The Effect of Non-covalent Interactions on the *n*-Butylbenzene…Ar Cluster Studied by Mass Analyzed Threshold Ionization Spectroscopy and *ab initio* Computations

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6. Supplement Material

6.1 Calculated XYZ Coordinates of *n*-Butylbenzene Monomer and *n*-Butylbenzene-V…Ar Cluster on Neural Ground State

All values are in Angstroms.

BB-I at cc-pVTZ level of theory			
C	-1.058123000	-0.642755000	1.058295000
C	-0.526982000	0.530507000	0.516895000
C	-1.184525000	1.117418000	-0.569126000
C	-2.338074000	0.548154000	-1.102068000
C	-2.854855000	-0.624764000	-0.553521000
C	-2.212485000	-1.218671000	0.530415000
C	0.745540000	1.130728000	1.045322000
C	1.941855000	0.840343000	0.132118000
C	2.253038000	-0.644285000	0.002903000
C	3.452816000	-0.902752000	-0.898984000
H	-3.751461000	-1.068160000	-0.964276000
H	-2.834924000	1.019811000	-1.939187000
H	-2.608909000	-2.126497000	0.964874000
H	-0.790483000	2.032306000	-0.995929000
H	-0.562390000	-1.106508000	1.902452000
H	0.624591000	2.210938000	1.147740000
H	0.949602000	0.734695000	2.042487000
H	2.821666000	1.361981000	0.517892000
H	1.741007000	1.253951000	-0.860043000
H	2.440947000	-1.057617000	0.997380000
H	1.377134000	-1.164755000	-0.388106000
H	4.344922000	-0.410312000	-0.511921000
H	3.270610000	-0.516822000	-1.901912000
H	3.668461000	-1.966553000	-0.984950000
BB-V at cc-pVTZ level of theory			
C	0.715170000	-0.448789000	0.000000000
C	0.714758000	-1.164449000	1.200446000
C	0.714758000	-2.557415000	1.204519000
C	0.713702000	-3.258036000	0.000000000

C	0.714758000	-2.557415000	-1.204519000
C	0.714758000	-1.164449000	-1.200446000
C	0.650726000	1.051192000	0.000000000
C	-0.793195000	1.556493000	0.000000000
C	-0.889951000	3.076077000	0.000000000
C	-2.332543000	3.564460000	0.000000000
H	0.717018000	-4.339321000	0.000000000
H	0.719600000	-3.093882000	2.143766000
H	0.719600000	-3.093882000	-2.143766000
H	0.720325000	-0.623209000	2.139152000
H	0.720325000	-0.623209000	-2.139152000
H	1.167823000	1.443954000	0.878429000
H	1.167823000	1.443954000	-0.878429000
H	-1.310596000	1.154119000	0.875216000
H	-1.310596000	1.154119000	-0.875216000
H	-0.366460000	3.468493000	0.874860000
H	-0.366460000	3.468493000	-0.874860000
H	-2.863415000	3.201272000	0.879737000
H	-2.863415000	3.201272000	-0.879737000
H	-2.389230000	4.651807000	0.000000000

BB-I…Ar(IU) at cc-pVTZ(BB)/aug-cc-pVTZ(Ar) level of theory			
C	0.356952226	-0.178666636	2.814124011
C	1.417604326	0.339003433	2.073960681
C	1.167231973	1.108498256	0.939027453
C	-0.140747620	1.369978873	0.521425592
C	-1.194926945	0.845212799	1.276031343
C	-0.952863851	0.079461461	2.413490995
C	-0.425088643	2.153179574	-0.729126016
C	-0.649604841	1.243154956	-1.943010905
C	0.607147987	0.507079875	-2.386453824
C	0.339016726	-0.436079077	-3.551699795
H	0.548699034	-0.772604546	3.697163092
H	-1.782453624	-0.312331237	2.986557997
H	2.437106468	0.148700954	2.381404578
H	-2.215005224	1.045963986	0.970078944
H	1.995170051	1.517467955	0.372808861
H	-1.312122876	2.769494362	-0.572296756
H	0.404873071	2.832029194	-0.938105219
H	-1.025357904	1.842612865	-2.776351314
H	-1.430259035	0.516344535	-1.700609091
H	1.366348175	1.240662408	-2.670050352
H	1.016534864	-0.053930592	-1.545457108
H	-0.057127112	0.107243583	-4.409753089

H	-0.393229543	-1.193505769	-3.272211048
H	1.245289492	-0.949130559	-3.869797310
Ar	-0.177914697	-2.334458369	-0.142988477

BB-I…Ar(ID) at cc-pVTZ(BB)/aug-cc-pVTZ(Ar) level of theory			
C	-0.860527957	-1.607183885	1.120745590
C	-0.079640173	-0.452837135	1.141076795
C	0.276284100	0.196007359	-0.043711997
C	-0.170081412	-0.341698772	-1.255148882
C	-0.950374698	-1.494464355	-1.283836566
C	-1.297509192	-2.131742532	-0.093406933
C	1.153791424	1.415896547	-0.035148524
C	2.591866083	1.092884834	-0.455563692
C	3.287310287	0.118895326	0.485292509
C	4.715874747	-0.179371089	0.049764772
H	-1.906033239	-3.025379802	-0.112578919
H	-1.291559855	-1.891287210	-2.230549559
H	-1.128370534	-2.093062340	2.049339845
H	0.090145382	0.154043124	-2.183073547
H	0.255206811	-0.045580752	2.087393705
H	0.740401680	2.167355199	-0.710928031
H	1.160823243	1.853487710	0.965539339
H	3.167527433	2.020752592	-0.506524436
H	2.581766568	0.673195505	-1.465297009
H	3.287069318	0.536516559	1.495602994
H	2.713965798	-0.808424536	0.533666540
H	5.312452279	0.732333913	0.018048274
H	4.730128887	-0.619131813	-0.947427379
H	5.205061082	-0.876037090	0.728650983
Ar	-3.234648579	1.048163707	0.118246768

BB-V…Ar(VU) at cc-pVTZ(BB)/aug-cc-pVTZ(Ar) level of theory			
C	1.263237661	-0.316395555	-0.001854941
C	1.074597730	-1.004289791	1.200020472
C	0.705019561	-2.347311585	1.206770945
C	0.516975761	-3.024704453	0.003558362
C	0.703579426	-2.351745195	-1.202332052
C	1.073030652	-1.008643755	-1.200939966
C	1.595821602	1.147754472	-0.004573739
C	0.335581123	2.015073046	0.001262042
C	0.642022237	3.506481517	-0.003162880
C	-0.621691229	4.356559664	0.004284435

H	0.232112319	-4.067830426	0.005645344
H	0.567311247	-2.864031987	2.147054305
H	0.564733977	-2.871893445	-2.140555500
H	1.223368147	-0.481946794	2.137695928
H	1.220571445	-0.489683858	-2.140676192
H	2.202426021	1.391337803	0.870609226
H	2.193425799	1.389926910	-0.886298489
H	-0.264791482	1.764924925	0.880281668
H	-0.275055408	1.761811685	-0.869746501
H	1.256228549	3.748997244	0.867072886
H	1.244122607	3.746234994	-0.882567471
H	-1.222918693	4.147270115	0.888800908
H	-1.235712724	4.143711818	-0.870544940
H	-0.390944696	5.420664335	0.000451387
Ar	-2.375902026	-0.714856662	-0.001094074

BB-V…Ar(VD) at cc-pVTZ(BB)/aug-cc-pVTZ(Ar) level of theory			
C	-0.177513647	-0.193628495	0.001069708
C	0.368467177	-0.657376970	1.201041942
C	1.432918858	-1.555830682	1.204093959
C	1.967695639	-2.007110991	-0.001023430
C	1.431724891	-1.554457174	-1.205105417
C	0.367296739	-0.656005588	-1.199978972
C	-1.360606559	0.730429344	0.002085513
C	-2.681486499	-0.041374527	-0.000087748
C	-3.901813501	0.869083216	0.000750026
C	-5.207791576	0.085463721	-0.001595549
H	2.796943026	-2.701081528	-0.001829148
H	1.846908381	-1.898269145	2.142941007
H	1.844788837	-1.895828332	-2.144748443
H	-0.040202817	-0.303306232	2.140099885
H	-0.042276686	-0.300851125	-2.138237898
H	-1.324432085	1.377098602	0.881759579
H	-1.323469708	1.380277443	-0.875212108
H	-2.710578019	-0.697705644	0.873932607
H	-2.709497626	-0.694609098	-0.876459575
H	-3.862675995	1.520445877	0.876826579
H	-3.861462391	1.523664974	-0.872869878
H	-5.275001742	-0.555909335	0.876888750
H	-5.273759805	-0.552698795	-0.882508978
H	-6.073478302	0.745829959	-0.001001310
Ar	2.989769659	1.574609695	-0.000365276

6.2 Calculated XYZ Coordinates of *n*-Butylbenzene Monomer and *n*-Butylbenzene-V…Ar Cluster on Cationic Ground State

The values are in Angstroms.

BB-I at cc-pVDZ level of theory			
C	-2.199318000	-1.310296000	0.409259000
C	-1.045027000	-0.813003000	1.006683000
C	-0.527373000	0.440380000	0.601217000
C	-1.216317000	1.166361000	-0.445855000
C	-2.360221000	0.699790000	-1.051452000
C	-2.859947000	-0.533022000	-0.637709000
C	0.724112000	1.015048000	1.169144000
C	1.915969000	0.833023000	0.181877000
C	2.267658000	-0.633108000	-0.081826000
C	3.508769000	-0.771448000	-0.966732000
H	-3.767794000	-0.940795000	-1.097183000
H	-2.864824000	1.272855000	-1.832661000
H	-2.629498000	-2.272184000	0.704109000
H	-0.801313000	2.134426000	-0.752454000
H	-0.543662000	-1.381851000	1.795264000
H	0.580560000	2.095610000	1.353805000
H	0.965359000	0.529210000	2.128514000
H	2.781483000	1.357451000	0.624557000
H	1.691353000	1.348940000	-0.771563000
H	2.439224000	-1.143553000	0.884893000
H	1.411838000	-1.145036000	-0.562107000
H	4.385049000	-0.302625000	-0.489263000
H	3.353221000	-0.284350000	-1.944021000
H	3.749176000	-1.830448000	-1.149526000

BB-V at cc-pVDZ level of theory			
C	0.716072000	-2.520954000	1.254704000
C	0.714672000	-3.218091000	0.000000000
C	0.716072000	-2.520954000	-1.254704000
C	0.716072000	-1.166702000	-1.235725000
C	0.734027000	-0.440158000	0.000000000
C	0.716072000	-1.166702000	1.235725000
C	0.682089000	1.048105000	0.000000000
C	-0.800712000	1.526115000	0.000000000
C	-0.900993000	3.055351000	0.000000000
C	-2.356784000	3.527133000	0.000000000

H	0.710003000	-4.314969000	0.000000000
H	0.715582000	-3.096798000	2.184089000
H	0.715582000	-3.096798000	-2.184089000
H	0.718833000	-0.607916000	2.177869000
H	0.718833000	-0.607916000	-2.177869000
H	1.186534000	1.452514000	0.894200000
H	1.186534000	1.452514000	-0.894200000
H	-1.314553000	1.112668000	0.888392000
H	-1.314553000	1.112668000	-0.888392000
H	-0.373741000	3.452251000	0.886657000
H	-0.373741000	3.452251000	-0.886657000
H	-2.891628000	3.161760000	0.892650000
H	-2.891628000	3.161760000	-0.892650000
H	-2.411592000	4.627159000	0.000000000

BB-I…Ar(IU) at cc-pVDZ(BB)/aug-cc-pVDZ(Ar) level of theory			
C	2.022212000	-0.429990000	1.331311000
C	0.755270000	-1.002476000	1.312738000
C	0.198928000	-1.444684000	0.086722000
C	0.969739000	-1.271465000	-1.125336000
C	2.224626000	-0.714954000	-1.137264000
C	2.760429000	-0.285266000	0.078793000
C	-1.167582000	-2.030905000	-0.008166000
C	-2.190898000	-0.967547000	-0.510118000
C	-2.399344000	0.185266000	0.474674000
C	-3.454397000	1.176750000	-0.021883000
H	3.757092000	0.170492000	0.108749000
H	2.791401000	-0.603982000	-2.064647000
H	2.484657000	-0.084133000	2.260660000
H	0.523468000	-1.614301000	-2.066979000
H	0.192089000	-1.124390000	2.242793000
H	-1.156013000	-2.875311000	-0.721037000
H	-1.489812000	-2.411640000	0.974796000
H	-3.145571000	-1.495730000	-0.682879000
H	-1.865966000	-0.576029000	-1.493524000
H	-2.705839000	-0.228202000	1.454130000
H	-1.443235000	0.716678000	0.640178000
H	-4.427059000	0.677271000	-0.164217000
H	-3.156123000	1.620136000	-0.986968000
H	-3.597916000	1.996831000	0.699114000
Ar	0.829163000	2.585775000	-0.171611000

BB-V…Ar(IU) at cc-pVDZ(BB)/aug-cc-pVDZ(Ar) level of theory			
C	1.366534000	-0.066388000	0.080237000
C	1.393796000	-0.824478000	1.275633000
C	1.362378000	-2.213535000	1.214044000
C	1.285631000	-2.873131000	-0.087863000
C	1.250769000	-2.140890000	-1.272680000
C	1.279046000	-0.769328000	-1.181918000
C	1.337386000	1.420979000	0.086327000
C	-0.139014000	1.911930000	-0.004587000
C	-0.223877000	3.442367000	-0.021423000
C	-1.673732000	3.925848000	-0.099279000
H	1.256106000	-3.968544000	-0.117655000
H	1.396774000	-2.829869000	2.117491000
H	1.195316000	-2.646632000	-2.239422000
H	1.457177000	-0.317639000	2.243473000
H	1.245675000	-0.167713000	-2.098664000
H	1.794532000	1.812629000	1.009705000
H	1.897199000	1.820997000	-0.777689000
H	-0.703480000	1.507941000	0.856266000
H	-0.609377000	1.499616000	-0.917950000
H	0.260556000	3.840478000	0.888595000
H	0.351992000	3.827650000	-0.882517000
H	-2.256325000	3.571185000	0.767365000
H	-2.165266000	3.558566000	-1.015774000
H	-1.719076000	5.026179000	-0.109436000
Ar	-2.096988000	-1.481560000	0.282774000

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