2.131478	-12.884197
O	-1.776847	2.973814	-14.350540
O	3.463822	0.051888	-14.350540
O	-1.686975	-3.025702	-14.350540
O	3.172319	1.857160	-16.611052
C	2.003592	2.095991	-17.174569
O	1.764533	3.136629	-17.677943
C	0.986196	0.986354	-17.144918
C	1.341715	-0.352532	-17.153556
C	0.361110	-1.347248	-17.144918
C	-0.976159	-0.985693	-17.153556
C	-1.347306	0.360893	-17.144918
C	-0.365556	1.338225	-17.153556

```
 C    -2.816977     0.687166   -17.174569
 O    -3.598668    -0.040184   -17.677943
 C     0.813385    -2.783157   -17.174569
 O     1.834134    -3.096446   -17.677943
 O    -3.194507     1.818729   -16.611052
 O     0.022188    -3.675889   -16.611052
 H     2.378859    -0.655548   -17.178053
 H    -1.757151    -1.732378   -17.178053
 H    -0.621708     2.387927   -17.178053
 H    -2.566569     2.217046   -16.006077
 H     3.203303     1.114191   -16.006077
 H    -0.636734    -3.331237   -16.006077
 H     1.670211     1.818211   -13.443276
 H     0.739511    -2.355550   -13.443276
 H    -2.409722     0.537339   -13.443276
 H    -3.075507    -1.483757   -12.174258
 H     0.252782     3.405345   -12.174258
 H     2.822725    -1.921588   -12.174258
 H     2.461614    -0.191927    -9.639767
 H    -1.397021    -2.035856    -9.639767
 H    -1.064593     2.227784    -9.639767
 H    -3.086512     1.485558    -8.369798
 H     2.829787     1.930219    -8.369798
 H     0.256725    -3.415777    -8.369798
 H     1.061999     2.229221    -5.839161
 H     1.399563    -2.034329    -5.839161
 H    -2.461562    -0.194893    -5.839161
 H    -2.487676    -2.362892    -4.568027
 H    -0.802486     3.335837    -4.568027
 H     3.290163    -0.972945    -4.568027
 H     2.396305     0.596164    -2.038177
 H    -0.681859    -2.373343    -2.038177
 H    -1.714445     1.777179    -2.038177
 H    -1.572949    -3.054935     3.030429
 H    -1.859177     2.889682     3.030429
 H     3.432126     0.165253     3.030429
 H    -3.409225     0.414985    -0.769012
 H     2.064000     2.744983    -0.769012
 H     1.345225    -3.159968    -0.769012
 H    -2.262655    -0.989089     1.761803
 H     1.987904    -1.464973     1.761803
 H     0.274752     2.454062     1.761803
```

$(B3CA)_{10}$

UHF/def-SV(P) geometry of the ^{3}CT state (μ= -29.3 Debye).

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  210
FINAL HEAT OF FORMATION = -7928.980840
 C    -0.960745     1.071255    16.672899
 C     0.485614     1.227420    16.655766
 C     1.268379     0.089575    16.602066
 C     0.745943    -1.204334    16.591995
 C    -0.700059    -1.356688    16.634712
 C    -1.502378    -0.215432    16.648046
 C     1.050336     2.536510    16.366270
```

O	2.306436	2.777112	16.721886
C	1.638055	-2.297135	16.277628
O	1.230954	-3.530570	16.560383
C	-2.974059	-0.382166	16.470858
O	-3.448222	-1.157650	15.699477
O	0.452043	3.403397	15.781816
O	2.711771	-2.171353	15.735427
O	-3.758103	0.399840	17.181464
O	-1.097910	3.588611	13.619595
C	-1.416855	2.571629	12.893591
C	-0.686330	1.274097	13.087798
C	-1.425089	0.080316	13.078720
C	-0.765481	-1.150229	13.078446
C	0.638874	-1.194912	13.094045
C	1.374476	-0.007743	13.096259
C	0.709678	1.230053	13.097774
C	-1.525662	-2.426509	12.870729
O	-1.148437	-3.216911	12.056539
C	2.865730	-0.023010	12.911310
O	3.357587	0.679608	12.075167
O	-2.253849	2.650763	12.040463
O	-2.613408	-2.626976	13.543961
O	3.584320	-0.821818	13.623901
O	0.383141	-3.668089	9.860140
C	0.920091	-2.714583	9.171744
O	1.748628	-2.935106	8.339448
C	0.442365	-1.306492	9.385829
C	1.387114	-0.267395	9.391805
C	0.961857	1.063247	9.384576
C	-0.410320	1.362338	9.381616
C	-1.350341	0.328840	9.376209
C	-0.922760	-1.009196	9.382707
C	-2.807118	0.619441	9.151514
O	-3.368997	1.562917	9.832847
C	1.944296	2.178756	9.167884
O	1.726134	2.999067	8.326405
O	-3.406507	0.009219	8.316746
O	3.033122	2.194994	9.862979
O	-3.333281	-1.571232	6.100654
C	-2.250393	-1.754423	5.417707
C	-1.086015	-0.831990	5.643033
C	-1.264864	0.553623	5.646126
C	-0.148363	1.406051	5.643356
C	1.140972	0.867999	5.648887
C	1.320692	-0.525058	5.647437
C	0.210230	-1.372664	5.649718
C	-0.364413	2.875952	5.418059
O	-1.137549	3.235154	4.581630
C	2.701843	-1.073662	5.426982
O	3.082754	-2.100472	6.114900
O	-2.173787	-2.605861	4.583747
O	0.333453	3.722437	6.102828
O	3.402230	-0.585884	4.591671
O	3.624247	0.977567	2.362994
C	2.594088	1.349337	1.674344
O	2.674740	2.197678	0.838140
C	1.282191	0.650796	1.895971
C	1.209190	-0.744385	1.896954

C	-0.042243	-1.382372	1.891971
C	-1.213972	-0.621653	1.892156
C	-1.140848	0.781045	1.890489
C	0.103849	1.415519	1.896796
C	-0.093003	-2.867030	1.666544
O	-0.931985	-3.574441	2.351668
C	-2.400665	1.567634	1.662699
O	-2.596198	2.646329	2.349501
O	0.602991	-3.359215	0.830634
O	-3.172451	1.212382	0.823870
O	2.143344	-3.049207	-1.407595
C	2.149015	-1.951621	-2.092416
C	1.055928	-0.946722	-1.861870
C	-0.283980	-1.341400	-1.862485
C	-1.301359	-0.373062	-1.869300
C	-0.973248	0.984612	-1.863165
C	0.373983	1.381590	-1.862929
C	1.385764	0.418590	-1.855327
C	-2.717163	-0.816378	-2.106953
O	-3.667148	-0.266177	-1.422547
C	0.698698	2.830152	-2.094856
O	0.111902	3.436165	-2.939684
O	2.971157	-1.743422	-2.932646
O	-2.944839	-1.628430	-2.951956
O	1.647926	3.375490	-1.405602
O	-1.431847	3.431337	-5.196192
C	-1.637969	2.358011	-5.887729
O	-2.478484	2.311848	-6.734539
C	-0.754935	1.164354	-5.656772
C	0.635444	1.298682	-5.647830
C	1.451445	0.155541	-5.648581
C	0.872507	-1.115790	-5.646073
C	-0.525542	-1.250951	-5.655135
C	-1.337027	-0.113904	-5.655148
C	2.927869	0.324146	-5.871681
O	3.750668	-0.394530	-5.179328
C	-1.116447	-2.613315	-5.885248
O	-2.154070	-2.968944	-5.199850
O	3.312507	1.078707	-6.713281
O	-0.650585	-3.321234	-6.726357
O	2.806205	2.544689	-8.957959
C	1.724803	2.388166	-9.648166
O	1.405478	3.166262	-10.496210
C	0.885138	1.163454	-9.417237
C	1.467439	-0.106386	-9.409577
C	0.654222	-1.251741	-9.415543
C	-0.736563	-1.121102	-9.413676
C	-1.321937	0.155815	-9.421794
C	-0.513467	1.295110	-9.416562
C	-2.801409	0.267976	-9.659461
C	1.295449	-2.590827	-9.647120
O	0.888152	-3.607119	-8.960327
O	2.130990	-2.701741	-10.493377
O	0.061785	3.773948	-12.778075
C	-0.517247	2.853606	-13.471102
O	-1.264909	3.109928	-14.367304
C	-0.190641	1.409789	-13.198523
C	1.135265	0.967719	-13.201573

C	1.416606	-0.409828	-13.203823
C	0.371097	-1.335681	-13.197114
C	-0.962205	-0.890167	-13.199248
C	-1.242529	0.477709	-13.186722
C	-2.053303	-1.885283	-13.483421
C	2.826952	-0.861489	-13.470789
O	3.324429	-1.821397	-12.767546
O	3.432584	-0.357386	-14.368455
O	-2.981568	2.303554	-16.408180
C	-2.800592	1.104233	-16.890099
O	-3.660138	0.448997	-17.354372
C	-1.389325	0.546558	-16.869625
C	-1.238013	-0.831628	-16.952984
C	0.067874	-1.448451	-16.979587
C	1.212827	-0.651839	-16.966273
C	1.073531	0.727025	-16.900436
C	-0.247893	1.325595	-16.876147
C	2.239843	1.691831	-16.992773
O	3.387184	1.329988	-16.508765
C	0.230398	-2.954587	-17.128444
O	2.041529	2.710244	-17.553960
O	-0.677551	-3.717749	-16.591870
O	1.141935	-3.346401	-17.759217
O	-3.131026	-1.864904	-12.780016
O	-1.911608	-2.637605	-14.403364
O	-3.482393	1.128238	-8.977040
O	-3.310845	-0.402874	-10.506722
H	-1.585544	1.952297	16.621479
H	2.343522	0.177834	16.505100
H	-1.171567	-2.325772	16.543170
H	0.473930	-3.536301	17.134647
H	-3.270572	0.925939	17.808260
H	2.638999	2.128215	17.331461
H	1.286395	2.144390	13.068982
H	1.141747	-2.151878	13.067872
H	-2.504937	0.124351	13.038349
H	-2.804686	-2.029017	14.284594
H	-0.522080	3.438440	14.396078
H	3.169822	-1.287968	14.380494
H	-0.729474	2.394630	9.337808
H	2.441165	-0.506621	9.357751
H	-1.657036	-1.802065	9.341579
H	-0.171304	-3.417380	10.616798
H	-2.882444	1.919304	10.595293
H	3.083516	1.600148	10.630263
H	2.006093	1.515419	5.605146
H	0.338667	-2.445680	5.608495
H	-2.258310	0.979028	5.605271
H	-3.286052	-0.966471	6.857391
H	0.829759	3.380746	6.862986
H	2.536098	-2.355620	6.874258
H	2.184833	-1.118701	-17.026534
H	-2.124644	-1.448087	-17.019858
H	-0.301911	2.405188	-16.880327
H	-2.342189	2.627423	-15.762804
H	3.397250	0.650752	-15.818011
H	-1.180845	-3.357525	-15.849588
H	1.949787	1.678600	-13.249191

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 H     0.579451    -2.396497   -13.240564
 H    -2.265454     0.827909   -13.227527
 H    -3.139785    -1.306557   -11.985227
 H     0.551635     3.496580   -11.987763
 H     2.834362    -2.102429   -11.978721
 H     2.542667    -0.217640    -9.445237
 H    -1.370267    -1.996687    -9.452127
 H    -0.954528     2.281704    -9.459146
 H    -3.048153     1.534938    -8.211464
 H     2.935093     1.963590    -8.192734
 H     0.316735    -3.429908    -8.197473
 H     1.092588     2.278008    -5.689419
 H     1.492348    -2.001224    -5.686078
 H    -2.413441    -0.207754    -5.703401
 H    -2.393882    -2.420361    -4.438023
 H    -0.841271     3.361464    -4.431178
 H     3.390747    -0.874309    -4.418355
 H     2.425368     0.714239    -1.894886
 H    -0.547573    -2.389310    -1.908767
 H    -1.748766     1.736984    -1.910379
 H    -1.359370    -3.147652     3.109584
 H    -2.013436     2.802735     3.107889
 H     3.466925     0.393150     3.119913
 H    -3.410320     0.273146    -0.659665
 H     1.984746     2.880223    -0.644029
 H     1.543600    -3.096250    -0.648109
 H    -2.181013    -1.103176     1.841203
 H     2.109825    -1.341239     1.849612
 H     0.170497     2.494087     1.852953
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$(B2CA)_{10}$

HF/def-SV(P) geometry of the S_0 state (μ= 77.1 Debye).

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  180
FINAL HEAT OF FORMATION = -6054.483070
 C    -0.542402    -1.279760    17.474782
 C     0.837975    -1.103341    17.427538
 C     1.749049    -2.273237    17.199911
 O     2.607113    -2.240580    16.383540
 C     1.380183     0.176920    17.441333
 O     1.530302    -3.358450    17.908815
 O     3.565517    -0.967194    14.019071
 C     2.872995    -0.137602    13.290761
 O     3.393195     0.535095    12.458317
 C     1.385806    -0.078558    13.495164
 C     0.624992    -1.242869    13.537443
 C     0.758115     1.162808    13.497247
 O     3.050179     2.077285    10.138202
 C     1.976613     2.090183     9.402518
 C     0.962288     0.999902     9.598822
 C     1.350152    -0.335564     9.640913
 O     1.809788     2.923610     8.567929
 C    -0.388318     1.332431     9.599659
 O     0.419702     3.665534     6.260302
 C    -0.289166     2.862176     5.522374
```

O	-1.026700	3.281382	4.685477
C	-0.127585	1.381769	5.717422
C	1.136482	0.802300	5.759900
C	-1.262083	0.577149	5.718181
O	-2.497788	2.714523	2.384441
C	-2.354252	1.653413	1.645919
C	-1.128649	0.807230	1.839504
C	-1.262015	-0.577202	1.840128
O	-3.154431	1.370169	0.809277
C	0.136426	1.384425	1.881930
O	-3.686287	-0.117431	-1.488625
C	-2.789814	-0.703338	-2.227201
O	-3.098989	-1.495993	-3.061734
C	-1.348429	-0.327503	-2.035642
C	-0.959266	1.007451	-1.993707
C	-0.387118	-1.332621	-2.035506
O	-2.311267	-2.872993	-5.359434
C	-1.281117	-2.576582	-6.097604
O	-0.878811	-3.330553	-6.927837
C	-0.628860	-1.237010	-5.908844
C	-1.389170	-0.072748	-5.867806
C	0.759886	-1.161121	-5.909349
O	0.693987	-3.619506	-9.227541
C	1.139645	-2.643278	-9.966239
C	0.537597	-1.279509	-9.783566
C	1.377068	-0.170621	-9.785457
O	1.981602	-2.826241	-10.788255
C	-0.842246	-1.107015	-9.744177
O	3.218441	-1.795003	-13.104801
C	2.762798	-0.813477	-13.836181
C	1.328134	-0.404869	-13.657459
C	1.012025	0.949607	-13.660076
O	3.451070	-0.274364	-14.642298
C	0.312492	-1.355007	-13.619640
O	3.243588	1.646738	-16.802576
C	2.133762	1.962454	-17.442855
C	1.044096	0.923450	-17.475056
C	-0.277076	1.358672	-17.515233
O	2.002783	3.016526	-17.959270
C	1.316600	-0.442019	-17.485789
H	2.452373	0.309183	17.395618
H	-0.973383	-2.272963	17.459947
H	0.906812	-3.235768	18.617894
H	1.352679	2.064771	13.444898
H	3.108101	-1.375894	14.760462
H	-0.685414	2.371202	9.550059
H	2.399208	-0.601414	9.643878
H	3.062176	1.462545	10.881391
H	2.023298	1.422495	5.764778
H	-2.242422	1.031363	5.669509
H	0.890851	3.273568	7.006204
H	2.338375	-0.797529	-17.484398
H	-0.481383	2.419214	-17.550803
H	3.193504	0.889876	-16.214516
H	1.803259	1.684946	-13.713323
H	0.549882	-2.410748	-13.619885
H	2.659619	-2.086194	-12.375588
H	2.448490	-0.309059	-9.835149

H	-1.501487	-1.965142	-9.740904
H	0.117855	-3.381455	-8.490919
H	1.346856	-2.068206	-5.957627
H	-2.501300	-2.285553	-4.617058
H	-0.693774	-2.368650	-2.083584
H	-1.702061	1.794376	-1.987962
H	-1.893135	2.814077	3.130875
H	-3.365758	0.406595	-0.743356
H	-2.246849	-1.021660	1.792226
H	0.247220	2.460879	1.887815
H	-2.470049	-0.124566	-5.862792
H	1.106407	-2.212246	13.535250
C	0.542402	1.279760	17.474782
C	-0.837975	1.103341	17.427538
C	-1.749049	2.273237	17.199911
O	-2.607113	2.240580	16.383540
C	-1.380183	-0.176920	17.441333
O	-1.530302	3.358450	17.908815
O	-3.565517	0.967194	14.019071
C	-2.872995	0.137602	13.290761
O	-3.393195	-0.535095	12.458317
C	-1.385806	0.078558	13.495164
C	-0.624992	1.242869	13.537443
C	-0.758115	-1.162808	13.497247
O	-3.050179	-2.077285	10.138202
C	-1.976613	-2.090183	9.402518
C	-0.962288	-0.999902	9.598822
C	-1.350152	0.335564	9.640913
O	-1.809788	-2.923610	8.567929
C	0.388318	-1.332431	9.599659
O	-0.419702	-3.665534	6.260302
C	0.289166	-2.862176	5.522374
O	1.026700	-3.281382	4.685477
C	0.127585	-1.381769	5.717422
C	-1.136482	-0.802300	5.759900
C	1.262083	-0.577149	5.718181
O	2.497788	-2.714523	2.384441
C	2.354252	-1.653413	1.645919
C	1.128649	-0.807230	1.839504
C	1.262015	0.577202	1.840128
O	3.154431	-1.370169	0.809277
C	-0.136426	-1.384425	1.881930
O	3.686287	0.117431	-1.488625
C	2.789814	0.703338	-2.227201
O	3.098989	1.495993	-3.061734
C	1.348429	0.327503	-2.035642
C	0.959266	-1.007451	-1.993707
C	0.387118	1.332621	-2.035506
O	2.311267	2.872993	-5.359434
C	1.281117	2.576582	-6.097604
O	0.878811	3.330553	-6.927837
C	0.628860	1.237010	-5.908844
C	1.389170	0.072748	-5.867806
C	-0.759886	1.161121	-5.909349
O	-0.693987	3.619506	-9.227541
C	-1.139645	2.643278	-9.966239
C	-0.537597	1.279509	-9.783566
C	-1.377068	0.170621	-9.785457

O	-1.981602	2.826241	-10.788255
C	0.842246	1.107015	-9.744177
O	-3.218441	1.795003	-13.104801
C	-2.762798	0.813477	-13.836181
C	-1.328134	0.404869	-13.657459
C	-1.012025	-0.949607	-13.660076
O	-3.451070	0.274364	-14.642298
C	-0.312492	1.355007	-13.619640
O	-3.243588	-1.646738	-16.802576
C	-2.133762	-1.962454	-17.442855
C	-1.044096	-0.923450	-17.475056
C	0.277076	-1.358672	-17.515233
O	-2.002783	-3.016526	-17.959270
C	-1.316600	0.442019	-17.485789
H	-2.452373	-0.309183	17.395618
H	0.973383	2.272963	17.459947
H	-0.906812	3.235768	18.617894
H	-1.352679	-2.064771	13.444898
H	-3.108101	1.375894	14.760462
H	0.685414	-2.371202	9.550059
H	-2.399208	0.601414	9.643878
H	-3.062176	-1.462545	10.881391
H	-2.023298	-1.422495	5.764778
H	2.242422	-1.031363	5.669509
H	-0.890851	-3.273568	7.006204
H	-2.338375	0.797529	-17.484398
H	0.481383	-2.419214	-17.550803
H	-3.193504	-0.889876	-16.214516
H	-1.803259	-1.684946	-13.713323
H	-0.549882	2.410748	-13.619885
H	-2.659619	2.086194	-12.375588
H	-2.448490	0.309059	-9.835149
H	1.501487	1.965142	-9.740904
H	-0.117855	3.381455	-8.490919
H	-1.346856	2.068206	-5.957627
H	2.501300	2.285553	-4.617058
H	0.693774	2.368650	-2.083584
H	1.702061	-1.794376	-1.987962
H	1.893135	-2.814077	3.130875
H	3.365758	-0.406595	-0.743356
H	2.246849	1.021660	1.792226
H	-0.247220	-2.460879	1.887815
H	2.470049	0.124566	-5.862792
H	-1.106407	2.212246	13.535250

$(B2CA)_{10}$

UHF/def-SV(P) geometry of the ^{3}LE state (μ= 77.0 Debye).

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  180
FINAL HEAT OF FORMATION = -6054.398510
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C	-0.685693	-1.270897	17.557681
C	0.715625	-1.241024	17.482705
C	1.506016	-2.389673	16.994643
O	2.456487	-2.231013	16.296497
C	1.415257	0.097684	17.587502

O	1.104343	-3.604466	17.309754
O	3.574881	-0.938259	14.030116
C	2.874259	-0.112936	13.305478
O	3.386183	0.566760	12.473553
C	1.386831	-0.066822	13.515031
C	0.635349	-1.237518	13.557053
C	0.748534	1.169233	13.518301
O	3.022092	2.115652	10.161577
C	1.952514	2.112733	9.420043
C	0.950746	1.010755	9.615698
C	1.353885	-0.320138	9.658608
O	1.779239	2.941645	8.582351
C	-0.403541	1.327940	9.616934
O	0.374445	3.669253	6.279448
C	-0.320492	2.859133	5.535705
O	-1.058911	3.271379	4.696193
C	-0.142496	1.380285	5.728701
C	1.127752	0.814568	5.771344
C	-1.268246	0.563433	5.729197
O	-2.528196	2.684507	2.399559
C	-2.371554	1.629209	1.655389
C	-1.136902	0.795607	1.846824
C	-1.255987	-0.590149	1.846725
O	-3.167588	1.341165	0.816495
C	0.122164	1.385772	1.889125
O	-3.683150	-0.161154	-1.474779
C	-2.782562	-0.732983	-2.219301
O	-3.085305	-1.525595	-3.056165
C	-1.344907	-0.341699	-2.029939
C	-0.969857	0.997280	-1.988290
C	-0.373031	-1.336632	-2.030342
O	-2.272821	-2.901540	-5.345183
C	-1.251004	-2.591745	-6.089289
O	-0.843386	-3.340590	-6.921502
C	-0.614430	-1.244228	-5.902816
C	-1.388239	-0.088915	-5.861611
C	0.773369	-1.152227	-5.903177
O	0.743098	-3.608275	-9.213626
C	1.173445	-2.628719	-9.956920
C	0.553856	-1.272506	-9.776086
C	1.379174	-0.153051	-9.777919
O	2.015750	-2.802918	-10.780387
C	-0.828070	-1.117643	-9.736431
O	3.242312	-1.749476	-13.092158
C	2.773481	-0.776738	-13.826937
C	1.333333	-0.387223	-13.649362
C	0.999354	0.962956	-13.652067
O	3.454548	-0.230606	-14.634410
C	0.330409	-1.350744	-13.611268
O	3.218009	1.692606	-16.787319
C	2.106369	1.991779	-17.432277
C	1.031282	0.937686	-17.466006
C	-0.295765	1.354724	-17.506108
O	1.962318	3.043388	-17.950234
C	1.322582	-0.423882	-17.476420
H	2.492371	0.109953	17.664243
H	-1.222172	-2.211681	17.533043
H	0.441338	-3.627438	17.992028

H	1.335237	2.076268	13.465214
H	3.113649	-1.360361	14.761282
H	-0.712371	2.363286	9.566969
H	2.405917	-0.574003	9.662164
H	3.039868	1.497843	10.902042
H	2.007825	1.444319	5.777313
H	-2.253388	1.007127	5.680194
H	0.850932	3.280279	7.023496
H	2.349185	-0.765270	-17.473395
H	-0.514386	2.412450	-17.540507
H	3.177371	0.932928	-16.202124
H	1.780809	1.708613	-13.706421
H	0.581778	-2.403265	-13.611177
H	2.684577	-2.048731	-12.365454
H	2.452228	-0.277913	-9.828701
H	-1.476298	-1.984146	-9.733941
H	0.161001	-3.375461	-8.480136
H	1.370798	-2.052462	-5.951688
H	-2.469841	-2.312992	-4.605567
H	-0.668757	-2.375786	-2.079787
H	-1.720926	1.776339	-1.982842
H	-1.921944	2.789380	3.143919
H	-3.365464	0.367900	-0.731921
H	-2.236174	-1.044649	1.797431
H	0.221914	2.463313	1.896599
H	-2.468467	-0.153345	-5.857087
H	1.124444	-2.202811	13.554913
C	0.685693	1.270897	17.557681
C	-0.715625	1.241024	17.482705
C	-1.506016	2.389673	16.994643
O	-2.456487	2.231013	16.296497
C	-1.415257	-0.097684	17.587502
O	-1.104343	3.604466	17.309754
O	-3.574881	0.938259	14.030116
C	-2.874259	0.112936	13.305478
O	-3.386183	-0.566760	12.473553
C	-1.386831	0.066822	13.515031
C	-0.635349	1.237518	13.557053
C	-0.748534	-1.169233	13.518301
O	-3.022092	-2.115652	10.161577
C	-1.952514	-2.112733	9.420043
C	-0.950746	-1.010755	9.615698
C	-1.353885	0.320138	9.658608
O	-1.779239	-2.941645	8.582351
C	0.403541	-1.327940	9.616934
O	-0.374445	-3.669253	6.279448
C	0.320492	-2.859133	5.535705
O	1.058911	-3.271379	4.696193
C	0.142496	-1.380285	5.728701
C	-1.127752	-0.814568	5.771344
C	1.268246	-0.563433	5.729197
O	2.528196	-2.684507	2.399559
C	2.371554	-1.629209	1.655389
C	1.136902	-0.795607	1.846824
C	1.255987	0.590149	1.846725
O	3.167588	-1.341165	0.816495
C	-0.122164	-1.385772	1.889125
O	3.683150	0.161154	-1.474779

C	2.782562	0.732983	-2.219301
O	3.085305	1.525595	-3.056165
C	1.344907	0.341699	-2.029939
C	0.969857	-0.997280	-1.988290
C	0.373031	1.336632	-2.030342
O	2.272821	2.901540	-5.345183
C	1.251004	2.591745	-6.089289
O	0.843386	3.340590	-6.921502
C	0.614430	1.244228	-5.902816
C	1.388239	0.088915	-5.861611
C	-0.773369	1.152227	-5.903177
O	-0.743098	3.608275	-9.213626
C	-1.173445	2.628719	-9.956920
C	-0.553856	1.272506	-9.776086
C	-1.379174	0.153051	-9.777919
O	-2.015750	2.802918	-10.780387
C	0.828070	1.117643	-9.736431
O	-3.242312	1.749476	-13.092158
C	-2.773481	0.776738	-13.826937
C	-1.333333	0.387223	-13.649362
C	-0.999354	-0.962956	-13.652067
O	-3.454548	0.230606	-14.634410
C	-0.330409	1.350744	-13.611268
O	-3.218009	-1.692606	-16.787319
C	-2.106369	-1.991779	-17.432277
C	-1.031282	-0.937686	-17.466006
C	0.295765	-1.354724	-17.506108
O	-1.962318	-3.043388	-17.950234
C	-1.322582	0.423882	-17.476420
H	-2.492371	-0.109953	17.664243
H	1.222172	2.211681	17.533043
H	-0.441338	3.627438	17.992028
H	-1.335237	-2.076268	13.465214
H	-3.113649	1.360361	14.761282
H	0.712371	-2.363286	9.566969
H	-2.405917	0.574003	9.662164
H	-3.039868	-1.497843	10.902042
H	-2.007825	-1.444319	5.777313
H	2.253388	-1.007127	5.680194
H	-0.850932	-3.280279	7.023496
H	-2.349185	0.765270	-17.473395
H	0.514386	-2.412450	-17.540507
H	-3.177371	-0.932928	-16.202124
H	-1.780809	-1.708613	-13.706421
H	-0.581778	2.403265	-13.611177
H	-2.684577	2.048731	-12.365454
H	-2.452228	0.277913	-9.828701
H	1.476298	1.984146	-9.733941
H	-0.161001	3.375461	-8.480136
H	-1.370798	2.052462	-5.951688
H	2.469841	2.312992	-4.605567
H	0.668757	2.375786	-2.079787
H	1.720926	-1.776339	-1.982842
H	1.921944	-2.789380	3.143919
H	3.365464	-0.367900	-0.731921
H	2.236174	1.044649	1.797431
H	-0.221914	-2.463313	1.896599
H	2.468467	0.153345	-5.857087

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 H    -1.124444     2.202811    13.554913
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$(B2CA)_{10}$

UHF/def-SV(P) geometry of the ^{1}CT state (μ= -72.3 Debye).

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  180
FINAL HEAT OF FORMATION = -6054.304730
 C    -0.520498    -1.296923    17.060476
 C     0.899618    -1.107687    16.976584
 C     1.806650    -2.162590    16.616175
 O     2.862579    -1.998979    16.043548
 C     1.374075     0.240896    17.021025
 O     1.448719    -3.423563    16.885723
 O     3.639395    -0.576286    13.944128
 C     2.874942     0.142815    13.193755
 O     3.335270     0.847491    12.337801
 C     1.386270     0.056396    13.363850
 C     0.743379    -1.175363    13.406286
 C     0.640027     1.229214    13.362382
 O     2.863612     2.318633    10.130647
 C     1.813284     2.232294     9.380684
 C     0.882118     1.070192     9.569849
 C     1.371652    -0.230662     9.615917
 O     1.598802     3.036043     8.519946
 C    -0.489523     1.298016     9.571829
 O     0.192304     3.683307     6.283774
 C    -0.450923     2.839799     5.540765
 O    -1.195351     3.212665     4.682610
 C    -0.207690     1.371459     5.738284
 C     1.087705     0.867048     5.784805
 C    -1.293332     0.502497     5.741413
 O    -2.617677     2.600693     2.432194
 C    -2.417300     1.556593     1.691543
 C    -1.160827     0.759422     1.892491
 C    -1.236786    -0.629164     1.896032
 O    -3.190457     1.248458     0.833818
 C     0.078745     1.388850     1.939189
 O    -3.684707    -0.214994    -1.423329
 C    -2.772203    -0.761170    -2.163372
 O    -3.057193    -1.540876    -3.023116
 C    -1.340255    -0.357735    -1.959749
 C    -0.981801     0.985514    -1.912688
 C    -0.356825    -1.341036    -1.955794
 O    -2.306774    -2.882715    -5.281392
 C    -1.292787    -2.567088    -6.022070
 O    -0.906981    -3.296403    -6.887304
 C    -0.632461    -1.234495    -5.815050
 C    -1.389538    -0.068469    -5.767030
 C     0.756454    -1.163464    -5.810243
 O     0.574493    -3.648639    -9.140057
 C     1.014534    -2.688313    -9.884673
 C     0.481189    -1.300747    -9.672589
 C     1.368733    -0.229931    -9.666377
 O     1.800693    -2.895035   -10.763020
 C    -0.889759    -1.069838    -9.622842
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O	3.039288	-2.123170	-13.025107
C	2.626810	-1.162761	-13.777782
C	1.266672	-0.568393	-13.534023
C	1.124441	0.815387	-13.521540
O	3.273419	-0.768990	-14.706036
C	0.139937	-1.384828	-13.479518
O	3.546862	1.133314	-16.668908
C	2.464331	1.625432	-17.200788
C	1.227079	0.746953	-17.197857
C	-0.020089	1.379814	-17.252394
O	2.395751	2.693581	-17.690427
C	1.250640	-0.629672	-17.212806
H	2.442396	0.414208	17.015637
H	-0.944651	-2.295266	17.071646
H	0.710470	-3.455317	17.481661
H	1.143656	2.185745	13.332888
H	3.245179	-1.046058	14.711912
H	-0.866193	2.311242	9.536137
H	2.437840	-0.413171	9.638054
H	2.923052	1.723202	10.899569
H	1.935893	1.538585	5.802226
H	-2.298985	0.898638	5.702183
H	0.674306	3.329889	7.049489
H	2.185182	-1.173611	-17.201320
H	-0.056899	2.459533	-17.311551
H	3.442390	0.423365	-16.019553
H	2.001408	1.448594	-13.552685
H	0.245124	-2.461865	-13.450300
H	2.523574	-2.328133	-12.224976
H	2.434044	-0.413679	-9.704102
H	-1.584270	-1.899506	-9.604167
H	0.040273	-3.408461	-8.365241
H	1.341516	-2.072325	-5.850364
H	-2.491442	-2.319834	-4.513084
H	-0.639539	-2.384233	-1.996740
H	-1.742720	1.754680	-1.897633
H	-2.033319	2.724695	3.196710
H	-3.388172	0.301798	-0.658025
H	-2.202410	-1.114713	1.855445
H	0.143744	2.468813	1.954753
H	-2.470365	-0.118022	-5.751021
H	1.318724	-2.091158	13.432807
C	0.520498	1.296923	17.060476
C	-0.899618	1.107687	16.976584
C	-1.806650	2.162590	16.616175
O	-2.862579	1.998979	16.043548
C	-1.374075	-0.240896	17.021025
O	-1.448719	3.423563	16.885723
O	-3.639395	0.576286	13.944128
C	-2.874942	-0.142815	13.193755
O	-3.335270	-0.847491	12.337801
C	-1.386270	-0.056396	13.363850
C	-0.743379	1.175363	13.406286
C	-0.640027	-1.229214	13.362382
O	-2.863612	-2.318633	10.130647
C	-1.813284	-2.232294	9.380684
C	-0.882118	-1.070192	9.569849
C	-1.371652	0.230662	9.615917

O	-1.598802	-3.036043	8.519946
C	0.489523	-1.298016	9.571829
O	-0.192304	-3.683307	6.283774
C	0.450923	-2.839799	5.540765
O	1.195351	-3.212665	4.682610
C	0.207690	-1.371459	5.738284
C	-1.087705	-0.867048	5.784805
C	1.293332	-0.502497	5.741413
O	2.617677	-2.600693	2.432194
C	2.417300	-1.556593	1.691543
C	1.160827	-0.759422	1.892491
C	1.236786	0.629164	1.896032
O	3.190457	-1.248458	0.833818
C	-0.078745	-1.388850	1.939189
O	3.684707	0.214994	-1.423329
C	2.772203	0.761170	-2.163372
O	3.057193	1.540876	-3.023116
C	1.340255	0.357735	-1.959749
C	0.981801	-0.985514	-1.912688
C	0.356825	1.341036	-1.955794
O	2.306774	2.882715	-5.281392
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C	0.632461	1.234495	-5.815050
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C	-1.014534	2.688313	-9.884673
C	-0.481189	1.300747	-9.672589
C	-1.368733	0.229931	-9.666377
O	-1.800693	2.895035	-10.763020
C	0.889759	1.069838	-9.622842
O	-3.039288	2.123170	-13.025107
C	-2.626810	1.162761	-13.777782
C	-1.266672	0.568393	-13.534023
C	-1.124441	-0.815387	-13.521540
O	-3.273419	0.768990	-14.706036
C	-0.139937	1.384828	-13.479518
O	-3.546862	-1.133314	-16.668908
C	-2.464331	-1.625432	-17.200788
C	-1.227079	-0.746953	-17.197857
C	0.020089	-1.379814	-17.252394
O	-2.395751	-2.693581	-17.690427
C	-1.250640	0.629672	-17.212806
H	-2.442396	-0.414208	17.015637
H	0.944651	2.295266	17.071646
H	-0.710470	3.455317	17.481661
H	-1.143656	-2.185745	13.332888
H	-3.245179	1.046058	14.711912
H	0.866193	-2.311242	9.536137
H	-2.437840	0.413171	9.638054
H	-2.923052	-1.723202	10.899569
H	-1.935893	-1.538585	5.802226
H	2.298985	-0.898638	5.702183
H	-0.674306	-3.329889	7.049489
H	-2.185182	1.173611	-17.201320
H	0.056899	-2.459533	-17.311551
H	-3.442390	-0.423365	-16.019553

H	-2.001408	-1.448594	-13.552685
H	-0.245124	2.461865	-13.450300
H	-2.523574	2.328133	-12.224976
H	-2.434044	0.413679	-9.704102
H	1.584270	1.899506	-9.604167
H	-0.040273	3.408461	-8.365241
H	-1.341516	2.072325	-5.850364
H	2.491442	2.319834	-4.513084
H	0.639539	2.384233	-1.996740
H	1.742720	-1.754680	-1.897633
H	2.033319	-2.724695	3.196710
H	3.388172	-0.301798	-0.658025
H	2.202410	1.114713	1.855445
H	-0.143744	-2.468813	1.954753
H	2.470365	0.118022	-5.751021
H	-1.318724	2.091158	13.432807